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Distributional Monte Carlo Methods for the Boltzmann Equation

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DISTRIBUTIONAL MONTE CARLO METHODS FOR THE BOLTZMANN EQUATION

DISSERTATION

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Abstract

Stochastic particle methods (SPMs) for the Boltzmann equation, such as the Direct Simulation Monte Carlo (DSMC) technique, have gained popularity for the prediction of flows in which the assumptions behind the continuum equations of fluid mechanics break down; however, there are still a number of issues that make SPMs computationally challenging for practical use. In traditional SPMs, simulated particles may possess only a single velocity vector, even though they may represent an extremely large collection of actual particles. This limits the method to converge only in law to the Boltzmann solution. This document details the development of new SPMs that allow the velocity of each simulated particle to be distributed. This approach has been termed Distributional Monte Carlo (DMC).

A technique is described which applies kernel density estimation to Nanbu's DSMC algorithm. It is then proven that the method converges not just in law, but also in solution for $L^{\infty}\left(\mathbb{R}^3\right)$ solutions of the space homogeneous Boltzmann equation. This provides for direct evaluation of the velocity density function. The derivation of a general Distributional Monte Carlo method is given which treats collision interactions between simulated particles as a relaxation problem. The framework is proven to converge in law to the solution of the space homogeneous Boltzmann equation, as well as in solution for $L^{\infty}\left(\mathbb{R}^3\right)$ solutions. An approach based on the BGK simplification is presented which computes collision outcomes deterministically.

Each technique is applied to the well-studied Bobylev-Krook-Wu solution as a numerical test case. Accuracy and variance of the solutions are examined as functions of various simulation parameters. Significantly improved accuracy and reduced variance are observed in the normalized moments for the Distributional Monte Carlo technique employing discrete BGK collision modeling.

To my wife and son - May your thirst for discovery never be quenched.
It is your support and encouragement which gave me the strength to complete this effort
and for your sacrifices I am forever grateful.

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DISTRIBUTIONAL MONTE CARLO METHODS FOR THE BOLTZMANN EQUATION

I. Introduction

The study of the thermodynamic properties of gas flows is critical in many fields of engineering and the sciences. The field of computational fluid mechanics has in recent years made ever increasing strides in the analysis of fluids governed by the continuum equations of fluid mechanics (e.g. the Navier-Stokes and Euler equations). Numerical methods for solving these equation sets have found their way into many practical engineering tools and practices, and many recent developments in applied aerodynamics can be attributed to their use.

Unfortunately, the continuum equation sets cannot provide a complete description of the physical phenomena taking place within a fluid under all circumstances. Notable departures from the predicted solutions of these equations occur whenever the "continuum hypothesis" is violated. Examples of such violations arise in rarefied gas dynamics, hypersonic flows, and micro-scale flows. Additionally, there is an "equilibrium hypothesis" inherent to the so-called "continuum" equation sets, as it can be shown that these equation sets may be derived by assuming various forms of a perturbation from local thermodynamic equilibrium [32].

To obtain accurate solutions in such cases, models based on kinetic theory are used. Kinetic theory attempts to relate the molecular interactions occurring at the microscopic level to macroscopic fluid properties such as pressure, temperature, viscosity, etc. The most common governing equation employed is the Boltzmann equation, which is an integro-differential equation which describes the evolution of the probability density function

(PDF) of molecular velocities throughout the gas. This function is commonly referred to in the literature as the velocity *distribution* function, but to be more mathematically precise this document will utilize the term velocity *density* function when referring to the Boltzmann solution.

Unlike the continuum equation sets, few practical solution methods for the Boltzmann equation have found their way into practical engineering settings. This is not for a lack of solution algorithms, but rather due to the complexity and computational demands of such algorithms. By far, the Direct Simulation Monte Carlo (DSMC) method, originally developed by Bird [14], has become the dominant approach for examining flows governed by the Boltzmann equation and has gained general acceptance for practical applications in rarefied gas dynamics.

The DSMC technique approximates the physics of the Boltzmann equation using a stochastic simulation of the interactions of a fraction of the molecules in the gas. In DSMC, each simulated particle possesses a single velocity vector and energy state. As only a fraction of the number of particles in the gas can be simulated, each simulated particle is assumed to represent $W = \frac{N}{N_p}$ actual particles, where N is the total number of actual particles in the gas and N_p is the number of simulated particles. In practice W may be quite large (10^6 or more), therefore restricting to only a single velocity vector per simulated particle is equivalent to assuming that millions of actual particles all share the exact velocity vector. This assumption is non-physical in the sense that kinetic theory tells us that the probability that any two molecules share the exact velocity is zero. Mathematically, this representation leads to what is known as a point measure approximation of the density function, f, as illustrated by

$$f(v) = \frac{1}{N_p} \sum_{i=1}^{N_p} \delta(v - v_i) \tag{1.1}$$

where v_i is the velocity vector of the i^{th} simulated particle, and δ is the Dirac distribution. This representation restricts the method to converge only *in law*. Another undesirable

feature of the DSMC method stems from the stochastic nature of the technique. Namely, flow solutions are subject to a significant amount of variance. In practice this variance is reduced by creating an ensemble averaged solution, combining the results of potentially thousands of simulations (or time steps in steady-state cases). The present work seeks to address these limitations through the development of Distributional Monte Carlo methods. Although the Boltzmann equation and DSMC will be discussed in greater detail in Chapters 2 and 3, a brief introduction is warranted here to provide a more comprehensive view of the motivation and contribution of the work presented herein.

1.1 Kinetic Theory and Rarefied Gas Dynamics

Although the continuum equations are capable of providing fairly accurate flowfields under relatively benign conditions, two specific regimes in which they fail are rarefied flows and flows containing non-equilibrium phenomena. Applications of rarefied gas dynamics typically involve high-altitude flight and microscale flows (e.g. Micro Electro-Mechanical devices(MEMs)). In the former, the atmospheric density is low enough that the large intermolecular spacing invalidates the continuum hypothesis. In the latter, the physical scale of interest is small enough that the flow appears rarefied even at standard densities.

Non-equilibrium phenomena typically result from the propensity of the constituent molecules to undergo changes in their internal energy state during a collision with a material surface or another molecule, as well as their ability to react chemically with other molecules upon collision. These events occur at some finite rate in the fluid, and not every encounter results in such changes. If these events occur in such a way as to alter the macroscopic properties of the fluid over timescales which are longer than some local flow timescale, they may be regarded as non-equilibrium phenomena. These effects can be responsible for causing a number of fluid properties that might normally be treated as constants to vary at a finite rate. Among these are fluid composition, viscosity, thermal conductivity, specific heats, etc. The variable nature of these properties in regions of non-

equilibrium changes the manner in which energy and momentum are transferred in the fluid, which alters the macroscopic thermodynamic and flow variables throughout the flow. Such effects are commonly observed in high temperature or high energy flow fields such as those generated in hypersonic flight.

The traditional continuum equations of fluid mechanics do nothing in and of themselves to address these effects. In fact, these equations permit only small departures from equilibrium in the translational energy mode, but must be augmented with additional equations to compensate for other forms of non-equilibrium. Integration of such models with the continuum equations in some cases is not well understood.

To illustrate the need for a noncontinuum based approach, consider a blunt body in a hypersonic flow, as illustrated in Figure 1.1. The physics involved with the associated strong shocks invalidate the continuum equations through the generation of non-equilibrium phenomena. Close to the body, strong gradients exist across the boundary layer and may generate non-equilibrium phenomena which invalidate the continuum equations. Further downstream the flow may expand around the body to the point at which the density is too low for the continuum equations to hold. Clearly the continuum equations are not sufficient for dealing with such flows.

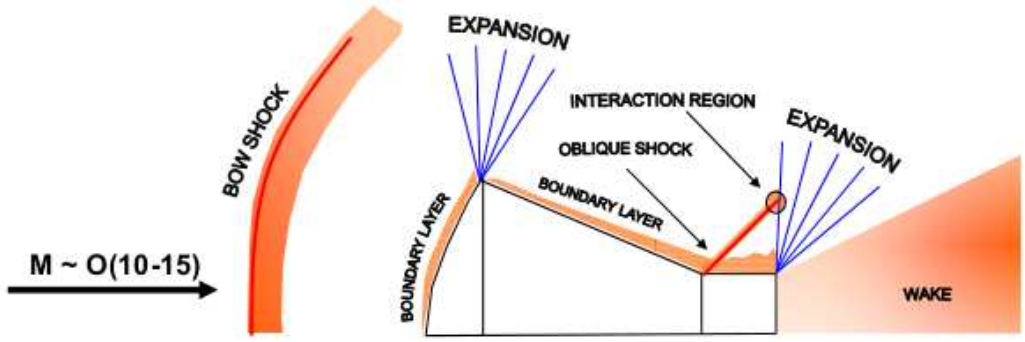


Figure 1.1: Hypersonic Flow over a Blunt Body

A common parameter used to examine the validity of the continuum equations is the Knudsen Number, Kn, defined by

$$Kn = \frac{\lambda}{L} \tag{1.2}$$

Here, λ represents the mean free path of a molecule in the gas and L is a characteristic length. The characteristic length of importance depends upon the situation under consideration. For example, to obtain a general idea of the validity of the continuum equations in the overall flowfield around a physical object, L could be set to some characteristic physical dimension of the object (e.g. the chord of a wing on an aircraft). On the other hand, to obtain an understanding of the validity of the continuum equations in approximating the fluid physics of the flow field, L should be set to a characteristic gradient length of a fluid property, e.g. $\frac{p}{|\nabla p|}$. Figure 1.2 illustrates generally accepted bounds on the regions of validity for the continuum equation sets. Note that the Boltzmann equation, the governing equation of kinetic theory, exhibits no Knudsen number dependence for sufficiently dilute gases.

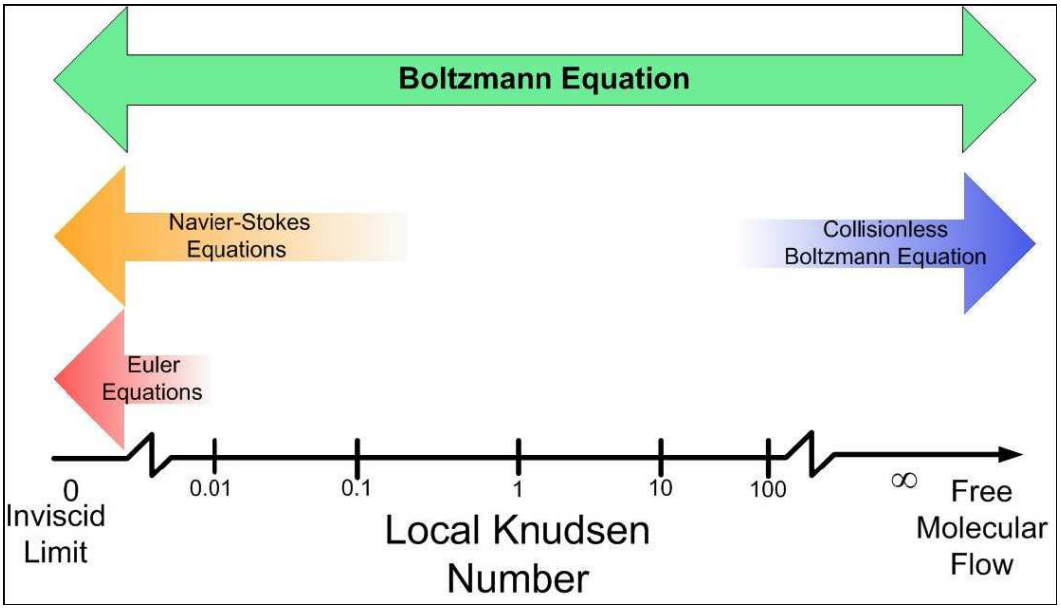


Figure 1.2: Knudsen Number Validity Ranges for Various Equation Sets [65]

The branch of gas dynamics which is formally concerned with accounting for changes in the gas which occur due to interactions at the molecular level is kinetic theory. Although the basic ideas of kinetic theory originated in the mid-1800's with Ludwig Boltzmann [23], the practical solution and application of these methods remain areas ripe for mathematical research. The complexity involved with performing a kinetic analysis of a gas has presented a challenging problem from the day these methods were conceived.

Kinetic theory attempts to track, at least statistically, the energy state, momenta and position of every particle in the gas as a function of time, and accounts for the variation of these properties due to collisions. This information can then be integrated over the collection of particles to obtain the macroscopic properties of the gas. No inherent assumptions regarding equilibrium are required and only the particle collision dynamics require modeling. The assumptions which go into such models typically do not exhibit restricted validity in regions of non-equilibrium.

Like continuum fluid mechanics, various governing equations have been derived to describe the behavior of molecules in a gas with various assumptions regarding interactions and collision dynamics. The most popular and well studied of these is the Boltzmann equation (alternatives include for example the Kac master equation [45]).

Unfortunately, the great flexibility afforded by kinetic theory is not without cost. The Boltzmann equation is a nonlinear integro-differential equation for a probability density function which statistically describes the energy state of the particles as a function of time. For a monatomic gas, this equation must be solved in a space of dimension no less than seven. For polyatomic molecules, which may possess several components of angular momentum and vibrational degrees of freedom, the dimension of the space grows even higher.

The present work considers a gas which is monatomic and further assumes that the internal energy capacity of such molecules is negligible. In other words, particles will

be assumed to possess only translational energy. This restriction allows study of the phenomena of interest without adding unnecessary complexity. Under this assumption, recall that the translational kinetic energy of a particle, ϵ, is related to its velocity via

$$\epsilon = \frac{1}{2} m \|v\|^2 \tag{1.3}$$

Here, $\|\cdot\|$ represents the standard Euclidean norm. In light of (1.3), one may equivalently examine thermodynamic properties in terms of the distribution of molecular velocities rather than energy.

Consider a gas occupying some physical region $V \subseteq \mathbb{R}^3$ during some interval of time. The velocity density function, $f : V \times \mathbb{R}^3 \times \mathbb{R}^+ \to \mathbb{R}^+$, is a probability density function that describes the distribution of velocity over the collection of particles. The function is defined such that

$$f(r, v, t)\, dr dv \tag{1.4}$$

represents the probability of finding a particle in the differential element of physical space, dr centered at r, which possesses velocity in the differential element of velocity space, dv centered at v, at time t. Here, and in all integrals to follow, the use of the notation dr is used to mean $dr_1 dr_2 dr_3$ and likewise the term dv is used for $dv_1 dv_2 dv_3$.

It is at this point that one first may begin to grasp the large dimensionality associated with examining a gas at the microscopic level as f is seen to be defined over a seven-dimensional space. In comparison, the variables involved in the partial differential equations modeling the gas at the macroscopic level are defined at most over a four-dimensional space. The six dimensions of physical and velocity space are commonly referred to as the "phase space". It should also be noted that many variations of f appear in the literature with some authors referring to Nf or nf as the distribution function, where N is the number of molecules in the gas and n is the number density of molecules in the gas. For clarity in this work, f will always be taken as the probability density function for

molecular velocity, or what some authors have referred to as the *normalized distribution function*.

For any function, Q, of molecular velocity, v, we define the expectation value $\bar{Q}$ at position r and time t as

$$\bar{Q}(r,t) = \int_{\mathbb{R}^3} Q(v)\, f(r,v,t)\, dv \tag{1.5}$$

Such functions are of great importance, as they allow for the computation of the macroscopic thermodynamic properties of the gas. This is illustrated in Table 1.1 [41].

Table 1.1: Expectation Values Related to Macroscopic Properties.

$Q(r,v,t)$	$\bar{Q}$	Description
N	n	Number Density
mN	ρ	Mass Density
$\frac{Nv}{n}$	u	Fluid Velocity
$-k_B \ln[f]$	S	Entropy
$\frac{m}{3nk_B}\|v-u\|^2$	T	Temperature
$\frac{m}{3}\|v-u\|^2$	P	Pressure

One can therefore see the importance of the density function in determining the macroscopic thermodynamic properties of interest in the fluid. It is with this in mind that one seeks a relation to describe the evolution of the density function throughout phase space. One such description is provided by the Boltzmann equation which accounts for changes to f due to three influences: particle advection, 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

$$\frac{\partial}{\partial t} f(r,v,t) + v \cdot \nabla_r f(r,v,t) + F \cdot \nabla_v f(r,v,t) = J[f](r,v,t) \tag{1.6}$$

Here, F is any externally applied force, and ∇_r and ∇_v represent the gradient with respect to position and velocity variables, respectively. That is, $\nabla_r = \left(\frac{\partial}{\partial r_1}, \frac{\partial}{\partial r_2}, \frac{\partial}{\partial r_3}\right)$, and $\nabla_v = \left(\frac{\partial}{\partial v_1}, \frac{\partial}{\partial v_2}, \frac{\partial}{\partial v_3}\right)$. The collision integral J is defined as

$$\begin{aligned} J[f](r,v,t) \quad = \quad & \int_{\mathbb{R}^3} \int_{S^+} \left[f\left(r, v'(v,w,n), t\right) f\left(r, w'(v,w,n), t\right) - \right. \\ & \left. f(r,v,t)\, f(r,w,t) \right] B\left(\theta, \|v-w\|\right) d\theta d\epsilon dw \end{aligned}$$

where S^+ denotes the positive half of the unit sphere in $\mathbb{R}^3$, n is the unit vector defining the collision orientation, θ and ϵ are the azimuth and elevation angles of n, respectively, and B is the collision cross section. The post-collision velocities v', w' are given by

$$v'(v,w,n) = v - [n \cdot (v-w)]\, n \tag{1.7}$$

$$w'(v,w,n) = w + [n \cdot (v-w)]\, n \tag{1.8}$$

Given the complexity inherent to (1.6), it is not difficult to understand why closed form solutions of the Boltzmann equation for flows of practical interest are difficult to obtain. The Boltzmann equation will be discussed in greater detail in Chapter 2.

1.2 Computational Methods for the Boltzmann equation

Computational methods for the Boltzmann equation continue to be developed; however, due to the inherent complexity of the equation itself, such methods are correspondingly complicated. This section summarizes the strengths and weaknesses of a few of the methods currently employed in this field. These methods can largely be broken into two categories: deterministic methods and stochastic methods.

1.2.1 Deterministic Methods.

Deterministic methods for the Boltzmann equation are typically plagued by two issues over their stochastic counterparts, namely, increased complexity and degraded physical

fidelity. On the other hand, they avoid the introduction of variance due to stochastic processes.

1.2.1.1 Direct Boltzmann CFD.

A class of methods known as Direct Boltzmann solvers or Direct Boltzmann Computational Fluid Dynamics (CFD) borrows from the methods of continuum CFD. These methods attempt to track the evolution of the velocity distribution function by performing finite difference or finite volume computations over a grid in phase space.

A number of issues arise with such an approach. Developing a numerical grid in the six-dimensional phase space is much more complex than simply gridding physical space as in continuum CFD. When discretized over a velocity grid, the distribution function is constrained to have compact support. In general, this is not physically accurate and it is non-trivial to establish appropriate bounds on the support region a priori. Furthermore, grid refinement in velocity space is non-trivial, and as of yet an area of open research, leading to the requirement of including a large number of grid points in order to obtain an accurate representation.

Even with these drawbacks, these methods have a number of desirable features that are not necessarily present in other computational schemes. First, they are directly traceable to the Boltzmann equation. Second, the numerical methods employed, although tailored to the Boltzmann equation, are well understood in general from a mathematical viewpoint, and are directly amenable to stability and error analysis.

Work on such methods began in the late-1960's and has continued to the present [7, 48]. Due to the associated complexities and computational demands required for accuracy, these methods have not yet gained popular acceptance as practical engineering tools but have been successfully employed to solve basic, fundamental flows.

1.2.1.2 Molecular Dynamics.

Molecular dynamics methods have been employed since the late 1950's [6, 16]. The idea behind such methods is to simulate the evolution of a very large collection of particles throughout the flowfield. Particle interactions and collisions are computed deterministically.

The complexity associated with such methods is fairly substantial. First, as these methods seek to *deterministically* describe the evolution of the particles, each particle's trajectory must be advanced by computing all of the possible field interactions with all other particles. Secondly, as collision interactions are computed deterministically, selection of an appropriate collision partner cannot be decoupled from particle advection/field interactions. Finally, scatter due to the finite sample size decreases only as one over the square root of the sample size [16]. Therefore, in order to achieve accuracy, a large number of particles must be simulated.

As such, molecular dynamics approaches are more frequently employed when the number of simulated particles can be nearly on the order of the number of actual particles in the flow. In these cases, the molecular dynamics method yields accurate results and has been applied to the study of elementary physical problems.

1.2.1.3 Discretization Methods.

There is a class of deterministic methods known as discretization methods which seek to "discretize" the behavior of the gas molecules. One such method is known as the Lattice Gas Automata Method. In this method, particle advection through phase space is viewed as motion from one node to an adjacent node in physical and velocity space. A similar method known as the Discrete Velocity Method discretizes only velocity space. That is, a finite set of possible particle velocities is specified [17].

Such methods, while interesting in their own right, cannot fully replicate the physics represented in the Boltzmann equation. Namely, it is impossible to totally conserve mass,

momentum, and energy over a finite velocity set [17]. This leads to a requirement for inclusion of a large number of potential velocities and the computations associated with determining the most appropriate post collision velocities over such a set is quite complex. Although consistency is an issue for such methods it has been shown that when a large enough set of possible velocities is taken, these methods can be accurate for elementary problems. Their associated complexity has, however, rendered them impractical for engineering applications at this time [38].

1.2.2 Stochastic Methods.

Stochastic methods for the Boltzmann equation typically employ a simulation algorithm of relatively lower complexity than deterministic methods to model intermolecular interactions. For this reason, initial attempts at developing such methods were aimed not at preserving mathematical consistency with the Boltzmann equation as much as accurately simulating the physics of particle interactions. For this reason, convergence results on such methods are somewhat limited. Additionally, the incorporation of various stochastic processes in such simulations leads to the introduction of variance in the solution that is not present in their deterministic counterparts.

1.2.2.1 The Direct Simulation Monte Carlo Method.

The Direct Simulation Monte Carlo (DSMC) method was originally developed in the mid-1960's by Bird [15]. The method relies on the Monte Carlo method originally developed by von Neumann and Ulam (although published in 1950 by Forsythe and Liebler [40]). The method is based on a stochastic simulation of a fraction of the actual number of particles in the gas. Each simulated particle is taken to represent N/N_p actual particles.

Unlike the molecular dynamics method, particle interactions are computed *probabilistically*. The principal approximation is termed the uncoupling principle, which allows intermolecular collisions to be decoupled from particle advection. Collision interactions

appropriate for the time increment are computed probabilistically after which particles are advected along their velocity vectors. Each simulated collision represents N/N_p actual collisions. Use of a grid in physical space ensures that the selected collision interactions are between near neighbors [17]. Specifically, one can view this as a two-stage splitting scheme with collisionless advection integrating

$$\frac{\partial f}{\partial t} + v \cdot \nabla_r f = 0 \tag{1.9}$$

and the collision simulation integrating

$$\frac{\partial f}{\partial t} = J[f](r, v, t) \tag{1.10}$$

Initially, the DSMC method was met with some consternation. Although remaining true to the principles of kinetic theory, the method itself was not formally derived from the Boltzmann equation. Without a proof of consistency or convergence, this raised questions as to the validity of the method itself. By the early 1980's, however, Nanbu [58] and others had proposed methods derived from the Boltzmann equation itself, and by 1992 Bird's method had been proven to be consistent with the Boltzmann equation as well [75].

The DSMC method is not without its drawbacks. First, a significant number of particles must be simulated to achieve results representative of reality. 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 significant burden on the simulation process. Secondly, the stochastic nature of the simulation introduces a significant amount of variation in the results and in practice data must be averaged over an ensemble to reduce the variance in the solution. Even with these drawbacks, DSMC is the standard computational method employed when increased accuracy over the continuum equation sets is required and has gained acceptance in the field of hypersonic aerodynamics [24, 44, 73], flows involving micro electromechanical systems (MEMS) [37], and semiconductor manufacturing processes such as film deposition processes [71].

With only a single velocity vector per simulated particle, DSMC approximates the velocity density function utilizing a point measure approximation as illustrated by

$$f(v) = \frac{1}{N_p} \sum_{i=1}^{N_p} \delta(v - v_i) \tag{1.11}$$

where v_i is the velocity vector of the i^{th} particle.

Equation 1.11 was the starting point for Nanbu's derivation of an algorithm consistent with the Boltzmann equation. Within each cell of the grid, the solution is assumed to be space homogeneous. Beginning with the weak form of the space homogeneous Boltzmann equation, Nanbu was able to develop appropriate stochastic processes that governed selection of collision pairs and collision outcomes within a given cell. Such methods will be discussed in greater detail in Chapter 3.

1.2.2.2 Stochastic Particle Methods.

Recently, Wagner sought to generalize the DSMC method into a class of methods he termed Stochastic Particle Methods [61, 62, 76]. His approach was motivated by a desire to allow simulated particles to have a varying level of influence, possibly depending on their location in the flowfield. This technique would potentially improve the ability of DSMC to handle flowfields which contain both low and high density regions of simulated particles. Specifically, as flow expands around an obstacle, it is common that the density of simulated particles in the wake region fall to levels that exorbitantly increase the level of scatter present in the solution [62]. This is predominantly due to the fact that although very few simulated collisions are being calculated, they will have tremendous impact on the approximation to the density function, since each simulated collision may in fact represent millions of actual collisions. Secondly, the very assumption that several million particles share the same velocity vector in a region where very few simulated particles exist leads to a gross underrepresentation of the density function itself. While the stochastic particle method developed by Wagner attempts to address the first of these issues, it does little to combat the second, as the method continues to employ point measures. This is a goal of

the work presented herein that will be discussed in much greater detail throughout this document.

Specifically, the stochastic particle method approximates the density function as illustrated by

$$f(v,t) = \sum_{i=1}^{N_p(t)} g_i(t)\,\delta(v - v_i) \tag{1.12}$$

where g_i is a weighting term on the influence of the i-th particle. Also, note that N_p is now allowed to vary with time. The reason for this is due to another feature of the method, namely a collision softening effect that requires N_p in general to grow as more collisions are computed. Specifically, each collision generates two new particles which are assigned a weight and post-collision velocity, while the two original particles persist with their velocities unaltered, but with their weighting reduced. The post-collision weightings of the four particles must be chosen in such a way as to ensure conservation of mass, momentum, and energy. The key criticism of the method is that because of this, the number of simulated particles grows with time which is highly undesirable from an implementation standpoint. To combat this, a method was proposed by which particles would be discarded after their weight fell below a certain threshold [61]. Nevertheless, perhaps because of the complexity associated with the creation and destruction of simulated particles, the method has not seen widespread application.

1.2.2.3 Low Variance Deviational Simulation Monte Carlo.

Recently, Baker, Homolle, and Hadjiconstatinou have developed a simulation method which employs Monte Carlo techniques only to simulate the departure from thermodynamic equilibrium [10, 43]. This method is termed Low Variance Deviational Simulation Monte Carlo (LV-DSMC). The method was specifically developed to handle low Mach number flows (e.g. microscale applications) in such a way as to attempt to ensure the variance is independent of the magnitude of the departure from thermodynamic equilibrium. With traditional DSMC, a limiting factor is that for near-equilibrium solutions,

large numbers of simulated particles must be employed to reduce the variance to the point that the deviation is observable.

This technique is based on defining the deviation, f^d, from an arbitrary Maxwell-Boltzmann (equilibrium) density function as

$$f^d \equiv f - f_{MB} \tag{1.13}$$

where f_{MB} is a Maxwell-Boltzmann density of the form given by

$$f_{MB}(v) = \frac{n_{MB}}{\left(\frac{2\pi k T_{MB}}{m}\right)} \exp\left[-\frac{m(v-u_{MB})^2}{2kT_{MB}}\right] \tag{1.14}$$

where n_{MB}, T_{MB}, and u_{MB} are the number density, temperature and mean velocity associated with the Maxwell-Boltzmann density function. As shown in any text on kinetic theory, the Maxwell-Boltzmann density is the solution of the Boltzmann equation in translational equilibrium. Substituting (1.13) into the (1.6), a new form of the collision integral is obtained. Baker, Homolle, and Hadjiconstantinou were then able to develop a particle scheme with particle advection and collision substeps to simulate the transformed equation.

The process is more complicated than traditional DSMC, as particles do not necessarily advect according to (1.9), and their advection behavior is dependent upon how f_{MB} is chosen. As for the collision substep, it is viewed as having a two step effect: first, a net change to f_{MB}, and second, a change to f^d with the goal being to lump as much of the change as possible into f_{MB} and then regenerate deviational particles with velocities corresponding to the new f^d. Therefore, like the stochastic particle method, LVDSMC also relies on particle creation and destruction at each time step.

The summary of methods provided here is in no way totally comprehensive. In fact, many methods currently being developed blur the lines of distinction outlined here [16] (e.g. Monte Carlo based Discrete Velocity Methods [56]). Each method presents unique challenges in its implementation and representation of the Boltzmann solution. In this

work, we focus on developing a stochastic particle based method which borrows from the ideas of DSMC, but removes the point measure representation of the density function.

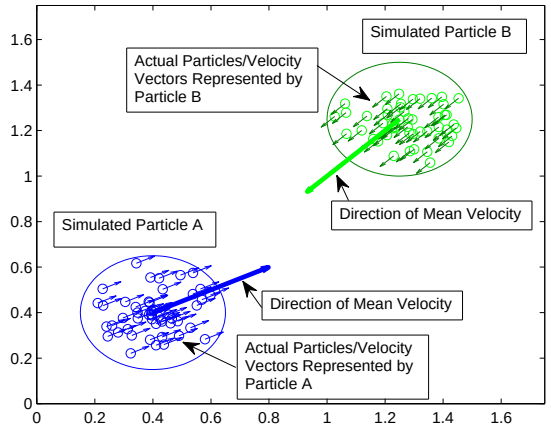
1.3 Overview of Current Approach – Distributional Monte Carlo

This work outlines the development of a new approach for the solution of the Boltzmann equation which has been termed "Distributional Monte Carlo". This method falls under the category of stochastic particle methods, but unlike attempts by prior authors, the Distributional Monte Carlo method removes the point measure approximation of the density function by allowing each simulated particle to possess not just a single velocity vector, but rather, a complete velocity distribution function. Binary collisions computed between simulated particles have the effect of altering the particles' density function. Specifically, a binary collision between two simulated particles is viewed as a space homogeneous relaxation of the distribution function of the potentially millions of actual particles represented by the two simulated particles; rather than assuming that millions of collisions each have the same outcome (as in traditional DSMC).

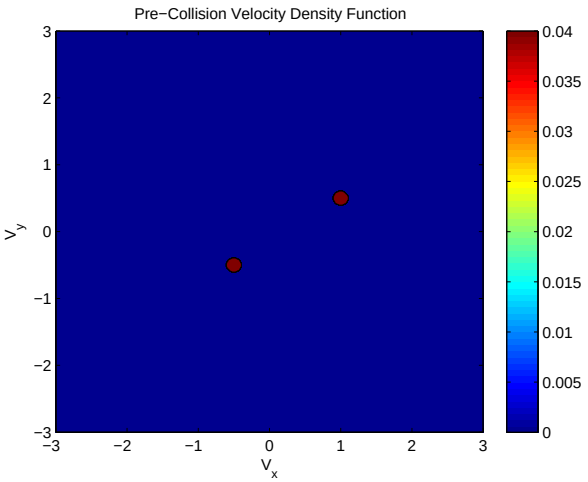
The reasons for such modifications are many. First, the assumption that the millions of actual particles represented by a single simulated particle all possess the same velocity vector, is nonphysical. Kinetic theory tells us that intermolecular collisions will drive the velocity density function of the collection towards the Maxwell-Boltzmann density function. Second, in addition to being nonphysical, this assumption has the effect of over emphasizing collision effects and introducing additional variance in the solution particularly in areas where the density of simulated particles is low as observed by Wagner [76]. Third, the point measure approximation limits convergence to occur only in the weak sense to the Boltzmann solution.

To illustrate the restrictive nature of the point measure representation, consider an arbitrary collision pair of simulated particles. Figure 1.3(a) is a 2-dimensional conceptual illustration of the two simulated particles as well as the collection of actual particles

represented by each simulated particle. Note that every particle represented by a given simulated particle possesses the same velocity vector. Figure 1.3(b) illustrates the velocity density function of the entire collection of actual particles prior to collision. The function is singular exactly at the velocities of the two simulated particles and identically zero everywhere else.



(a) A Collision Pair Prior to Collision



(b) Velocity Density Function of Actual Particles

Figure 1.3: DSMC Pre-Collision Modeling

Figure 1.4(a) illustrates the same collision pair post collision. Note that the collision process changes the velocity vectors of all the particles and all of the actual particles represented by a simulated particle are assumed to possess the same velocity vector post collision. Figure 1.4(b) illustrates the velocity density function of the collection of actual particles post-collision. The function is still singular at the new post-collision velocities and identically zero elsewhere. The locus of possible collision outcomes is given by the overlaid circle. That is to say, any two velocities which lie on the circle directly across from one another represent a possible collision outcome. As there are infinitely many possible outcomes, the selection of a single outcome is performed stochastically.

The Distributional Monte Carlo Methods developed by the author represent the density function not as in (1.11) or (1.12), but rather as

$$f(v) = \frac{1}{N_p} \sum_{i=1}^{N_p} f_i(v) \tag{1.15}$$

where f_i is the density function of the i^{th} simulated particle. In developing such a scheme for the space homogeneous case, the most important choices one must consider are how to approximate f_i and how to compute collision interactions between particle pairs. The current work presents the results for two specific schemes.

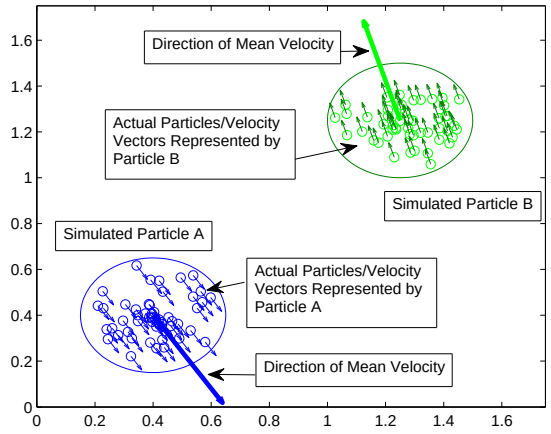
The first scheme is an approach which employs a fixed functional form of f_i, and is termed DMC-KDE, where KDE stands for Kernel Density Estimator. In this case, each particle's density function assumes a prescribed form, namely

$$f_i(v) = \frac{1}{h^3} K\left(\frac{v - v_i}{h}\right) \tag{1.16}$$

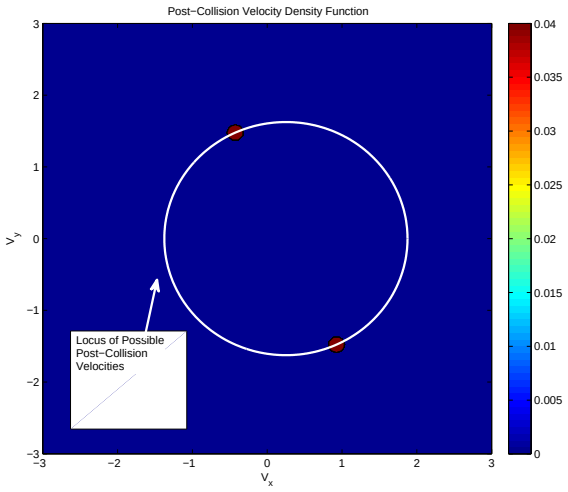
where, $K \in L^2\left(\mathbb{R}^3\right)$ satisfies

$$\int_{\mathbb{R}^3} K(v)\, dv = 1 \tag{1.17}$$

$$\int_{\mathbb{R}^3} vK(v)\, dv = 0 \tag{1.18}$$



(a) A Collision Pair Prior to Collision



(b) Velocity Density Function of Actual Particles

Figure 1.4: DSMC Post-Collision Modeling

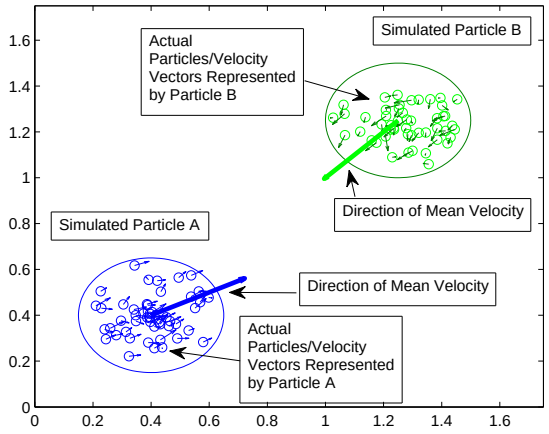
and $h \in \mathbb{R}^+$. Under these conditions, (1.15) assumes the form of a Kernel Density Estimator, where K is the kernel function and h is the bandwidth. Unlike a point measure approximation, it will be shown that an approach based on this technique achieves convergence for $L^\infty\left(\mathbb{R}^3\right)$ solutions of the space homogeneous Boltzmann equation, as well as pointwise convergence for bounded solutions, whereas DSMC converges only in law (or

weakly). A sufficient criteria for convergence of the method will be shown that h must be chosen as a function of N_p in such a way that $h \to 0$ as $N_p \to \infty$.

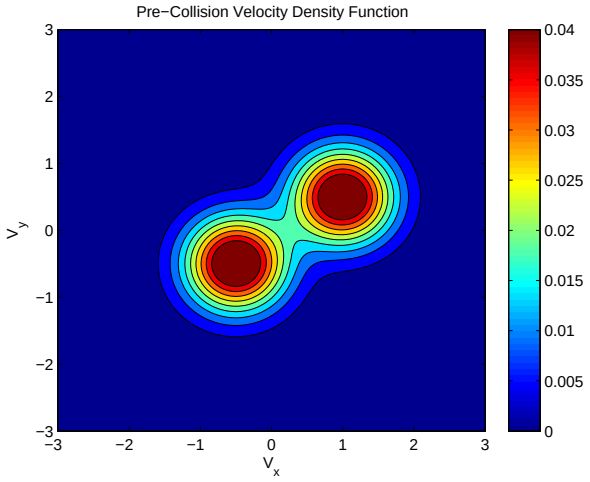
An intuitive choice for K is a Maxwellian density, in which case the actual particles represented by a single particle are no longer assumed to possess the exact same velocity, but rather have velocities distributed according to a Maxwellian distribution. The physical interpretation of this approach is that the actual particles represented by a simulated particle are in thermodynamic equilibrium with one another. This situation is illustrated in Figure 1.5(a). Note that the actual particles are no longer constrained to possess the same velocities. The velocity density function prior to collision of the actual particles represented by the simulated collision pair is illustrated in Figure 1.5(b). Note that unlike DSMC, the distribution function is no longer singular, but rather bimodal, being a sum of Maxwellians.

As will be discussed later, the DMC-KDE method represents a kernel density estimator applied to the DSMC technique. While simulated particles are allowed to posses non-singular distributions, collision simulation is still performed using similar rules to DSMC to assign the mean of the post-collision Maxwellian distributions. The post-collision situation is outlined in Figure 1.6(a). In this case the actual particles are not assumed to possess the exact same velocity, but note that the mean velocity of the collection is the same as the post-collision velocity computed in DSMC (Figure 1.4(a)). The post-collision velocity density function is given in Figure 1.6(b). In this case, valid solutions for the center points of the Maxwellian density functions will lie on opposite sides of the locus of the overlaid circle.

As will be discussed, the replacement of the point measure representation with the non-singular DMC-KDE form allowed the author to prove strong convergence of the method for $L^\infty\left(\mathbb{R}^3\right)$ and bounded solutions of the space homogeneous Boltzmann equation. This was the first time that a stochastic particle simulation was shown to converge in this



(a) A Collision Pair Prior to Collision

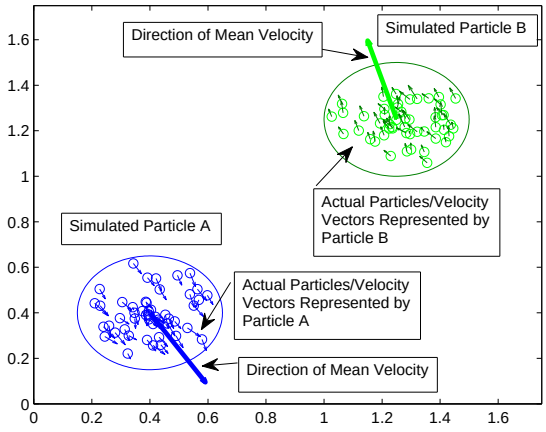


(b) Velocity Density Function of Actual Particles

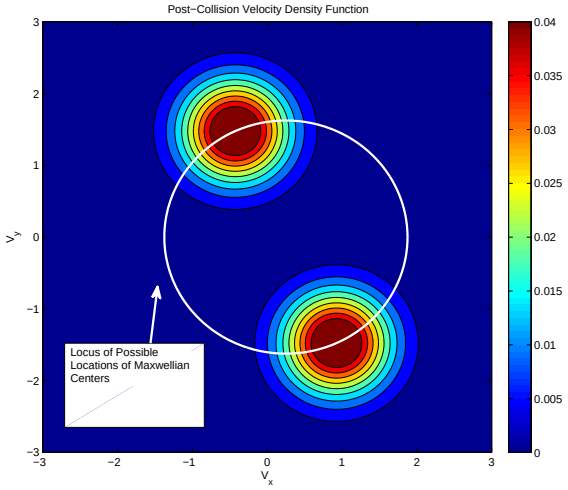
Figure 1.5: DMC-KDE Pre-Collision Modeling

sense, as opposed to simply in law. Unfortunately, it will be observed that the method does not achieve a significant variance reduction over traditional DSMC. Even so, the method is valuable from a practical perspective in that it allows for direct evaluation of the velocity density function.

Although valuable in its own right, DMC-KDE does not fully embody the Distributional Monte Carlo concept envisioned by this research. In the general Distributional Monte



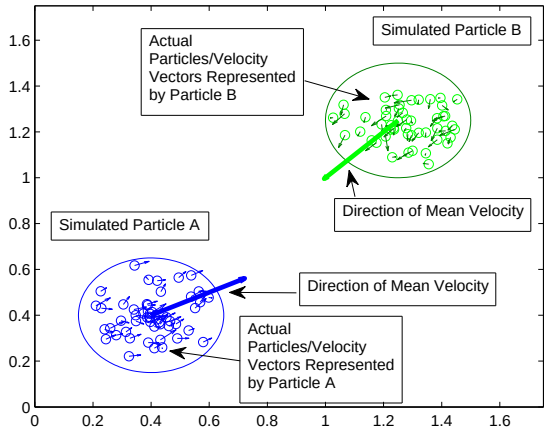
(a) A Collision Pair Post Collision



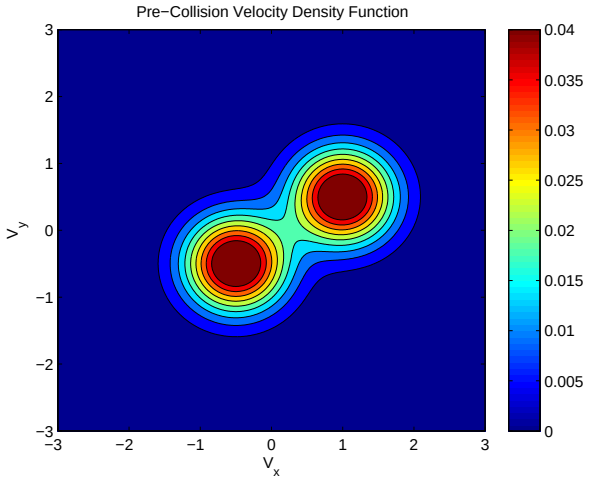
(b) Velocity Density Function of Actual Particles

Figure 1.6: DMC-KDE Post-Collision Modeling

Carlo approach, particles may possess arbitrary velocity density functions, and interactions are computed as a space homogeneous relaxation over the current time step of the combined density function of the two simulated particles involved in a collision. Figures 1.7(a) and 1.7(b) illustrate the pre-collision conditions for two simulated particles each possessing Maxwellian distribution functions prior to collision.



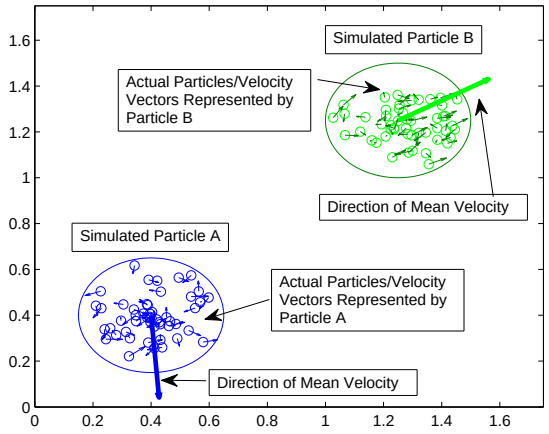
(a) A Collision Pair Pre Collision



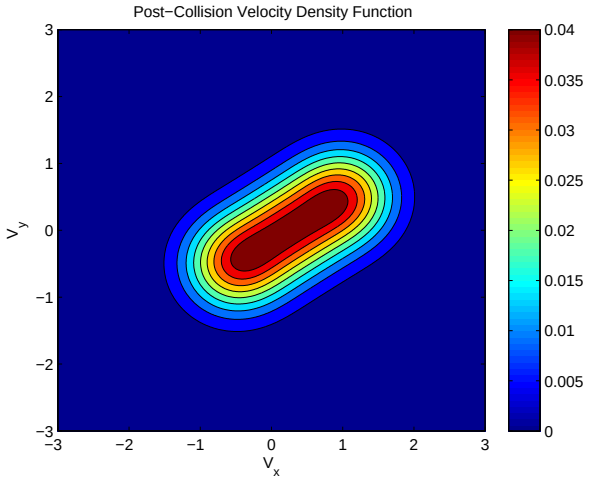
(b) Velocity Density Function of Actual Particles

Figure 1.7: DMC Pre-Collision Modeling

Instead of basing the collision modeling on a binary collision between the simulated particles, the method computes the post-collision velocity density function of both particles by computing an approximate space homogeneous relaxation of the initial density function over the current time step. As the time step is increased the post collision solution tends toward a Maxwellian. This is illustrated in Figures 1.8(a) and 1.8(b).



(a) A Collision Pair Post Collision



(b) Velocity Density Function of Actual Particles

Figure 1.8: DMC Post-Collision Modeling

In this work, the author derives and proves that so long as the binary collision relaxation calculation is consistent with the Boltzmann equation, the Distributional Monte Carlo method converges in law to the Boltzmann solution. Additionally, the method exhibits strong convergence for $L^{\infty}\left(\mathbb{R}^3\right)$ solutions. This marks the first development of a non-point measure based stochastic particle method for the Boltzmann equation, as well

as the first proof of such a method's convergence. This is the main contribution of this work.

Finally, in order to obtain numerical results, the method was implemented using a BGK [11] approximation for collision simulation. This approach is termed DMC-BGK. Although not completely consistent with the Boltzmann equation, the BGK approximation is commonly applied in rarefied gas dynamics. It should be noted that this does not detract from the theoretical proof previously discussed, as many suitable approaches exist which are consistent with the space-homogeneous Boltzmann equation (e.g. moment methods, spectral methods, etc.); the BGK approximation was chosen simply because its ease of coding allowed for rapid generation of numerical solutions. The approach is applied to the well-studied Bobylev-Krook-Wu [22, 50] problem, where it is observed to have significantly reduced variance over traditional DSMC.

The remainder of this work is outlined as follows: Chapters 2 and 3 provide the necessary background and results on the space-homogeneous Boltzmann equation and the Direct Simulation Monte Carlo Method. Chapter 4 presents the DMC-KDE method, proof of convergence of the method, and numerical results on the Bobylev-Krook-Wu problem. Chapter 5 presents the general Distributional Monte Carlo approach in detail as well as proof of its convergence in law to the Boltzmann solution. Also in Chapter 5, the DMC-BGK approach is detailed and applied numerically to the Bobylev-Krook-Wu problem. Chapter 6 summarizes the conclusions and findings of this work and outlines potential areas of fertile research for future investigators.

II. The Boltzmann equation

The Boltzmann equation (1.6) is the governing equation of kinetic theory. As introduced in Chapter 1, the fundamental assumption of kinetic theory is that all macroscopic properties of a gas can be deduced from a knowledge of the interactions and internal structure of its constituent molecules [41]. Remarkably, the fundamentals of kinetic theory were first formally postulated by Ludwig Boltzmann [23] at a time when the atomic makeup of matter was not an accepted concept. Modern physics realizes Boltzmann's vision as the application of statistical mechanics to a gas. Although the development of these concepts can be traced back nearly 150 years, it has been only over the last 50 years that significant contributions have been made to understanding some of the mathematical properties (e.g. existence and uniqueness of solutions) of the Boltzmann equation [1, 2, 26, 46, 54]. Numerical methods for the Boltzmann equation were successfully developed and applied to the study of basic physical flows over the last 30 years [14, 18, 57], but have only recently made significant inroads to applications of practical interest in both hypersonic/high altitude flight [24, 44] and microscale flows [37].

To understand and appreciate the development of the methods described in this work, it is necessary to begin with a brief general discussion of the Boltzmann equation (1.6). This chapter briefly outlines the assumptions behind and derivation of the Boltzmann equation, before simplifying to the space homogeneous Boltzmann equation which is the basis for the remainder of this work. The chapter concludes with the presentation of a well known solution [22, 50] of the space homogeneous Boltzmann equation which has been employed in numerous studies [52, 64] to examine the performance of various numerical methods.

The Boltzmann equation is a probabilistic representation of the evolution of the energy state of the molecules comprising the gas under consideration. In general, a molecule may store its energy in a number of modes. It may possess energy in translational and rotational

motion. It may also store energy in a vibrational mode along one or more chemical bonds. Additionally, the molecule may become electronically excited. To simplify the analysis of the present work, it will henceforth be assumed that the gas under consideration is monatomic and further, that the internal energy capacity of such molecules is negligible. In other words, particles will be assumed to possess only translational energy. This restriction allows study of all of the phenomena of interest without adding unnecessary complexity and does not prohibit later generalization to molecules with internal structure.

As the Boltzmann equation is a probabilistic model of the gas, some basic concepts from probability theory must be introduced before continuing with a brief derivation of the Boltzmann equation. The following definitions motivate the concept of a probability space.

Definition 2.1. *Given a set Ω and a σ-algebra $\mathcal{S}$ of subsets of X, a countably additive function, μ, from $\mathcal{S}$ into $[0, \infty]$ is called a measure and $(\Omega, \mathcal{S}, \mu)$ is called a measure space.*

Definition 2.2. *A measurable space $(\Omega, \mathcal{S})$ is a set Ω with a σ-algebra $\mathcal{S}$ of subsets of Ω.*

Definition 2.3. *Given a measurable space $(\Omega, \mathcal{S})$, a probability measure, P, is a measure on $\mathcal{S}$ with $P(\Omega) = 1$. $(\Omega, \mathcal{S}, P)$ is called a probability space. Elements of $\mathcal{S}$ are called events.*

Definition 2.4. *A law is a Borel probability measure; that is a probability measure defined on the Borel σ-algebra.*

The Boltzmann equation is a relation describing the evolution of a law on the measurable space $(D, \mathcal{D})$, where $D = V \times \mathbb{R}^3$, and $\mathcal{D}$ is the Borel σ-algebra defined on D. Here, $V \subset \mathbb{R}^3$ is the physical volume occupied by the gas, and the remaining dimensions of D represent three components of velocity. In rarefied gas dynamics, D is commonly referred to as the phase space. The following theorem is necessary to motivate the concept of probability density.

Theorem 2.1. *(Radon-Nikodym) [35] On the measurable space $(X, \mathcal{S})$ let μ be a σ-finite measure. Let ν be a finite measure, absolutely continuous with respect to μ. Then for some $h \in \mathcal{L}^1(X, \mathcal{S}, \mu)$,*

$$\nu(E) = \int_E h d\mu \tag{2.1}$$

for all $E \in \mathcal{S}$. Any two such h are equal μ-almost everywhere. h is called the Radon-Nikodym derivative or density of ν with respect to μ, and is written $h = \frac{d\nu}{d\mu}$.

Definition 2.5. *A law P on $\mathbb{R}^k$ is said to have a density f if P is absolutely continuous with respect to Lebesgue measure λ^k and has Radon-Nikodym derivative $\frac{dP}{d\lambda^k} = f$. In other words, $P(A) = \int_A f(x)\, d\lambda^k(x)$ for all Borel sets A.*

For purposes of this work, the term *probability density* will be used to describe the Radon-Nikodym derivative as given in Definition 2.5 so as to avoid confusion with the physical properties of the gas of mass density or number density. As mentioned above, the Boltzmann equation describes the evolution of a probability law for molecular velocity. To be more precise, the Boltzmann equation is an integro-differential equation over the space D for the evolution of the probability density of the law for molecular velocity. Physically speaking, the probability of a molecule existing in a given subset of phase space $A \subset D$ is given by $P(A) = \int_A f(x)\, dx$, where dx denotes the Lebesgue measure in the phase space. This is equivalent to the more common differential description that $f(r, v)\, drdv$ represents the probability of molecule existing in the differential element dr centered at r in physical space, while possessing velocity in the differential element dv centered at v in velocity space. Having established the required mathematical definitions, a brief derivation of the Boltzmann equation based on physical reasoning is next presented.

2.1 Overview of Derivation of the Boltzmann Equation

A brief exposition of the origin of the Boltzmann equation and the development of relations that will later prove useful is discussed herein. Detailed derivations and

discussions of the Boltzmann equation can be found in numerous sources (see, for example Reference [23, 27–30, 32, 41, 74]).

There are a few important physical assumptions that are inherent to the Boltzmann equation. First, one must assume complete collisions. That is, the "dt" time interval involved in the equation is much larger than the collision interaction time [41]. This is somewhat more precise and restrictive than the more common interpretation that only binary collisions occur in the gas. The assumption implies, in fact, that the collisions occur so rapidly (instantaneously) that the probability of a tertiary collision is zero [41].

The next assumption is that f is slowly varying at small scales, i.e. on the order of molecular diameters[41]. This assumption is based on the concept of a thermodynamic limit, namely, that at the physical scales of interest the gas must be capable of being described in a statistically meaningful way. Unless the gas is quite dense this assumption has no implication on how f varies on the order of the mean free path. This assumption limits the Boltzmann equation to dilute gases.

The final assumption inherent to the Boltzmann equation is the existence of molecular chaos [41]. This means that no correlation can exist between the molecular velocities of any two particles which are outside of one another's field of influence. These assumptions can be shown to be consequential from a single assumption termed the Boltzmann-Grad limit [29, 30].

The Boltzmann equation accounts for changes to the density function throughout the phase space by three mechanisms: particle advection through physical space, particle acceleration by means of some external force, and intermolecular collisions. Let $drdv$ represent a differential element of phase space centered at (r, v). By accounting for these mechanisms, one can determine a balance equation for particle accumulation within the differential element of phase space over the differential time dt. Heuristically, we seek an

expression of the form

$$\frac{\partial f}{\partial t}(r,v,t) = \left(\frac{\partial f}{\partial t}\right)_{Adv}(r,v,t) + \left(\frac{\partial f}{\partial t}\right)_{Accel}(r,v,t) + \left(\frac{\partial f}{\partial t}\right)_{Coll}(r,v,t) \tag{2.2}$$

where, $\left(\frac{\partial f}{\partial t}\right)_{Adv}$ represents the rate of change of f due to particle advection, $\left(\frac{\partial f}{\partial t}\right)_{Accel}$ represents the rate of change of f due to particle acceleration, and $\left(\frac{\partial f}{\partial t}\right)_{Coll}$ represents the rate of change of f due to intermolecular collisions. Considering only elementary mechanics, it can be shown [29, 74] that the changes due to advection, and particle acceleration are given by

$$\left(\frac{\partial f}{\partial t}\right)_{Conv}(r,v,t) = -v \cdot \nabla_r f(r,v,t) \tag{2.3}$$

$$\left(\frac{\partial f}{\partial t}\right)_{Accel}(r,v,t) = -F(r,t) \cdot \nabla_v f(r,v,t) \tag{2.4}$$

where $F(r,t)$ is the total external force acting at r at time t.

The term resulting from collisions requires some additional considerations. At a given time and location in phase space, we must account for all possible collisions that result in particles with pre-collision velocities outside the differential element dv centered at v attaining a post-collision velocity within dv. Additionally, we must account for all possible collisions that result in particles with pre-collision velocities within the differential element dv centered at v attaining post-collision velocities outside dv. Generically, we will represent these gain and loss terms by the symbols G and L, respectively, and write

$$\left(\frac{\partial f}{\partial t}\right)_{Coll}(r,v,t) = G(r,v,t) - L(r,v,t) \tag{2.5}$$

In order to analyze G and L properly, one must first consider the mechanics of a binary collision between two particles. Conceptually, the easiest model to employ is the hard sphere, or billiard ball model of a molecule. Although the model is physically imperfect, it provides a credible starting point for this analysis and the modifications required for other molecular models will be discussed shortly.

To begin, consider two particles undergoing a collision with velocities v and w respectively. Denote the relative velocity of the particles by $V = v - w$. Denote the velocities of the two molecules post collision by v' and w', and the post collision relative velocity by $V' = v' - w'$.

During the collision, both momentum and kinetic energy must be conserved, which implies [30]

$$v + w = v' + w' \tag{2.6}$$

$$\|v\|^2 + \|w\|^2 = \|v'\|^2 + \|w'\|^2 \tag{2.7}$$

Let n be a unit vector directed along $v - v'$. Then the post-collision velocities are related to the pre-collision velocities via

$$v' = v - [n \cdot V]\, n \tag{2.8}$$

$$w' = w + [n \cdot V]\, n \tag{2.9}$$

which implies

$$V' = V - [2n \cdot V]\, n \tag{2.10}$$

From the reference frame of the first molecule, this means that the second molecule is specularly reflected and n is directed along the line of centers. This reference frame provides a convenient method for computing the gain and loss terms sought above. Specifically, let d represent the diameter of a single molecule. In this reference frame let particle 1 be a sphere at rest and endowed with diameter $2d$, and view the remaining particles as point masses moving with velocity $V = w - v$. Next, one must determine the probability that a particle possessing velocity w impacts the sphere at the differential surface element $dS = d^2 dn$ during the time interval $[t, t + dt]$. If a particle is to exhibit such a collision it must lie within the slant cylinder traced out by the differential element over dt which has height $\|V\|\, dt$ and volume $|V \cdot n|\, dS\, dt$. The probability that a molecule satisfies

these requirements is given by

$$f(r, w, t)\,|V \cdot n|\,dS\,dw dt \tag{2.11}$$

where dw represents a differential element of velocity space centered at w.

What we have established in (2.11) is the probability of a collision between a molecule with velocity in the differential element dw impacting a single molecule with velocity in the differential element dv, but have said nothing of the probability of the first molecule possessing a velocity in the differential element dv. Therefore the probability of any molecule with velocity in the differential element dw impacting any molecule with velocity in the differential element dv per unit time is given by [74]

$$f(r, v, t)\, f(r, w, t)\,|V \cdot n|\,dS\,dw dv \tag{2.12}$$

This is commonly referred to as a collision of class (v, w) [74]. The L term we seek in (2.5) is due to the loss of particles with velocity in the differential element dv due to collisions with particles of any other velocity. Therefore, we conclude

$$L(r, v, t) = \int_{\mathbb{R}^3} \int_{S^-} f(r, v, t)\, f(r, w, t)\, d^2\,|V \cdot n|\,dn dw \tag{2.13}$$

where S^- is the hemisphere corresponding to $V \cdot n < 0$, i.e. orientations over which particles are moving toward each other prior to the collision [29]. A similar analysis can be performed to determine an expression for G. To do this, one must consider the concept of *inverse collisions* or *replenishing collisions* for a given collision class. Given a collision between molecules with velocities v_1 and v_2, an inverse collision is any collision which has initial velocities equal to the final velocities of the original collision and the same direction of the line of centers [74]. Using this concept one can determine the G term we seek in (2.5), which represents the replenishment of particles in the differential element dv centered at v due to collisions, is given by [30, 74]

$$G(r, v, t) = \int_{\mathbb{R}^3} \int_{S^+} f(r, v', t)\, f(r, w', t)\, d^2\,|V \cdot n|\,dn dw \tag{2.14}$$

Therefore, we conclude that

$$\left(\frac{\partial f}{\partial t}\right)_{Coll}(r,v,t) = \int_{\mathbb{R}^3}\int_{S^+}\left[f(r,v',t)\,f(r,w',t) - f(r,v,t)\,f(r,w,t)\right] d^2\,|(v-w)\cdot n|\,dndw \tag{2.15}$$

where,

$$v' = v - [n\cdot(v-w)]\,n \tag{2.16}$$

$$w' = w + [n\cdot(v-w)]\,n \tag{2.17}$$

The right hand side of (2.15) is known as the collision integral and is the main source of complexity in the Boltzmann equation. Thus, the Boltzmann equation for a monatomic hard sphere gas is given by

$$\frac{\partial f}{\partial t}(r,v,t) + v\cdot\nabla_r f(r,v,t) + F(r,t)\cdot\nabla_v f(r,v,t) = \int_{\mathbb{R}^3}\int_{S^+}\left[f(r,v',t)\,f(r,w',t) - f(r,v,t)\,f(r,w,t)\right] d^2\,|(v-w)\cdot n|\,dndw \tag{2.18}$$

As previously mentioned, other molecular models beyond hard sphere exist; some of which are preferred due to improved physical accuracy and others because of mathematical simplicity. It can be shown [28, 29] that in such cases the only required modification to the above is to replace the term $d^2\,|(v-w)\cdot n|$ with a function of $\|v-w\|$, and θ, the angle between n and $v-w$. In this case, the Boltzmann equation becomes

$$\frac{\partial f}{\partial t}(r,v,t) + v\cdot\nabla_r f(r,v,t) + F(r,t)\cdot\nabla_v f(r,v,t) = \int_{\mathbb{R}^3}\int_{S^+}\left[f(r,v',t)\,f(r,w',t) - f(r,v,t)\,f(r,w,t)\right] B(\theta,\|v-w\|)\,dwd\theta d\epsilon \tag{2.19}$$

where ϵ is the second angle defining the orientation of n on the unit sphere, and B is called the collision cross section or collision kernel. In the case of hard spheres, $B(\theta,\|v-w\|) = \cos(\theta)\sin(\theta)\|v-w\|$. Another common model is called the inverse power law, in which the attractive force between two particles is assumed to vary as the n-th inverse power of the distance between them. In this case, B is given by

$$B(\theta,\|v-w\|) = \beta(\theta)\,\|v-w\|^{\frac{n-5}{n-1}} \tag{2.20}$$

where the function β incorporates the collision orientation. The case of $n = 5$ gives rise to the Maxwell molecule, in which case the dependence on $\|v - w\|$ vanishes [53].

2.1.1 Relation to the Continuum Equations of Fluid Mechanics.

During this general discussion of the Boltzmann equation, it is worth noting its connection to the continuum equations of fluid motion.

Upon taking the moment of the Boltzmann equation with respect to m, mv, and $\frac{1}{2}m\|v\|^2$, expressions for the conservation of mass, momentum, and energy in the gas will result. These expressions will vary with respect to the form of f. If f is locally Maxwellian, the resulting set of conservation equations reduces to the well known Euler equations of fluid mechanics.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u = 0 \tag{2.21}$$

$$\frac{\partial \rho u}{\partial t} + (\nabla \cdot \rho u)\, u + \nabla P = 0 \tag{2.22}$$

$$\frac{\partial e}{\partial t} + \nabla \cdot (e + P)\, u = 0 \tag{2.23}$$

where e is the specific energy. As stated previously, however, an equilibrium (locally Maxwellian) description is not sufficient to capture all of the phenomena of interest. A method which attempts to address this situation was proposed first by Hilbert [42] and later developed independently by Chapman and Enskog [31, 36]. The method expands the distribution function in a Hilbert series from a local Maxwellian.

$$f = f_M \left(1 + \Phi^{(1)} + \Phi^{(2)} + \cdots\right) \tag{2.24}$$

Truncating the expansion, one may develop expressions for the $\Phi^{(i)}$ terms. For example, including the first correction term one obtains the Navier-Stokes equations.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u = 0 \tag{2.25}$$

$$\frac{\partial \rho u}{\partial t} + (\nabla \cdot \rho u)\, u + \nabla p = \frac{1}{Re} \nabla \tau_{ij} \tag{2.26}$$

$$\frac{\partial e}{\partial t} + \nabla \cdot (e + p)\, u = -\frac{1}{RePr} \left[\nabla \cdot q\right] \tag{2.27}$$

The inclusion of the first correction term allows for the physical phenomena of viscosity and thermal conductivity in the gas. This results in the appearance of the shear stress tensor, τ_{ij}, the heat flux vector, q, as well as the Reynold's Number, Re, and Prandtl Number, Pr. Including the second order term yields the Burnett equations, the third yields the Super-Burnett equations and so forth. It is important to note however that while the connection is seen to exist to the continuum equation sets, there is no guarantee that such a truncated approximation will be a good one. In fact, open debate continues over whether the Burnett and higher order sets add any accuracy over the Navier-Stokes equations, and it has been shown that there are situations in which they violate the second law of thermodynamics [34, 39].

2.2 The Space Homogeneous Boltzmann equation

Clearly, much of the complexity associated with the Boltzmann equation is inherent to the right-hand side which is known as the collision integral. For this reason, it is common to study the space homogeneous version of the equation. It is also common to neglect the influence of external forces, in which case the equation reduces to

$$\frac{\partial f}{\partial t}(v,t) = \int_{\mathbb{R}^3}\int_{S^+}\left[f(v',t)\,f(w',t) - f(v,t)\,f(w,t)\right]B(\theta,\|v-w\|)\,dwd\theta d\epsilon \tag{2.28}$$

The equation is solved subject to the initial condition $f(v,0) = f_0(v)$, where $f_0 \in L^1\left(\mathbb{R}^3\right)$ is a non-negative function which satisfies the normalization condition

$$\int_{\mathbb{R}^3} f(v)\,dv = 1 \tag{2.29}$$

Additionally, in order to maintain finite energy, the boundary condition,

$$\lim_{\|v\|\to\infty} f(v,t) = 0 \text{ for all } t \geq 0 \tag{2.30}$$

is imposed. In the space homogeneous case, any changes to f are solely due to intermolecular collisions. Existence and uniqueness of solutions of (2.28) was established by Akeryd [1, 2].

Another common notation is to denote the collision integral by $Q(f, f)$ where Q is the functional defined by [30]

$$\begin{aligned} Q(f, g) = \int_{\mathbb{R}^3} \int_{S^+} & \left[f(v', t)\, g(w', t) + f(w', t)\, g(v', t) \right. \\ & \left. - f(v, t)\, g(w, t) - f(w, t)\, g(v, t) \right] B(\theta, \|v - w\|)\, dw d\theta d\epsilon \end{aligned} \tag{2.31}$$

In this case the space homogeneous equation can be written as

$$\frac{\partial f}{\partial t}(v, t) = Q(f, f) \tag{2.32}$$

A fundamental solution is the case when $Q(f, f) = 0$. In this case, the density function is constant and depleting collisions are exactly balanced by replenishing collisions for all collision classes. This state is known as translational thermodynamic equilibrium. It can be shown [74] that the solution for which this criteria holds is the Maxwell-Boltzmann density function

$$f(v) = \alpha_1 \exp\left[-\alpha_2 \|v - u\|^2 \right] \tag{2.33}$$

where $\alpha_{1,2}$ are constants that depend upon the physical characteristics of the gas, and u represents the bulk fluid velocity. One frequently considers the case where $u = 0$ which is known as a nondrifting Maxwellian [29].

Let ϕ be a real valued function over $\mathbb{R}^3$ such that $\int_{\mathbb{R}^3} \phi(v)\, Q(f, f)\, dv$ exists. Cercignani shows [29]

$$\begin{aligned} \int_{\mathbb{R}^3} \phi(v)\, Q(f, f)\, dv = \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^+} & \left[f(v')\, f(w') - f(v)\, f(w) \right] \cdot \\ & \left[\phi(v) + \phi(w) - \phi(v') - \phi(w') \right] B(\theta, \|v - w\|)\, dw dv dn \end{aligned} \tag{2.34}$$

as well as the more compact form

$$\begin{aligned} \int_{\mathbb{R}^3} \phi(v)\, Q(f, f)\, dv = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^+} & f(v)\, f(w) \cdot \\ & \left[\phi(v') + \phi(w') - \phi(v) - \phi(w) \right] B(\theta, \|v - w\|)\, dw dv dn \end{aligned} \tag{2.35}$$

The right-hand side of (2.35), can be made to be zero independent of f if

$$\phi(v) + \phi(w) = \phi(v') + \phi(w') \tag{2.36}$$

almost everywhere in velocity space [29]. Since the left-hand side of (2.35) represents the net rate of change of the average value of ϕ due to collisions, any ϕ for which $\int_{\mathbb{R}^3} \phi(v) Q(f,f)\, dv = 0$ for any f is termed a collision invariant.

It can be shown [29] that there exists a five-dimensional subspace of continuous functions which are collision invariants that is spanned by the functions, $\{\psi_i\}_{i=1}^5$, given by

$$\psi_1(v) = 1 \tag{2.37}$$

$$\psi_2(v) = v_x \tag{2.38}$$

$$\psi_3(v) = v_y \tag{2.39}$$

$$\psi_4(v) = v_z \tag{2.40}$$

$$\psi_5(v) = \|v\|^2 \tag{2.41}$$

This is not a surprising result, as the appearance of ψ_1 is a statement of the conservation of mass, whereas (ψ_2, ψ_3, ψ_4) result from the conservation of momentum in each of the cardinal directions and ψ_5 is a statement of the conservation of energy.

Next, we note that a special case exists when $\phi = \log f$. If $\int_{\mathbb{R}^3} \log(f) Q(f,f)\, dv$ exists, it can be shown [74] that

$$\int_{\mathbb{R}^3} \log(f) Q(f,f)\, dv \leq 0 \tag{2.42}$$

This is known as the Boltzmann inequality and is required to prove the Boltzmann H-Theorem, which applies not just to the space homogeneous equation but to the general Boltzmann equation as well.

Theorem 2.2. *Boltzmann's H-Theorem. Let* $\mathcal{H}(t) = \int_{\mathbb{R}^3} f(v,t) \log(f(v,t))\, dv$ *Then*

$$\frac{d\mathcal{H}}{dt}(t) \leq 0 \tag{2.43}$$

Further, $\frac{d\mathcal{H}}{dt} = 0$ *if and only if* f *is a Maxwell-Boltzmann density function.*

The function $\mathcal{H}$ is commonly referred to as Boltzmann's H-function. This theorem is the analogue of the second law of thermodynamics at the microscopic level, in fact,

it can be shown [47, 74] that the entropy of the gas is related to the H-function by $S = -k_B\mathcal{H}$. This is important because it demonstrates that the Boltzmann equation possesses the basic thermodynamic feature of irreversibility [30]. It also indicates that the Maxwellian distribution is the prevailing distribution in thermodynamic equilibrium, a state characterized by zero entropy generation.

2.2.1 Results on Existence and Uniqueness of Solutions.

Existence and uniqueness of solutions for the space homogeneous Boltzmann equation (2.28) is a well studied area. Carleman [25] proved existence and uniqueness of solutions for continuous initial conditions which satisfied $(1 + \|v\|^\kappa) f_0(v) \in L^\infty\left(\mathbb{R}^3\right)$ for some $\kappa > 6$. Morgenstern [54, 55] proved the same for Maxwellian molecules with a truncated collision kernel and initial conditions $f_0 \in L^1\left(\mathbb{R}^3\right)$. Povzner [59] proved existence and uniqueness for continuous collision kernels that obey $B(\theta, V) \leq C(1 + V)$, where $C \in \mathbb{R}^+$ and initial conditions f_0 with $\left(1 + \|v\|^4\right) f_0(v) \in L^1\left(\mathbb{R}^3\right)$. The results presented herein are due to Akeryd [1, 2], and represent a more general result for bounded collision kernels. The following theorem combines several of Akeryd's results.

Theorem 2.3. *Suppose that*

$$0 \leq B(\theta, \|v - w\|) \leq K_k \tag{2.44}$$

for all $v, w \in \mathbb{R}^3$, $\theta \in [0, 2\pi]$. *Here,* $K_k \in \mathbb{R}^+$. *If* $f_0 \in L^1\left(\mathbb{R}^3\right)$, *with* $f_0 \geq 0$ *and* $\int_{\mathbb{R}^3} f_0(v)\, dv = 1$, *then there exists a unique, nonnegative solution* $f(v,t) \in L^1\left(\mathbb{R}^3\right)$ *of the space homogeneous Boltzmann equation (2.28) with* $f(v,0) = f_0(v)$.

Furthermore, if $\left(1 + \|v\|^2\right) f_0(v) \in L^1\left(\mathbb{R}^3\right)$, *then* $f(v,t)\left(1 + \|v\|^2\right) \in L^1\left(\mathbb{R}^3\right)$ *for all* $t > 0$ *and*

$$\int_{\mathbb{R}^3} f(v,t)\, dv = \int_{\mathbb{R}^3} f_0(v)\, dv \tag{2.45}$$

$$\int_{\mathbb{R}^3} v f(v,t)\, dv = \int_{\mathbb{R}^3} v f_0(v)\, dv \tag{2.46}$$

$$\int_{\mathbb{R}^3} \|v\|^2 f(v,t)\, dv = \int_{\mathbb{R}^3} \|v\|^2 f_0(v)\, dv \tag{2.47}$$

for all $t > 0$*. Also, if* $f_0 \log f_0 \in L^1\left(\mathbb{R}^3\right)$*, then* $f(v,t)\log f(v,t) \in L^1\left(\mathbb{R}^3\right)$ *for all* $t > 0$*, and*

$$\mathcal{H}(t) = \int_{\mathbb{R}^3} f(v,t)\log\left(f(v,t)\right) dv \tag{2.48}$$

is a nonincreasing decreasing function in t.

2.2.2 The Bobylev, Krook, and Wu Solution.

Although many of the fundamental mathematical properties such as existence and uniqueness of solutions of the Boltzmann equation have been solved, and several approximate approaches exist, a characterizing feature of the equation has been the nearly complete absence of exact analytical results [22]. One well known exception is the Bobylev-Krook-Wu solution of the space homogeneous equation, first published by Bobylev [19–21] and later independently by Krook and Wu [49, 50]. The problem has thus served as a useful test case for various schemes (e.g. [52, 58]) and will be utilized in the same capacity by the work presented herein. For this reason, a brief background on the solution is presented here.

The solution is specific to Maxwellian Molecules. Without loss of generality, Bobylev considered the following initial conditions

$$\int_{\mathbb{R}^3} v f_0(v)\, dv = 0 \tag{2.49}$$

$$\int_{\mathbb{R}^3} \|v\|^2 f_0(v)\, dv = 3 \tag{2.50}$$

which by (2.41) will hold for all $t > 0$. These moments correspond to the net momentum and energy of the gas, and thus by utilizing (2.33) the corresponding Maxwell-Boltzmann density function (the solution as $t \to \infty$) can immediately be determined to be

$$f_{MB}(v) = (2\pi)^{-3/2}\exp\left(-\frac{\|v\|^2}{2}\right) \tag{2.51}$$

Bobylev's approach was to perform a Fourier transform on the space homogeneous Boltzmann equation. Under this representation, the velocity density function is replaced

by the Fourier variable Φ defined as,

$$\Phi(k,t) = \int_{\mathbb{R}^3} f(v,t) \exp(-ik \cdot v)\, dv \tag{2.52}$$

where $k \in \mathbb{R}^3$ is the variable in the Fourier domain. The transformed space homogeneous equation becomes

$$\begin{aligned} \frac{\partial \Phi}{\partial t} &= \int_{\mathbb{R}^3} Q(f,f) \exp(-ik \cdot v)\, dv \\ &= \int_{S^+} \beta\left(\frac{k \cdot n}{\|k\|}\right)\left[\Phi\left(\frac{k + \|k\| n}{2}\right)\Phi\left(\frac{k - \|k\| n}{2}\right) - \Phi(0)\,\Phi(k)\right] dn \end{aligned} \tag{2.53}$$

Note the drastic simplification that results from taking the Fourier transform, namely the five dimensional integral in (2.28) is reduced to a two dimensional integral. The strategy, therefore, is to determine the solution of (2.53) and invert the transformation to obtain the density function via the inversion formula

$$f(v,t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \Phi(k,t) \exp(ik \cdot v)\, dk \tag{2.54}$$

(2.53) must be solved subject to the transformed initial and normalization conditions

$$\Phi_0(k) = \int_{\mathbb{R}^3} f_0(v) \exp(-ik \cdot v)\, dv \tag{2.55}$$

Also, the transformed Maxwellian, Φ_{MB}, can be determined by direct substitution of (2.51) into (2.52) and is given by

$$\Phi_{MB}(k) = \exp\left(-\frac{\|k\|^2}{2}\right) \tag{2.56}$$

Bobylev then sought to determine a similarity solution of (2.53) of the form

$$\Phi(k,t) = \Phi_0\left(ke^{-\mu t}\right) \exp\left[-\frac{\|k\|^2}{2}\left(1 - e^{-2\mu t}\right)\right] \tag{2.57}$$

where $\mu \in \mathbb{R}^3$. This is further simplified by seeking an isotropic solution, the simplest of which can be written as

$$\Phi(x,t) = \left(1 - \Theta x e^{-\lambda t}\right) \exp\left[-x\left(1 - \Theta e^{-\lambda t}\right)\right] \tag{2.58}$$

where $x = \frac{\|k\|^2}{2}$ and the parameter Θ is any real number in the interval $\left[0, \frac{2}{5}\right]$. Note the dependence on x versus k clearly exhibits the isotropic property of the solution. The variable $\lambda \in \mathbb{R}^+$ is dependent upon the collision cross section and is given by

$$\lambda = \frac{\pi}{2} \int_0^{2\pi} \beta(\theta) \left(1 - \cos(\theta)^2\right) d\theta \tag{2.59}$$

Applying the inverse transform to (2.58) results in the final expression for the density function

$$f(v,t) = \frac{1}{(1\pi\tau(t))^{-3/2}} \exp\left(-\frac{\left\|v^2\right\|}{2\tau(t)}\right)\left[1 + \frac{1-\tau(t)}{\tau(t)}\left(\frac{\|v\|^2}{2\tau} - \frac{3}{2}\right)\right] \tag{2.60}$$

where $\tau(t) = 1 - \Theta e^{-\lambda t}$. This was the first known nontrivial closed form solution of the space homogeneous Boltzmann equation [22]. Bobylev defines the following normalized even moments of the distribution function

$$z_n(t) = \frac{1}{(2n+1)!!} \int_{\mathbb{R}^3} \|v\|^{2n} f(v,t)\, dv \; n = 1, 2, \ldots \tag{2.61}$$

where,

$$(2n+1)!! = \prod_{i=1}^{n} (2i+1) \tag{2.62}$$

In the process of obtaining his solution, Bobylev was able to exploit the isotropic nature of the solution and determine expressions for these moments fairly simply in the Fourier domain. The resulting normalized moments, z_n are given by

$$z_n(t) = \left(1 - \Theta e^{-\lambda t}\right)^{n-1} \left[1 + (n-1)\Theta e^{-\lambda t}\right] \tag{2.63}$$

The simplicity of this closed form solution lends it to great use in evaluating numerical schemes for the Boltzmann equation (e.g. [52, 56, 58, 63, 64]), and will be used towards that end in the present work as well. The present work will utilize the solution for $\lambda = 1/6$ and $\Theta = 2/5$. Visualizing the velocity density function can be difficult given its inherent dimensionality, however, as the present solution is spherically symmetric one can readily derive the density function for molecular speed by moving to spherical polar coordinates

and integrating out the directional dependence from (2.60)

$$F(\|v\|,t)=\frac{4\pi}{(2\pi)^{-3/2}}\|v\|^2\exp\left(-\frac{\|v\|^2}{2\tau(t)}\right)\left[1+\frac{1-\tau(t)}{\tau(t)}\left(\frac{\|v\|^2}{2\tau(t)}-\frac{3}{2}\right)\right] \tag{2.64}$$

The speed density function is shown in Figure 2.1 below. In many situations it is not

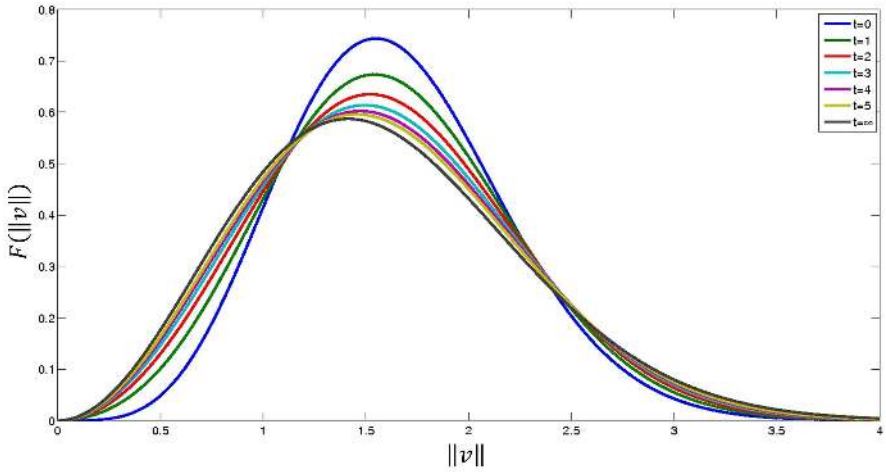


Figure 2.1: Molecular Speed Density Function of Bobylev-Krook-Wu Solution

practical to directly compare the density function (e.g. DSMC, which converges in law but does not directly produce a convergent density function), and therefore it is common to employ a comparison of the even moments of the Bobylev-Krook-Wu solution. The first four moments are illustrated in Figure 2.2.

These results have been employed in the current work as a numerical test case for the various algorithms under development and represent a standard benchmark problem for Boltzmann simulators and solvers.

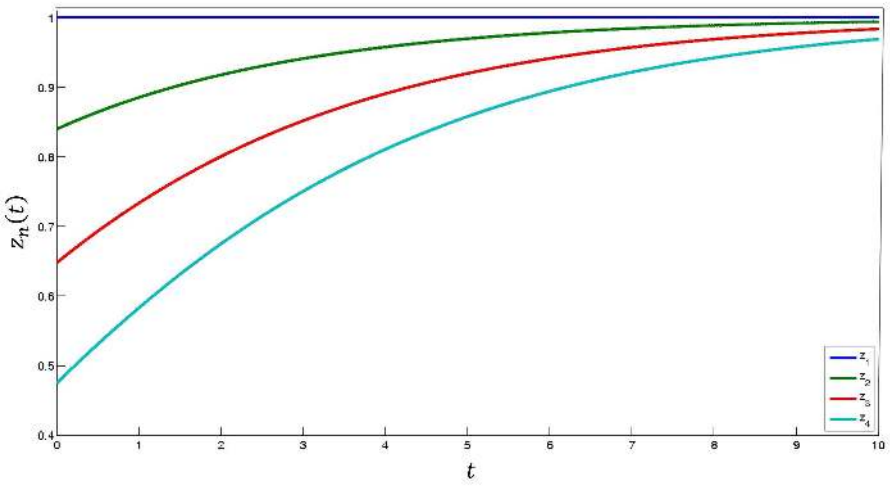


Figure 2.2: First Four Even Moments of Bobylev-Krook-Wu Solution

III. The Direct Simulation Monte Carlo Method

3.1 Overview

The Direct Simulation Monte Carlo Method was originally proposed by Bird in 1963 [14]. Bird entitled the method *Direct Simulation* to distinguish from methods which would be characterized as *Direct Solution* techniques. In other words, Bird's original development of DSMC was never intended to be a numerical solution technique for the Boltzmann equation. Bird argued that a computational simulation of the physics of rarefied gas interactions without explicitly incorporating the Boltzmann equation was more tractable and perhaps more valuable than applying numerical techniques to the equation itself [17].

Others were not as content to accept the simulation process without a connection to the underlying equation and in 1980 Nanbu proposed a DSMC scheme directly derived from the Boltzmann equation [58]. By 1987, Babovsky [8] had proven that Nanbu's scheme was in fact convergent in law to the space homogeneous Boltzmann solution. Two years later, Babovsky and Illner proved the same for the nonhomogeneous equation [9]. Interestingly, as Bird's method itself argues from the same physical assumptions (e.g. dilute gas, molecular chaos, etc.) inherent to the Boltzmann equation, Wagner was later able to prove that in spite of the procedure's ignorance of the Boltzmann equation itself, it did in fact converge to the solution of the Boltzmann equation in law [75].

We utilize results which stem from Nanbu's technique and Babovsky's proof of its convergence, both of which are presented in this chapter. The approaches could be applied equally well to develop techniques that are more like Bird's approach, but the direct traceability to the Boltzmann equation of Nanbu's technique results in a relatively easier path to proving convergence. For this reason, we utilize results from Nanbu's technique over those of Bird's.

3.2 Nanbu's Simulation Technique

In this section, an overview of the original derivation [58] of Nanbu's method is provided while in Section 3.3 an explanation [8] is given which is more amenable to analyzing convergence of the method. Although other DSMC schemes exist which are in more widespread usage, Nanbu's method is presented here due to the clarity with which it can be derived from the Boltzmann equation.

The basic premise of any DSMC scheme is the uncoupling principle, namely, that particle convection and particle collisions are treated independently. In non-homogeneous problems, physical space is discretized by means of a volume grid, and within a cell the solution is assumed to be space homogeneous. For this reason, the original derivation of Nanbu's scheme focused on developing the stochastic relations to simulate the space homogeneous Boltzmann equation. Simulated particle convection is a more trivial problem, as particles simply convect along their velocity vectors for the current time step by $\Delta r = v\Delta t$. The space-homogeneous simulation of the collision operator is therefore the central problem in DSMC. As such, proof of convergence of Nanbu's method was originally obtained for the space homogeneous equation [8] and subsequently for the full Boltzmann equation [9]. With this in mind, the current work focuses solely on space homogeneous results.

Nanbu's derivation seeks to develop a set of stochastic rules governing collision pair selection and collision outcomes for a set of N particles each possessing a velocity vector v_i. Nanbu begins by writing the initial density function for molecular velocity as a point measure approximation

$$f^k(v) = \frac{1}{N_p} \sum_{i=1}^{N_p} \delta\left(v - v_i^k\right) \tag{3.1}$$

where the superscript indicates the k^{th} time step of the simulation. Expanding the temporal derivative in the space homogeneous Boltzmann equation using a forward Euler

discretization in time and solving for f^{k+1} yields

$$f^{k+1}(v) = f^k(v) + Q\left(f^k, f^k\right)\Delta t \tag{3.2}$$

Upon substituting (3.1) into (3.2), Nanbu [58] shows that the collision integral is given by

$$Q\left(f^k, f^k\right) = \frac{1}{N_p^2}\sum_{i=1}^{N_p}\sum_{j=1}^{N_p}\left(S_{ij}^k - T_{ij}^k\right) \tag{3.3}$$

where,

$$S_{ij}^k = \int_{\mathbb{R}^3}\int_{S^+}\delta\left(v' - v_i^k\right)\delta\left(w' - v_j^k\right)\|v-w\|\,B\left(\|v-w\|,\theta\right)dndw \tag{3.4}$$

$$T_{ij}^k = \int_{\mathbb{R}^3}\int_{S^+}\delta\left(v - v_i^k\right)\delta\left(w - v_j^k\right)\|v-w\|\,B\left(\|v-w\|,\theta\right)dndw \tag{3.5}$$

which represent the replenishing and depleting collision contributions, respectively. Note that T_{ij}^k has a somewhat simpler form than S_{ij}^k and may be evaluated directly,

$$T_{ij}^k = \left\|v_i^k - v_j^k\right\| B_{ij}^k \delta\left(v - v_i^k\right) \tag{3.6}$$

where B_{ij}^k is sometimes referred to as the total collision cross section and is given by

$$B_{ij}^k = \int_{S^+} B\left(\left\|v_i^k - v_j^k\right\|,\theta\right)dn \tag{3.7}$$

In order to simplify S_{ij}^k, Nanbu resorts to approximating the delta function as

$$\delta(v) = \lim_{\epsilon\to 0}\frac{1}{(\pi\epsilon)^3}\exp\left[-\frac{\|v\|^2}{\epsilon}\right] \tag{3.8}$$

Upon substituting (3.8) and (2.9) into (3.4), one obtains

$$\begin{aligned} S_{ij}^k = &\lim_{\epsilon\to 0}\frac{1}{(\pi\epsilon)^3}\int_{\mathbb{R}^3} G_{ij}^k(v,w)\cdot \\ &\exp\left\{-\frac{1}{\epsilon}\left[\|v\|^2 + \|w\|^2 + \left\|v_i^k\right\|^2 + \left\|v_j^k\right\|^2 - \left(v_i^k + v_j^k\right)\cdot(v+w)\right]\right\}\|v-w\|\,dw \end{aligned} \tag{3.9}$$

where G_{ij}^k is defined by

$$G_{ij}^k(v,w) = \int_{S^+}\exp\left(a_{ij}^k\cdot n\right)B\left(\|v-w\|,\theta\right)dn \tag{3.10}$$

and $a_{ij}^k = \frac{1}{\epsilon}\|v-w\|\left(v_j^k - v_i^k\right)$. As stated previously, θ is the angle between $(v-w)$ and n. Next, introduce the spherical-polar coordinate system with the axis directed along a_{ij}^k. Denote the angle between a_{ij}^k and n by ω and the azimuth angle of n about the new axis by ξ. Then $dn = sin(\omega)\, d\omega d\xi$ and $\theta = \theta(\omega, \xi)$. Substituting into (3.10)

$$G_{ij}^k(v,w) = \int_0^{2\pi}\int_0^{\pi} \exp\left[\left\|a_{ij}^k\right\|\cos(\omega)\right] B\left(\|v-w\|, \theta(\omega,\xi)\right)\sin(\omega)\, d\omega d\xi \tag{3.11}$$

Nanbu [58] next asserts that since $\left\|a_{ij}^k\right\| \to \infty$ as $\epsilon \to 0$, the range of small ω is the dominant contributor in (3.11). This allows him to utilize the following approximations

$$\exp\left[\left\|a_{ij}^k\right\|\cos(\omega)\right] \approx \exp\left[\left\|a_{ij}^k\right\|\left(1-\frac{\omega^2}{2}\right)\right] \tag{3.12}$$

$$\theta(\omega,\xi) \approx \theta(0,\xi) = \chi \tag{3.13}$$

$$\sin(\omega) \approx \omega \tag{3.14}$$

where χ is the angle between $(v-w)$ and a_{ij}^k. Nanbu then substitutes these approximations into (3.11), along with one additional approximation, obtained by changing the upper limit of integration from π to ∞ on $d\omega$ to obtain

$$G_{ij}^k(v,w) \approx \int_0^{2\pi}\int_0^{\infty} \exp\left[\left\|a_{ij}^k\right\|\left(1-\frac{\omega^2}{2}\right)\right]\omega B\left(\|v-w\|,\chi\right) d\omega d\xi \tag{3.15}$$

$$= 2\pi B\left(\|v-w\|,\chi\right)\frac{\exp\left(\left\|a_{ij}^k\right\|\right)}{\left\|a_{ij}^k\right\|} \tag{3.16}$$

Substituting (3.16) into (3.9), and using the fact that $\|a\| = \frac{\|v-w\|\left\|v_i-v_j\right\|}{\epsilon}$, one obtains

$$S_{ij}^k = \lim_{\epsilon\to 0}\frac{2}{(\pi\epsilon)^2}\int_{\mathbb{R}^3}\exp\left\{-\frac{1}{2\epsilon}\left[\left(v+w-v_i^k-v_j^k\right)^2 + \left(\|v-w\| - \left\|v_i-v_j\right\|\right)^2\right]\right\}\cdot B\left(\|v-w\|,\xi\right) dw \tag{3.17}$$

Recalling (3.8), this expression can be rewritten as

$$S_{ij}^k = \frac{8}{\left\|v_i^k - v_j^k\right\|}\int_{\mathbb{R}^3}\delta\left(v+w-v_i-v_j\right)\delta\left(\|v-w\| - \left\|v_i-v_j\right\|\right) B\left(\|v-w\|,\chi\right) dw$$

$$= \frac{4}{\left\|v_i^k - v_j^k\right\|}\delta\left(\left\|v_{ij}^{*\,k}\right\| - \frac{\left\|v_i^k - v_j^k\right\|}{2}\right) B\left(\left\|v_i^k - v_j^k\right\|, \chi_{ij}^k\right) \tag{3.18}$$

where

$$v_{ij}^{*\,k} = v - \frac{v_i^k + v_j^k}{2} \tag{3.19}$$

and χ_{ij}^k is the angle between $\left(v_i^k - v_j^k\right)$ and $v_{ij}^{*\,k}$. Substituting (3.9), (3.6), and (3.3), into (3.2) yields the final expression for f^{k+1}

$$f^{k+1}(v) = \frac{1}{N_p} \sum_{i=1}^{N_p} \left[\left(1 - P_i^k\right) \delta\left(v - v_i^k\right) + Q_i^k\right] \tag{3.20}$$

where

$$P_i^k = \frac{\Delta t}{N_p} \sum_{j=1}^{N_p} \left\|v_i^k - v_j^k\right\| B_{ij}^k \tag{3.21}$$

$$Q_i^k = \frac{4\Delta t}{N_p} \sum_{j=1}^{N_p} \delta\left(\left\|v_{ij}^{*\,k}\right\| - \frac{\left\|v_i^k - v_j^k\right\|}{2}\right) \frac{B\left(\left\|v_i^k - v_j^k\right\|, \chi_{ij}^k\right)}{\left\|v_i^k - v_j^k\right\|} \tag{3.22}$$

Rewriting P_i^k as

$$P_i^k = \sum_{i=1}^{N_p} P_{ij}^k \tag{3.23}$$

where,

$$P_{ij}^k = \frac{\Delta t}{N} \left\|v_i^k - v_j^k\right\| B_{ij}^k \tag{3.24}$$

Nanbu bases his scheme on the interpretation that P_i^k represents the probability that the i^{th} simulated particle undergoes a collision during the time interval $[t_k, t_{k+1}]$, while P_{ij}^k represents the probability that particle i collides with particle j during Δt. Under this interpretation, the $j = i$ terms must be omitted from the summation, as a simulated particle cannot collide with itself.

Assuming that particle i collides with particle j, Nanbu then shows that the conditional probability density function for collision angle, g, is given by

$$g(\chi) = \frac{B\left(\left\|v_i^k - v_j^k\right\|, \chi\right) \sin(\chi)}{B_{ij}^k} \tag{3.25}$$

Note that the absence of ξ from the expression implies that the azimuthal dependence is of uniform probability.

Based on these results, Nanbu developed the following stochastic scheme to evolve the molecular velocities during a given time step:

- For each particle, calculate P_i^k. Generate a random number r_1 in the interval $(0, 1)$. If $P_i^k > r_1$, accept the particle for collision.

- Sample a collision partner j from the conditional probability distribution $P_{im}^* = \frac{P_{im}^k}{P_i^k}$, by sampling a second random number r_2 uniformly from the interval $(0, 1)$ and identifying the j which satisfies $\sum_{m=1}^{j-1} P_{im}^* < r_2 < \sum_{m=1}^{j} P_{im}^*$

- Sample the direction of v^* based on (3.25), and compute the post collision velocity of the i^{th} particle, According to

$$v_i' = \frac{1}{2}\left(\left\|v_i^k - v_j^k\right\| R + v_i^k + v_j^k\right) \tag{3.26}$$

  where the vector R is a unit vector computed by sampling the densities for azimuthal and elevation angles, namely

$$\tilde{\xi} = 2\pi r_3 \tag{3.27}$$

  where $r_3 \in (0, 1)$ is another random number, $\tilde{\chi}$ is determined by generating a random number $r_4 \in (0, 1)$ until $g(\tilde{\chi}) \geq r_4$ where $\tilde{\chi} = \pi r_4$, and R is computed as

$$R = \begin{bmatrix} \sin\left(\tilde{\xi}\right)\cos\left(\tilde{\chi}\right) \\ \sin\left(\tilde{\xi}\right)\sin\left(\tilde{\chi}\right) \\ \cos\left(\tilde{\xi}\right) \end{bmatrix} \tag{3.28}$$

In general $P_i^k \neq P_j^k$, but Nanbu points out that in the special case of Maxwell molecules, the collision probabilities are all equal, namely

$$P_i^k = \pi\beta_0^2\left(\frac{8b}{m}\right)^{\frac{1}{2}}\left(\frac{N_p - 1}{N_p}\right)\Delta t \forall i \tag{3.29}$$

where β_0 and b are parameters which define the collision cross section. In this case, collision partners can be chosen randomly simplifying the second step of the procedure significantly.

Note, however, that the procedure developed by Nanbu does not exactly produce the solution at time step $k+1$ from equation 3.20. Specifically, note that the effect of collisions, namely the Q_i^k term, does not lend itself to be written as a simple delta function involving two distinct post collision velocities. Rather the form of this term indicates that the post collision velocities for a collision pair are distributed over a sphere. DSMC techniques such as Nanbu's method simply sample discrete post collision velocities from this sphere. In so doing, much of the information contained in equation 3.20 is destroyed. If one considers the fact that each simulated particle represents a large number of actual particles, the solution indicates that the collision interaction will distribute the velocities of the actual particles over the sphere post collision. Further, the appearance of the first term in equation 3.20 indicates that a portion of the molecules are unaffected by the collision interaction. As DSMC allows for only a single velocity per simulated particle, the sampling cannot account for all of these effects.

3.3 Proof of Convergence of Nanbu's Method

The previous section provided an overview of Nanbu's method which followed Nanbu's original derivation fairly closely [58]. This section will follow Babovsky's proof, which showed Nanbu's method converged in law to the solution of the space homogeneous Boltzmann equation (2.28) [8]. Much of the details of Babovsky's work will be included here, as the work serves as a good template for completing such proofs, and the following section lays out many of the details omitted from Babovsky's original paper. Before continuing we define this form of convergence concretely as follows.

Definition 3.1. *Let $(S,\mathcal{T})$ be a topological space, with Borel σ-algebra $\mathcal{B}$. Define $C_b(S) \coloneqq C_b(S,\mathcal{T})$ to be the set of all bounded, continuous, real-valued functions on S. A sequence of laws $\{P_n\}$ is said to converge to a law P if $\int_S f dP_n \to \int_S f dP$ as $n \to \infty$ for every f in $C_b(S)$ [35].*

To begin, it is necessary to develop a few additional relations and consider Nanbu's approach in a somewhat more rigorous setting. Recalling the expressions for the post-collision velocities (2.9), here we define the more compact notation

$$T_{v,w}(n) \coloneqq v - [n \cdot (v - w)]\, n \tag{3.30}$$

to more explicitly indicate the dependence on the pre-collision velocities and the orientation angle. It should be noted that the Jacobian of the transformation which maps $(v, w) \rightarrow (v', w')$ is unity [30]. Further, $T_{v',w'}(n) = v$. Babovsky begins his explanation of Nanbu's method by developing a weak form of the time discretized Boltzmann equation [8]. Rewriting (3.2) using (2.31), one obtains

$$\begin{aligned} f^{k+1}(v) = \left(1 - \Delta t \int_{\mathbb{R}^3}\int_{S^+} B(\|v - w\|, \theta)\, f^k(w)\, dS(n)\, dw\right) f^k(v) + \\ \Delta t \int_{\mathbb{R}^3}\int_{S^+} B(\|v - w\|, \theta)\, f^k(v')\, f^k(w')\, dS(n)\, dw \end{aligned} \tag{3.31}$$

which, so long as B is bounded, is an approximation to the solution of (2.28) with truncation error on the order of $O(\Delta t)$.

Let $\phi \in C_b\left(\mathbb{R}^3\right)$. By multiplying (3.31) by ϕ and integrating over velocity space, i.e. $\mathbb{R}^3$, one obtains a weak form of the equation. Utilizing the properties discussed above, it can be shown [8] that this expression can be written as

$$\int_{\mathbb{R}^3} \phi(v)\, f^{k+1}(v)\, dv = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K_{v,w}(\phi)\, f^k(v)\, f^k(w)\, dw dv \tag{3.32}$$

where, $K_{v,w}$

$$\begin{aligned} K_{v,w}(\phi) = \left[1 - \Delta t \int_{S^+} B(\|v - w\|, \theta)\, d\theta d\epsilon\right] \phi(v) + \\ \Delta t \int_{S^+} B(\|v - w\|, \theta)\, \phi(v')\, d\theta d\epsilon \end{aligned} \tag{3.33}$$

is called the transition kernel. Note that the kernel itself exhibits no dependence on f^k. Also, as Babovsky points out, there is no guarantee that (3.31) preserves non-negativity of solutions. To ensure non-negativity is preserved one must assume

$$1 - \Delta t \int_{S^+} B(\|v - w\|, \theta)\, d\theta d\epsilon \geq 0 \;\forall v, w \in \mathbb{R}^3 \tag{3.34}$$

This establishes a restriction on the time step and typically also requires that B be truncated in velocity space.

Babovsky [8] proves the following lemma which allows the transition kernel to be written more compactly.

Lemma 3.1. *For all $v, w \in \mathbb{R}^3$, there exists a continuous mapping, $\Phi_{v,w} : D \to S^+$, where D is the disk in $\mathbb{R}^2$ centered at the origin with radius $\frac{1}{\sqrt{\pi}}$, such that*

$$K_{v,w}(\phi) = \int_D \phi\left(T_{v,w} \circ \Phi_{v,w}(x)\right) dx \tag{3.35}$$

for any $\phi \in C_b\left(\mathbb{R}^3\right)$.

Using this property, and assuming B is bounded and continuous, we define the function, $\Psi : D \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ as

$$\Psi(x, v, w) = T_{v,w} \circ \Phi_{v,w}(x) \tag{3.36}$$

It can be shown [8] that because B is assumed to be bounded and continuous, Ψ is continuous almost everywhere (a.e.) in $D \times \mathbb{R}^3 \times \mathbb{R}^3$. Physically, Ψ is a function which takes two velocities and a 2-parameter orientation as inputs and maps to a single velocity. The following definitions motivate the concept of a point measure approximation, which is the framework by which DSMC constructs a weak solution to the Boltzmann equation.

Definition 3.2. *Let μ be a measure on the measurable space $(\Omega, \mathcal{S})$. The support of μ is the set of all points $\omega \in \Omega$ for which every open neighborhood of ω has a positive measure and is denoted* $\operatorname{supp}(\mu)$.

Definition 3.3. *Let P be a probability measure on the measurable space $(\Omega, \mathcal{S})$. P is called a discrete probability measure if* $\operatorname{supp}(P)$ *is countable.*

Lemma 3.2. *Let P be a disrete probability measure on the measurable space $(\Omega, \mathcal{S})$ with* $\operatorname{supp}(P) = \{\omega_i\}$. *Then there exists $\{a_i\}$, with $a_i \in \mathbb{R}^+$ such that for any $A \subset \Omega$,*

$$P(A) = \sum_i a_i \delta_{\omega_i}(A) \tag{3.37}$$

where δ_{ω_i} is the delta measure supported at ω_i, and,

$$\sum_i a_i = 1 \tag{3.38}$$

Definition 3.4. *Let P be a probability measure on the measurable space $(\Omega, \mathcal{S})$, and let $\{P_N\}$ be a sequence of discrete probability measures on $(\Omega, \mathcal{S})$ with $\text{card}(\text{supp}(P_N)) = N$. If $\{P_N\}$ converges to P in law, then $\{P_N\}$ is called a point measure approximation to P. Further, denoting $supp(P_N)$ by $\{\omega_i\}_{i=1}^N$, if*

$$P_N(A) = \frac{1}{N} \sum_{i=1}^{N} \delta_{\omega_i}(A) \tag{3.39}$$

for every $A \subset \Omega$, then P_N is said to possess uniform weights.

We also require the following definitions and results regarding image measures.

Definition 3.5. *Let $(X, \mathcal{S})$ and $(Y, \mathcal{B})$ be measurable spaces, and let f be a transformation from X into Y. If $f^{-1}(B) \in \mathcal{S}$ for all $B \in \mathcal{B}$ then f is called a measurable transformation.*

Definition 3.6. *Let $(X, \mathcal{S}, \mu)$ be a measure space and $(Y, \mathcal{B})$ a measurable space. Let T be a measurable transformation from X into Y. Let $\left(\mu \circ T^{-1}\right)(A) = \mu\left(T^{-1}(A)\right)$ for all $A \in \mathcal{B}$. Since $A \mapsto T^{-1}(A)$ preserves all set operations and preserves disjointedness, $\mu \circ T^{-1}$ is a countably additive measure and is called the image measure of μ by T.[35]*

Lemma 3.3. *Let f be any measurable function from Y into $[-\infty, \infty]$. Then $\int f d\left(\mu \circ T^{-1}\right) = \int f \circ T d\mu$ if either integral is defined, (possibly infinite) [35].*

Lemma 3.4. *Let $(X, \mathcal{S}, P)$ be a measure space and $(Y, \mathcal{B})$ a measurable space. Let T be a transformation from X into Y, and let T be continuous a.e. Let $\left\{P^N\right\}$ be a sequence of probability measures on $(X, \mathcal{S})$ which converges to P in law. Then, the sequence $\left\{P^N \circ T^{-1}\right\}$ converges in law to the image measure $P \circ T^{-1}$ [13].*

The following theorem, proven by Babovsky [8] employs these results to develop a sufficiency criteria for a point measure scheme to converge in law to the space homogeneous Boltzmann solution.

Theorem 3.1. *Let $P2^k$ be the probability measure on $D \times \mathbb{R}^3 \times \mathbb{R}^3$ defined by*

$$P2^k(B) = \int_B f^k(v) f^k(w) \, dxdwdv \text{ for any } B \subset D \times \mathbb{R}^3 \times \mathbb{R}^3 \tag{3.40}$$

where f^k is the solution of the space homogeneous Boltzmann equation at $t = t_k$. Let P^{k+1} be the probability measure on $\mathbb{R}^3$ defined by

$$P^{k+1}(A) = \int_A f^{k+1}(v) \, dv \text{ for any } A \subset \mathbb{R}^3 \tag{3.41}$$

Suppose a sequence of probability measures $\{P2_N\}$ is a point measure approximation with uniform weights to $P2^k$, with support denoted by

$$\operatorname{supp}(P2_N) = \left\{\left(x_i^N, v_i^N, w_i^N\right)\right\}_{i=1}^N \tag{3.42}$$

Then define a probability measure P_N on $\mathbb{R}^3$ by

$$P_N(A) = \frac{1}{N} \sum_{i=1}^N \delta_{\Psi\left(x_i^N, v_i^N, w_i^N\right)}(A) \text{ for any } A \subset \mathbb{R}^3 \tag{3.43}$$

where Ψ is defined as in (3.36). Then, $\{P_N\}$ is a point measure approximation to P^{k+1}.

Proof. By definition, $\operatorname{card}(\operatorname{supp}(P_N)) = N$. We will show that $\{P_N\}$ converges to P^{k+1} in law. Take any $\phi \in C_b\left(\mathbb{R}^3\right)$. Then

$$\begin{aligned}
\int_{\mathbb{R}^3} \phi(v) \, dP_N &= \frac{1}{N} \sum_{i=1}^N \int_{\mathbb{R}^3} \phi(v) \, \delta\left(v - \Psi\left(x_i^N, v_i^N, w_i^N\right)\right) dv \\
&= \frac{1}{N} \sum_{i=1}^N \phi\left(\Psi\left(x_i^N, v_i^N, w_i^N\right)\right) \\
&= \frac{1}{N} \sum_{i=1}^N \int_D \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \phi \circ \Psi(x, v, w) \, \delta\left(x - x_i^N\right) \cdot \delta\left(v - v_i^N\right) \cdot \\
&\quad \delta\left(w - w_i^N\right) dxdwdv \\
&= \int_D \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \phi \circ \Psi(x, v, w) \, dP2_N \\
&= \int_{\mathbb{R}^3} \phi(v) \, d\left(P2_N \circ \Psi^{-1}\right) \text{ by Lemma 3.3}
\end{aligned} \tag{3.44}$$

Thus, $P_N = P2_N \circ \Psi^{-1}$. Recall that by assumption $\{P2_N\}$ converges in law to $P2^k$ as $N \to \infty$. Since Ψ is continuous a.e., by Lemma 3.4 we have $\left\{P2_N \circ \Psi^{-1}\right\}$ converges to $P2^k \circ \Psi^{-1}$ in law as $N \to \infty$. By (3.44) this implies that $\{P_N\}$ converges to $P2^k \circ \Psi^{-1}$ in law as $N \to \infty$. Next, for any $\phi \in C_b\left(\mathbb{R}^3\right)$, we have

$$\begin{aligned}
\int_{\mathbb{R}^3} \phi(v)\, d\left(P2_N \circ \Psi^{-1}\right) &= \int_D \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \phi(\Psi(x,v,w))\, dP2^k \text{ by Lemma 3.3} \\
&= \int_D \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \phi(\Psi(x,v,w))\, f^k(v)\, f^k(w)\, dxdwdv \\
&= \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, f^k(v)\, f^k(w)\, dwdv \text{ by (3.35) and (3.36)} \\
&= \int_{\mathbb{R}^3} \phi(v)\, f^{k+1}(v)\, dv \text{ by (3.32)} \\
&= \int_{\mathbb{R}^3} \phi(v)\, dP^{k+1} \qquad (3.45)
\end{aligned}$$

Thus, $P2^k \circ \Psi^{-1} = P^{k+1}$ and hence we conclude that $\{P_N\}$ converges to P^{k+1} in law as $N \to \infty$. □

Theorem 3.1 provides a sufficient criterion for the convergence of a point-measure based simulation scheme for the space homogeneous Boltzmann equation in law. Namely, if one can show that a scheme constructs a point measure approximation, $\{P2_N\}$ to $P2^k$ at $t = t^k$, then one can construct a point mesure approximation, $\{P_N\}$, to P^{k+1} by defining its support to be given by $\text{supp}(P_N) = \Psi(\text{supp}(P2_N))$.

Babovsky [8] summarizes Nanbu's scheme more compactly than the overview described in the prior section. Babovsky's description lends itself better to the proofs that follow while retaining the important characteristics of the scheme. Nanbu's scheme is summarized as follows:

- Let P_N^0 be a point measure approximation to P^0 defined by

$$P^0(A) = \int_A f^0(v)\, dv \qquad (3.46)$$

  where f^0 is the initial condition for the Boltzmann equation, and let $\text{supp}\left(P_N^0\right) = \left\{v_i^N\right\}_{i=1}^N$.

- For a fixed N, choose a set of N uniformly distributed random numbers $\{r_i\}_{i=1}^N$, $r_i^N \in [0,1]$ and a set of N uniformly distributed random vectors $\left\{x_i^N\right\}_{i=1}^N$, $x_i \in D$.
- Define collision partners $C(i,N) = \left\lfloor Nr_i^N \right\rfloor + 1$ with velocities given by $w_i^N = v_{C(i,N)}^N$.
- Define the sequence of discrete probability measures P_N^{k+1} by

$$P_N^{k+1}(A) = \frac{1}{N}\sum_{i=1}^{N} \delta_{\Psi\left(x_i^N, v_i^N, w_i^N\right)}(A) \text{ for all } A \subset \mathbb{R}^3 \tag{3.47}$$

  This sequence will be shown to be a point measure approximation to P^1 defined by

$$P^1(A) = \int_A f^1(v)\,dv \tag{3.48}$$

  where f^1 is the Boltzmann solution at time $t = \Delta t$
- Repeat the process with f^1 as the new initial condition.

Before continuing, a few additional definitions and results on random variables and probability theory are required.

Definition 3.7. *If $(\Omega, \mathcal{A}, P)$ is a probability space and $(S, \mathcal{B})$ is any measurable space, a function X from Ω into S is called a random variable. The law of the random variable X, denoted $\mathcal{L}(X)$, is the image measure $P \circ X^{-1}$ defined by*

$$\left(P \circ X^{-1}\right)(B) \coloneqq P\left(X^{-1}(B)\right) \text{ for any } B \subset S \tag{3.49}$$

The notation $X^{-1}(B)$ is used to indicate the pre-image of B, that is $X^{-1}(B) \coloneqq \{\omega \in \Omega : X(\omega) \in B\}$. [35]

Definition 3.8. *The expected value of a random variable X on (Ω, σ, P) is denoted EX and is defined by $EX \coloneqq \int X dP$.[35]*

Theorem 3.2. *For any two random variables, X and Y such that EX and EY are both defined and finite, and any constant c, $E(cX + Y) = cEX + EY$.*

Definition 3.9. *The variance of a random variable X is denoted by var (X) or $\sigma^2(X)$, and is defined by*

$$var(X) := \sigma^2(X) := \begin{cases} E(X - EX)^2 = EX^2 - (EX)^2 & \text{if } EX^2 < \infty \\ 0 & \text{otherwise} \end{cases}$$

If $EX^2 < \infty$, then $\sigma(X) := \sqrt{\sigma^2(X)}$ is called the standard deviation of X.

Definition 3.10. *Given a random variable X on a probability space $(\Omega, \mathcal{S}, P)$ with values in $\mathbb{R}^k$, (i.e. $X : \Omega \to \mathbb{R}^k$), the distribution function of X on $\mathbb{R}^k$ is defined by*

$$F(x) := P(X \leq x) \tag{3.50}$$

where "$\leq$" is defined on $\mathbb{R}^k$ by $x \leq y$ if and only if $x_i \leq y_i$ for $i = 1, \ldots, k$.

These definitions motivate defining convergence not just for probability measures, but for random variables as well. In this case, several forms of convergence are important.

Definition 3.11. *Let $\{X_n\}$ be a sequence of random variables with distribution functions $\{F_n\}$, and X be a random variable with distribution function, F. If $F_n \to F$, then $\{X_n\}$ is said to converge in distribution to X.*

It should be noted that convergence in distribution is equivalent to convergence in law for random variables, that is, $F_n \to F$ if and only if $\mathcal{L}(X_n) \to \mathcal{L}(X)$ [12].

Theorem 3.3. *(Central Limit Theorem [12]) Suppose that $\{X_n\}$ is a sequence of independent random variables having the same distribution with mean c and finite positive variance σ^2. If $S_n = X_1 + \cdots + X_n$, then the random variable*

$$\frac{S_n - nc}{\sigma\sqrt{n}} \tag{3.51}$$

is distributed according to the standard normal distribution, $\mathcal{N}(0, 1)$.

Definition 3.12. *Let* $(\Omega, \mathcal{S}, P)$ *be a probability space. Any event with probability* 1 *is said to happen almost surely (a.s.). A sequence of random variables* $\{X_n\}$ *is said to converge almost surely to a random variable* X *if* $P(\{\omega \in \Omega : \lim_{n\to\infty} X_n(\omega) = X(\omega)\}) = 1$. *[35]*

The following definition and theorem are useful in considering the convergence of stochastic schemes.

Definition 3.13. *Given a probability space,* $(\Omega, \mathcal{S}, P)$ *and a sequence of events* $\{A_n\}$*, define* $\limsup A_n$ *as the event*

$$\limsup A_n = \cap_{m\geq 1} \cup_{n\geq m} A_n \tag{3.52}$$

The event $\limsup A_n$ *is also referred to as* A_n *infinitely often (i.o.), as* $\omega \in \limsup A_n$ *if and only if* $\omega \in A_n$ *for infinitely many values of* n.

Theorem 3.4. *(Borel-Cantelli Lemma) If* $\{A_n\}$ *are any events with* $\sum_n P(A_n) < \infty$*, then* $P(\limsup A_n) = 0$. *If the* $\{A_n\}$ *are independent and* $\sum_n P(A_n) = \infty$ *then* $P(\limsup A_n) = 1$ *[35].*

With these results, one may proceed to prove the following theorem.

Theorem 3.5. *Let* $\{P_N\}$ *be a point-measure approximation with uniform weights to the probability measure* P *on* $\mathbb{R}^3$*, defined by* $P(A) = \int_A f(v)\, dv$ *for any* $A \subset \mathbb{R}^3$. *Further, let* $\hat{P}$ *be the probability measure on* $\mathbb{R}^3 \times \mathbb{R}^3$ *defined by* $\hat{P}(B) = \int_B f(v) f(w)\, dwdv$.

Denote $\operatorname{supp}(P_N)$ *by* $\{v_i\}_{i=1}^N$. *Define the probability measure,* $\hat{P}_N$ *on* $\mathbb{R}^3 \times \mathbb{R}^3$ *by*

$$\hat{P}_N(B) = \frac{1}{N} \sum_{i=1}^{N} \delta_{v_i, w_i}(B) \text{ for any } B \in \mathbb{R}^3 \times \mathbb{R}^3 \tag{3.53}$$

where w_i *is as defined in Nanbu's method (i.e.* $w_i = v_{C(i,N)}$*, where* $C(i, N) = \lfloor N r_i \rfloor + 1$*). Then,* $\hat{P}_N$ *is a point measure approximation to* $\hat{P}$.

Proof. Define the following distribution functions,

$$F(v) = \int_{v' \leq v} f(v')\, dv' \tag{3.54}$$

$$G(v,w) = \int_{v' \le v} \int_{w' \le w} f(v') f(w') \, dv' dw' = F(v) F(w) \tag{3.55}$$

which are the distribution functions associated with the laws P and $\hat{P}$ respectively. Define the distribution functions for P_N and $\hat{P}_N$ by

$$F_N(v) = \int_{v' \le v} \frac{1}{N} \sum_{i=1}^{N} \delta(v' - v_i) \, dv' \tag{3.56}$$

and

$$G_N(v,w) = \int_{v' \le v} \int_{w' \le w} \frac{1}{N} \sum_{i=1}^{N} \delta(v' - v_i) \, \delta(w' - w_i) \, dw' dv' \tag{3.57}$$

respectively. Recall, by Definition 3.11 a sequence of probability laws $\{P_n\}$ with distribution functions $\{F_n\}$ converge to a law P with distribution function F if and only if $\{F_n\}$ converges to F. By assumption, we have P_N converges to P in law, which implies $F_N \to F$. We will prove that for any $(a,b) \in \mathbb{R}^3 \times \mathbb{R}^3$, $G_N(a,b) \to G(a,b)$ and hence $\hat{P}_N$ converges to $\hat{P}$ in law. To begin, define the following variables,

$$k_N(v) = \text{card}(\{i \le N : v_i \le v\}) \tag{3.58}$$

$$m_N(v,w) = \text{card}(\{i \le N : (v_i, w_{C(i,N)}) \le (v,w)\}) \tag{3.59}$$

Then,

$$F_N(v) = \frac{k_N(v)}{N} \tag{3.60}$$

$$G_N(v) = \frac{m_N(v,w)}{N} \tag{3.61}$$

Let $(a,b) \in \left(\mathbb{R}^3 \times \mathbb{R}^3\right)$. Define

$$S_i = \begin{cases} 1 & \text{if } v_i \le a \\ 0 & \text{otherwise} \end{cases} \tag{3.62}$$

Then,

$$\begin{aligned} G_N(a,b) &= \frac{m_N(a,b)}{N} \\ &= \frac{1}{N} \sum_{i=1}^{N} \int_{v \le a} \int_{w \le b} \delta(v - v_i) \, \delta(w - w_i) \, dw dv \\ &= \frac{1}{N} \sum_{i=1}^{N} S_i \int_{w \le b} \delta(w - v_{C(i,n)}) \, dw \end{aligned}$$

Let $\{i(s)\}_{s=1}^{k_N(a)}$ be the set of $k_N(a)$ integers such that $v_{i(s)} \leq a$. Define

$$X_s = \begin{cases} 1 & \text{if } v_{C(i(s),N)} \leq b \\ 0 & \text{otherwise} \end{cases} \tag{3.63}$$

Then,

$$G_N(a,b) = \frac{1}{N} \sum_{s=1}^{k_N(a)} X_s \tag{3.64}$$

Substituting the above into (3.61) we find

$$m_N(a,b) = \sum_{s=1}^{k_N(a)} X_s \tag{3.65}$$

Let $\Omega_n = (0,1)$. Then $(\Omega_n, \mathcal{S}_n, \lambda)$ is a probability space, where $\mathcal{S}_n$ is the standard $\sigma-$algebra on $(0,1)$ and λ is the Lebesgue measure. Define Ω to be the Cartesian product

$$\Omega = \prod_{n=1}^{N} \Omega_n \tag{3.66}$$

The elements of Ω are thus N-tuples $\{\omega_n\}_{n=1}^N$ with $\omega_n \in \Omega_n$. Defining π_m to be the natural projection of Ω onto Ω_m (i.e. $\pi_m\left(\{\omega_n\}_{n=1}^N\right) = \omega_m$), let $\mathcal{S}$ be the smallest $\sigma-$ algebra of subsets of Ω containing all sets $\pi_n^{-1}(A)$ for all n and all $A \subset \Omega_n$. Here, $\pi_n^{-1}(A)$ denotes the pre-image of A (namely, $\pi_n^{-1}(A) \coloneqq \{\omega \in \Omega : \pi(\omega) \in A \subset \Omega_n\}$) . Then $(\Omega, \mathcal{S}, Prob)$ is a product probability space with $Prob = \lambda^N$. Now, given an N-tuple $\{\omega_n\}_{i=1}^N \in \Omega$, X_s maps the N-tuple to either 0 or 1. That is, $X_s : \Omega \to \{0,1\}$, which implies X_s is a random variable on the probability space $(\Omega, \mathcal{S}, Prob)$. Furthermore, the set of random variables $\{X_s\}_{s=1}^{k_N(a)}$ are independent, and identically distributed (i.i.d.). Furthermore,

$$\begin{aligned} EX_s &= \int X_s dProb \\ &= \int_{\Omega_1} \cdots \int_{\Omega_s} \cdots \int_{\Omega_N} X_s d\lambda^N \\ &= 1 \cdot \lambda(\Omega_s') + 0 \cdot \lambda(\Omega_s - \Omega_s') \end{aligned}$$

where $\Omega'_s = \{x \in (0,1) : v_{\lfloor xN \rfloor + 1} \leq b\}$ Thus, $N\lambda(\Omega') = \text{card}(\{i \leq N : v_i \leq b\})$. Therefore,

$$\begin{aligned} EXs &= \lambda(\Omega'_s) \\ &= \frac{N\lambda(\Omega'_s)}{N} \\ &= \frac{\text{card}(\{i \leq N : v_i \leq b\})}{N} \\ &= \frac{k_N(b)}{N} \end{aligned} \tag{3.67}$$

Also,

$$\begin{aligned} Var(X_s) &= EX_s^2 - (EX_s)^2 \\ &= \int X_s^2 dProb - \left(\frac{k_N(b)}{N}\right)^2 \\ &= \int_{\Omega_1} \cdots \int_{\Omega_s} \cdots \int_{\Omega_N} X_s^2 d\lambda^N - \left(\frac{k_N(b)}{N}\right)^2 \\ &= 1^2 \cdot \lambda(\Omega'_s) + 0^2 \cdot \lambda(\Omega_s - \Omega'_s) - \left(\frac{k_N(b)}{N}\right)^2 \\ &= \lambda(\Omega'_s) - \left(\frac{k_N(b)}{N}\right)^2 \\ &= \frac{N\lambda(\Omega'_s)}{N} - \left(\frac{k_N(b)}{N}\right)^2 \\ &= \frac{\text{card}(\{i \leq N : v_i \leq b\})}{N} - \left(\frac{k_N(b)}{N}\right)^2 \\ &= \frac{k_N(b)}{N} - \left(\frac{k_N(b)}{N}\right)^2 \\ &= \frac{k_N(b)}{N}\left(1 - \frac{k_N(b)}{N}\right) \end{aligned} \tag{3.68}$$

Combining (3.65) and (3.67) we have

$$Em_N(a,b) = \sum_{s=1}^{k_N(a)} EX_s = \frac{k_n(a)\,k_n(b)}{N^2} \tag{3.69}$$

Define the set (or event) $A_N \subset \Omega$ as

$$A_N = \left\{\{r_i\}_{i=1}^N : \left|\frac{m_N(a,b)}{N} - F(a,b)\right| > \epsilon(N)\right\} \tag{3.70}$$

where $\epsilon(N)$ is some positive real number. In this expression, note that the m_N term is dependant upon $\{r_i\}_{i=1}^N$, via equation 3.65 . We next develop an upper bound on $Prob(A_N)$. By the triangle inequality,

$$\begin{aligned} A_N \subset & \left\{ \{r_i\}_{i=1}^N : \left| \frac{m_N(a,b)}{N} - \frac{k_N(a)}{N}\frac{k_N(b)}{N}) \right| > \frac{\epsilon(N)}{2} \right\} \\ & \cup \left\{ \{r_i\}_{i=1}^N : \left| \frac{k_N(a)}{N}\frac{k_N(b)}{N} - F(a)F(b) \right| > \frac{\epsilon(N)}{2} \right\} \end{aligned} \tag{3.71}$$

Thus,

$$\begin{aligned} Prob(A_N) \leq & Prob\left(\left\{ \{r_i\}_{i=1}^N : \left| \frac{m_N(a,b)}{N} - \frac{k_N(a)}{N}\frac{k_N(b)}{N}) \right| > \frac{\epsilon(N)}{2} \right\} \right) + \\ & Prob\left(\left\{ \{r_i\}_{i=1}^N : \left| \frac{k_N(a)}{N}\frac{k_N(b)}{N} - F(a)F(b) \right| > \frac{\epsilon(N)}{2} \right\} \right) \end{aligned} \tag{3.72}$$

Notice that by equations 3.56 and 3.60, the term $\left| \frac{k_N(a)}{N}\frac{k_N(b)}{N} - F(a)F(b) \right|$ does not depend on $\{r_i\}_{i=1}^N$, and is simply a constant for a given N. Define $\epsilon_2(N)$ to be

$$\epsilon_2(N) = 2\left| \frac{k_N(a)}{N}\frac{k_N(b)}{N} - F(a)F(b) \right| \tag{3.73}$$

and thus,

$$Prob\left(\left\{ \{r_i\}_{i=1}^N : \left| \frac{k_N(a)}{N}\frac{k_N(b)}{N} - F(a)F(b) \right| > \frac{\epsilon_2(N)}{2} \right\} \right) = 0 \tag{3.74}$$

Note that since $P_N \to P$ implies $F_N \to F$, we have $\epsilon_2(N) \to 0$ as $N \to \infty$.

Since m_N is the summation of the k_N i.i.d random variables X_s, by the central limit theorem (Theorem 3.3), we have that

$$\frac{m_N(a,b) - k_N(a)EX_s}{\sqrt{k_N(a)VarX_s}} \tag{3.75}$$

is distributed according to the standard normal distribution $\mathcal{N}(0,1)$. This implies that

$$\frac{1}{N}\sum_{s=1}^{k_N(a)}(X_s - EXs) = \frac{m_N(a,b)}{N} - \frac{k_N(a)}{N}\frac{k_N(b)}{N} \tag{3.76}$$

is distributed according to $\mathcal{N}(0,\sigma_N)$, where

$$\begin{aligned} \sigma_N &= \frac{\sqrt{k_N(a)Var(X_s)}}{N} \\ &= \frac{\sqrt{\frac{k_N(a)}{N}\frac{k_N(b)}{N}\left(1 - \frac{k_N(b)}{N}\right)}}{\sqrt{N}} \end{aligned} \tag{3.77}$$

Now, since $E\left[\frac{m_N(a,b)}{N} - \frac{k_N(a)}{N}\frac{k_N(b)}{N}\right] = 0$, and σ_N is finite, choose $\epsilon_1(N)$ to be the smallest positive number such that

$$Prob\left(\left\{\{r_i\}_{i=1}^N : \left|\frac{m_N(a,b)}{N} - \frac{k_N(a)}{N}\frac{k_N(b)}{N}\right| > \frac{\epsilon_1(N)}{2}\right\}\right) \leq \frac{1}{N^2} \tag{3.78}$$

The existence of such a value follows from the conditions on the expected value and variance of $\frac{m_N(a,b)}{N} - \frac{k_N(a)}{N}\frac{k_N(b)}{N}$. Furthermore, $\epsilon_1(N) \to 0$ as $N \to \infty$ since

$$\begin{aligned}
\lim_{N\to\infty} \sigma_N &= \lim_{N\to\infty} \frac{\sqrt{\frac{k_N(a)}{N}\frac{k_N(b)}{N}\left(1 - \frac{k_N(b)}{N}\right)}}{\sqrt{N}} \\
&= \left(\lim_{N\to\infty} \frac{1}{\sqrt{N}}\right)\left(\lim_{N\to\infty} \sqrt{\frac{k_N(a)}{N}\frac{k_N(b)}{N}\left(1 - \frac{k_N(b)}{N}\right)}\right) \\
&= (0)\sqrt{F(a)F(b)(1-F(b))} \\
&= 0
\end{aligned}$$

Let $\epsilon(N) = \max\{\epsilon_1(N), \epsilon_2(N)\}$. Then, $\epsilon(N) \to 0$ as $N \to \infty$ and

$$\begin{aligned}
Prob(A_N) &\leq Prob\left(\left\{\{r_i\}_{i=1}^N : \left|\frac{m_N(a,b)}{N} - \frac{k_N(a)}{N}\frac{k_N(b)}{N}\right| > \frac{\epsilon(N)}{2}\right\}\right) \\
&\quad + Prob\left(\left\{\{r_i\}_{i=1}^N : \left|\frac{k_N(a)}{N}\frac{k_N(b)}{N} - F(a)F(b)\right| > \frac{\epsilon(N)}{2}\right\}\right) \\
&= Prob\left(\left\{\{r_i\}_{i=1}^N : \left|\frac{m_N(a,b)}{N} - \frac{k_N(a)}{N}\frac{k_N(b)}{N}\right| > \frac{\epsilon(N)}{2}\right\}\right) + 0 \\
&\leq \frac{1}{N^2}
\end{aligned}$$

Thus, we have,

$$\sum_{N=1}^{\infty} Prob(A_N) \leq \sum_{N=1}^{\infty} \frac{1}{N^2} < \infty \tag{3.79}$$

Thus defining A to be the event A_N i.o., as given in (3.52), by the Borel-Cantelli Lemma (Theorem 3.4) we have $Prob(A) = 0$. Thus,

$$\lim_{N\to\infty} \left|\frac{m_N(a,b)}{N} - F(a)F(b)\right| = 0 \tag{3.80}$$

for almost all $\underline{r}$. Combining this result with (3.55) and (3.61) yeilds that

$$\lim_{N\to\infty} |G_N(a,b) - G(a,b)| = 0 \text{ almost surely} \tag{3.81}$$

for all $(a, b) \in \mathbb{R}^3 \times \mathbb{R}^3$. Hence $\hat{P}_N$ converges in law to $\hat{P}$ as $N \to \infty$ almost surely. □

The next result incorporates the distribution of collision orientations; the proof will be omitted as it follows the same technique as Theorem 3.5.

Theorem 3.6. *Let $\{P_N\}$ be a point measure approximation to the probability measure P on $\mathcal{R}^3$, defined by $P(A) = \int_A f(v)\,dv$ for any $A \in \mathcal{R}^3$. Further, let $\tilde{P}$ be the probability measure on $D \times \mathbb{R}^3 \times \mathbb{R}^3$ defined by $\tilde{P}(B) = \int_B f(v)\, f(w)\, dxdwdv$ for any $B \in D \times \mathbb{R}^3 \times \mathbb{R}^3$.*

Denote $\operatorname{supp}(P_N)$ *by $\{(v_i, w_i)\}_{i=1}^N$. Let $\{x_i\}_{i=1}^N$ be a sequence of uniformly distributed random numbers on $D = \left\{x \in \mathbb{R}^2 : \|x\| \leq \frac{1}{\sqrt{pi}}\right\}$, where $\|\cdot\|$ represents the Euclidean norm. Define the probability measure $\tilde{P}_N$ on $D \times \mathbb{R}^3 \times \mathbb{R}^3$ by*

$$\tilde{P}_N(B) = \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i, v_i, w_i}(B) \text{ for any } B \in D \times \mathbb{R}^3 \times \mathbb{R}^3 \tag{3.82}$$

Then $\tilde{P}_N$ is a point measure approximation to $\tilde{P}$.

Theorem 3.7. *Nanbu's scheme converges in law almost surely to the solution of the time discretized space homogeneous Boltzmann equation (3.2) for all timesteps.*

Proof. Combing Theorems 3.1,3.5, and 3.6 yields the desired result. □

3.4 Nanbu's DSMC Scheme Applied to the Bobylev-Krook-Wu Problem

To provide a numerical baseline for comparison with the schemes developed by the author, Nanbu's DSMC technique was applied to the Bobylev-Krook-Wu Problem. As Nanbu's scheme converges only in law, it is not possible to directly evaluate the error present in the solution (e.g. in terms of $L^1\left(\mathbb{R}^3\right)$ norm, etc.). For this reason, the moment expressions for the Bobylev-Krook-Wu solution presented in Chapter 2 provide a very valuable and commonly exploited tool for evaluating the effectiveness of various DSMC schemes. Utilizing the Nanbu approximation to the distribution function, these normalized

moments can easily be computed as

$$z_n(t) = \frac{1}{(2n+1)!!} \sum_{i=1}^{N_p} \frac{1}{N_p} \int_{\mathbb{R}^3} \delta(v - v_i(t)) \|v\|^{2n} dv = \frac{1}{N_p (2n+1)!!} \sum_{i=1}^{N_p} v_i^{2n}(t) \qquad (3.83)$$

Figure 3.1 presents a comparison of the first four normalized moments of the density function for the case in which $N_p = 100$. The results have been averaged over an ensemble of 600 runs. This is common practice to reduce the variance present in the solution.

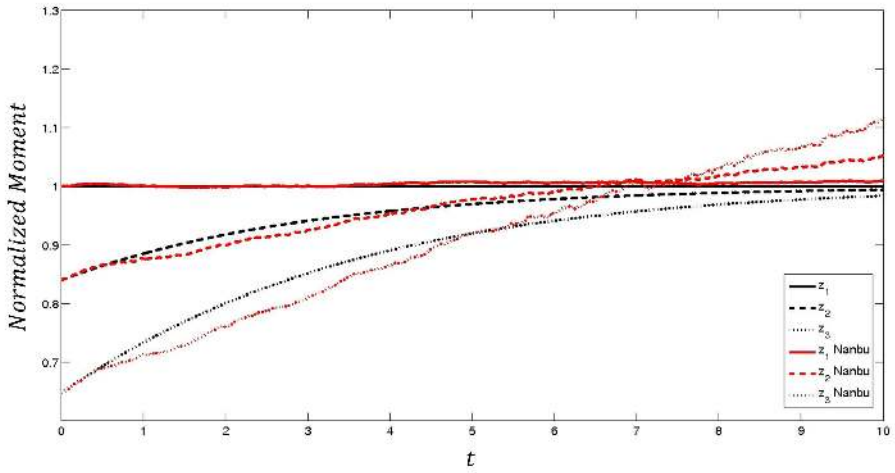


Figure 3.1: Normalized Moments of Bobylev-Krook-Wu Solution ($N_p = 100$, 600 run ensemble)

Notice the significant amount of variance present in the solution and that the solution tends to diverge more significantly for the higher order moments. A particularly concerning effect for which Nanbu's method has received much criticism is apparent in examining z_1. Note that the exact solution for z_1 is unity for all time. This moment is in fact a multiple of the energy in the gas which must be conserved for all time. Nanbu's method does not exactly conserve energy with each collision, but rather only on average. This leads to some variation in z_1 throughout the simulation.

The results illustrated in Figures 3.2 and 3.3 illustrate results for the first and second normalized moments for varying values of N_p. These results were derived from an

ensemble of 400 samples, and the time step was chosen as $\Delta t = 1/N_p$. Notice that as the number of simulated particles is increased, both the accuracy and variance are improved; however, even at the largest number of particles simulated, the variance is still substantial. Higher order moments exhibit similar features, however the divergence from the exact solution increases as higher moments are considered.

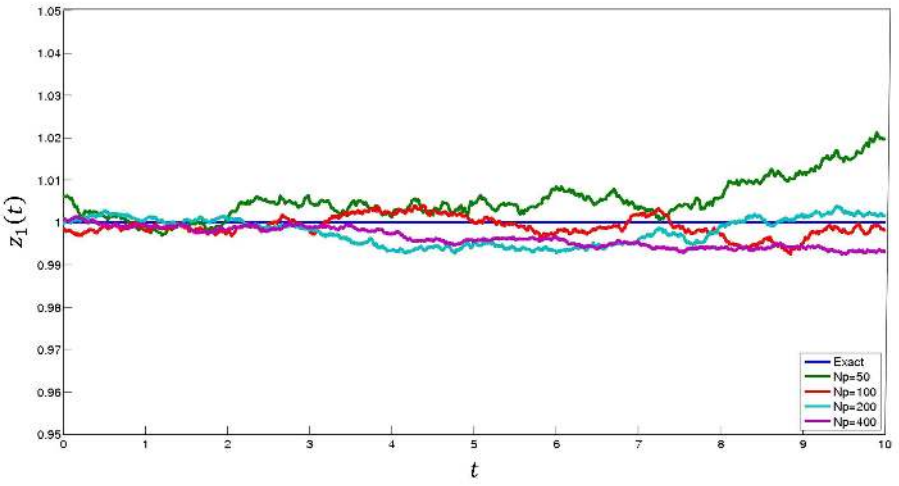


Figure 3.2: First Normalized Moment with Varying N_p (400 run sample)

To measure the effect of the simulation parameters on the variance in the solution, one technique is to consider the total variation of each moment. For the current problem we define the total variation of the n^{th} moment as

$$V(z_n) = \int_0^{t_{final}} |\dot{z}_n(t)|\, dt \tag{3.84}$$

For the current work, $t_{final} = 10$. The total variation for $N_p = 100$ is plotted against the number of runs in the ensemble average in Figure 3.4 along with the exact solution for the total variation of each moment. Notice that the only moment whose total variation is identically zero for all time is z_1 which again is a statement of the conservation of energy.

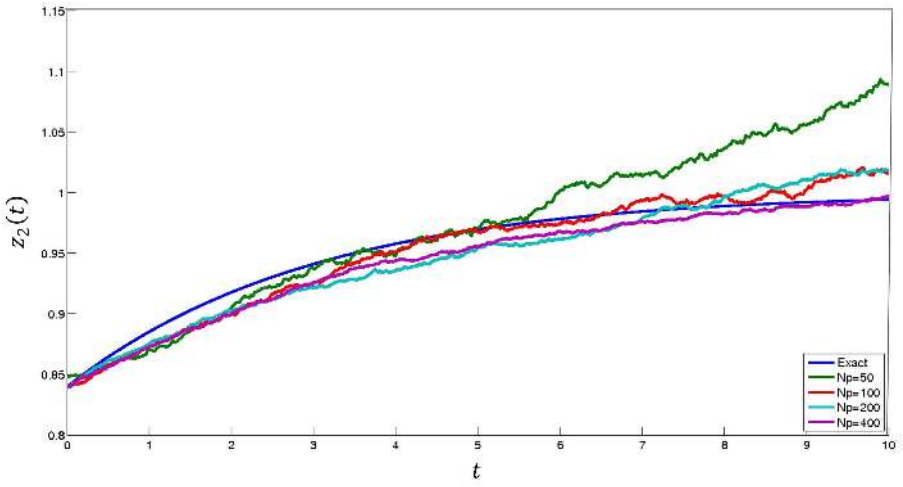


Figure 3.3: Second Normalized Moment with Varying N_p (400 run sample)

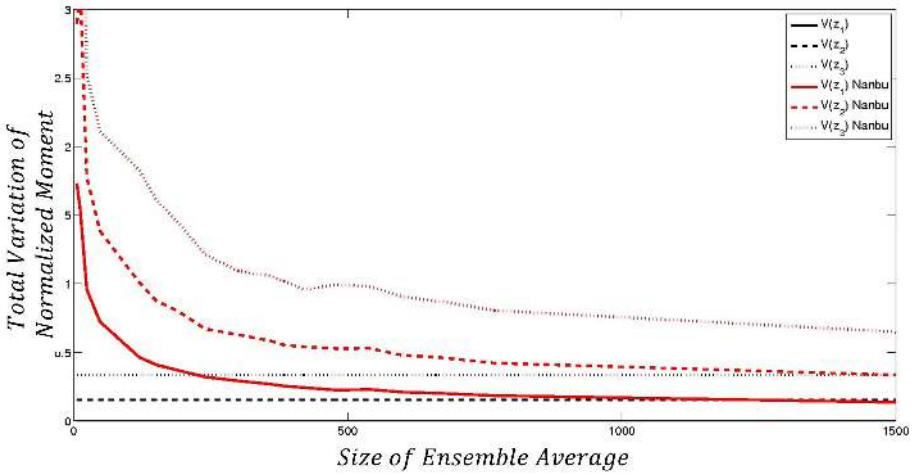


Figure 3.4: Total Variation of Nanbu Method as a Function of Sample Size for $N_p = 100$

While increasing the number of samples in a DSMC simulation is the primary approach for variance reduction, it does not improve the accuracy of the solution itself. To improve the accuracy of a simulation one must increase the number of simulated particles. Since it is not possible to directly analyze the distribution function, consider the $L^1\left(\mathbb{R}^3\right)$

error for each of the moments defined by

$$Error\left(z_n\right) = \int_0^{t_{final}} \left|\hat{z_n}\left(t\right) - z_n\left(t\right)\right| dt \tag{3.85}$$

Fixing the number of samples at 1000, Figure 3.5 shows the effect of increasing the number of particles on the $L^1\left(\mathbb{R}^3\right)$ error in the solution.

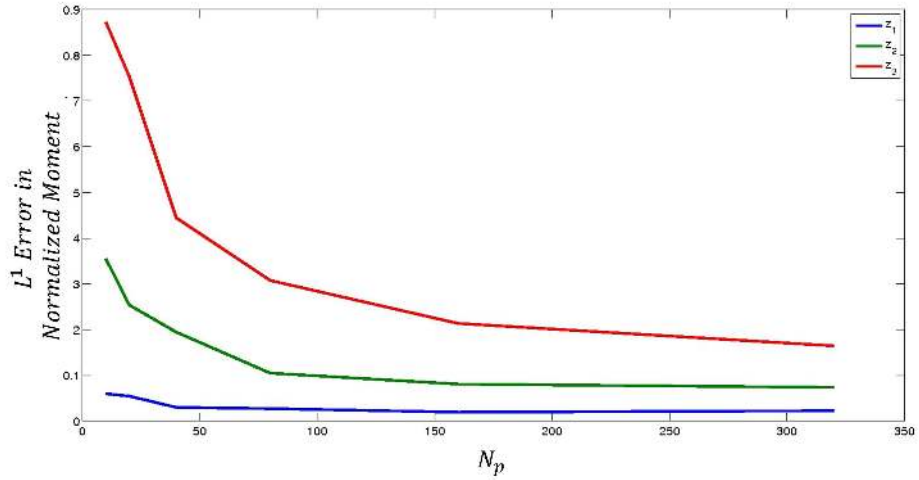


Figure 3.5: $L^1\left(\mathbb{R}^3\right)$ Error in Normalized Moments as a Function of the Number of Simulated Particles, Nanbu Method (1000 run ensemble)

IV. A Distributional Monte Carlo Algorithm Based on Kernel Density Estimation

As a first attempt towards a distributional approach, the concept of Kernel Density Estimation was applied to the DSMC framework. As outlined in Chapter 1, the Distributional Monte Carlo method advocated by the author replaces the point measure representation of the velocity density function with one in which each simulated particle is allowed to possess an entire velocity density function versus only a single velocity vector. One interesting limiting case is the case in which particle velocity density functions are all assumed to have the same functional form. Perhaps the simplest such representation is obtained by writing the particle density functions as

$$f_i(v) = \frac{1}{h^3} K\left(\frac{v - \bar{v}_i}{h}\right) \tag{4.1}$$

where K is a specified probability density function, $h \in \mathbb{R}^+$, and $\bar{v}_i$ is the mean velocity of the i^{th} simulated particle. The problem then becomes one of determining a suitable stochastic scheme for altering $\bar{v}_i$ to account for the collisional process. In this chapter, such a scheme is developed, which is equivalent to applying kernel density estimation to Nanbu's DSMC scheme. It will be shown that with an appropriately chosen value of K, the scheme converges in law, as well as in solution for $L^\infty\left(\mathbb{R}^3\right)$ and bounded solutions of the space homogeneous Boltzmann equation. These latter two forms of convergence have never previously been demonstrated for a stochastic particle scheme. The method could therefore be viewed as a bridge from Direct Simulation to Direct Solution.

The remainder of this chapter is outlined as follows. First, a brief explanation of kernel density estimation is presented, as the development of the scheme draws significantly upon the concept. Next, a brief derivation of the technique is presented, followed by proof of its convergence in law, as well as in solution for $L^\infty\left(\mathbb{R}^3\right)$ and bounded solutions of the space homogeneous Boltzmann equation. The chapter concludes with some numerical results obtained by applying the technique to the Bobylev-Krook-Wu solution.

4.1 Overview of 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 [77].

$$\hat{f}(x;h) = \frac{1}{Nh^d} \sum_{i=1}^{N} K\left(\frac{x - X_i}{h}\right) \tag{4.2}$$

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 $K \in L^2\left(\mathbb{R}^d\right)$ the kernel function. The kernel function must satisfy the following conditions

$$\int_{\mathbb{R}^d} K(x)\, dx = 1 \tag{4.3}$$

$$\int_{\mathbb{R}^d} xK(x)\, dx = 0 \tag{4.4}$$

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 [77] shows that the asymptotic mean square error between f and $\hat{f}$ is minimized when

$$h = \left[\frac{m(K)}{(\mu_2(K))^2 m(f'') N}\right]^{\frac{1}{5}} \tag{4.5}$$

where,

$$m(g) = \int_{\mathbb{R}^d} [g(x)]^2\, dx$$

$$\mu_2(g) = \int_{\mathbb{R}^d} x^2 g(x)\, dx$$

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, (4.5) becomes,

$$h = \left[\frac{8\sqrt{\pi} m(K)}{3(\mu_2(K))^2 N}\right]^{\frac{1}{5}} \sigma \tag{4.6}$$

4.2 Application to Distributional Monte Carlo (DMC-KDE)

Observe that a point measure approximation (as in DSMC, e.g. (1.11)) 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, a distributional Monte Carlo method employing some of the results from kernel density estimation was developed by the author [66, 67, 69]. The approach has been termed DMC-KDE. It should be noted that KDE has been applied in the Variance Reduced DSMC (VRDSMC) approach proposed by Al-Mohssen and Hadjiconstantinou [3–5] though in that application it was employed only as a smoothing and stabilization technique.

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

$$f = \frac{1}{N_p} \sum_{i=1}^{N_p} f_i \tag{4.7}$$

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

$$f_i(v) = \frac{1}{h^3} K\left(\frac{v - \bar{v}_i}{h}\right) \tag{4.8}$$

The mean of each particle's distribution function $\bar{v}_i$ 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

$$\tilde{f}(v; h) = \frac{1}{N_p h^3} \sum_{i=1}^{N_p} K\left(\frac{v - \bar{v}_i}{h}\right) \tag{4.9}$$

Choosing $h : \mathbb{N} \to \mathbb{R}^+$ with the property

$$\lim_{N_p \to \infty} h\left(N_p\right) = 0 \tag{4.10}$$

and choosing K with properties as described in the previous section, (4.9) 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 (4.6) to determine h.

$$K(x) = (2\pi)^{-3/2} \exp\left(-\frac{\|x\|^2}{2}\right) \tag{4.11}$$

$$h\left(N_p\right) = \left[\frac{32}{3\sqrt{2}N_p}\right]^{\frac{1}{5}} \sigma_{est} \tag{4.12}$$

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 $N_p \to \infty$, (4.9) 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 physical interpretation therefore is that although the collection of particles, which a simulated particle represents, all possess different velocities, as a collection, the particles represented by a single simulated particle are in translational 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 [58].

Beginning with (4.9) 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

$$f(v, t + \Delta t) = f(v, t) + \Delta t \frac{\partial f}{\partial t}(v, t) \tag{4.13}$$

where, $\frac{\partial f}{\partial t}$ is obtained from the space homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t}(v, t) = Q(f, f)(v, t) \tag{4.14}$$

and Q is defined by (2.31). Substituting (4.9) into (4.14), one obtains

$$\frac{\partial f}{\partial t} = \frac{1}{N_p^2} \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} \left(S_{ij} - T_{ij}\right) \tag{4.15}$$

where,

$$S_{ij} = \frac{1}{h^6} \int_{\mathbb{R}^3} \int_{S^+} K\left(\frac{v' - \bar{v}_i}{h}\right) K\left(\frac{w' - \bar{v}_j}{h}\right) \cdot \|v - w\| \, B\left(\|v - w\|, \theta\right) dndw \tag{4.16}$$

$$T_{ij} = \frac{1}{h^6} \int_{\mathbb{R}^3} \int_{S^+} K\left(\frac{v - \bar{v}_i}{h}\right) K\left(\frac{w - \bar{v}_j}{h}\right) \cdot \|v - w\| \, B\left(\|v - w\|, \theta\right) dndw \tag{4.17}$$

Substituting (4.11), (1.7) and (1.8) into (4.16), one obtains

$$\begin{aligned} S_{ij} = \frac{1}{2\pi h^6} \int_{\mathbb{R}^3} G(v, w) \exp\Bigg\{ -\frac{1}{4h^2} \Big[\|w\|^2 + \|v\|^2 + \\ \|\bar{v}_i\|^2 + \left\|\bar{v}_j\right\|^2 - \left(\bar{v}_i + \bar{v}_j\right) \cdot (w + v) \Big] \Bigg\} \|v - w\| \, dw \end{aligned} \tag{4.18}$$

where,

$$G(v, w) = \int_{S^+} \exp\left[a \cdot n\right] B\left(\|v - w\|, \theta\right)$$

$$a = \frac{\|v - w\| \left(\bar{v}_j - \bar{v}_i\right)}{4h^2}$$

Nanbu [58] shows that G may be approximated for small h by the following

$$G(v, w) \approx 2\pi B\left(\|v - w\|, \chi\right) \frac{e^{\|a\|}}{\|a\|} \text{ for } h \text{ small}$$

Substituting this expression for G into (4.18) yields

$$\begin{aligned} S_{ij} = \frac{2}{\left\|v_i - v_j\right\|} \int_{\mathbb{R}^3} \left\{ \frac{(2\pi)^{-3/2}}{h^3} \exp\left[-\frac{\left(v + w - \bar{v}_i - \bar{v}_j\right)^2}{4h^2} \right] \right\} \cdot \\ \left\{ \frac{1}{\sqrt{2\pi} h} \exp\left[-\frac{\left(\|v - w\| - g_{ij}\right)^2}{4h^2} \right] \right\} B\left(\|v - w\|, \chi\right) dw \end{aligned} \tag{4.19}$$

where $g_{ij} = \left\|\bar{v}_j - \bar{v}_i\right\|$. Next, we consider (4.13) under the limit as $h \to 0$ with $\frac{\partial f}{\partial t}$ as in (4.15).

$$f(v, t + \Delta t) = f(v, t) + \frac{\Delta t}{N_p^2} \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} \left(S_{ij}^* - T_{ij}^*\right) \tag{4.20}$$

where,

$$S_{ij}^* = \lim_{h \to 0} S_{ij}$$

$$T_{ij}^* = \lim_{h \to 0} T_{ij}$$

Definition 4.1. *Let* $\{g_\alpha\}$ *be a family of locally integrable functions on* $\mathbb{R}^n$ *with parameter* $\alpha \in \mathbb{R}$. $\{g_\alpha\}$ *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 [72].

For any bounded and continuous function ϕ on $\mathbb{R}^3$, it can be shown that It can be shown that

$$\lim_{h \to 0} \int_{\mathbb{R}^3} \phi(w) \left\{ \frac{(2\pi)^{-3/2}}{h^3} \exp\left[-\frac{\left(v + w - \bar{v}_i - \bar{v}_j\right)^2}{4h^2} \right] \right\} dw = \phi\left(\bar{v}_i + \bar{v}_j - v\right) \tag{4.21}$$

Thus, the first bracketed term in (4.19) is a three-dimensional delta family. Utilizing this property, it can be shown

$$S^*_{ij} = \frac{4}{g_{ij}} \delta\left(\|v^*\| - \frac{1}{2} g_{ij} \right) \sigma\left(g_{ij}, \chi\right) \tag{4.22}$$

where,

$$v^* = v - \frac{1}{2}\left(\bar{v}_i - \bar{v}_j\right) \tag{4.23}$$

Using (4.17) and performing a similar analysis, it can be shown

$$T^*_{ij} = g_{ij} B_{ij} \delta\left(v - \bar{v}_i\right) \tag{4.24}$$

where,

$$B_{ij} = \int_{S^+} B\left(g_{ij}, \theta\right) dn \tag{4.25}$$

Substituting these terms into (4.20), one obtains

$$f(v, t + \Delta t) = \frac{1}{N_p} \sum_{i=1}^{N_p} \left[\left(1 - P_i\right) \delta\left(f - \bar{v}_i\right) + Q_i(v) \right]$$

where,

$$P_i = \frac{\Delta t}{N} \sum_{j=1, j\neq i}^{N} g_{ij} B_{ij} \tag{4.26}$$

$$Q_i(v) = \frac{4\Delta t}{N} \sum_{j=1, j\neq i}^{N} \frac{B\left(g_{ij}, \chi\right)}{g_{ij}} \delta\left(\|v^*\| - \frac{1}{2} g_{ij}\right) \tag{4.27}$$

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

$$P_{ij} = \frac{\Delta t}{N} g_{ij} B_{ij}$$

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 [58] 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, $\bar{v}_i$ now represents the mean velocity of the i^{th} simulated particle. Collision interactions therefore have the effect of shifting the individual Maxwellian densities 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 $P^*_{ik} = \frac{P_{ik}}{P_i}$, 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 v^* based on (4.27), 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 demonstrating the benefits of such an approach, and a number of practical 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), it is proven that the DMC-KDE approach results in convergence in solution (strong convergence) for $L^{\infty}\left(\mathbb{R}^3\right)$ 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.

4.3 Proof of Convergence of DMC-KDE Approach

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 [8, 9] this is not unreasonable to expect. Although in the previous section specific functions for h and K were chosen, the proof is for the more general case.

Let $\{\bar{v}_i\}_{i=1}^{N_p}$ 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

$$\tilde{f}(v) = \frac{1}{N_p h^3} \sum_{i=1}^{N_p} K\left(\frac{v - \bar{v}_i}{h}\right)$$

where

$$K \in \left\{ g \in L^2\left(\mathbb{R}^3\right) : g(x) \geq 0 \ \forall x; \int_{\mathbb{R}^3} g(x)\, dx = 1; \int_{\mathbb{R}^3} x g(x)\, dx = 0 \right\},$$

and $h : \mathbb{N} \to \mathbb{R}^+$ defined as in (4.10). Define $\{f_h\}$ by

$$f_h(x) = \frac{1}{h^3} K\left(\frac{x}{h}\right)$$

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

$$\tilde{f}(v) = \frac{1}{N_p} \sum_{i=1}^{N_p} f_h(v - \bar{v}_i) \tag{4.28}$$

Lemma 4.1. *$\{f_h\}$ is a delta family as $h \to 0^+$.*

Proof. [72] Let $u = \frac{x}{h}$. we have

$$\int_{\mathbb{R}^3} f_h(x)\, dx = \frac{1}{h^3} \int_{\mathbb{R}^3} K\left(\frac{x}{h}\right) dx = \int_{\mathbb{R}^3} K(u)\, du = 1.$$

Also, for any $A > 0$,

$$\begin{aligned} \lim_{h\to 0} \int_{\|x\|>A} f_h(x)\, dx &= \lim_{h\to 0} \frac{1}{h^3} \int_{\|x\|>A} K\left(\frac{x}{h}\right) dx \\ &= \lim_{h\to 0} \int_{\|u\|>\frac{A}{h}} K(u)\, du \\ &= 0 \end{aligned}$$

and,

$$\begin{aligned} \lim_{h\to 0} \int_{\|x\|<A} f_h(x)\, dx &= \lim_{h\to 0} \frac{1}{h^3} \int_{\|x\|<A} K\left(\frac{x}{h}\right) dx \\ &= \lim_{h\to 0} \int_{\|u\|<\frac{A}{h}} K(u)\, du \\ &= 1 \end{aligned}$$

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

$$\begin{aligned} \lim_{h\to 0} \int_{\mathbb{R}^3} f_h(x)\phi(x)\, dx - \phi(0) &= \lim_{h\to 0} \left[\int_{\mathbb{R}^3} f_h(x)\phi(x)\, dx - \phi(0) \int_{\mathbb{R}^3} f_h(x)\, dx \right] \\ &= \lim_{h\to 0} \int_{\mathbb{R}^3} f_h(x) \left[\phi(x) - \phi(0)\right] dx \end{aligned}$$

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

$$\int_{\mathbb{R}^3} f_h(x)\,\eta(x)\,dx = \int_{\|x\|<B} f_h(x)\,\eta(x)\,dx + \int_{\|x\|>B} f_h(x)\,\eta(x)\,dx$$

Choose $M > 0$ such that $|\eta(x)| \leq M\ \forall x$. Let $p(B) = \max_{\|x\|<B} |\eta(x)|$. We have,

$$\begin{aligned}
\left|\int_{\mathbb{R}^3} f_h(x)\,\eta(x)\,dx\right| &\leq \left|\int_{\|x\|\leq B} f_h(x)\,\eta(x)\,dx\right| + \left|\int_{\|x\|>B} f_h(x)\,\eta(x)\,dx\right| \\
&\leq p(B)\left|\int_{\|x\|\leq B} f_h(x)\,dx\right| + M\left|\int_{\|x\|>B} f_h(x)\,dx\right| \\
&\leq p(B) + M\left|\int_{\|x\|>B} f_h(x)\,dx\right|
\end{aligned}$$

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

$$\left|\int_{\|x\|>B} f_h(x)\,dx\right| < \frac{\epsilon}{2M}$$

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

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

whenever $0 < h < \alpha$. Therefore, $\lim_{h\to 0}\int_{\mathbb{R}_3} f_h(x)\,\eta(x)\,dx = 0$. Which implies $\lim_{h\to 0}\int_{\mathbb{R}_3} f_h(x)\,\phi(x)\,dx = \phi(0)$, 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 $\lim_{N_p\to\infty} h\left(N_p\right) = 0$. Then $\left\{f_{h\left(N_p\right)}\right\}$ is a delta family as $N_p \to \infty$ by Lemma 4.1. Denote this family by $\left\{f_{N_p}\right\}$. Next it is proven 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 4.2. *For any bounded and continuous ϕ on $\mathbb{R}^3$,*

$$\lim_{N_p\to\infty}\int_{\mathbb{R}^3}\phi(v)\,\tilde{f}(v)\,dv=\lim_{N_p\to\infty}\int_{\mathbb{R}_3}\phi(v)\,\hat{f}(v)\,dv$$

where,

$$\hat{f}(v)=)\frac{1}{N_p}\sum_{i=1}^{N_p}\delta(v-\bar{v}_i) \tag{4.29}$$

Proof. Choose any $\epsilon>0$. Then by Lemma 4.1, for any bounded and continuous ϕ, there exists M such that

$$\left|\int_{\mathbb{R}^3}\phi(v)\,f_{N_p}(v-\bar{v}_i)\,dv-\phi(\bar{v}_i)\right|<\epsilon$$

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

$$\begin{aligned}\left|\int_{\mathbb{R}^3}\phi(v)\left(\tilde{f}(v)-\hat{f}(v)\right)dv\right| &= \left|\int_{\mathbb{R}^3}\phi(v)\,\frac{1}{N_p}\left(\sum_{i=1}^{N_p}f_{N_p}(v-\bar{v}_i)-\delta(v-\bar{v}_i)\right)dv\right|\\ &\le \frac{1}{N_p}\sum_{i=1}^{N_p}\left|\int_{\mathbb{R}^3}\phi(v)\left(f_{N_p}(v-\bar{v}_i)-\delta(v-\bar{v}_i)\right)dv\right|\\ &< \frac{1}{N_p}\sum_{i=1}^{N_p}\epsilon\\ &= \epsilon\end{aligned}$$

for all $N_p>M$. □

Combining this result with Theorem 3.7, yields the following result.

Theorem 4.1. *If the time discretized space homogeneous Boltzmann equation (3.2) has a non-negative solution $f\in L^1\left(\mathbb{R}^3\right)$, then the solution $\tilde{f}$ 4.9 of the DMC-KDE method converges in law (see Definition 3.1) at each timestep.*

Proof. Take any $\phi\in C_b\left(\mathbb{R}^3\right)$. Choose any $\epsilon>0$. Then, by the triangle inequality,

$$\begin{aligned}\left|\int_{\mathbb{R}^3}\phi(v)\left(\tilde{f}(v)-f(v)\right)dv\right| \le &\left|\int_{\mathbb{R}^3}\phi(v)\left(\tilde{f}(v)-\hat{f}(v)\right)dv\right|\\ &+\left|\int_{\mathbb{R}^3}\phi(v)\left(\hat{f}(v)-f(v)\right)dv\right|\end{aligned}$$

where $\hat{f}$ is as defined in (4.29). Applying Lemma 4.2 and Theorem 3.7 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 law to the space homogeneous Boltzmann solution. We next prove that stronger forms of convergence are possible compared with Nanbu's method, specifically for solutions which are $L^\infty\left(\mathbb{R}^3\right)$ or bounded. Such solutions arise frequently in kinetic theory and are of greater practical interest than $L^1\left(\mathbb{R}^3\right)$ solutions.

Corollary 4.1. *If the time discretized space homogeneous Boltzmann equation (3.2) has a non-negative solution $f \in L^\infty\left(\mathbb{R}^3\right)$, then the solution $\tilde{f}$ (4.9) of the DMC-KDE method converges in $L^\infty\left(\mathbb{R}^3\right)$ to f at each timestep. That is,*

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

Proof. Take any $\epsilon > 0$. Since $\tilde{f}, f \in L^\infty\left(\mathbb{R}^3\right)$, there exist $B_1, B_2 \in \mathbb{R}^+$ such that $\left|\tilde{f}(x)\right| \le B_1$, and $|f(x)| \le B_2$ 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 $x' \in \mathbb{R}^3 - S$, define $\phi_h : \mathbb{R}^3 \to \mathbb{R}$ by

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

where $h \in \mathbb{R}^+$. By Lemma 4.1, ϕ_h is a delta family as $h \to 0^+$ centered at x'. Therefore, there exists $H_1 > 0$ such that

$$\left|\int_{\mathbb{R}^3} \phi_h(x)\, \tilde{f}(x)\, dx - \tilde{f}(x')\right| < \frac{\epsilon}{3} \tag{4.30}$$

for all $h < H_1$. Likewise, there exists $H_2 > 0$ such that

$$\left|\int_{\mathbb{R}^3} \phi_h(x)\, f(x)\, dx - f(x')\right| < \frac{\epsilon}{3} \tag{4.31}$$

Note that ϕ_h is everywhere continuous and $|\phi_h(x)| \leq \frac{1}{\sqrt{2\pi h^3}}$ for all $x \in \mathbb{R}^3$. Thus by Theorem 4.1, there exist $N > 0$ such that

$$\left| \int_{\mathbb{R}^3} \phi_h(x) \left(\tilde{f}(x) - f(x) \right) dx \right| < \frac{\epsilon}{3} \tag{4.32}$$

for all $N_p > N$. Choose $H < \min\{H_1, H_2\}$, then for any $N_p < N$ we have,

$$\begin{aligned}
\left\| \tilde{f} - f \right\|_\infty &= \operatorname{ess\,sup} \left| \tilde{f} - f \right| \\
&= \sup_{x' \in \mathbb{R}^3 - S} \left| \tilde{f}(x') - f(x') \right| \\
&\leq \sup_{x' \in \mathbb{R}^3 - S} \left| \tilde{f}(x') - \int_{\mathbb{R}^3} \phi_h(x) \tilde{f}(x)\, dx \right| + \\
&\quad \left| \int_{\mathbb{R}^3} \phi_h(x) \tilde{f}(x)\, dx - f(x') \right| \text{ by the triangle inequality} \\
&\leq \sup_{x' \in \mathbb{R}^3 - S} \left| \tilde{f}(x') - \int_{\mathbb{R}^3} \phi_h(x) \tilde{f}(x)\, dx \right| + \left| \int_{\mathbb{R}^3} \phi_h(x) \left(\tilde{f}(x) - f(x) \right) dx \right| + \\
&\quad \left| \int_{\mathbb{R}^3} \phi_h(x) f(x)\, dx - f(x') \right| \text{ by the triangle inequality} \\
&< \frac{\epsilon}{3} + \frac{\epsilon}{3} + \frac{\epsilon}{3} \text{ by inequalities (4.30), (4.31), and (4.32)} \\
&= \epsilon
\end{aligned}$$

□

Corollary 4.2. *If the time discretized space homogeneous Boltzmann equation (3.2) has a non-negative bounded solution f, then the solution $\tilde{f}$ (4.9) of the DMC-KDE method converges pointwise to f.*

Proof. The proof follows naturally from Corollary 4.1. □

The current work represents the first time these forms of convergence have been proven for a stochastic particle method, and illustrates that DMC-KDE transforms DSMC from a Boltzmann simulator to a Boltzmann solver, allowing direct evaluation of the velocity density function.

4.4 Application to Bobylev, Krook, and Wu Problem

To provide a numerical demonstration of the DMC-KDE technique, the method was applied to the Bobylev-Krook-Wu problem. As with Nanbu's DSMC technique, it is possible to compute the normalized moments by substituting the DMC-KDE distribution function into (2.61)

$$z_n(t) = \frac{1}{(2n+1)!!} \sum_{i=1}^{N_p} \frac{1}{N_p h^3} \int_{\mathbb{R}^3} K\left(\frac{v - \bar{v}_i(t)}{h}\right) \|v\|^{2n} \, dv \tag{4.33}$$

from which closed form expressions for the moments can be derived. The first three moments are given by

$$z_1(t) = \frac{1}{3N_p} \sum_{i=1}^{N_p} \bar{v}_i^2(t) + \frac{1}{2}h^2$$

$$z_2(t) = \frac{1}{15N_p} \sum_{i=1}^{N_p} \bar{v}_i^4(t) + \frac{1}{4}h^4$$

$$z_3(t) = \frac{1}{105N_p} \sum_{i=1}^{N_p} \bar{v}_i^6(t) + \frac{107}{840}h^6$$

One may therefore see that the Nanbu solution and the DMC-KDE solution for the normalized moments vary only by a term involving h^{2n}. Since $h \to 0$ as $N_p \to \infty$ these terms become negligible as the number of simulated particles become large and are rapidly diminishing for higher order moments.

Figure 4.1 presents a comparison of the first three normalized moments of the density function for the case in which $N_p = 100$. The results have been averaged over an ensemble of 600 runs. Note that like the DSMC results, there is a significant amount of variance present in the solution and that the solution tends to diverge more significantly for the higher order moments. Additionally, note that the moments are offset by the h^{2n} term, which is most visible for the first moment.

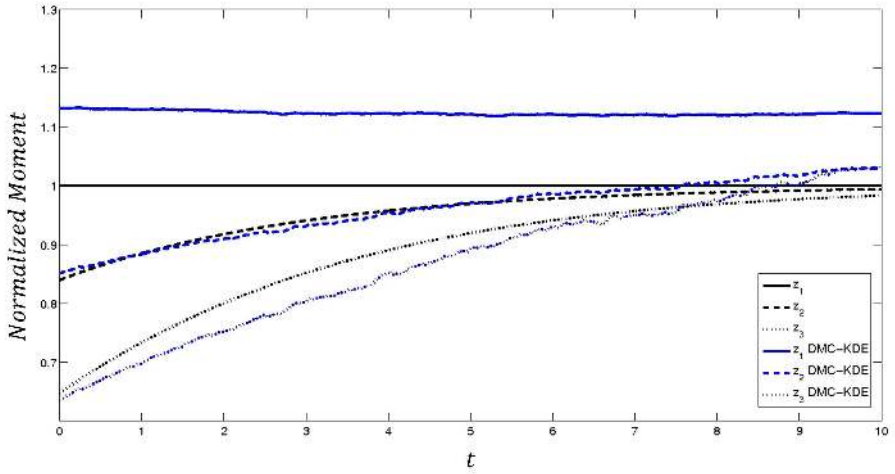


Figure 4.1: Normalized Moments of Bobylev-Krook-Wu Solution (N_p = 100, 600 run ensemble)

Figures 4.2 and 4.3 illustrate the same normalized moments for the DMC-KDE solution of the Bobylev problem for an ensemble of 400 samples. Notice that in comparison to Figures 3.2 and 3.3, the moments are offset by an amount proportional to h^{2n}. As predicted theoretically, the offset diminishes rapidly with increasing

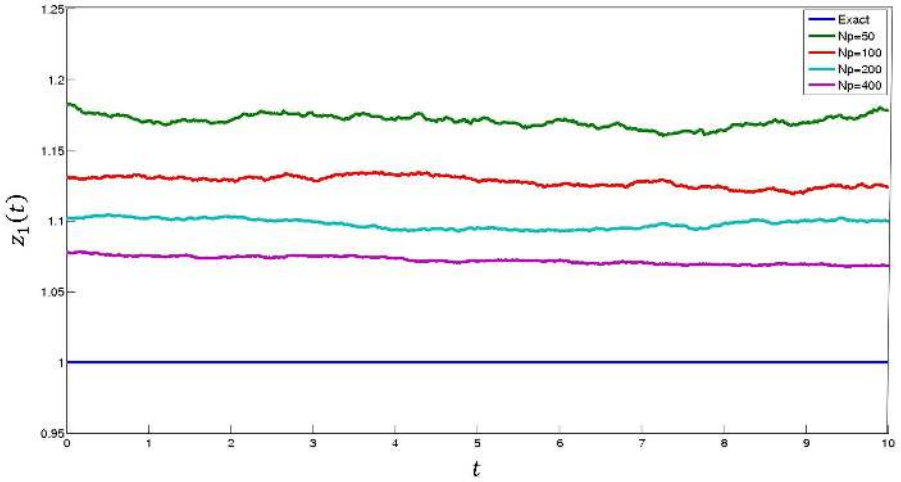


Figure 4.2: First Normalized Moment with Varying N_p (400 run sample)

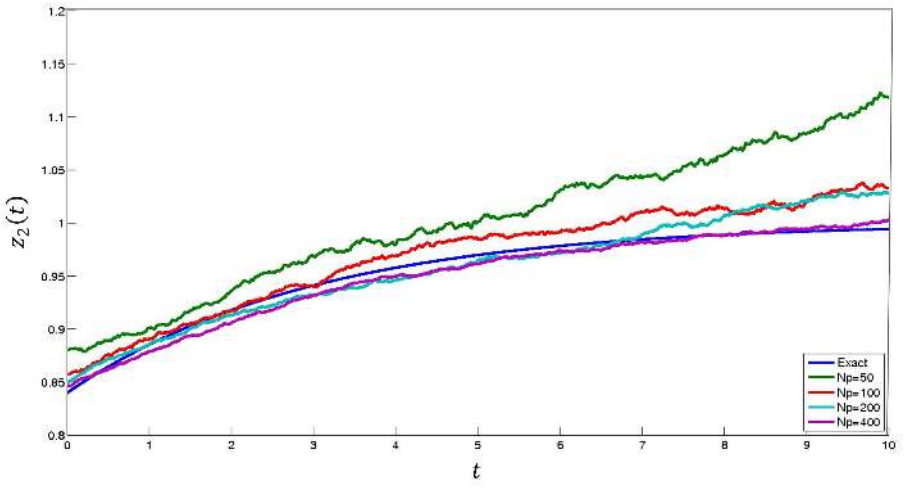


Figure 4.3: Second Normalized Moment with Varying N_p (400 run sample)

moment orders and as the number of simulated particles is increased. Strictly speaking, however, notice that neither method performs particularly well in capturing the evolution of the higher order moments. The advantage of DMC-KDE is that it allows for direct computation/visualization of the distribution function, but when only examining moments this advantage is not observable.

To better exhibit this advantage consider the $L^1\left(\mathbb{R}^3\right)$ error between the approximate and actual solution defined by

$$Error\,(t) = \int_{\mathbb{R}^3} \left|\tilde{f}\,(v) - f\,(v)\right| dv \tag{4.34}$$

As the Bobylev-Krook-Wu solution is bounded and continuous for all t, Corollary 4.2 guarantees that $\tilde{f}\,(v) \rightarrow f\,(v)$ for all $v \in \mathbb{R}^3$. Since $\tilde{f}$ is also bounded and continuous it is trivial to prove that in this case convergence in the $L^1\left(\mathbb{R}^3\right)$ norm is also guaranteed. Figure 4.4 presents the results for the $L^1\left(\mathbb{R}^3\right)$ error as it varies with the number of simulated particles for a 1000 run sample.

Notice that the convergence is fairly monotonic with some exception at larger values of t. As stated in the previous section, this form of convergence has never previously been

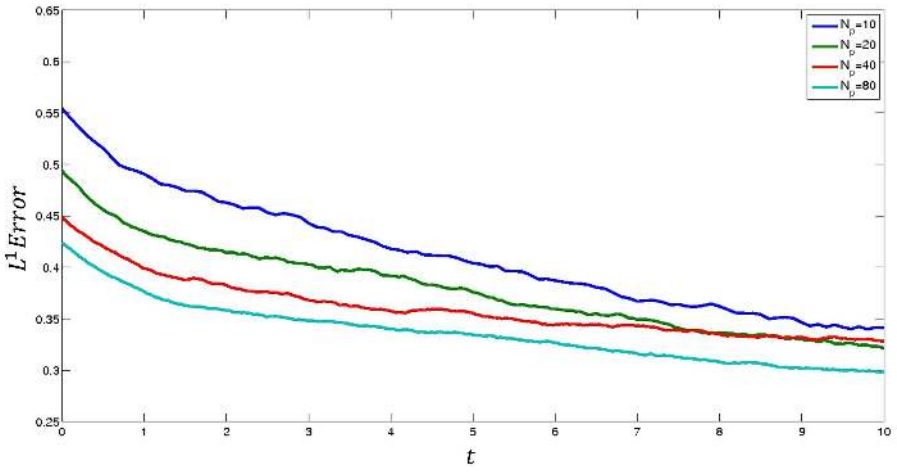


Figure 4.4: $L^1\left(\mathbb{R}^3\right)$ Error for DMC-KDE Bobylev-Krook-Wu Solution with Varying N_p (100 run sample)

proven for a stochastic particle scheme for the Boltzmann equation. The present work has demonstrated that by applying principles from kernel density estimation such schemes can be taken from the realm of Boltzmann simulators to the realm of Boltzmann solvers.

V. A General Approach for Distributional Monte Carlo (DMC) Methods for the Space Homogeneous Boltzmann Equation

As observed in the previous chapter, the DMC-KDE approach allowed for stronger forms of convergence than traditional DSMC and provides a means for recovering the velocity density function. The fixed functional form of the particle velocity density functions, however, precludes it from being considered a fully distributional method as envisioned by the author. A Distributional Monte Carlo method for the Boltzmann equation is a particle simulation which employs a non-singular representation of the velocity density function by allowing each simulated particle to posess a velocity density function throughout the simulation instead of just a single velocity. Collision outcomes for a given pair are determined by computing an approximate space homogeneous relaxation of the velocity density functions of the two simulated particles participating in a collision.

From a physically intuitive point of view, this approach makes sense. As each simulated particle represents a very large number of actual particles, kinetic theory tells us that intermolecular collisions occurring within the collection will drive the density function toward equilibrium. What is perhaps somewhat suprising is that it can be shown that such an approach arises naturally from the time discretized, space homogeneous Boltzmann equation when nonsingular particle distributions with arbitrary forms are employed.

In this case, the velocity density function of the gas is modelled by

$$f(v) = \frac{1}{N_p} \sum_{i=1}^{N_p} g_i(v) \tag{5.1}$$

where g_i is the velocity density function of the i^{th} simulated particle. No particular functional form of g_i is assumed in the general approach. Let f, g be density functions such that $f(v)(1 + \|v\|) \in L^1\left(\mathbb{R}^3\right)$, $g(v)(1 + \|v\|) \in L^1\left(\mathbb{R}^3\right)$, $f(v)\log(f(v)) \in L^1\left(\mathbb{R}^3\right)$, and $g(v)\log(g(v)) \in L^1\left(\mathbb{R}^3\right)$. Then by Theorem 2.3 the space homogeneous Boltzmann

equation has a unique solution over the time interval Δt for the initial condition $f_0 = \frac{1}{2}(f+g)$. Denote this solution by $\mathcal{G}(f,g)$.

To illustrate the mathematical motivation for treating collision interactions as a relaxation problem, recall the weak transition kernel formulation of the space homogeneous Boltzmann equation from Chapter 2

$$\int_{\mathbb{R}^3} \phi(v) f^{k+1}(v)\, dv = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K_{v,w}(\phi) f^k(v) f^k(w)\, dwdv \tag{5.2}$$

By definition we have

$$\begin{aligned}
\int_{\mathbb{R}^3} \phi(v)\mathcal{G}(f,g)\, dv &= \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K_{v,w}(\phi)(f(v)+g(v))(f(w)+g(w))\, dwdv \\
&= \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K_{v,w}(\phi)(f(v)f(w)+f(v)g(w)+g(v)f(w)+ \\
&\quad g(v)g(w))\, dwdv \\
&= \frac{1}{4}\left(\int_{\mathbb{R}^3}\mathcal{G}(f,f)\, dv + 2\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K_{v,w}(\phi) f(v) g(w)\, dwdv + \right. \\
&\quad \left. \int_{\mathbb{R}^3}\mathcal{G}(g,g)\, dv\right)
\end{aligned} \tag{5.3}$$

Rearraging, one obtains

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K_{v,w}(\phi) f(v) g(w)\, dwdv = \int_{\mathbb{R}^3}\phi(v)\left(2\mathcal{G}(f,g) - \frac{1}{2}\mathcal{G}(f,f) - \frac{1}{2}\mathcal{G}(g,g)\right)dv \tag{5.4}$$

Allowing f^k to have the form of equation 5.1, upon direct substitution into Equation 5.2, one obtains

$$\int_{\mathbb{R}^3} \phi(v) f^{k+1}(v)\, dv = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K_{v,w}(\phi) g_i^k(v) g_j^k(w)\, dwdv \tag{5.5}$$

Note that each particle pair contibutes a term similar in form to Equation 5.4 to the solution, therefore one obtains

$$\int_{\mathbb{R}^3} \phi(v) f^{k+1}(v)\, dv = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\int_{\mathbb{R}^3}\phi(v)\left(2\mathcal{G}\left(g_i^k, g_j^k\right) - \frac{1}{2}\mathcal{G}\left(g_i^k, g_i^k\right) - \frac{1}{2}\mathcal{G}\left(g_j^k, g_j^k\right)\right)dv \tag{5.6}$$

This demonstrates that the solution at the next time step can be written as a summation of space homogeneous relaxation solutions for the particle pairs. This expression can be further simplified to

$$\int_{\mathbb{R}^3} \phi(v) f^{k+1}(v)\, dv = \frac{2}{N^2} \sum_{\substack{i=1 \\ i\neq j}}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left(g_i^k, g_j^k\right) dv + \frac{1}{N} \sum_{i=1}^{N} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left(g_i^k, g_i^k\right) dv \tag{5.7}$$

In this form, the evolved solution is clearly decomposed into two contributions. The first term on the right side represents space homogeneous relaxation among the particle pairs while the second term represents the self-evolution of the individual particle distribution function due to intermolecular collisions only between the actual particles it represents. In the special case where the g_i^k terms are Maxwellian, $\mathcal{G}\left(g_i^k, g_i^k\right) = g_i^k$, and thus

$$\begin{aligned} \int_{\mathbb{R}^3} \phi(v) f^{k+1}(v)\, dv &= \frac{2}{N^2} \sum_{\substack{i=1 \\ i\neq j}}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left(g_i^k, g_j^k\right) dv + \frac{1}{N} \sum_{i=1}^{N} \int_{\mathbb{R}^3} \phi(v)\, g_i^k(v)\, dv \\ &= \frac{2}{N^2} \sum_{\substack{i=1 \\ i\neq j}}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left(g_i^k, g_j^k\right) dv + \int_{\mathbb{R}^3} \phi(v) f^k(v)\, dv \end{aligned} \tag{5.8}$$

which is somewhat analguous to the form obtained by Nanbu in Equation 3.20 in that it is decomposed into a binary interaction term and the original density function.

In principle, any stochastic scheme which emulates the density function on the right-hand side of Equation 5.6 should be a valid simulation scheme for the space-homogeneous Boltzmann equation. Within the Distributional Monte Carlo framework, one such choice is as follows

- Choose a set of velocity density functions $\{g_i\}_{i=1}^N$ for which the probability measure, P_N on $\mathbb{R}^3$ defined by

$$P_N(A) = \frac{1}{N} \sum_{i=1}^{N} \int_A g_i(v)\, dv \tag{5.9}$$

converges in law to P_0 defined by

$$P_0(A) = \int_A f_0(v)\, dv \tag{5.10}$$

where f_0 is the initial condition for the Boltzmann equation.

- Choose a sequence of equidistributed random numbers $\{r_i\}$, $r_i \in [0, 1]$.

- Define the indices of collision partners

$$C(i, N) = \lfloor N r_i \rfloor + 1 \tag{5.11}$$

with velocity density functions given by

$$h_i(v) = g_{C(i,N)}(v) \tag{5.12}$$

- Compute the set of velocity density functions $\{p_i\}_{i=1}^N$ where p_i is given by

$$p_i = 2\mathcal{G}(g_i, h_i) - \frac{1}{2}\mathcal{G}(g_i, g_i) - \frac{1}{2}\mathcal{G}(h_i, h_i) \tag{5.13}$$

The overall density function is given by

$$\check{f} = \frac{1}{N}\sum_{i=1}^{N} p_i \tag{5.14}$$

The sequence of probability measures $\left\{\hat{P}_N\right\}$ on $\mathbb{R}^3$ defined by

$$\hat{P}_N(A) = \int_A \check{f}(v)\, dv = \frac{1}{N}\sum_{i=1}^{N}\int_A p_i(v)\, dv \text{ for any } A \subset \mathbb{R}^3 \tag{5.15}$$

will be shown to converge in law to P_1 defined by

$$P_1(A) = \int_A f_1(v)\, dv \tag{5.16}$$

as $N \to \infty$. Here f_1 is the Boltzmann solution at time $t = \Delta t$

- Repeat the process with f_1 as the new initial condition.

5.1 Proof of Convergence of DMC Approach

In developing this approach, it became necessary to develop a generalization of one of Babovsky's theorems. Namely, the following theorem provides a sufficient condition for the convergence of <u>any</u> numerical scheme for the Boltzmann equation; that is, no assumptions are made regarding the use of a point measure approximation to the density function.

Theorem 5.1. *Let f^k be the solution of the time discretized space homogeneous Boltzmann equation (3.2) at $t = t_k$, and let P^k be the probability measure defined by*

$$P^k(A) = \int_A f^k(v)\,dv \text{ for any } A \subset \mathbb{R}^3 \tag{5.17}$$

Define $P2^k$ to be the probability measure on $D \times \mathbb{R}^3 \times \mathbb{R}^3$ given by

$$P2^k(B) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_D f^k(v)\,f^k(w)\,dxdwdv \tag{5.18}$$

If a sequence of probability measures $\left\{\tilde{P2}_N\right\}$ converges to $P2^k$ as $N \to \infty$, then the sequence of probability measures, $\left\{\tilde{P2}_N \circ \Psi^{-1}\right\}$, on $\mathbb{R}^3$ converges to P^{k+1} in law as $N \to \infty$.

Proof. Since Ψ is absolutely continuous and $\tilde{P2}_N \to P2^k$ in law as $N \to \infty$, we have that $\tilde{P2}_N \circ \Psi^{-1} \to P2^k \circ \Psi^{-1}$ in law as $N \to \infty$ by Lemma 3.4. Take any $\phi \in C_b\left(\mathbb{R}^3\right)$. Then,

$$\begin{aligned}
\int_{\mathbb{R}^3} \phi(v)\, d\left(P2^k \circ \Psi^{-1}\right) &= \int_{\mathbb{R}^3} \phi(\Psi(x,v,w))\, dP2^k \text{ by Lemma 3.3} \\
&= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_D \phi(\Psi(x,v,w))\, f^k(v)\, f^k(w)\, dxdwdv \text{ by (5.18)} \\
&= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K_{v,w}(\phi)\, f^k(v)\, f^k(w)\, dxdwdv \text{ by (3.35) and (3.36)} \\
&= \int_{\mathbb{R}^3} \phi(v)\, f^{k+1}(v)\, dv \text{ by (3.32)}
\end{aligned}$$

Thus, $P2^k \circ \Psi^{-1} = P^{k+1}$ and hence, $\tilde{P2}_N \circ \Psi^{-1}$ converges in law to P^{k+1} as $N \to \infty$. □

Thus, any scheme which can be shown to be constructed in such a way that the above theorem is satisfied will be convergent.

The following results will be needed for the convergence proofs that follow.

Theorem 5.2. *(Kolmogorov's Convergence Criterion) [60] Suppose $\{X_n\}$ is a sequence of independent random variables. If*

$$\sum_{j=1}^{\infty} Var\left(X_j\right) < \infty \tag{5.19}$$

then

$$\sum_{j=1}^{\infty} \left(X_j - EX_j\right) \text{ converges almost surely.} \tag{5.20}$$

Lemma 5.1. *(Kronecker's Lemma) [60] Given two sequences $\{x_k\}$ and $\{a_k\}$ such that $x_k, a_k \in \mathbb{R}$ and $0 < a_k \uparrow \infty$. If*

$$\sum_{k=1}^{\infty} \frac{x_k}{a_k} \text{ converges,} \tag{5.21}$$

then

$$\lim_{n\to\infty} a_n^{-1} \sum_{k=1}^{n} x_k = 0 \tag{5.22}$$

While the traditional strong law of large numbers typically is stated as applying to only sequences of independent, identically distributed random variables, by combining Theorem 5.2 and Lemma 5.1 one can derive the following Corollary for independent sequences of random variables (not neccessarily identically distributed), which is sometimes labelled as Kolmogorov's Strong Law of Large Numbers.

Corollary 5.1. *(Kolmogorov's Strong Law of Large Numbers) [60] Let $\{X_n\}$ be a sequence of independent random variables satisfying $E\left(X_n^2\right) < \infty$. If $\{b_n\}$ is a monotonic sequence such that $b_n \uparrow \infty$, and if*

$$\sum_{k} Var\left(\frac{X_k}{b_k}\right) < \infty \tag{5.23}$$

then

$$\frac{S_n - ES_n}{b_n} \to 0 \text{ almost surely as } n \to \infty \tag{5.24}$$

where $S_n = \sum_{k=1}^{n} X_k$.

This result allows one to prove the following.

Theorem 5.3. *Let f^k be the solution to the time discretized space homogeneous Boltzmann equation (3.2), and define P to be the probability measure on $\mathbb{R}^3$ given by*

$$P(A) = \int_A f(v)\,dv \text{ for any } A \subset \mathbb{R}^3 \tag{5.25}$$

Define the probability measure, $\hat{P}$ on $\mathbb{R}^3 \times \mathbb{R}^3$ by

$$\hat{P}(B) = \int_B f(v) f(w)\,dvdw \text{ for any } B \subset \mathbb{R}^3 \times \mathbb{R}^3 \tag{5.26}$$

Let P_N be the probability measure defined on $\mathbb{R}^3$ by

$$P_N(A) = \frac{1}{N}\sum_{i=1}^{N} \int_A g_i(v)\,dv \text{ for any } A \subset \mathbb{R}^3 \tag{5.27}$$

where $\{g_i\}_{i=1}^N$ is a set of density funtions. Also define the probability measure $\hat{P}_N$ on $\mathbb{R}^3 \times \mathbb{R}^3$ to be

$$\hat{P}_N(B) = \frac{1}{N}\sum_{i=1}^{N} \int_B g_i(v)\, h_i(w)\,dvdw \text{ for any } B \subset \mathbb{R}^3 \times \mathbb{R}^3 \tag{5.28}$$

where h_i are defined as in (5.12). If P_N converges to P in law as $N \to \infty$, then $\hat{P}_N$ converges in law to $\hat{P}$ as $N \to \infty$.

Proof. Define the distribution functions associated with P and $\hat{P}$ to be

$$F(v) = \int_{v' \le v} f(v')\,dv' \tag{5.29}$$

$$G(v,w) = \int_{v' \le v}\int_{w' \le w} f(v') f(w')\,dv'dw' = F(v) F(w) \tag{5.30}$$

respectively. Also define the distribution functions associated with P_N and $\hat{P}_N$ to be

$$F_N(v) = \int_{v' \le v} \frac{1}{N}\sum_{i=1}^{N} g_i(v')\,dv' \tag{5.31}$$

$$G_N(v,w) = \int_{v' \le v}\int_{v' \le w} \frac{1}{N}\sum_{i=1}^{N} g_i(v')\, h_i(w')\,dv'dw' \tag{5.32}$$

Take any $(a,b) \in \mathbb{R}^3 \times \mathbb{R}^3$. We will prove $G_N(a,b) \to G(a,b)$ as $N \to \infty$, and thus $\hat{P}_N$ converges to $\hat{P}$ in law as $N \to \infty$. Define the particle distribution functions

$$\mathcal{F}_i(v) = \int_{v' \leq v} g_i(v')\, dv' \tag{5.33}$$

Note that

$$F_N(v) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{F}_i(v) \tag{5.34}$$

Let $\Omega_n = (0,1)$. Then $(\Omega_n, \mathcal{S}_n, \lambda)$ is a probability space, where $\mathcal{S}_n$ is the standard $\sigma-$algebra on $(0,1)$ and λ is Lebesgue measure. Define Ω to be the cartesian product

$$\Omega = \prod_{n=1}^{N} \Omega_n \tag{5.35}$$

The elements of Ω are thus N-tuples $\{\omega_n\}_{n=1}^N$ with $\omega_n \in \Omega_n$. Defining π_m to be the natural projection of Ω onto Ω_m (i.e. $\pi_m\left(\{\omega_n\}_{n=1}^N\right) = \omega_m$), let $\mathcal{S}$ be the smallest $\sigma-$ algebra of subsets of Ω containing all sets $\pi_n^{-1}(A)$ for all n and all $A \subset \Omega_n$. Here, $\pi_n^{-1}(A)$ denotes the pre-image of A (namely, $\pi_n^{-1}(A) \coloneqq \{\omega \in \Omega : \pi(\omega) \in A \subset \Omega_n\}$) . Then $(\Omega, \mathcal{S}, Prob)$ is a product probability space with $Prob = \lambda^N$. Define the sequence of random variables $X_i : \Omega \to [0,1]$ by

$$\begin{aligned} X_i(\omega) &= \int_{v \leq a} \int_{w \leq b} g_i(v)\, h_i(w)\, dvdw \\ &= \int_{v \leq a} g_i(v)\, dv \int_{w \leq b} g_{C(i,N)}(w)\, dw \\ &= \mathcal{F}_i(a) \int_{w \leq b} g_{C(i,N)}(w)\, dw \\ &= \mathcal{F}_i(a)\, \mathcal{F}_{C(i,N)}(b) \\ &= \mathcal{F}_i(a)\, Y_i(\omega) \end{aligned} \tag{5.36}$$

where

$$Y_i(\omega) = \mathcal{F}_{C(i,N)}(b) \tag{5.37}$$

Note that by Equation 5.32,

$$G_N(a,b) = \frac{1}{N} \sum_{i=1}^{N} X_i \tag{5.38}$$

Unlike in Babovsky's proof for Nanbu's scheme, the variables $\{X_i\}$ are independent, but *not* identically distributed. Therefore, we cannot employ the same arguments based on the Central Limit Theorem that Babovsky utilized, but rather will employ Kolmogorov's Strong Law of Large Numbers. To begin, recall $EX_i = \mathcal{F}_i(a)\, EY_i$, thus consider

$$\begin{aligned} EY_i &= \int_\Omega Y_i d\lambda^N \\ &= \int_{\Omega_1} \cdots \int_{\Omega_i} \cdots \int_{\Omega_N} \mathcal{F}_{C(i,N)}(b)\, d\lambda^N \text{ by (5.37)} \\ &= \int_{\Omega_i} \mathcal{F}_{C(i,N)}(b)\, d\lambda \end{aligned} \tag{5.39}$$

Recall from (5.11) that $\mathcal{F}_{C(i,N)}(b)$ can be written piecewise over the intervals $\left[\frac{j-1}{N}, \frac{j}{N}\right]$ for $j = 1, \ldots, N$, namely,

$$\mathcal{F}_{C(i,N)}(b) = \mathcal{F}_j(b) \text{ for } \omega_i \in \left[\frac{j-1}{N}, \frac{j}{N}\right] \tag{5.40}$$

Substituting (5.40) into (5.39),

$$\begin{aligned} EY_i &= \int_0^{1/N} \mathcal{F}_1(b)\, d\lambda + \int_{1/N}^{2/N} \mathcal{F}_2(b)\, d\lambda + \cdots + \int_{(N-1)/N}^{1} \mathcal{F}_N(b)\, d\lambda \\ &= \frac{1}{N} \sum_{i=1}^{N} \mathcal{F}_i(b) \\ &= F_N(b) \end{aligned} \tag{5.41}$$

Thus,

$$EX_i = \mathcal{F}_i(a)\, F(b) \tag{5.42}$$

Also, recall $Var(X_i) = (\mathcal{F}_i(a))^2 Var(Y_i)$. Thus we have

$$\begin{aligned}
Var(Y_i) &= E\left(Y_i^2\right) - (EY_i)^2 \\
&= \int_\Omega Y_i^2(\omega)\, d\lambda^N - (F(b))^2 \text{ by (5.39)} \\
&= \int_{\Omega_1} \cdots \int_{\Omega_i} \cdots \int_{\Omega_N} (\mathcal{F}_{C(i,N)}(b))^2\, d\lambda^N - (F(b))^2 \text{ by (5.37)} \\
&= \int_{\Omega_i} (\mathcal{F}_{C(i,N)}(b))^2\, d\lambda - (F_N(b))^2 \\
&= \int_0^{1/N} (\mathcal{F}_1(b))^2\, d\lambda + \int_{1/N}^{2/N} (\mathcal{F}_2(b))^2\, d\lambda + \cdots + \\
&\quad \int_{(N-1)/N}^{1} (\mathcal{F}_N(b))^2\, d\lambda_i - (F_N(b))^2 \text{ by (5.40)} \\
&= \frac{1}{N} \sum_{i=1}^{N} (\mathcal{F}_i(b))^2 - (F_N(b))^2 \\
&\leq 1 - (F_N(b))^2 \\
&\leq 1 \qquad (5.43)
\end{aligned}$$

Consider

$$\begin{aligned}
\sum_{k=1}^{N} \frac{1}{k^2} Var(X_k) &= \sum_{k=1}^{N} \frac{(\mathcal{F}_k(a))^2}{k^2} Var(Y_k) \\
&\leq \sum_{k=1}^{N} \frac{(\mathcal{F}_k(a))^2}{k^2} \text{ by (5.43)} \\
&\leq \sum_{k=1}^{N} \frac{1}{k^2} < \infty
\end{aligned}$$

Therefore, having satified the requirements of Corollary 5.1, we conclude

$$\frac{S_N - ES_N}{N} \to 0 \text{ almost surely} \qquad (5.44)$$

where $S_N = \sum_{i=1}^{N} X_i = NG_N(a,b)$. Thus,

$$\begin{aligned}
ES_N &= \sum_{i=1}^{N} \mathcal{F}_i(a)\, F_N(b) \\
&= NF_N(a)\, F_N(b)
\end{aligned}$$

By Equation 5.44 we have that

$$G_N(a,b) \to F_N(a) F_N(b) \text{ almost surely.} \tag{5.45}$$

Recall that by assumption F_N converges to F. Thus,

$$F_N(a) F_N(b) \to F(a) F(b) = G(a,b) \tag{5.46}$$

Combining this with Equation 5.45 yeilds

$$G_N(a,b) \to G(a,b) \text{ almost surely} \tag{5.47}$$

for all $(a,b) \in \mathbb{R}^3 \times \mathbb{R}^3$, which implies $\hat{P}_N$ converges to $\hat{P}$ in law as $N \to \infty$. □

We are now ready to prove our main result.

Theorem 5.4. *Let f^k be the solution of the time discretized space homogeneous Boltzmann equation (3.2) and define the probability measure P^k on $\mathbb{R}^3$ by*

$$P^k(A) = \int_A f^k(v)\, dv \text{ for any } A \subset \mathbb{R}^3 \tag{5.48}$$

Given a set of density functions $\{g_i\}_{i=1}^N$ define the sequence of probability measures $\left\{P_N^k\right\}$ on $\mathbb{R}^3$ by

$$P_N^k(A) = \frac{1}{N} \sum_{i=1}^{N} \int_A g_i(v)\, dv \tag{5.49}$$

Let

$$p_i = 2\mathcal{G}(g_i, h_i) - \frac{1}{2}\mathcal{G}(g_i, g_i) - \frac{1}{2}\mathcal{G}(h_i, h_i) \tag{5.50}$$

with h_i as given in (5.12). Define the sequence of probability measures $\left\{P_N^{k+1}\right\}$ on $\mathbb{R}^3$ by

$$P_N^{k+1}(A) = \frac{1}{N} \sum_{i=1}^{N} \int_A p_i(v)\, dv \tag{5.51}$$

If P_N^k converges to P^k in law as $N \to \infty$, then P_N^{k+1} converges to P^{k+1} in law as $N \to \infty$ almost surely.

Proof. Take any $\phi \in C_b\left(\mathbb{R}^3\right)$. Then,

$$\int_{\mathbb{R}^3} \phi(v) = \int_{\mathbb{R}^3} \phi(v) \left[\frac{1}{N} \sum_{i=1}^{N} 2\mathcal{G}\left[g_i, g_{C(i,N)}\right](v) - \frac{1}{2}\mathcal{G}\left[g_i, g_i\right](v) - \frac{1}{2}\mathcal{G}\left[g_{C(i,N)}, g_{C(i,N)}\right](v) \right] dv \tag{5.52}$$

Employing (3.32), one may obtain,

$$\begin{aligned} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left[g_i, g_{C(i,N)}\right](v)\, dv = \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi) \left[g_i(v)\, g_i(w) + g_i(v)\, g_{C(i,N)}(w) + \right. \\ \left. g_i(w)\, g_{C(i,N)}(v) + g_{C(i,N)}(v)\, g_{C(i,N)}(w) \right] dvdw \\ = \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_i(v)\, g_i(w)\, dvdw + \\ \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_i(v)\, g_{C(i,N)}(w)\, dvdw + \\ \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_i(w)\, g_{C(i,N)}(v)\, dvdw + \\ \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_{C(i,N)}(v)\, g_{C(i,N)}(w)\, dvdw \end{aligned} \tag{5.53}$$

Recall that $K_{v,w}(\phi) = K_{w,v}(\phi)$, thus (5.53) reduces to

$$\begin{aligned} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left[g_i, g_{C(i,N)}\right](v)\, dv = \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_i(v)\, g_i(w)\, dvdw + \\ \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_i(v)\, g_{C(i,N)}(w)\, dvdw + \\ \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_{C(i,N)}(v)\, g_{C(i,N)}(w)\, dvdw \end{aligned}$$

Recalling the definition of $\mathcal{G}$, we have

$$\begin{aligned} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left[g_i, g_{C(i,N)}\right](v)\, dv = \frac{1}{4} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left[g_i, g_i\right](v)\, dv + \\ \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_i(v)\, g_{C(i,N)}(w)\, dvdw + \\ \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left[g_{C(i,N)}, g_{C(i,N)}\right](v)\, dv \end{aligned} \tag{5.54}$$

Rearranging, yields

$$\begin{aligned} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_i(v)\, g_{C(i,N)}(w)\, dvdw = 2 \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left[g_i, g_{C(i,N)}\right](v)\, dv - \\ \frac{1}{2} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left[g_i, g_i\right](v)\, dv - \frac{1}{2} \int_{\mathbb{R}^3} \phi(v)\, \mathcal{G}\left[g_{C(i,N)}, g_{C(i,N)}\right](v)\, dv \end{aligned} \tag{5.55}$$

Substituting (5.55) into (5.52) yields,

$$\begin{aligned}\int_{\mathbb{R}^3} \phi(v)\, dP_N^{k+1} &= \frac{1}{N}\sum_{i=1}^{N} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} K_{v,w}(\phi)\, g_i(v)\, g_{C(i,N)}(w)\, dvdw \\ &= \frac{1}{N}\sum_{i=1}^{N} \int_D \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \phi(\Psi(x,v,w))\, g_i(v)\, h_i(w)\, dxdvdw \qquad (5.56)\end{aligned}$$

by Lemma 3.35. Denote by $P2_N$ the probability measure on $D \times \mathbb{R}^3 \times \mathbb{R}^3$ given by

$$P2_N(B) = \int_B \frac{1}{N}\sum_{i=1}^{N} g_i(v)\, h_i(w)\, dxdvdw \text{ for any } B \subset D \times \mathbb{R}^3 \times \mathbb{R}^3 \qquad (5.57)$$

Recalling (5.56) we have

$$\begin{aligned}\int_{\mathbb{R}^3} \phi(v)\, dP_N^{k+1} &= \int_D \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \phi(\Psi(x,v,w))\, dP2_N \text{ by (5.57)} \\ &= \int_{\mathbb{R}^3} \phi(v)\, d\left(P2_N \circ \Psi^{-1}\right) \text{ by Lemma 3.3} \qquad (5.58)\end{aligned}$$

Thus, we have shown that $P_N^{k+1} = P2_N \circ \Psi^{-1}$. Denote by $P2$ the probability measure on $D \times \mathbb{R}^3 \times \mathbb{R}^3$ given by

$$P2(B) = \int_B f(v)\, f(w)\, dxdwdv \text{ for any } B \subset D \times \mathbb{R}^3 \times \mathbb{R}^3 \qquad (5.59)$$

Also, denote by $\hat{P}_N$ the probability measure on $\mathbb{R}^3 \times \mathbb{R}^3$ given by

$$\hat{P}_N(C) = \frac{1}{N}\sum_{i=1}^{N} \int_C g_i(v)\, h_i(w)\, dvdw \text{ for any } C \subset \mathbb{R}^3 \times \mathbb{R}^3 \qquad (5.60)$$

Likewise, denote by $\hat{P}$ the probability measure on $\mathbb{R}^3 \times \mathbb{R}^3$ given by

$$\hat{P}_N(C) = \int_C f(v)\, f(w)\, dvdw \text{ for any } C \subset \mathbb{R}^3 \times \mathbb{R}^3 \qquad (5.61)$$

Consider,

$$\begin{aligned}\lim_{N\to\infty} \int_D \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \phi(x,v,w)\, dP2_N &= \lim_{N\to\infty} \int_D \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \phi(x,v,w)\, \frac{1}{N}\sum_{i=1}^{N} g_i(v)\, h_i(w)\, dxdvdw \\ &= \lim_{N\to\infty} \int_D \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \phi(x,v,w)\, dxd\hat{P}_N \text{ by (5.60)} \\ &= \int_D \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \phi(x,v,w)\, dxd\hat{P} \text{ a.s. by Theorem 5.3} \\ &= \int_D \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \phi(x,v,w)\, f(v)\, f(w)\, dxdvdw \\ &= \int_D \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \phi(x,v,w)\, dP2\end{aligned}$$

Thus, $P2_N$ converges in law to $P2$ as $N \to \infty$. Therefore, by Lemma 5.1 we have that $P_N^{k+1} = P2_N \circ \Psi^{-1}$ converges to P^{k+1} in law as $N \to \infty$. □

While the previous theorem proved convergence in law to the time discretized space homogeneous Boltzmann solution, the following Corollaries prove convergence in solution for solutions which are $L^\infty\left(\mathbb{R}^3\right)$ or bounded.

Corollary 5.2. *If the time discretized space homogeneous Boltzmann equation (3.2) has a non-negative solution $f \in L^\infty\left(\mathbb{R}^3\right)$, then the solution $\check{f}$ of the DMC method (5.14) converges in $L^\infty\left(\mathbb{R}^3\right)$ to f at each timestep. That is,*

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

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

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

where $h \in \mathbb{R}^+$. By Lemma 4.1, ϕ_h is a delta family as $h \to 0^+$ centered at x'. Therefore, there exists $H_1 > 0$ such that

$$\left| \int_{\mathbb{R}^3} \phi_h(x) \check{f}(x)\, dx - \check{f}(x') \right| < \frac{\epsilon}{3} \tag{5.62}$$

for all $h < H_1$. Likewise, there exists $H_2 > 0$ such that

$$\left| \int_{\mathbb{R}^3} \phi_h(x) f(x)\, dx - f(x') \right| < \frac{\epsilon}{3} \tag{5.63}$$

Note that ϕ_h is everywhere continuous and $|\phi_h(x)| \leq \frac{1}{\sqrt{2\pi}h^3}$ for all $x \in \mathbb{R}^3$. Thus by Theorem 5.4, there exists $N > 0$ such that

$$\left| \int_{\mathbb{R}^3} \phi_h(x) \left(\check{f}(x) - f(x)\right) dx \right| < \frac{\epsilon}{3} \tag{5.64}$$

for all $N_p > N$. Choose $H < \min\{H_1, H_2\}$, then for any $N_p < N$ we have,

$$\begin{aligned}
\left\|\check{f} - f\right\|_\infty &= \operatorname{ess\,sup}\left|\check{f} - f\right| \\
&= \sup_{x' \in \mathbb{R}^3 - S} \left|\check{f}(x') - f(x')\right| \\
&\leq \sup_{x' \in \mathbb{R}^3 - S} \left|\check{f}(x') - \int_{\mathbb{R}^3} \phi_h(x)\, \check{f}(x)\, dx\right| + \\
&\quad \left|\int_{\mathbb{R}^3} \phi_h(x)\, \check{f}(x)\, dx - f(x')\right| \text{ by the triangle inequality} \\
&\leq \sup_{x' \in \mathbb{R}^3 - S} \left|\check{f}(x') - \int_{\mathbb{R}^3} \phi_h(x)\, \check{f}(x)\, dx\right| + \left|\int_{\mathbb{R}^3} \phi_h(x) \left(\check{f}(x) - f(x)\right) dx\right| + \\
&\quad \left|\int_{\mathbb{R}^3} \phi_h(x)\, f(x)\, dx - f(x')\right| \text{ by the triangle inequality} \\
&< \frac{\epsilon}{3} + \frac{\epsilon}{3} + \frac{\epsilon}{3} \text{ by inequalities (5.62), (5.63), and (5.64)} \\
&= \epsilon
\end{aligned}$$

□

Corollary 5.3. *If the time discretized space homogeneous Boltzmann equation (3.2) has a non-negative bounded solution f, then the solution $\check{f}$ of the DMC method (5.14) converges pointwise to f.*

Proof. The proof follows naturally from Corollary 5.2. □

Note that as mentioned previously, the current work represents the first time such forms of convergence have ever been proven for a stochastic particle method for the Boltzmann equation.

5.2 Distributional Monte Carlo using the Bhatnagar-Gross-Krook Approximation (DMC-BGK)

Note that the proofs presented in the prior section assumed the space homogenous relaxation problem between the two particles was solved in a way which is consistent with the Boltzmann solution. In practice, this will necesitate some numerical approximation

technique; however, so long as the technique is consistent with the Boltzmann equation the prior theorems guarantee the DMC approach will converge in law to the Boltzmann solution.

A number of appropriate techniques could be applied toward this end. Such techniques could be either stochastic or deterministic. Some possible choices include moment methods, spectral methods, linearization of the collision operator, or even simplified stochastic particle schemes. In practice, it would be desirable to reduce the complexity of the scheme as a large number of simulated collisions will require computation. A complementing aspect, however, is that since a large number of collisions will be computed, and each particle already carries a significant amount of information in its distribution function, the actual collision calculation can be rather coarse.

As a demonstration case, the present work employs the Bhatnagar-Gross-Krook (BGK) equation [11] to compute the outcome of intermolecular collisions. The space homogeneous BGK equation is a model equation for the Boltzmann equation which replaces the complex collision integral with a simple relaxation form.

$$\frac{\partial}{\partial t} f(v,t) = -\nu \left[f(v,t) - f_M(v) \right] \tag{5.65}$$

Here, ν is the collision frequency and f_M is the Maxwellian which possesses the same energy and momentum as f. In the case where ν is constant with respect to molecular velocity, equation 5.65 becomes a linear, ordinary differential equation in t. Given initial data f_0, the solution of equation 5.65 is given by

$$f(v,t) = e^{-\nu t} f_0(v) + \left(1 - e^{-\nu t}\right) f_M(v) \tag{5.66}$$

Though the BGK equation is not fully consistent with the Boltzmann equation, various BGK implementations have served as an appropriate approximation in many investigations of rarefied gases [33, 78], including variance reduced DSMC schemes [51] and therefore represents an appropriate choice to demonstrate the benefits of a distributional approach.

The above solution is employed to approximate the solution $\mathcal{G}$ of the previous sections. Denoting the respective velocity distributions as g and h, the initial condition is given by $f = 1/2\,(g + h)$. The Maxwellian which corresponds to this density function can be determined by matching the first and second moments.

$$f_M(v) = \alpha_1 e^{-\alpha_2 (v-u)^2} \tag{5.67}$$

Where the mean velocity $u = \int v f(v)\, dv$, $\alpha_1 = \left[\frac{8\left(M_2 - \|u\|^2\right)}{\pi}\right]^{3/2}$, $\alpha_2 = 8\left(M_2 - \|u\|^2\right)$, and $M_2 = \int \|v\|^2 f(v)\, dv$. The space homogeneous evolution of the combined distribution function may then be obtained utilizing (5.66).

$$\mathcal{G}[g,h](v) = \frac{e^{-\nu\Delta t}}{2}\left[g(v) + h(v)\right] + \left(1 - e^{-\nu\Delta t}\right)\alpha_1 e^{-\alpha_2 (v-u)^2} \tag{5.68}$$

Equation 5.68 is a closed form expression for the evolution of the joint distribution function of the two simulated particles involved in a collision interaction. Although an exact expression, one must determine an appropriate way to represent the distribution functions g, h numerically. Several approaches exist. For simplicity, the current study represents the distribution function as a set of values evaluated on a three dimensional grid in velocity space. Although conceptually simple, this approach would be suboptimal for implementation in a production code as a large amount of data is tied to each particle. In a parallel implementation the latency associated with convecting a particle from one processing domain to another could become nontrivial because of the amount of data to be transferred to the new processing unit. A better approach would be to approximate the distribution function in closed form. For example, if one expanded the distribution functions utilizing Hermite polynomials (as suggested by Grad [41]), Equation 5.68 could then be used to evolve each of the Hermite coefficients in time. The polynomial coefficients are then the only data carried with each particle and the latency associated with a parallel implementation would be significantly reduced.

Computation of the distribution function over a discrete grid as described above presents the method with another tunable parameter, namely, the grid spacing. Grid

refinement in velocity space is a problem that is common with other numerical techniques for the Boltzmann equation (e.g. direct solvers) but is not currently well understood. For this reason, the results and techniques described in this work are based only on uniform grid spacing in velocity space.

Before continuing, it should be noted that the method described here represents a hybrid stochastic-deterministic scheme. That is to say, collision pair selections continue to be performed stochastically using the Monte Carlo scheme previosly discussed. Collision outcomes, however, are computed deterministically using equation 5.68. This hybridization is made possible by the fact that particles possess distributed velocities. If the scheme restriced them to a finite set of velocities, a stochasic approach would be required to sample from equation 5.68 (such a scheme was presented by the author in Reference [67]). The hybridization of the current scheme, however, will be observed in the subsequent section to result in a drastic reduction in variance.

5.3 Application to the Bobylev-Krook-Wu Problem

To provide a numerical demostration of the DMC-BGK technique, the method was applied to the Bobylev-Krook-Wu problem. As the solution is computed over a discrete grid in velocity space, simple quadrature was utilied to compute the normalized moments as defined by Equation 2.61. Figure 5.1 presents a comparison of the first three normalized moments of the density function for the case in which $N_p = 100$. The cell width on the velocity grid was chosen to be $\Delta v = 2/3$ over the region $[-5, 5] \times [-5, 5] \times [-5, 5]$. Outside of this region the value of the density function was assumed to be zero. The results have been averaged over an ensemble of 600 runs.

Note that unlike the DSMC results or the DMC-KDE results, the current method does not display large amounts of variance. This effect is due to the fact that collision outcomes are determined deterministically which was facilitated by the distributed particle velocities.

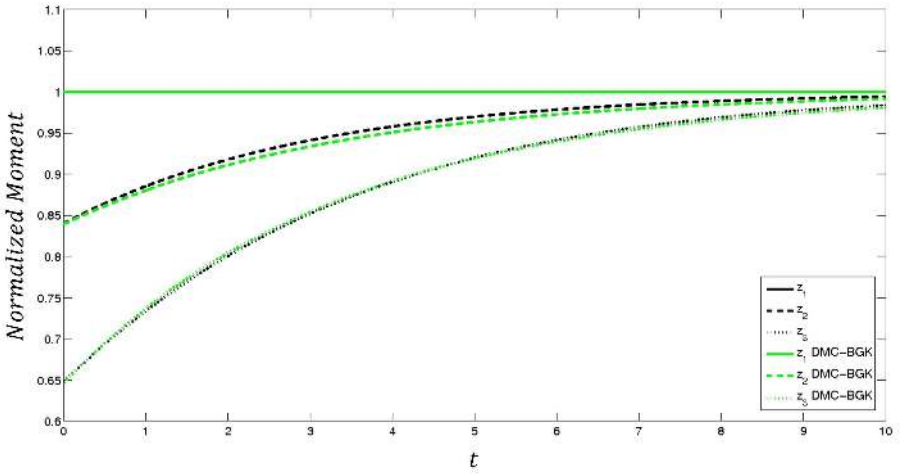


Figure 5.1: Normalized Moments of Bobylev-Krook-Wu Solution ($N_p = 100$, $\Delta v = 2/3$, 600 run ensemble)

Furthermore, note that not only does the current solution display reduced variance, but is also much more accurate than the prior methods discused. As each particle possesses an entire distribution function of unrestricted form, a tremendous amount of information is represented with each particle which allows for the overall density function to be calculated much more accurately for the same number of particles. Finally, also note that as a result of the variance reduction previously discussed, the scheme conserves energy much better that the prior schemes as evidenced by the nearly constant first normalized even moment z_1.

Figures 5.2 and 5.3 illustrate the results for the first and second normalized moments obtained by varying N_p while holding the cell size constant at $\Delta v = 2/3$ and using an ensemble of 400 runs.

Note that in this case, Figure 5.2 shows that the total fluctuation in energy throughout the simulation is less that one-tenth of one percent. In contrast, the results for Nanbu's method (Figure 3.1) displayed about an order of magnitude greater fluctuation in this

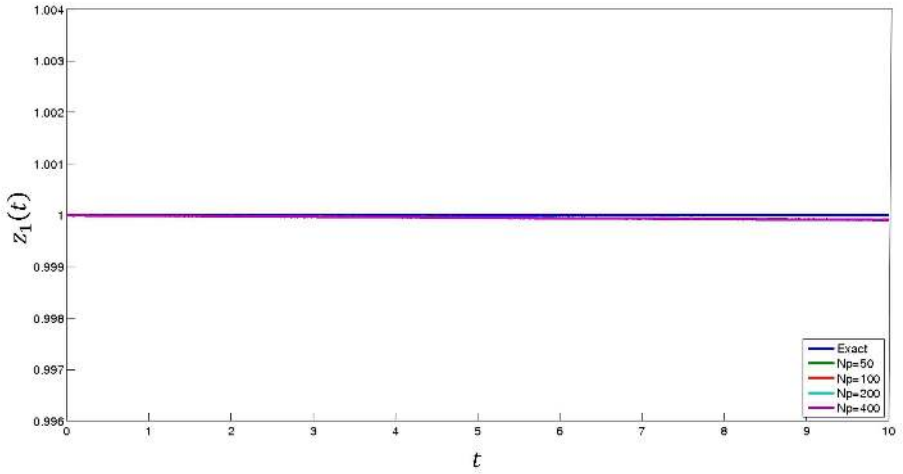


Figure 5.2: First Normalized Moment with Varying N_p ($\Delta v = 2/3$, 400 run sample)

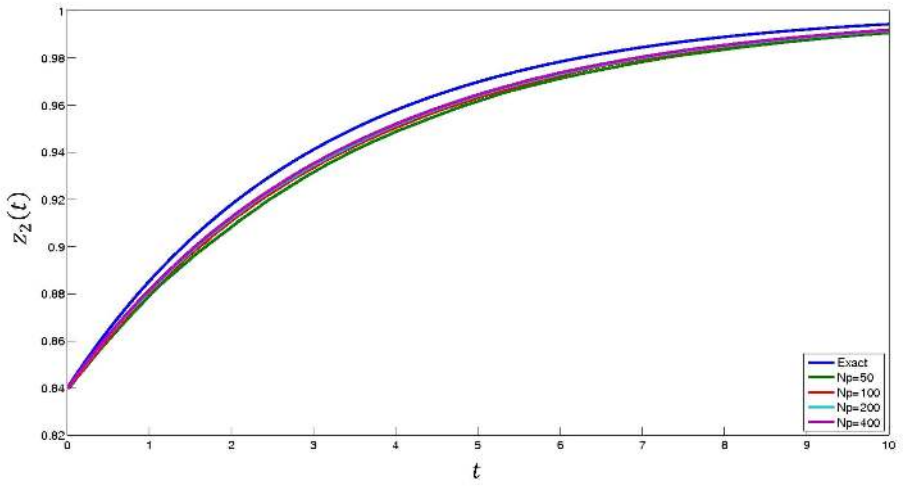


Figure 5.3: Second Normalized Moment with Varying N_p ($\Delta v = 2/3$, 400 run sample)

moment. The results for the second moment in Figure 5.3 show very little variance as well and nearly monotonic convergence.

As the entire distribution function is computed, like DMC-KDE it is possible to compute the $L^1\left(\mathbb{R}^3\right)$ error via Equation 4.34. Figure 5.4 shows how the $L^1\left(\mathbb{R}^3\right)$ error

varies as a function of the number of simulated particles with $\Delta v = 2/3$. Note that

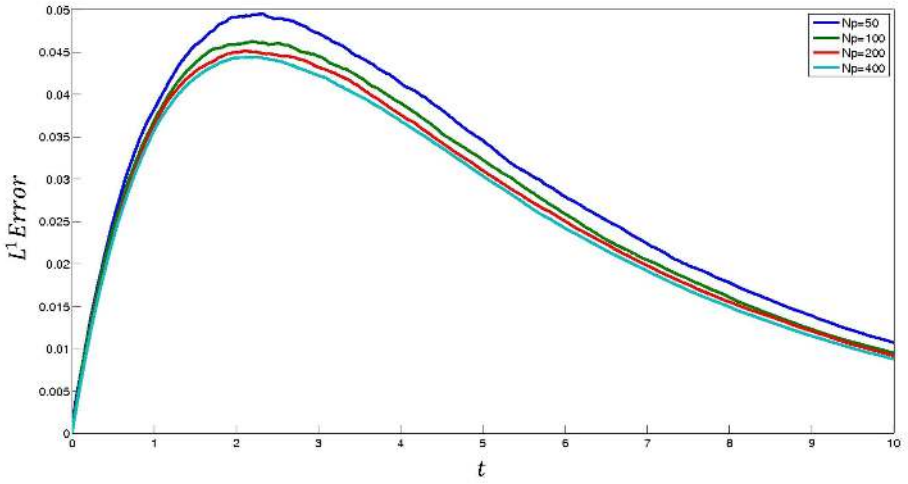


Figure 5.4: $L^1\left(\mathbb{R}^3\right)$ Error for DMC-BGK Bobylev-Krook-Wu Solution with Varying N_p (100 run sample)

the convergence is monatonic, and the maximum error throughout the simulation is about one order of magnitude smaller than the DMC-KDE approach (Figure 4.4). Also, unlike the DMC-KDE approach, note that the error is nearly zero at $t = 0$. This is due to the fact that the initial condition can be much better represented with non-gaussian particle distributions.

Figure 5.5 presents the results for the $L^1\left(\mathbb{R}^3\right)$ error as it varies with velocity grid cell size. The simulations employed 50 simulated particles and were ensemble averaged over 100 runs. Here, the expected general trend is observed, namely that reduced cell size results in reduced error, however the results are not necessarily monatonic. This is likely owed to the fact that as domain was finite and held constant, at some point the error in approximating the quadrature becomes smaller than the stochastic variance introduced by collision pair selection over a collection of only 50 particles.

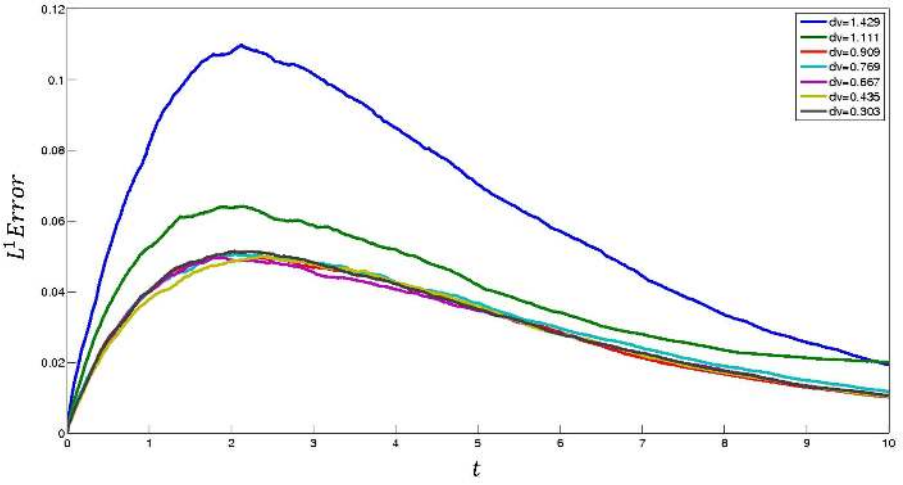


Figure 5.5: $L^1\left(\mathbb{R}^3\right)$ Error for DMC-BGK Bobylev-Krook-Wu Solution with Varying Δv (100 run sample)

The total variation for the first three moments as a function of the size of the ensemble average is given in Figure 5.6. Here $N_p = 100$ and $\Delta v = 2/3$. Notice the drastic improvement over Figure 3.4. The total variation is very nearly equal to the analytical value even for a very modest number of samples. This is owed in large part to the fact that the stochastic step predicting collision outcomes has been replaced by a deterministic calculation, which due to the ability of particles to posess distributed velocities accounts for all possible collision outcomes. This represents the first use of deterministic collision modeling within a stochastic particle method.

It should be noted that although the numerical solutions presented in this section compare well to the Boltzmann solution, it should not be assumed that the scheme employing the BGK approximation is convergent to the Boltzmann solution. Although in many cases the BGK model can be a useful surrogate, it cannot be directly derived by simplification of the Boltzmann collision integral. Nevertheless, the results presented here suggest that so long as an appropriate number of collisions are calculated, some simplification of the collision operator is tolerable.

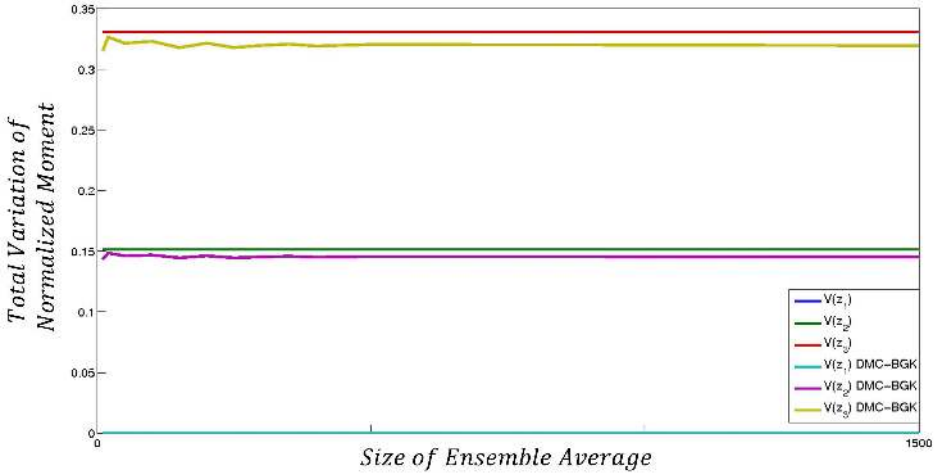


Figure 5.6: Total Variation of DMC-BGK Method as a Function of Sample Size for $N_p = 100$, $\Delta v = 2/3$

VI. Conclusion

The work presented herein has contributed a number of important discoveries and developments to the stochastic solution of the Boltzmann equation. First and foremost, this research has introduced the Distributional Monte Carlo concept for the Boltzmann equation. The framework derived by the author represents the first stochastic particle based method which does not employ a point measure based approximation of the velocity density function, but rather allows each simulated particle to possess an entire velocity density function of its own. Allowing the simulated particle velocities to be distributed enables the modeling of collision events between simulated particles to be treated as a space homogeneous relaxation problem over the collection of actual particles they represent. While physically intuitive, the author was able to prove that such a representation results naturally from the weak time discretized space homogeneous equation when particle velocities are distributed. In addition to deriving the general DMC approach, it was also proven that the technique was convergent to the solution of the space homogeneous Boltzmann equation in law, and in solution for $L^{\infty}\left(\mathbb{R}^3\right)$ solutions.

The distributional framework derived by the author is quite general, and the present work established a sufficiency criterion by which any distributional scheme will converge so long as collision modeling is consistent with the space homogeneous solution. This facilitates possible employment of both stochastic and deterministic schemes. The author presented one such scheme based on the BGK simplification of the collision operator which employed deterministic modeling of collision effects. Note that while collision outcomes were determined deterministically, collision pair selection was performed stochastically. In contrast to DSMC which performs both steps stochastically, the technique is observed to have drastically reduced variance. This is due to three sources. First, replacement of the stochastic process for selecting collision outcomes with a deterministic one tends to reduce

variability. Second, the use of distributed velocities and particle distribution functions of general form allows for the calculation of not just one possible collision outcome, but computes the effects of all possible collision interactions. Finally, the mere fact that particle velocities are distributed means that each simulated particle carries with it significantly more information than it would in a traditional DSMC approach, allowing for the overall distribution function to be represented much more accurately. Reduced variance in solution translates to a reduction in the number of particles required to accurately simulate a given problem which can have a drastic impact on computational time to solution.

The author also applied kernel density estimation to DSMC to develop a new approach called DMC-KDE. It was shown that through the application of kernel density estimation, the DSMC technique could be made to converge not just in law, but in solution for $L^{\infty}\left(\mathbb{R}^3\right)$ and bounded solutions of the space homogeneous equation. This represents the first time that such forms of convergence have been proven for a stochastic particle method for the Boltzmann equation. Simply put, the DMC-KDE approach turns a stochastic Boltzmann simulator into a stochastic Boltzmann solver. This facilitates the direct computation and/or visualization of the distribution function, something which is not directly available to Boltzmann simulators which converge only in law, such as DSMC.

Although the particle velocities were allowed to be distributed, they were constrained to be distributed by a prescribed form of a density function. In this case, particles were allowed to possess velocities distributed according to a Maxwellian distribution. This leads to the physical interpretation that the actual particles represented by a simulated particle do not all possess the same velocity vectors, but rather are in translational equilibrium with one another. Collision interactions were computed stochastically and had the effect of shifting the mean of the particle Maxwellians. The rules governing the selection of the new mean were shown to be identical to the rules Nanbu used to assign post collision velocities. Unfortunately, the restrictions placed on the form and evolution of the particle velocity

density functions eliminate any potential variance reduction by distributing velocities, and for the Bobylev-Krook-Wu solution it was observed that the total variation in the normalized moments was equal to that of Nanbu's scheme.

The current work has opened up a number of avenues for continued research in Distributional Monte Carlo methods for the Boltzmann equation. The next logical step for such methods is generalization to the full Boltzmann equation. The approach for such a technique would largely mirror DSMC, that is a grid will be employed in physical space to ensure collisions occur between simulated particles which are near neighbors. Particle advection and collision interactions will be decoupled via the uncoupling principle, and within a cell the solution will be presumed to be space homogeneous. The approach for handling particle advection is not necessarily determined, as simulated particles now possess not just a single velocity vector but an entire distribution function. Early experimentation by the author suggests one appropriate choice is to sample an advection velocity at each timestep with which to convect each particle from its density function.

There is great potential for distributional approaches in the nonhomogeneous case which arises from the fact that the distribution function is directly computed and available throughout the computation. When the distribution function of a given cell is Maxwellian or near-Maxwellian collisional effects can be neglected. To illustrate this, consider the problem of a one-dimensional shock wave. The typical approach for modeling such a case is to initialize the upstream half of the domain to an equilibrium distribution based on the freestream conditions. The downstream half of the domain is initialized to an equilibrium distribution based on the downstream conditions which can be computed via the normal shock relations. In the case of a distributional approach, at $t = 0$, the particles in upstream domain share a common Maxwellian density function, as do the particles in the downstream domain. As particles begin to advect, the cells near the middle of the domain become the first to possess non-Maxwellian distributions, and therefore become the only location where

collisions are required to be calculated. That is to say, collision calculations are clustered in the area of the shock wave itself. As the simulation continues, the region grows slightly but the majority of collisions are computed in the shock region. The method is therefore self adjusting to regions of non-equilibrium, in that it requires little to no computations in equilibrium regions and focuses its computational power in regions which are highly non-equilibrium.

In addition to generalization to the full Boltzmann equation, there are a number of potential research areas that can still be addressed in the space homogeneous setting. First, for the numerical results presented here, the current effort employed a grid in velocity space. This is suboptimal for use in a production code as each simulated particle carries with it an enormous amount of information which could introduce significant latency in a parallel environment as particles convect between processing domains. A better approach is likely to expand the particle velocity density functions using Hermite polynomials, in which case a handful of coefficients would be the only data required to fully describe each particles velocity density function. Second, in addition to the numerical representation of the density function, the exploration of methods to model the solution $\mathcal{G}$ used in the collision simulation of the Distributional Monte Carlo approach is an area which holds a number of interesting problems. The framework proven by the author made little restriction on the form of such modeling, allowing for both stochastic and deterministic techniques. Although the present work has demonstrated significant variance reductions are achievable with a deterministic approach, there is value in pursuing stochastic approaches as well. One such approach is to apply kernel density estimation to the particle distribution functions themselves (versus the overall distribution). The author has presented such a technique in the past [67], however, some additional work is required to make the approach consistent with the DMC framework presented in this effort.

While the DMC-KDE scheme presented did not exhibit variance reduction over DSMC, it did establish an interesting approach for turning Boltzmann simulators into Boltzmann solvers. There are a number of modifications that could be explored which could enhance the performance of such an approach. As mentioned above, the author has presented a scheme which applied kernel density estimation at the particle density function level [67] which allowed for multiple velocity samples per particle. This has the effect of unconstraining the particle density functions from a fixed form. Another, less drastic, approach might be to allow the kernel bandwidth to vary for each particle. In this case, particle densities would continue to be Maxwellian but each particle would have a unique mean and standard deviation. This is equivalent to allowing each particle to possess a translational temperature. Relations governing the collision modeling would need to be developed which not only determined a mean post-collision velocity, but post-collision temperature for each simulated particle.

When viewed as a whole, the current effort has provided a number of firsts in the area of stochastic particle schemes for the Boltzmann equation and has opened a new area of research with many interesting mathematical challenges for future researchers. In addition, the importance of hypersonic and rarefied flows has ensured that techniques for modeling the Boltzmann equation will remain relevant to Air Force problems for the foreseeable future.

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Vita

Christopher R. Schrock was raised in Ypsilanti, Michigan. He graduated from Willow Run High School in 1998. He attended Washtenaw Community College and soon transferred to the University of Michigan College of Engineering to pursue a degree in Aerospace Engineering. There he served as a research assistant in the Combustion Synthesis Laboratory, Department of Mechanical Engineering. In 2002 he graduated from with a Bachelor of Science in Engineering, Aerospace Engineering with academic minor in Mathematics and accepted a position with the Aerospace Systems Design and Analysis Branch of the USAF Aeronautical Systems Center (ASC) at Wright-Patterson AFB under the PALACE Acquire program. In 2003, he returned to full time study at the Air Force Institute of Technology (AFIT) to pursue a Master of Science in Aeronautical Engineering. His thesis on the use of entropy generation to quantify breakdown of the continuum fluid equations won both Best Fluid Mechanics Thesis and the Dean's Award, and he was recognized as a Distinguished Graduate. Upon returning from full-time study, Christopher served as lead aerodynamicist in the Future Systems Concept Branch, Capability Integration Directorate of ASC. In 2007, he returned to AFIT in pursuit of a Doctoral Degree in Applied Mathematics and was awarded long-term, full-time training status in 2008. After returning to the Capability Integration Directorate in 2009, Christopher continued to pursue his research while resuming duties as lead aerodynamicist. In 2011, his presentation at the Dayton Cincinnati Aerospace Sciences Symposium (DCASS) on Distributional Monte Carlo Methods was recognized as Best Technical Presentation in CFD Methods. Later that year, Christopher would accept a broadening position in the Air Force Research Laboratory where he now serves as a Research Aerospace Engineer specializing in Computational Fluid Dynamics in the Aerospace Systems Directorate's Computational Sciences Center of Excellence.

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14. ABSTRACT

Stochastic particle methods (SPMs) for the Boltzmann equation, such as the Direct Simulation Monte Carlo (DSMC) technique, have gained popularity for the prediction of flows in which the assumptions behind the continuum equations of fluid mechanics break down. In traditional SPMs, simulated particles may possess only a single velocity vector, even though they may represent an extremely large collection of actual particles. This limits the method to converge only in law to the Boltzmann solution. This document details the development of new SPMs that allow the velocity of each simulated particle to be distributed. This approach has been termed Distributional Monte Carlo (DMC). The derivation of a general DMC framework which treats collision interactions between simulated particles as a relaxation problem is given. The methods are proven to converge in law as well as in solution for L-infinity and bounded solutions. An approach based on the BGK simplification is presented which computes collision outcomes deterministically. Each technique is applied to the Bobylev-Krook-Wu solution as a test case. Accuracy and variance of solutions are examined as functions of simulation parameters. Significantly improved accuracy and reduced variance are observed for the Distributional Monte Carlo technique employing discrete BGK collision modeling.

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