Weighted Particle Variance Reduction of Direct Simulation Monte Carlo for the Bhatnagar-Gross-Krook Collision Operator

by

Colin Donald Landon

Submitted to the Department of Mechanical Engineering in partial fulfillment of the requirements for the degree of Master of Science at the MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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Abstract

Direct Simulation Monte Carlo (DSMC)—the prevalent stochastic particle method for high-speed rarefied gas flows—simulates the Boltzmann equation using distributions of representative particles. Although very efficient in producing samples of the distribution function, the slow convergence associated with statistical sampling makes DSMC simulation of low-signal situations problematic.

In this thesis, we present a control-variate-based approach to obtain a variance-reduced DSMC method that dramatically enhances statistical convergence for low-signal problems. Here we focus on the Bhatnagar-Gross-Krook (BGK) approximation, which as we show, exhibits special stability properties. The BGK collision operator, an approximation common in a variety of fields involving particle mediated transport, drives the system towards a local equilibrium at a prescribed relaxation rate.

Variance reduction is achieved by formulating desired (non-equilibrium) simulation results in terms of the difference between a non-equilibrium and a correlated equilibrium simulation. Subtracting the two simulations results in substantial variance reduction, because the two simulations are correlated. Correlation is achieved using likelihood weights which relate the relative probability of occurrence of an equilibrium particle compared to a non-equilibrium particle. The BGK collision operator lends itself naturally to the development of unbiased, stable weight evaluation rules.

Our variance-reduced solutions are compared with good agreement to simple analytical solutions, and to solutions obtained using a variance-reduced BGK based particle method that does not resemble DSMC as strongly. A number of algorithmic options are explored and our final simulation method, (VR)\(^2\)-BGK-DSMC, emerges as a simple and stable version of DSMC that can efficiently resolve arbitrarily low-signal flows.

Thesis Supervisor: Nicolas G. Hadjiconstantinou
Title: Associate Professor
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I am also deeply indebted to H. A. Al-Mohssen. His tremendous work developing the weighted particle variance reduction method made this research possible, and he was helpful throughout. G. Radtke and G. Fayad were the best of collaborators and their familiarity with the field was frequently a time-saving resource for me.

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<th>Symbol</th>
<th>Description</th>
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<tr>
<td>$\mathbf{c}$, $\mathbf{c}^{(j)}$</td>
<td>Velocity vector, velocity vector of particle $j$</td>
</tr>
<tr>
<td>$c_i$, $c_i^{(j)}$</td>
<td>Velocity in direction $i$, velocity of particle $j$ in direction $i$</td>
</tr>
<tr>
<td>$\mathbf{x}$, $x_i$</td>
<td>Spatial position vector, spatial position in direction $i$</td>
</tr>
<tr>
<td>$W$, $W^{(j)}$</td>
<td>Weight defined by ratio of distribution functions, weight of particle $j$</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$n$, $\hat{n}_0$</td>
<td>Dimensionless number density, dimensioned reference equilibrium number density</td>
</tr>
<tr>
<td>$A$</td>
<td>Arbitrary property</td>
</tr>
<tr>
<td>$L$</td>
<td>Length</td>
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<td>$T$</td>
<td>Temperature</td>
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<tr>
<td>$\mathbf{n}$</td>
<td>Inward pointing wall normal vector</td>
</tr>
<tr>
<td>$\mathbf{u}$</td>
<td>Mean flow velocity</td>
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<tr>
<td>$\mathbf{\tau}$</td>
<td>Pressure tensor</td>
</tr>
<tr>
<td>$q$</td>
<td>Heat flux</td>
</tr>
<tr>
<td>$N$</td>
<td>Number of particles per cell</td>
</tr>
<tr>
<td>$N_0$</td>
<td>Equilibrium number of particles per cell</td>
</tr>
<tr>
<td>$M$</td>
<td>Number of ensembles</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>$Kn$</td>
<td>Knudsen number</td>
</tr>
<tr>
<td>$k$</td>
<td>Modified Knudsen number, $k = \frac{\sqrt{\pi}}{2} Kn$</td>
</tr>
<tr>
<td>$Ma$</td>
<td>Mach number</td>
</tr>
<tr>
<td>$R$</td>
<td>Molar gas constant</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Mean free path</td>
</tr>
<tr>
<td>$a$, $b$, $d$</td>
<td>Constants for enforced conservation scheme</td>
</tr>
<tr>
<td>$\mathbf{c}_i$</td>
<td>Vector of $c_i$ (one entry per particle)</td>
</tr>
<tr>
<td>$\mathbf{W}$</td>
<td>Vector of $W$ (one entry per particle)</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

Recent interest in small-scale devices has driven demand for efficient hydrodynamic simulations in a regime intractable by traditional methods. For dilute gases, the simplest continuum description—the no slip, Navier-Stokes limit—is valid when the average distance traveled by a gas particle between collisions, $\lambda$, is small compared to a relevant length scale, $L$. When the Knudsen number, $Kn = \frac{\lambda}{L}$, is greater than about 0.1, the Navier-Stokes description fails as the ballistic motion of particles between collisions becomes significant. For a Knudsen number greater than about 10, simulation of such phenomena can be simplified by neglecting collision events entirely. The remaining range of Knudsen number ($0.1 < Kn < 10$), called the transition regime, may be correctly modeled using molecular dynamics, but the enormous number of particles even in small-scale devices, makes the explicit numerical integration of their equations of motion infeasible. Instead, Monte Carlo methods are used to perform the integration and model the distribution of particles probabilistically.

The most prevalent of the stochastic methods is Direct Simulation Monte Carlo (DSMC), which was developed for high-signal transitional flows (i.e. high Mach number, $Ma > 0.1$, rarefied gas flows) [12]. Unfortunately, in the limit of low-speed transitional flows, like those found in micro- or nano-scale devices, the computational requirements scale poorly—the samples required for a constant level of uncertainty scale with the inverse of the signal strength to the second power. This scaling relationship makes DSMC an unsuitable tool for modeling transitional flows with vanishing
A more efficient (lower variance) approach for simulating low-signal transitional flows is to exploit a nearby, analytically-described equilibrium. Achieving variance reduction by simulating the deviation from equilibrium was originally proposed by Baker and Hadjiconstantinou [8]. Since then, a number of variance-reduced methods have emerged. Chun and Koch [17] developed a variance-reduced particle simulation method for solving the linearized hard-sphere Boltzmann equation using particle weights. Baker and Hadjiconstantinou developed a variance-reduced particle method [9, 10] for simulating the non-linear Boltzmann equation, which is referred to as a deviational method because it uses particles to simulate only the deviation from equilibrium. Unfortunately, both methods [17, 9, 10] become very inefficient in the collision dominated limit due to numerical instability. This limitation has been overcome by Homolle and Hadjiconstantinou [22, 23] who showed that stability for all Knudsen numbers can be obtained by using a special (but exact) form of the hard-sphere collision operator first derived by Hilbert. This led to the development of LVDSMC (low variance deviational simulation Monte Carlo) [22, 23], which provides accurate variance-reduced solution of the Boltzmann equation while retaining most of the attributes of particle methods.

Recently, Al-Mohssen and Hadjiconstantinou have developed an alternative approach for obtaining variance-reduced solutions of the non-linear Boltzmann equation [1, 2, 3]. A correlated equilibrium is simulated by augmenting the DSMC particle description with an importance weight. The weight adds a single degree of freedom per particle and introduces minimal changes to the original DSMC algorithm, while significantly improving the signal-to-noise ratio. Like the deviational particle methods, Al-Mohssen’s weighted particle method also requires special treatment of the numerical instability, which slightly decreases the computational gains.

In the this thesis, we extend the approach of Al-Mohssen and Hadjiconstantinou to the Boltzmann equation under the relaxation-time approximation [13, 14, 21, 27, 38, 39], which is expected to improve the numerical behavior of the variance-reduced method. The relaxation-time approximation has found a number of applications in
fields involving particle mediated transport [16]. In the dilute gas community, the relaxation-time approximation is also known as the BGK model—a more detailed discussion of the BGK model can be found in Section 1.1.5.

Variance-reduced simulation methods for the BGK model have been proposed by Ramanathan and Koch [36], and Radtke and Hadjiconstantinou [20, 35]. In our approach, like the above methods, the structure of the BGK collision operator results in a stable, variance-reduced simulation for all Knudsen regimes. Unlike the previous BGK based methods, however, our approach uses the Al-Mohssen and Hadjiconstantinou variance reduction formulation that requires minimal modifications to the original DSMC algorithm. Hence we will refer to our method as a variance-reduced BGK-DSMC (VR-BGK-DSMC). A more efficient variant that we will refer to as (VR)$^2$-BGK-DSMC will also be developed. The background for these methods will be presented in Chapters 1-3; the methods will be developed in Chapter 4; results will be presented in Chapter 5, while Chapter 6 contains a summary and conclusions.

The treatment in this thesis is limited to dilute gas cases, although it is expected that the present work will extend in a straightforward manner to other applications of the BGK operator in phonon, electron, and radiative transport problems.

In summary, we present a new stochastic particle method for rarefied gas simulations that requires minimal modifications to the widely used DSMC algorithm. Unlike DSMC, our variance reduced algorithm efficiently models arbitrarily low-signal flows, and unlike more complex models, our approach requires no special treatment for stability over all ranges of the Knudsen number.

1.1 Dilute Gases

This section introduces the fundamentals of modeling rarefied gas systems using kinetic theory as well as introducing the notations that will be used throughout the remainder of this thesis.
1.1.1 Dimensionless units

Unless otherwise specified, all expressions are presented in dimensionless form, using the following definitions:

\[
\begin{align*}
  f &= \frac{j}{\hat{n}_0 (2\hat{R}_0)^{-3/2}} \\
  x_i &= \frac{x_i}{L} \\
  c_i &= \frac{c_i}{(2\hat{R}_0)^{1/2}} \\
  k &= \frac{\sqrt{\pi}}{2} \hat{K}n \\
  t &= \frac{i}{L (2\hat{R}_0)^{-1/2}} \\
  F_i &= \frac{\hat{F}_i L}{(2\hat{R}_0)^{1/2}} \\
  n &= \frac{\hat{n}}{\hat{n}_0} \\
  \hat{K}n &= \frac{\hat{\lambda}}{L}
\end{align*}
\]

where \([\cdot]\) indicates a dimensional quantity. Here, \(\hat{n}_0\), and \(\hat{T}_0\) are the reference number density and temperature, respectively; \(R = k_b/M\) is the gas constant where \(k_b\) is the Boltzmann constant and \(M\) is the molecular mass; \(L\) is a characteristic length-scale; \(\hat{F}_i\) is a body force acting on the gas; and \(\hat{\lambda}\) is the molecular mean free path. This scheme significantly simplifies numerical simulation.

1.1.2 Single-particle distribution functions

A dilute gas is a many body system where the mean free path between intermolecular collisions is significantly larger the molecular length scale (i.e. diameter of a particle). Intermolecular interactions are relatively rare and allow a dilute gas systems to be described [13] by the single-particle distribution function, \(f = f(x, c, t)\), which is defined as proportional to the probability of finding a particle at a location in phase space \((x, c)\) at a time, \(t\). Here, \(x\) is the position vector and \(c\) is the molecular velocity vector. Many common gases (e.g. air at atmospheric pressure) satisfy the dilute gas criteria [12]; a comprehensive discussion can be found in [12].

1.1.3 The Boltzmann equation

The evolution of the single-particle distribution function is described by the well-known Boltzmann transport equation [13] given here in non-dimensional form. We will also use Einstein notation (repeated indices indicate summation).

\[
\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + \frac{\partial F_i f}{\partial c_i} = \frac{1}{k} J(f, f)
\] (1.1)
This equation balances molecular advection and acceleration effects on the left hand side (LHS) with the effects of molecular collisions on the right hand side (RHS).

In the absence of collisions $J(f, f) = \left[ \frac{\partial f}{\partial t} \right]_{\text{coll}} = 0$. This implies that between collisions the distribution $f$ (or a sample from it) advects ballistically. This is particularly convenient for the development of particle simulation methods in which the distribution function is approximated using a number of particles sampling $f$.

Including the collision integral increases the complexity of the Boltzmann equation significantly. Since the form of the collision operator depends on the molecular interaction model, it will be discussed in more detail in Section 1.1.5.

1.1.4 The Maxwell-Boltzmann distribution

The distribution function that solves the equilibrium Boltzmann equation (i.e. $\left[ \frac{\partial f}{\partial t} \right]_{\text{coll}} = 0$) is known as the Maxwell-Boltzmann distribution

$$f^{\text{MB}}(c; u, n, T) = \frac{n}{(\pi T)^{3/2}} \exp \left( -\frac{||c - u||^2}{T} \right), \quad (1.2)$$

where $n(x, t), u(x, t), T(x, t)$ are free parameters, interpreted in the present context as the gas number density, flow velocity, and temperature, respectively. Note that $\frac{\partial f^{\text{MB}}}{\partial t} + c \frac{\partial f^{\text{MB}}}{\partial x} = 0$ is only satisfied when $n$, $u$, and $T$ are not functions of space and time. We call this equilibrium (i.e. one for which $n$, $u(= 0)$, and $T$ are not functions of space and time) global equilibrium, while (1.2) is usually referred to as local equilibrium.

The Maxwell-Boltzmann distribution is of central importance to our discussion of variance reduction, which exploits equilibrium distributions as controls. In our work, the reference (control) equilibrium distribution will be taken to be a global equilibrium: $f^{\text{eq}}(c) = f^{\text{MB}}(c; 0, n_0, T_0)$. 

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1.1.5 Collision operators

Boltzmann originally considered a hard-sphere gas [13], which can be described using the following collision operator:

\[ J(f, f) = \frac{1}{2} \int \int (f' f' + f_+ f' - f_+ f - f_+ f) \rho^2 \Omega(\alpha) d^3 c, \] \hspace{1cm} (1.3)

\[
\begin{align*}
    f &= f(x, c, t), \\
    c'_i &= c_i + \alpha_i \alpha_j (c_j - c_j), \\
    f' &= f(x, c', t), \\
    c'_{i*} &= c_i - \alpha_i \alpha_j (c_j - c_j), \\
    f_* &= f(x, c_{i*}, t), \\
    f'_{i*} &= f(x, c'_{i*}, t)
\end{align*}
\] \hspace{1cm} (1.4)

The unit vector \( \alpha \) expresses the variation of the direction of the molecular velocity due to a molecular collision, and \( d\Omega(\alpha) \) is the appropriate solid-angle element [38].

Due to the complexity associated with (1.3) and (1.4), simpler approximations of the collision term have often been employed. An important approximation was given by Bhatnagar, Gross, and Krook [11] (the BGK approximation). It states that the role of the collision operator is to drive the distribution function towards the local equilibrium distribution function, \( f^{\text{loc}} \); namely,

\[
\frac{J(f, f)}{k} = \left[ \frac{\partial f}{\partial t} \right]_{\text{coll}} (x, c, t) = \frac{n(x)}{k} \left( f^{\text{loc}}(x, c, t) - f(x, c, t) \right), \hspace{1cm} (1.5)
\]

where the local equilibrium distribution, \( f^{\text{loc}} \), is a Maxwell-Boltzmann distribution with properties \( n(x, t), u(x, t), \) and \( T(x, t) \) representative of the local gas properties (see Section 1.1.6).

Under the BGK approximation, the transport equation can be shown to obey the laws of mass, momentum and energy conservation, as well as satisfying the entropy generation inequality [6]. Moreover, the equilibrium distribution is a Maxwellian. By satisfying these conditions, the BGK collision operator captures the most important features of the hard-sphere Boltzmann equation, while having a much simpler form. The most notable weakness of this model is that it predicts a Prandtl number of 1 while dilute gases have \( Pr \approx \frac{2}{3} \). This is discussed further in Section 2.3.
As mentioned previously, this model is also used in electron, phonon, and radiative transport [16], where it is known as the relaxation-time approximation.

1.1.6 Moments of the distribution function

While the distribution function is a complete description of a dilute gas system, it is not directly of much practical use. Fortunately, the familiar physical properties of a system can be calculated by taking simple moments of (averages over) the distribution function. The expression for density, mean flow velocity, temperature, shear, and heat flux are given by [38]

\[ n = \int f \, d^3c, \]  
\[ u_i = \frac{1}{n} \int c_i f \, d^3c, \]  
\[ T = \frac{2}{3n} \int (c_i - u_i)^2 f \, d^3c, \]  
\[ \tau_{ij} = 2 \int (c_i - u_i) (c_j - u_j) f \, d^3c, \]  
\[ q_i = \int (c_i - u_i) (c_j - u_j)^2 f \, d^3c. \]

Therefore, complete characterization requires only to determine the distribution function. Analytically this can be an overwhelming task, but using stochastic particle approaches the appropriate distribution dynamics can be simulated in a relatively straightforward manner.

1.2 Particle Simulation of the Boltzmann Equation

Closed form solutions for the Boltzmann equation are available in relatively few limiting cases (equilibrium, simple boundaries, or linearized and low dimensional systems). However, stochastic particle approximations and Monte Carlo integration allow efficient generation of unbiased distribution function samples for a large class of problems.
of practical interest. This section gives a brief background for statistical simulation of the Boltzmann Equation.

1.2.1 Particle approximation of distribution functions

The continuous probability distribution function can be represented using \( N \) particles by writing

\[
\hat{f}(\mathbf{x}, \mathbf{c}, t) = N_{\text{eff}} \sum_{i=1}^{N} \delta^3(\mathbf{x} - \mathbf{x}^{(i)}) \delta^3(\mathbf{c} - \mathbf{c}^{(i)})
\]  

where \( N_{\text{eff}} \) is the number of real (physical) particles represented by every computational particle. Using the fact that \( \hat{n}_0 = \frac{N_0 N_{\text{eff}}}{V} \) we obtain the dimensionless expression,

\[
f(x, c, t) \approx \frac{1}{N_0} \sum_{i=1}^{N} \delta^3(x - x^{(i)}) \delta^3(c - c^{(i)}).
\]

In a simulation, each delta function is represented by simulation particle \( (i) \) at the location \( (x^{(i)}, c^{(i)}) \) in phase space. The number of particles can be tuned (by changing \( N_{\text{eff}} \)) to achieve the desired accuracy in approximating the distribution function. If at any time (e.g. the initial condition) the distribution function is known analytically, then a particle representation can be generated (see A.1), and evolved in time using a stochastic set of rules consistent with the Boltzmann equation (1.1).

1.2.2 Direct Simulation Monte Carlo

G.A. Bird developed a stochastic particle simulation method for the Boltzmann Equation that correctly models both the dynamics of discrete approximations of the velocity distribution function. His method, Direct Simulation Monte Carlo (DSMC) [12], exploits the structure of the Boltzmann equation to integrate it in time using a splitting scheme in which particles successively undergo collisionless advection and then collision steps. During the advection step, particles move ballistically according to the LHS of Equation (1.1). Bird’s insight into the particle behavior during the collision step is perhaps the most valuable feature of DSMC.
During the collision step for the hard-sphere collision operator, random trial collision pairs are selected such that the number of pairs chosen is greater than the actual number of expected collisions. Each collision pair will collide with a probability proportional to their relative speed (see Equation (1.3)), so acceptance/rejection is used to determine which pairs will undergo a collision. If a collision is accepted, the velocities are updated with a randomly chosen scattering angle to preserve linear momentum and energy; if rejected, velocities are left unmodified.

When a particle reaches the system boundaries, appropriate boundary conditions are applied; for example in the case of a partially accommodating wall, a particle is either diffusely or specularly reflected based on the value of the accommodation coefficient (see [4] for more complete details).

In this manner the dynamics of Equations (1.1) and (1.3) are simulated correctly. At any time, the computational particles (or a subset of them) can be sampled according to the discussion that follows to obtain estimates for the physical properties of the gas.

### 1.2.3 Moments of the particle distribution function

The properties of the simulated gas can be recovered by applying the approximated distribution function (Equation (1.12)) to the moment expressions (1.6) to (1.10). The spatial dependence is captured by considering cell-averaged properties $A$, given by $\bar{A} = \frac{1}{V} \int_{x \in \text{Cell}} A(x) d^3x$. With the discrete representation of the distribution function, the integral moment expressions become summations over the $N$ particles in the domain. In other words, the spatial dependence of these properties is captured by sampling particles using local bins, and the definitions (1.6) to (1.10):

\[
\bar{n} = \frac{N}{N_0}, \quad (1.13)
\]

\[
\bar{u}_i = \frac{1}{N} \sum_{j=1}^{N} c_i^{(j)}, \quad (1.14)
\]
\[
\bar{T} = \frac{2}{3N} \sum_{j=1}^{N} \left( c_i^{(j)} - u_i \right)^2,
\]

(1.15)

\[
\bar{r}_{ij} = \frac{2}{N_0} \sum_{k=1}^{N} \left( c_i^{(k)} - u_i \right) \left( c_j^{(k)} - u_j \right),
\]

(1.16)

\[
q_i = \frac{1}{N_0} \sum_{k=1}^{N} \left( c_i^{(k)} - u_i \right) \left( c_j^{(k)} - u_j \right)^2.
\]

(1.17)

### 1.2.4 Statistical uncertainty in hydrodynamic quantities

Estimates of the uncertainty associated with the estimators of Section 1.2.3 are given by Hadjiconstantinou et al. [19]. In general, the fractional error (statistical error normalized by the quantity of interest) scales with the inverse of the signal strength times the square root of the number of particles. For instance, the fractional error in flow velocity, \( E_u \), is inversely proportional to the square root of the number of samples and the Mach number, \( E_u \propto \left( Ma\sqrt{MN} \right)^{-1} \), where \( M \) is the number of ensembles, and \( Ma \) is the Mach number. DSMC has been remarkably successful in the field of aeronautics where the signal is large (i.e. \( Ma > 0.1 \)). However, in the limit of small scale devices and low-signal flows, DSMC suffers from severely unfavorable scaling requirements to achieve useful levels of accuracy—a decrease of a flow signal strength by a factor of 10 requires a factor of 100 more samples in order to maintain the same level of fractional error. Flows in micro- and nano-scale devices are inherently low-signal and have driven the need for a more efficient modeling in the regime where DSMC fails.
Chapter 2

Particle Simulations of the Bhatnagar-Gross-Krook Collision Operator

Particle simulations of the BGK model were developed by at least four groups from 1981 to 2001. In chronological order they are: Nanbu [31, 32], Montanero [24], Gallis [18], and Macrossan [29]. Our implementation follows most closely the work of Macrossan which is the most complete treatment of those listed here.

As seen in Section 1.1.5, the BGK collision operator by design is significantly simpler than the hard-sphere operator. Extending the DSMC simulation procedure to the BGK collision operator is conceptually straightforward, but requires subtle treatment of issues, such as momentum and energy conservation. This chapter develops the BGK based DSMC simulation (BGK-DSMC) to which variance reduction will be applied in Chapter 4.
2.1 Bhatnagar-Gross-Krook Collision Rules

The BGK approximation essentially states that collisions drive a distribution function towards its local equilibrium state. In a relaxation problem, this can be written as

$$\left[ \frac{\partial f}{\partial t} \right]_{\text{coll}} = \frac{n(x)}{k} (f^{\text{loc}} - f). \quad (2.1)$$

Defining a new function $\Delta f(x, c, t) = f^{\text{loc}}(x, c) - f(x, c, t)$, allows direct solution of (2.1),

$$f(x, c, t) = \Delta f(x, c, 0) \left( 1 - \exp \left( \frac{-n(x)t}{k} \right) \right) + f(x, c, 0). \quad (2.2)$$

The solution shows the distribution decaying exponentially towards equilibrium with time constant $\nu(x) = \frac{n(x)}{k}$. This feature is exploited in DSMC simulations in which within each collision step the dynamics resemble a homogeneous relaxation. This relaxation can be implemented in particle simulations with time step $\delta t$ by redrawing an appropriate fraction $(1 - \exp(-\nu \delta t))$ of the particles in a cell from the local equilibrium distribution. In a typical implementation involving $N$ particles, $N(1 - \exp(-\nu \delta t))$ particles are chosen randomly and their velocities are updated ($c \to c'$) by drawing the new velocities ($c'$) from the local equilibrium distribution, $f^{\text{loc}}(x, c)$. It is important to note that particles are chosen independently, so that the probability of a collision for any particle (not collision pairs as in Section 1.2.2) is the same$^2$ and equal to

$$P_{\text{coll}} = (1 - \exp (-\delta \nu)) = \left( 1 - \exp \left( \frac{-\delta tn(x)}{k} \right) \right). \quad (2.3)$$

This probability will be used when weight update rules are discussed in Section 4.1.

---

$^1$The simpler first order approximation for the number of particles to relax is $N \delta t \nu$. This is also used in the literature, but it is an unnecessary approximation.

$^2$Macrossan also developed a particle implementation of a BGK collision operator (and other collision models) based on choosing collision pairs [28] which results in the correct gaseous Prandtl number and eliminates the conservation concerns discussed in Section 2.2. However, the similarity of Macrossan's algorithm with DSMC also makes it subject to numerical instabilities when used in a control variate formulation that is the major inconvenience of variance-reduced DSMC (see Section 3.2.2) and that can be avoided in methods where collision particles are chosen independently.
2.2 Schemes for Enforcing Conservation

Unlike the standard DSMC collision rules (and the analytic form of the BGK operator), the BGK particle scheme described in the preceding section does not strictly enforce conservation of momentum or energy (momentum and energy are conserved on average). In the limit of a low number of particles \( N \lesssim 2000 \), random walks in the properties are significant. To control the walks and enforce the prescribed conservation, one of two approaches is usually followed: 1) the velocities of all of the particles in a cell or 2) the velocities of the particles that underwent a collision in a cell are shifted and scaled to exactly preserve the pre-collision mean cell velocity and its variance. While both approaches have worked in practice, the error associated with these methods is unclear.

An alternative is to enforce conservation using information from previous time-steps. This approach will be referred to as the residual-corrector method\(^3\). Let

\[
\bar{M}_j^n(t) = \frac{\int c_j^n d^3 c d^3 x}{\int d^3 x}
\]

(2.4)

denote the moment \( M \) of the \( j^{th} \) component of the molecular velocity raised to the \( n^{th} \) power at time \( t \) averaged over a computational cell \( cell \). In the residual corrector method, instead of drawing particles from a Maxwell-Boltzmann distribution with the moments as measured at time \( t \), we ensure conservation by drawing particles from a Maxwellian with the residual-corrected moments

\[
\bar{CM}_j^n(t) = \bar{M}_j^n(t) - [\Delta \bar{M}_j^n(t - \delta t)]_{coll}
\]

(2.5)

where

\[
[\Delta \bar{M}_j^n(t - \delta t)]_{coll} = \bar{M}_j^n(t - \delta t)_{post\ collision} - \bar{CM}_j^n(t - \delta t)
\]

(2.6)

In words, this scheme measures the discrepancy/residual between the desired mo-

\(^3\)This approach was first suggested and implemented by Gregg Radtke in the Fall of 2009. His implementation was for a deviational particle method [34], and the author adapted it for use in this work.
ments \((\bar{C}M^n_j(t - \delta t))\) and the actual moments \((M^n_j(t - \delta t)|_{\text{post collision}})\) and applies this as a correction on the next time step. It is noteworthy that in the absence of advection (i.e. for homogeneous relaxation problems) this scheme ensures exact conservation since \(\bar{M}^n_j(t) = M^n_j(t - \delta t)|_{\text{post collision}}\).

The primary advantage of this scheme is that the distribution from which particles are drawn is known, which facilitates the variance-reduced algorithm that will be described in Chapter 4. For a standard (not variance-reduced) BGK-DSMC simulation any of these three methods should perform adequately to enforce conservation; in this work we will employ the residual-corrector method.\(^4\)

2.3 Ellipsoidal Statistical Model

As discussed in Section 1.1.5, the BGK operator captures most of the important physics of the more complex hard-sphere operator. The most notable difference is that the Prandtl number (the ratio of momentum diffusivity to thermal diffusivity) under the relaxation time approximation is unity, while for the Boltzmann equation with the hard-sphere collision operator \(\Pr \approx \frac{2}{3}\).

To exploit the computational efficiencies that arise from the BGK approximation, but also capture the correct Prandtl number, the Ellipsoidal Statistical (ES-BGK) model [13] has been proposed, in which an anisotropic Gaussian

\[
f^G = \frac{n(x)}{\pi^{\frac{3}{2}}} \sqrt{\det \mathbf{A}} \exp \left[ -\mathbf{A}_{ij}(c_i - u_i)(c_j - u_j) \right]
\]  

\[
\mathbf{A}_{ij} = \frac{1}{\Pr} \delta_{ij} - \frac{(1 - \Pr)\tau_{ij}}{n(x) \Pr} \]  

\[
\mathbf{A} = \mathbf{A}^{-1}
\]

is chosen instead of \(f^{loc}\) in (1.5).

The transport equation that results when applying the Ellipsoidal Statistical

\(^4\)In our final algorithm, \((\text{VR})^2\)-BGK-DSMC, we will exploit the variance reduction method to effectively eliminate the noise in local property estimates that gives rise to the random walks, and the enforced conservation is not needed.
model satisfies the four major properties of the hard-sphere Boltzmann equation collision term [30]:

1. It conserves mass, momentum, and energy

2. It satisfies the H-theorem [6]

3. The equilibrium distribution is a Maxwellian

4. The Prandtl number, $Pr$, can be chosen to be $\frac{2}{3}$

Because calculation and inversion of the matrix $A$ is computationally expensive, the remainder of this work implements the BGK model without the Ellipsoidal Statistical correction, but its inclusion in the variance-reduced scheme will be briefly discussed in Chapter 6.

### 2.4 BGK-DSMC and DSMC Comparison

In summary, the advection, sorting, and sampling routines of DSMC remain unchanged in BGK-DSMC. The BGK-DSMC collision routine, on the other hand, is a simpler homogeneous relaxation. This relaxation is implemented by selecting the appropriate fraction of particles and redrawing their velocities from the local equilibrium (as measured from the simulation). The primary advantage of BGK-DSMC is that this simplified collision routine eliminates acceptance-rejection (a major computational cost of DSMC). Redrawing particles can be made to conserve the lower moments (mass, momentum and energy) of the distribution function by shifting and scaling particle velocities or by drawing from a residual-corrected local distribution. The correct Prandtl number dependence can also be achieved in BGK-DSMC by using the Ellipsoidal Statistical model.

BGK-DSMC should prove to be a more efficient alternative to standard DSMC, but despite the modest efficiency gains achieved in the collision routine, BGK-DSMC will also suffer from the same unfavorable statistical convergence that makes simulation of low-signal problems problematic. A variance reduction method that en-
ables DSMC to model arbitrarily low-signal flows is presented next (Chapter 3); our variance-reduced BGK-DSMC is unveiled in Chapter 4.
Chapter 3

Variance Reduction in DSMC Simulations

The focus of this thesis is the application of the Al-Mohssen and Hadjiconstantinou weighted particle approach [3] to variance reduction of DSMC simulations because of its ability to provide substantial variance reduction without altering the simulation method significantly. We start with a discussion of control variates which is the basic principle behind the variance reduction approach used here. We then discuss the application of these ideas to the general DSMC algorithm. Our variance-reduced BGK collision operator and simulation method is then presented in Chapter 4.

3.1 Control Variates

The control variate [7] approach exploits the knowledge of a correlated function to reduce the statistical uncertainty in the evaluation of a function of interest. In the guise used here, sometimes referred to as correlated sampling, two correlated simulations (essentially using the same random numbers) run in parallel. By ensuring that one of the simulations has moments that are analytically known, the moments of the second simulation can be recovered with reduced statistical uncertainty.

In the case of a kinetic flow, an equilibrium simulation is a convenient choice for the control simulation with analytically known properties. If an equilibrium simu-
lation can remain correlated with a non-equilibrium simulation, the non-equilibrium estimators can be variance reduced using the method of correlated random numbers as described above.

The simplest, perhaps, way to force two simulations to be correlated is to make the particles in both simulations have the same velocities and positions. Clearly the probability of a particle existing at a given state in either simulation is different, but this difference can be quantified by a weight $W = W(x, c, t)$, defined as the quotient of the two distribution functions

$$W = \frac{f_{eq}}{f}. \quad (3.1)$$

Assigning these weights to the particles in a DSMC simulation, allows concurrent simulation of two correlated stochastic processes sampling two distributions: $f_{eq}$ with known moments, and $f$, the unknown non-equilibrium distribution function.

To show how variance reduced properties are obtained using these weights, consider an arbitrary property of the non-equilibrium simulation, $A$. Properties of interest take the form

$$\langle A \rangle = \int A(c) f(x, c, t) d^3 c. \quad (3.2)$$

In order to obtain variance-reduced estimators, simply subtract the noisy estimator for the equilibrium property and add the analytical value,

$$\langle A \rangle = \int A(c) (f - f_{eq} + f_{eq}) d^3 c. \quad (3.3)$$

The standard control variate method (see [37] for details) is formulated more generally as,

$$\bar{A}^{VR} = \bar{A} - \beta (\bar{A}^{eq} - \langle A \rangle^{eq}). \quad (3.4)$$

where, $\bar{A}$ is a volume averaged approximation of $\langle A \rangle$ found by summing over samples in a region, and the optimal value of the constant. $\beta$ is given by $\beta = \frac{\text{cov}(A, A^{eq})}{\text{var}(A^{eq})} = \frac{\text{cov}[W(x, c)A(x, c), A(x, c)]}{\text{var}[W(x, c)A(x, c)]}$. This expression cannot normally be evaluated a priori, but in near-equilibrium flows, the value of $W$ will be close to unity such that $\beta \approx 1$, whereby Equation (3.4) reduces to Equation (3.3). In practice, the value of $\beta$ may be estimated.
using regressions. In one of our experiments, an estimate of the optimal $\beta$ obtained from simulation data doubled the variance reduction. However, every moment of the velocity distribution function requires a different coefficient $\beta$, which at least doubles the computational cost of the sampling routine. For this reason we will proceed with $\beta = 1$.

### 3.2 Weight Update Rules

As stated above, variance reduction is achieved by utilizing an equilibrium simulation that is correlated with the non-equilibrium simulation of interest. The two simulations remain correlated by using the same particles (namely those of the non-equilibrium simulation) and a set of weights $\{W^{(i)}\}$ which account for the relative probability of finding particle $(i)$ in the equilibrium simulation relative to the non-equilibrium simulation. When we discuss equilibrium particles we refer to imaginary particle that would exist in an equilibrium simulation, but are instead represented by weights.

In the present work, the reference equilibrium simulated by the equilibrium simulation is the global equilibrium

$$f^{eq}(c) = f^{MB}(c; 0, n_0, T_0) = \frac{n_0}{(\pi T_0)^{3/2}} \exp \left( -\frac{||c||^2}{T_0} \right). \quad (3.5)$$

Knowledge of the (non-equilibrium) initial condition $f(x, c, t = 0)$ implies knowledge of the initial condition for the weights, $W(x, c, t = 0)$, through (3.1) and (3.5). As the two simulations evolve in time, the update rules for equilibrium particles and non-equilibrium particles may differ, and the weights must be updated accordingly. Below we present rules for following the evolution of the weights. Since DSMC is divided into advection and collision steps, the weight updates are similarly considered separately.
3.2.1 Advection step

During the advection step, the non-equilibrium transport equation reduces to Equation (3.6),

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + \frac{\partial F_i f}{\partial c_i} = 0,$$

while the equilibrium simulation is governed by a different advection equation:

$$\frac{\partial f^{eq}}{\partial t} + c_i \frac{\partial f^{eq}}{\partial x_i} = 0.$$  \hspace{1cm} (3.7)

In the absence of body forces ($F = 0$) and by substituting $f^{eq} = W f$ into (3.7), it can be shown [1] that the weights advect normally (i.e. weights do not update during ballistic motion because equilibrium particles and non-equilibrium particles of the same velocity and position move together).

In the presence of external forces, update rules are more complex. In particular, a space and time dependent external force $F$ makes it difficult to derive a closed form solution for the weight evolution. Instead we consider the case of a constant force that is useful in a variety of situations, such as gravity, or pressure driven flows. A pressure driven flow is further discussed in Section 5.3.

In the presence of a constant body force, the particle positions and velocities are updated according to

$$c' = c(t + \delta t) = c(t) + F \delta t$$  \hspace{1cm} (3.8)

and

$$x' = x(t + \delta t) = x(t) + c(t) \delta t + \frac{1}{2} F \delta t^2.$$  \hspace{1cm} (3.9)

The weight at the end of the advection step is given by definition as

$$W' = \frac{f^{eq}(c')}{f(x', c', t')}.$$  

Since $f(x', c', t') = f(x, c, t)$ from (3.6) and with $F$ constant,

$$W' = \frac{f^{eq}(c + F \delta t)}{f(x, c, t)}.$$
From Equation (3.1), we obtain a usable weight update rule for particles experiencing a constant body force:

$$W' = \frac{f_{eq}(c + F\delta t)}{f_{eq}(c)} W.$$  

This update rule is equivalent to shifting the reference equilibrium to counteract the acceleration of the non-equilibrium particles as compared to the equilibrium particles.

**Boundary conditions**

During the advection step, if a particle crosses the boundaries of the simulation it can be handled in the traditional manner (open, toroidal, specular, or diffuse boundaries). For toroidal or specular boundaries the weights remain unchanged, because both equilibrium and non-equilibrium particles are updated identically.

For diffuse boundaries, which are the focus of this section, the boundary condition is given by [38]

$$f_{wall} = \frac{\sigma_w}{(\pi T_{wall})^{3/2}} \exp \left( - \frac{||c - u_{wall}||^2}{T_{wall}} \right) = \sigma_w f_{wall} \quad [(c - u_{wall}) \cdot n_{wall} < 0]$$  

(3.11)

where

$$\sigma_w = -2 \left( \frac{\pi}{T_{wall}} \right)^{1/2} \int_{(c - u_{wall}) \cdot n_{wall} < 0} (c - u_{wall}) \cdot n_{wall} f(x, c, t)d^3c.$$  

(3.12)

In the interest of simplicity, we consider here the case for which $u_{wall} \cdot n_{wall} = 0$, but motion of the boundaries in the direction of the normal has been discussed elsewhere [1].

The weight update for particles colliding with a wall can be derived by considering the definition of the weights (3.1)

$$W' = \frac{f_{eq,wall}(c')}{f_{wall}(c')}.$$  

(3.13)

Unfortunately, this is complicated by the fact that $\sigma_w$ in general needs to be evaluated from simulation data. An exception to this is isothermal, constant density flows for
which \( \sigma_w \) is known analytically (typically \( \sigma_w = 1 \)), in which case the weight update is simply

\[
W' = \frac{f^{eq}(c')}{\bar{f}^{wall}(c')}
\]  

(3.14)

where knowledge of the equilibrium distribution has been exploited to give \( f^{eq} = f^{eq,wall} \).

In the general case, where evaluation of the constant \( \sigma_w \) is required, Equation (3.13) leads to

\[
W' = \frac{f^{eq}(c')}{\bar{f}^{wall}(c')} \sum W \sum W'
\]  

(3.15)

or

\[
W' = \left( \frac{T^{wall}}{T_0} \right) \frac{1}{2} \frac{f^{eq}(c')}{\bar{f}^{wall}(c')} \sum W \sum W' N
\]  

(3.16)

where the summations run over particles that had a collision with the wall during the time step in question.

The difference between Equation (3.15) and Equation (3.16) lies in the approach of evaluating (3.12) [1]. Essentially, in (3.16), (3.12) is partially evaluated analytically, whereas in (3.15) it is completely evaluated by the simulation (particles acting as Monte Carlo samples)—see [1] for complete details. Care needs to be taken in implementing (3.15), since it is expected to be biased in the limit of few particles colliding with the wall during the time step. Equation (3.16) on the other hand, is theoretically unbiased even for a single particle-wall collision in a time step.

In both (3.15) and (3.16) the summation terms of the weights going into the wall and the weights going out of the wall can only be evaluated at the end of the advection step (after all particle-wall collisions have been processed). Only then can these terms be applied as a multiplicative constant on the weights of all particles that collided with the wall during the advection step. This additional bookkeeping is a relatively minor concern.
3.2.2 Collision step

The collision rules for variance-reduced, hard-sphere DSMC simulations are considerably different than for VR-BGK-DSMC simulations, so they will only be summarized here. The reader is referred to [1, 2, 3] for more details.

In brief, collision pairs in hard-sphere DSMC are chosen and accepted with a probability $\hat{c}_r$ (proportional to the relative velocity of the colliding pair), or rejected with probability $1 - \hat{c}_r$. If a collision is accepted, the post-collision weights of the collision pair, is related to the pre-collision weights, $W^{(1)}$ and $W^{(2)}$, by

$$ W'^{(2)} = W'^{(1)} = W^{(1)}W^{(2)}. \quad (3.17) $$

If the collision is rejected, the update rule is

$$ W'^{(1)} = W^{(1)} \frac{1 - W^{(2)} \hat{c}_r}{1 - \hat{c}_r}, \quad (3.18) $$

$$ W'^{(2)} = W^{(2)} \frac{1 - W^{(1)} \hat{c}_r}{1 - \hat{c}_r}. \quad (3.19) $$

Additional averaging is performed during the collision step to enforce stability (see [1]). One of the principal motivations for our VR-BGK-DSMC method (to be presented Chapter 4) is to eliminate the need for additional averaging for stability.

3.3 Variance Reduced Moments

Variance-reduced hydrodynamic properties (given below) may be obtained by applying the variance reduction formula (Equation (3.3)) to the moment expressions of Section 1.1.6. This yields

$$ \bar{n}^{VR} = \frac{\sum_i (1 - W^{(i)})}{N_0} + n_{eq} \quad (3.20) $$

$$ \bar{u}^{VR}_i = \frac{1}{\bar{n}^{VR}N_0} \sum_j (1 - W^{(j)}) c^{(j)}_i + \frac{n_0}{\bar{n}^{VR}} u^{VR}_{i,eq} \quad (3.21) $$
\[ \tilde{T}^{\text{VR}} = \frac{2}{3n^{\text{VR}}N_0} \sum_j (1 - W^{(j)}) \left( c^{(j)}_i \right)^2 - \frac{2}{3} \left( \bar{u}_i^{\text{VR}} \right)^2 + \frac{n_{\text{eq}}}{n^{\text{VR}}} T_0 \]  

(3.22)

\[ \tilde{\tau}^{\text{VR}}_{ij} = \frac{2}{N_0} \sum_k (1 - W_k) c^{(k)}_i c^{(k)}_j + \langle c_i c_j \rangle^\text{eq} - 2 \bar{u}_i^{\text{VR}} \bar{u}_j^{\text{VR}} n^{\text{VR}} \]  

(3.23)

\[ \tilde{q}_i^{\text{VR}} = -\bar{u}_i^{\text{VR}} \left( \frac{5}{2} + \left( \bar{u}_k^{\text{VR}} \right)^2 \right) + \frac{1}{N_0} \left( \sum_j c^{(j)}_i c^{(j)}_k \right)^2 + \left( c^{(j)}_i \bar{u}_k^{\text{VR}} + 2 \left( \bar{u}_i^{\text{VR}} c^{(j)}_k - c^{(j)}_i c^{(j)}_k \right) \right) \bar{u}_k^{\text{VR}} - \left( c^{(j)}_k \right)^2 \bar{u}_i^{\text{VR}} \]  

(3.24)

### 3.4 VR-DSMC Comparison with DSMC

Variance reduction of a DSMC simulation is obtained by adding a weight (defined by Equation (3.1)) to every particle. During the advection step, the weight of every particle is updated by Equation (3.10). During the collision step, the weights of trial collision particles are updated by Equation (3.17) or Equation (3.18) and (3.19). When properties are sampled, the variance-reduced moments of Section 3.3 are used.

This approach results in a simulation method with relative uncertainty that is independent of the signal strength [1], whereas traditional DSMC results in relative uncertainty that scales inversely with the signal strength [19]. For low signal flows, the computational gains of VR-DSMC may be several orders of magnitude.

This variance reduction method also has the desirable feature of requiring essentially no modification of the standard DSMC simulation. Data from the variance-reduced simulation and the standard DSMC simulation can both be outputted. This is very convenient for comparison and is a result of the fact that the DSMC algorithm is left intact—a favorable feature in its own right.
Chapter 4

Variance Reduced Particle Simulation of the Bhatnagar-Gross-Krook Collision Operator

This chapter is the keystone of this work, albeit nearly the shortest. Rather than diminishing the magnitude of this contribution, in the Author’s opinion it enhances it by adding simplicity to its list of virtues. In this chapter, we combine the BGK particle simulation method described in Chapter 2 with the control-variate variance reduction approach discussed in Chapter 3 to obtain a variance-reduced particle simulation of the BGK model, which we will refer to as VR-BGK-DSMC or (VR)²-BGK-DSMC, depending on whether or not variance-reduced properties are used in the collision step (see Section 4.2). The advection, sorting, and sampling routines of our variance-reduced BGK-DSMC schemes are the same as the variance-reduced DSMC [2] method which closely resembles DSMC itself. The collision routine is significantly simplified due to the different (simpler) weight update rules required for the BGK model. These rules are developed in this chapter, which also details the complete algorithm. Results and validation are presented in Chapter 5.
4.1 Particle-Particle Collisions

The fundamental difference between the variance-reduced approach presented here from the BGK-DSMC model of Chapter 2 is that each particle carries a weight which allows it to represent a sample of an equilibrium distribution function in addition to being a sample of a non-equilibrium distribution. In this section, we derive evolution rules for particle weights during the collision step under the BGK approximation. These rules are simpler than their variance-reduced DSMC counterparts, and also impart desirable stability to our method.

As described in Section 2.1, the collision routine for the BGK model consists of selecting a fraction of the particles in a cell according to Equation (2.3). Those particles’ velocities are then redrawn from the local equilibrium distribution (potentially with residual-corrected moments). In the variance-reduced case, the collision routine also requires a weight update because the local equilibria in the equilibrium and non-equilibrium simulations may be different.\footnote{The collision probability in an equilibrium simulation is arbitrary, because collisions have no effect on the distribution. Therefore, the collision probability has no effect on the weight update.}

Conveniently, both the non-equilibrium and the equilibrium distribution functions of collided particles are analytically known and the weights can be redefined independently from their history [1]. Specifically, using the definition of the weight in Equation (3.1), the update rule for collided particles is given by

\begin{equation}
W(c') = W' = \frac{f^{eq}(c')}{f^{loc}(c')}, \tag{4.1}
\end{equation}

where the local distribution is defined by the measured (and potentially corrected) moments. If we define temperature according to those measured moments as \( T = \frac{2}{3} (M^2 - M_i^1 M_i^1) \), then the expression for the local equilibrium distribution is

\begin{equation}
f^{loc} = \frac{M^0(t)}{(\pi T)^{3/2}} \exp \left( -\frac{(c_i - M_i^1)^2}{T} \right). \tag{4.2}
\end{equation}

The appropriate method for drawing the new particles based on the five measured
moments is discussed in Appendix A.1. The weights of particles that do not collide remain unchanged. These simple rules at once remove the need for acceptance rejection and additional averaging for stability. The only added cost comes from sampling the local properties (mass, momentum, and energy) every collision step rather than at some reduced frequency. Thus the VR-BGK-DSMC collision rules satisfy the principal motivation for developing a VR-BGK simulation—the instability inducing random walks in the weights are eliminated, because the weights are reevaluated at every time step from definition (3.1) and stochastic deviations do not accumulate as they do in the variance-reduced DSMC collision rules.

4.2 VR vs. (VR)²

In the sampling routine the variance-reduced property expressions from Section 3.3 are used to give lower noise results. When evaluating the local properties for (4.2) it is intuitively appealing to use the variance-reduced equations from Section 3.3 as well, rather than standard expressions of Section 1.2.3. Indeed the only drawback of this approach seems to be that the original BGK-DSMC simulation is no longer unmodified, but has a small amount of variance-reduction built in. If preservation of an unmodified underlying simulation is important then the standard moment expressions must be used. On the other hand, if a slight modification of the underlying BGK-DSMC simulation is allowable, then variance-reduction can be further enhanced. We will call the former VR-BGK-DSMC and the latter (VR)²-BGK-DSMC. Perhaps the most desirable feature of (VR)²-BGK-DSMC is not the additional variance reduction, but rather its effect on conservation. In the VR-BGK-DSMC algorithm, variance in the local property estimators causes random walks in the properties for small number of particles and requires an enforced conservation scheme; on the other hand, variance is essentially eliminated in (VR)²-BGK-DSMC—there are no observable problems with random walks, and enforced conservation is not needed.
4.3 Variance-Reduced BGK-DSMC Algorithm

There are three main algorithmic decisions that must be made when implementing a variance-reduced BGK-DSMC simulation. The first is whether or not to use variance-reduced estimators in estimating the local equilibrium distribution (VR vs. (VR)²). The second is whether or not to use the residual-corrector enforced conservation scheme of Section 2.2. The third is how to evaluate the weights after a wall collision (see Section 3.2.1). The first two decisions are interrelated: If the user decides to not use the (VR)² approach, then conservation is needed for simulations with low numbers of particles ($N \lesssim 10000$ per cell); otherwise it is not necessary. The choice of boundary condition enforcement depends on the problem being simulated. If the problem may be reasonably approximated as constant density at the boundaries, then Equation (3.14) may be used, which offers slight computational advantages. For more complex problems (e.g. non-isothermal) one of the other rules, Equation (3.15) or (3.16), needs to be used. The author sees no compelling reason to use the enforced conservation rule, Equation (3.15), but it is included in [1], so it will be evaluated as well as Equation (3.16) in Chapter 5.

In the algorithm that follows, items marked with * are only required if using the residual-corrector conservation scheme.

1. Initialize the system (as per standard DSMC procedure) by distributing particles in simulation space according to the initial conditions (Appendix A.1) and dividing the simulation into cells

2. Assign weights by definition (Equation (3.1)) to every particle.

3. *Measure residual moments (differences from exact) in each cell (Equation (2.5)).

4. Advection step:
   (a) Integrate particle positions and velocities (Equations (3.8) and (3.9)).
   (b) For particles that cross a boundary during $\delta t$:
i. Update weights for the up to the wall collision time (Equation (3.10)).

ii. Redraw particle velocities appropriately from the fluxal distribution (Appendix A.1)

iii. Update weights for the wall collision (see Section 3.2.1).

iv. Integrate position and velocity for remainder of time step (Equations (3.8) and (3.9)).

v. Update weights for the advection during the remainder of the time step (Equation (3.10)).

(c) For all particles that did not cross a boundary:

i. Update weights for the advection (Equation (3.10)).

5. Collision step (evaluated cell by cell):

(a) Measure the first five moments of the distribution function (*and add residual from previous step (Equation (2.5))).

(b) Select appropriate fraction of particles (Equation 2.3) to collide (do not select the same particle twice and round fractions of particles in an unbiased manner).

(c) For each collision particle, redraw its velocity (Appendix (A.1)) from the measured (*corrected) moments.

(d) Redefine weights for every collided particle (Equation (4.1)).

(e) *Measure the residual moments (Equation (2.5)).

6. Sample properties of interest (For BGK-DSMC use Equations (1.13) to (1.17) or for variance-reduced BGK-DSMC use Equations (3.20) to (3.24)).

7. Repeat advection and collision steps and include the sampling step as desired.
4.4 Symmetrized Algorithm

Rader and Gallis showed that convergence of a DSMC simulation can be improved by symmetrizing the sequence of the algorithm [33]. Their modified algorithm processes an advection step for half of the time step, $\frac{\Delta t}{2}$, followed by a collision step, the remaining half advection step, and then the sampling step. While no systematic comparison of the convergence has been performed, the symmetrized algorithm has been used to compare directly with another VR-BGK code [35] in Section 5.4 (Figure 5-5).
Chapter 5

Results and Comparisons

The primary feature of our new method that we desire to validate is the variance-reduced collision routine, which comes in two varieties, VR-BGK-DSMC and (VR)$^2$-BGK-DSMC where variance reduced estimators are not or are, respectively, used to measure the local properties in the collision routine. That validation is performed for relaxation, shear, pressure, and temperature driven problems. Additionally, this chapter will demonstrate the effects of enforced conservation (see Section 2.2) and boundary conditions rules (see Section 3.2.1). The most robust, efficient, and general method is shown to be (VR)$^2$-BGK-DSMC with no enforced conservation and semi-analytical boundaries (Equation (3.16)). Both analytic results and numerical results (for the temperature jump problem) will be used to validate each case.

5.1 Homogeneous Relaxation

The first problem studied is a homogeneous relaxation. This problem is convenient, because there is a simple analytic solution for the evolution of the distribution function. Additionally, the advection routine can be eliminated, so effects of the collision rules alone can be scrutinized.

The initial condition chosen was the sum of two displaced equilibrium distributions

$$f^i = \frac{1}{2} \left( f^{MB}(c; +u_0, n_i, T_i) + f^{MB}(c; -u_0, n_i, T_i) \right), \quad (5.1)$$
where \( u_0 = [u_{\text{offset}}, 0, 0] \) while \( n_i = 1 \) and \( T_i \) is given by

\[
T = \frac{1}{3} \sum_{i=1}^{3} c_i^2 f^i d^3 c = T_i + \frac{2}{3} u_{\text{offset}}^2 = 1. \tag{5.2}
\]

Under the BGK approximation, a time-dependent solution for the distribution function in the homogeneous case follows from

\[
\left[ \frac{\partial f(t)}{\partial t} \right]_{\text{coll}} = n_i \left( f^{\text{loc}} - f(t) \right) \tag{5.3}
\]

where \( f^{\text{loc}} = f^{eq} \) (due to judicious choice of \( f^i \)). The solution of this equation is:

\[
f(t) = (f^i - f^{eq}) e^{-t} + f^{eq} \tag{5.4}
\]

Using Equation (5.4), we may obtain an analytic result for any moment of the distribution function. The lower moments are conserved (mass, momentum, and energy), so we chose the fourth moment of the distribution function, which is given as

\[
M_x^4(t) = \frac{1}{4} \left( 3 T_0^2 - 3 + 12 u_{\text{offset}}^2 T_0 + 4 u_{\text{offset}}^4 + 3 e^t \right) e^{-t}. \tag{5.5}
\]

This provides an analytical solution for validating transient and steady state behavior. This moment will be denoted \( M_x^4(t) \) when calculated from simulation data and \( M_x^4(t) \) when given by (5.5).

When running homogeneous relaxation simulations we will look for two behaviors: stability and bias. Stability is defined here as the ability to run to long times while maintaining meaningful results. Instability occurs when the weights grow to infinity or decay to zero \([1]\). A simple measure of this instability is the rate of change of the variance of the weights at steady state.

\[\text{A related instability occurs when random walks in properties dominate the results, but this will be considered separately.}\]
To measure the bias, the percent error is used, given by

$$\text{Error} = \left| \frac{\hat{M}_x^4(t) - M_x^4(t)}{\hat{M}_x^4(0) - M_x^4(\infty)} \right|.$$  \hspace{1cm} (5.6)

If the error is clearly dominated by the effects of random walks in properties (not weights), then it will occlude our ability to evaluate the stability of the weights and no determination about the bias or stability can be made.

To scrutinize our proposed collision rules (VR vs. (VR)$^2$) a homogeneous relaxation as described above was run with no advection routine—any instability or bias must result from the collision rules alone. The specific simulation used was initiated with $u_{\text{offset}} = 0.1$. For comparison, the simulation was run with and without the enforced-conservation scheme. The simulation without the residual-corrector conservation was allowed to reach equilibrium by evolving to $t = 100$ with a time steps of size $\delta t = 0.1$. At this time, the analytical value of the fourth moment from (5.5) is the steady state value of $0.75$ to machine precision. Steady state conditions were simulated for another 1000 time steps of size $\delta t = 0.1$. The steady state value of the fourth moment was the average of these 1000 steady state time steps and averaged over 100 ensembles. A study of the variance-reduced simulation collision rules was conducted as specified in Table 5.1, and the results are included therein. We will discuss these results before proceeding to the enforced conservation simulations.

Table 5.1: Comparison of collision rules for a steady state homogeneous relaxation problem with no residual-corrector conservation, 2000 particles, and 100 ensembles.

<table>
<thead>
<tr>
<th>Method</th>
<th>$\frac{\partial \text{var}(W)}{\partial t}$</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>VR-BGK-DSMC</td>
<td>$&gt;0$</td>
<td>RW</td>
</tr>
<tr>
<td>(VR)$^2$-BGK-DSMC</td>
<td>$0$</td>
<td>$0.333$</td>
</tr>
</tbody>
</table>

There are several important features in the results obtained in Table 5.1. First, without conservation, for a simulation with 2000 particles per cell, VR-BGK-DSMC is dominated by random walks (denoted RW). The random walks arise from the variance of the local cell properties. When the fluctuations of the properties compound over
time the simulation properties walk away from the true values. The walks should be unbiased, but they grow in magnitude with time. Since the variance of the properties and the variance of the weights are linked, the growth of the variance at steady state can be attributed to the random walk problem, leaving us with little information about the stability of the weights.

In the \((VR)^2\)-BGK-DSMC simulation, the variance of the local property estimators is vanishingly small, so random walks were not apparent. As expected, the variance of the weights was constant at steady state and the error was very small (0.333%). This simple test validates the theory and implementation of the \((VR)^2\) collision routine. It should also be noted that the \((VR)^2\)-BGK-DSMC simulation shows little need for the enforce conservation scheme of Section 2.2.

Table 5.2: Comparison of collision rules for a steady state homogeneous relaxation problem with residual-corrector conservation, 2000 particles, and 100 ensembles.

<table>
<thead>
<tr>
<th>Method</th>
<th>(\frac{\partial \text{var}(W)}{\partial t})_{SS}</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>VR-BGK-DSMC</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>((VR)^2)-BGK-DSMC</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Next, the residual-corrector method of Section 2.2 is applied to the same relaxation problem. The results (Table 5.2) show stable variance and no bias for both of the simulation methods—a convincing argument for the validity of both collision routines at steady state. It may seem surprising that the conservation scheme has such a dramatic effect on the error. However, one needs to keep in mind that the homogeneous relaxation problem is particularly subtle in the sense that the local equilibrium in this case is not only time independent, but under the residual-corrector it coincides exactly with \(f^{\text{eq}}\). Without the residual-corrector, the estimate of the local distribution function had random fluctuations which led to the error reported in Table 5.1.

Both Tables 5.1 and 5.2 deal with the steady state behavior, so additional tests were run to validate the transient behavior. The relaxation problem described above
was simulated with 20000 particles and \( u_{\text{offset}} = 0.1 \) and compared to the analytic solution in Equation (5.5). All three simulations (BGK-DSMC, VR-BGK-DSMC, and \((VR)^2\)-BGK-DSMC) were run for 100 time steps of size \( \delta t = 0.1 \) and for \( M = 10 \) ensembles. In Figure 5-1 the transient behavior of the three simulations is shown. The variance-reduced solutions from Figure 5-1 converge rapidly (only 10 ensembles) in an unbiased manner to the analytical solution strongly supporting the validity (lack of bias) of the transient variance-reduced solutions in general. The BGK-DSMC solution suffers from large statistical errors, even in this case of relatively large deviation from equilibrium, which is a good demonstration of the advantages of variance-reduced methods.

![Figure 5-1](image.png)

Figure 5-1: Homogeneous relaxation of \( \tilde{M}_x^4(t) \), the estimator of the fourth moment of the velocity distribution. Variance-reduced methods show statistical errors significantly smaller than the standard method.

The homogeneous relaxation is a very simple test, but it targets the same behavior that occurs within every collision step of a full simulation. Since the advection
and sampling routines were validated previously [1] and this section provides strong evidence for the validity of the collisional model, we will move confidently forward to probing other aspects of our new methods.

5.2 Isothermal Couette Flow

We now add another layer of complexity to the testbed by allowing non-homogeneity, but still keeping temperature constant. We use these results from a Couette flow as a means of validating our boundary condition methodology as well as the complete (advection, collision, and sampling) simulation algorithm.

In Couette flow, a gas is sheared by two parallel walls moving in opposite directions. For our test, the wall velocity is allowed to be sufficiently low such that the flow is isothermal. Results will be presented for $u_{\text{wall}} = 0.01$ and for various values of $k$. In each simulation, the estimator for the shear is compared to analytic (for the collisionless case) or semi-analytical linearized results from the literature.

First we focus on the collisionless limit ($k \to \infty$) to study the boundary condition implementation, in the same manner as the collision rules were studied for the relaxation case in the previous section. The shear for the free molecular limit is easily derived from kinetic theory (see, for example, [39])

$$
\tau_{\text{fml}} = \frac{2u_{\text{wall}}}{\sqrt{\pi}}.
$$

Accordingly, the error reported for the collisionless limit is given as

$$
\text{Error} = \frac{\tilde{\tau}^{\text{VR}} - \tau_{\text{fml}}}{\tau_{\text{fml}}}. \quad (5.8)
$$

There are three boundary conditions from which one must be selected. They are Rule #0: known density, Equation (3.14); Rule #1: flux conserving, Equation (3.15); and Rule #2: semi-analytic flux, (3.16). For this isothermal problem all three are expected to perform equally well in the limit of many particles, but the flux conserving rule will be biased for a lower number of particles. We will confirm this behavior by
measuring the bias, Equation (5.8), for each case.

In all cases, the walls are impulsively started at $t = 0$, and the simulation runs for 20000 time steps of size $\delta t = 0.1$ to reach steady state. Then steady state averages of the variance-reduced shear are calculated over the next 980000 steps. Three simulations are run for $N = 200$, $N = 2000$, and $N = 20000$ with 100, 10, and 1 ensembles, respectively, so each case represents the same number of samples. Since there is no difference for the boundary conditions between VR-BGK-DSMC and (VR)$^2$-BGK-DSMC, no distinction is made in the results summary (Table 5.3).

Table 5.3: Comparison of boundary conditions in a steady state collisionless isothermal shear flow.

<table>
<thead>
<tr>
<th>Rule #</th>
<th>$W' = \frac{f_{eq}}{f_{wall}} \sum W/N$</th>
<th>$N = 200$</th>
<th>$N = 2000$</th>
<th>$N = 20000$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$-0.0044$</td>
<td>$-0.0079$</td>
<td>$0.0196$</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$-17.7$</td>
<td>$-1.78$</td>
<td>$-0.182$</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>$-0.0265$</td>
<td>$0.0231$</td>
<td>$0.0054$</td>
<td></td>
</tr>
</tbody>
</table>

The known-density rule, which we expect to perform well for this case, shows no dependence on the number of particles in the simulation. Its error is consistently on the order of 0.01%. We assume this is the statistical error associated with the finite sampling, and accept this as validation of the implementation.

The flux conservation rule (Rule #1) shows an error based on the number of particles as expected. Since the sign of the errors is the same for all three cases ($N = 200$, 2000, and 20000) it appears that this error is a systematic bias. This bias decreases rapidly, as the inverse of the number of particles colliding with the wall in each time step which is itself a random variable. The expected number of wall collisions per step $E[N_{wall}]$ for the isothermal Couette is the same as the equilibrium estimate for the flux, namely,

$$E[N_{wall}] = \frac{N\delta t}{2\sqrt{\pi}}$$

For $N = 200$, $N = 2000$, and $N = 20000$ the expected number of collisions per wall
was 56, 564, and 5642, respectively. These fluxes and the related biases should inform the user's particle number choices in order to achieve the desired accuracy.

The partially analytic rule (Rule #2) consistently has error less than 0.1% and is thus considered unbiased. A more detailed study would be necessary to identify the source of this error, but for the present it is insignificantly small and attributed to statistical sampling.

To test the complete algorithm (advection, collision, and sampling), a fine-scale study of the shear flow was performed with a simulation of 50 cells and 20000 particles per cell. A wall velocity of $u_{\text{wall}} = .01$ was applied at $t = 0$. Since the temperature generation is expected to be negligible, the isothermal boundary condition rule (Rule #0) is used. After the simulation reached steady state, the average flow velocity was calculated and compared to semi-analytical solutions for the linearized BGK approximation as tabulated by Loyalka [26]. The comparison is shown in Figure 5-2. For a broad range of Knudsen numbers $(VR)^2$-BGK-DSMC provides stable, unbiased, variance-reduced estimates of the shear. Although not shown, VR-BGK-DSMC performs similarly.
Figure 5-2: Isothermal Couette flow results for $\tau_{xy}$, the estimator of shear stress. For a range of Knudsen numbers, the variance-reduced BGK simulation converges to the linearized results in [25].
The isothermal Couette flow studied in this section demonstrated the behavior of the boundary conditions in an isothermal problem as well as validating the complete algorithm for a simple flow.

### 5.3 Poiseuille Flow

A more demanding test case is the pressure driven channel or Poiseuille flow. In this problem, a flow between two parallel plates is induced by a pressure gradient supported by a density gradient. Again we will restrict the flow to be isothermal in order to compare with results from the literature. Typically, in DSMC simulations these pressure gradients are simulated with particle reservoirs at the ends of the channel, but for steady state simulation of a pressure gradient that is small and constant, a simpler approach is suggested by Cercignani [15] in which pressure gradients are converted into body forces which are applied during the advection step. This approach is convenient for our model, since the body force can be specified using Equation (3.10).

To determine the magnitude of the body force let

\[ \kappa = \frac{\partial n}{\partial y} = \frac{\partial p}{\partial y} \]  \hspace{1cm} (5.10)

quantify the pressure gradient in the \( y \) direction (flow direction). The dimensionless pressure gradient is small (\( \kappa \ll 1 \)) for an isothermal flow. In this linearized case, the non-dimensional form of the Boltzmann relation is given by [5]

\[ \frac{\partial f}{\partial t} + c_x \frac{\partial f}{\partial x} + c_y \kappa f^{eq} = \left[ \frac{\partial f}{\partial t} \right]_{coll} \] \( (x, c, t) \),  \hspace{1cm} (5.11)

where we have assumed that the linearization takes place about the reference equilibrium, \( f^{eq} \). Taking advantage of the analytical expression for \( f^{eq} \), we can write

\[ \frac{\partial f^{eq}}{\partial c_y} = -2c_y f^{eq} \].

Using the splitting scheme of DSMC, the advection step can be rewritten as

\[ \frac{\partial f}{\partial t} + c_x \frac{\partial f}{\partial x} - \frac{\kappa}{2} \frac{\partial f^{eq}}{\partial c_y} = 0. \]  \hspace{1cm} (5.12)
Finally, by applying the linear approximation for the distribution function, \( f = f^{eq}(1 + h) \) where \( h \ll 1 \), the advection equation for the non-equilibrium distribution function emerges with a body force term,

\[
\frac{\partial f}{\partial t} + c_x \frac{\partial f}{\partial x} - \frac{\kappa}{2} \frac{\partial f}{\partial c_y} \approx 0.
\]  

(5.13)

The interpretation of this relationship is to apply a driving pressure gradient in the non-equilibrium simulation as a body force of magnitude \( F = -\frac{\kappa}{2} \).

As derived previously, weights in a simulation with an applied body force advect normally and the weights are then are updated by (3.10), which for the pressure case yields

\[
W' = W e^{(\kappa \delta t c_y - (\kappa \delta t/2)^2)}.
\]  

(5.14)

As outlined in Section 4.3, near the boundary, the time step for the weight update may be some fraction of the simulation time step. If a particle collides with a diffuse wall, its velocity and weight must be updated for the fraction of the time step it accelerates before the collision, then for the remaining fractional time step after the collision.

### 5.3.1 Poiseuille simulation results

A (VR)^2-BGK-DSMC Poiseuille flow was run with 20000 particles and 50 cells and compared to the flow rate \( Q_y = \frac{2w_y}{\kappa} \) from the Loyalka results [26]. Comparisons are made for the flow profile at a Knudsen number of \( k = 0.5 \) in Figure 5-3 and for the average flow \( Q = \frac{\int_0^L Q_y dx}{\int_0^L dx} \) for a range of Knudsen numbers in Figure 5-4.
Figure 5-3: Poiseuille flow profile for a Knudsen number of $k = 0.5$. The variance-reduced simulation produces a flow rate profile that agrees with the results in [25].
Figure 5-4: Poiseuille average flow results. The pressure driven flow rate shows good agreement with results in [25] for a broad range Knudsen numbers.
At a Knudsen of $k = 0.5$, the flow rate in each cell matches the profile from the Loyalka solutions and (though the calculation is not shown here) the average flow rate has an error of approximately 0.1%—considered unbiased for the present case. Figure 5-4 shows good agreement across the whole range of Knudsen numbers of interest.

5.4 Temperature Couette

Up to this point the flows studied have been isothermal. In this section, we study the flow induced by an impulsive change in the temperature between two parallel plates. First, the collisionless limit is used to study the boundary conditions for a non-isothermal problem. Then, a fine scale study is performed to validate the transient behavior of the variance-reduced method.

For the collisionless study, linearized conditions (i.e. small temperature jump) were simulated. At $t = 0$, one wall of the simulation is heated to $T = 1.005$, while the other wall is cooled to $T = .995$. Both walls are stationary and the simulation is initially at equilibrium at $T = 1$. To reach steady state conditions, the simulation is run for 20000 time steps of size $\delta t = 0.1$, and then the variance-reduced temperature is averaged over the next 980000 steps. The simulation was run with $N=200$, 2000, and 20000 and 100, 10, and 1 ensembles were used, respectively, to preserve the total number of samples.

In the linearized regime, this problem is expected to have constant heat flux [38] of

$$q_x = \frac{\Delta T}{\sqrt{\pi}},$$

(5.15)

so the error is measured as

$$\text{Error} = \frac{q_x^{\text{VR}} - q_x}{q_x}.$$  

(5.16)

Only the boundary condition rules that correctly account for the mass flux to and from the wall are expected to be unbiased. The known-density rule is shown to be biased as expected. Table 5.4 summarizes the results.

These results demonstrate that correct handling of the flux at the wall is vital.
Table 5.4: Comparison of boundary conditions in a steady state collisionless temperature jump flow.

| Rule #: | \( W' = \frac{f_{eq}}{f_{wall}} \sum W' \sqrt{\frac{T_{wall}}{T_0}} \frac{f_{eq}}{f_{wall}} \sum \frac{W'}{N} | \begin{array}{|c|c|c|c|} \hline N = 200 & N = 2000 & N = 20000 \\ \hline \% Error & \% Error & \% Error \\ \hline 0 & -12.50 & -12.51 & -12.49 \\ \hline 1 & -17.7 & -1.77 & -0.171 \\ \hline 2 & -0.030 & -0.0024 & 0.0178 \\ \hline \end{array} |

Table 5.4 shows an error of 12.5% if the mass flux is not correctly calculated at the wall (Rule #0). Rule #1 shows the same bias as in the shear flow study (which is dependent on the inverse of the number of samples). As in Table 5.3, Rule #2 demonstrates no discernible bias. There is no clear reason to prefer Rule #1 over Rule #2, so the latter is recommended. The known-density rule should only be used when physically reasonable.

As an investigation of the transient behavior of the variance reduced quantities, the temperature jump problem was compared to the results from another variance-reduced BGK simulation [35]. Out simulation was run with 50 cells and 20000 particles per cell. The semi-analytic boundary condition (Rule #2) is used. The temperature profiles for three different times (\( \tau_{advect} \) denoting the advective time scale) are given in Figure 5-5. The transient behavior of our variance reduced method is in good agreement with the results from the method developed in [35].

The temperature jump problem highlighted the need for judicious choice of boundary conditions. The known-density rule should only be used when the problem physically satisfies that condition (e.g. isothermal). The temperature jump problem also served as an opportunity to again validate the new simulation method. This time, no simple analytical solutions were available, so our method was compared with good agreement to another variance-reduced BGK particle method that does not as resemble BGK-DSMC as closely as \((VR)^2\)-BGK-DSMC.
Figure 5-5: Temperature jump problem. The \((\text{VR})^2\)-BGK-DSMC algorithm yields unbiased transient temperature profiles. The benchmark here is calculated using a deviational particle variance-reduced BGK simulation [35].

5.5 Results Summary

The variance-reduced BGK-DSMC method was compared favorable with analytical results for relaxation, shear, and pressure driven problems. For a more complex temperature jump problem the variance-reduce BGK-DSMC method compared well with another related method. These tests are strong evidence of the validity of the implementation and theory presented in the thesis. Additionally, the variance-reduced method shows significantly lower noise compared to the non-variance-reduced method under identical conditions. The VR-BGK-DSMC algorithm is shown to need enforced conservation at low number of particles per cell, and accordingly the \((\text{VR})^2\)-BGK-DSMC algorithm is preferable (with no enforced conservation). Of the three potential boundary conditions the no flux rule (Equation (3.14)) and the semi analytic flux rule (Equation (3.16)) perform equally well in isothermal problems, with the latter
being preferable when the isothermal restriction is relaxed. The flux conservation boundary rule (Equation 3.15) should only be used with a large number of particles ($N \geq 10000$).
Chapter 6

Conclusions

A stable, unbiased, variance-reduced algorithm for DSMC-like particle simulations of the relaxation time approximation has been presented. The general approach follows from the Al-Mohssen and Hadjiconstantinou DSMC variance-reduction scheme (VR DSMC). The method presented allows efficient modeling of transition regime flows. Although only simple geometric boundaries have been considered, this method is easily extended to boundaries of arbitrary complexity.

The greatest advantage associated with our approach is that it more closely resembles the DSMC implementation than the Ramanathan and Koch or the Radtke and Hadjiconstantinou [20, 35] variance-reduced BGK methods. Since DSMC is perhaps the most widely used particle simulation method, this similarity increases the accessibility of our approach. Furthermore, this similarity also makes our VR-BGK-DSMC and (VR)$^2$-BGK-DSMC easy to extend and modify in the same manner that BGK-DSMC simulations have been modified. For example, a variance-reduced Ellipsoidal Statistical BGK model (see Section 2.3) should be a straightforward extension of our algorithm. The important features remain unchanged (particles act independently during the collision step and the post-collision distribution function has an analytical form), so all weight updates should still be calculated analytically in a stable manner.

The VR-BGK-DSMC approach also has significant advantages over the parent VR DSMC implementation of Al-Mohssen and Hadjiconstantinou [1]; on the other hand, it models a lower fidelity approximation to collisional behavior. The VR DSMC
implementation requires additional averaging which introduces additional discretization error. VR-BGK-DSMC and (VR)$^2$-BGK-DSMC, on the other hand, define the weights during the collision routine in a stable and unbiased manner.

As in VR DSMC, our method benefits from rigorous handling of the boundary conditions. In cases where the isothermal boundary condition is applicable, it can provide an additional algorithmic simplification and speed-up, over the more generalized rules. Of the general rules, the semi-analytically derived rule of Section 3.2.1 performs the best. The mass conservation derived rule, shows a bias based on the number of particles colliding with the wall. While this bias is significant at low numbers of particles, it vanishes with increasing number of particles. In general, using the semi-analytically derived rule should give unbiased results.

The principal difference between the two variants of variance-reduced BGK-DSMC (VR and (VR)$^2$) is that the latter uses variance-reduced properties for the measured local equilibrium to further reduce the statistical noise of the simulation. In VR-BGK-DSMC a complete and unmodified BGK-DSMC simulation runs in parallel with the variance-reduced simulation, but the modification in (VR)$^2$-BGK-DSMC does not preserve that feature; instead, the non-equilibrium simulation modeled by particles alone is slightly variance-reduced by using the lower variance estimators, and problems with random walks are eliminated. While both of these features are beneficial, the parallel particle simulation can no longer be used to estimate the gains of the variance reduced method over the standard method. Apart from that slight inconvenience, (VR)$^2$-BGK-DSMC maintains all of the beneficial features of VR-BGK-DSMC, which make both of these methods valuable tools for modeling gaseous flows (or other related physics) in the low-signal regime.
Appendix A

Discrete Representation of Distribution Functions

A.1 Drawing from a Distribution

At several points in the BGK-DSMC algorithm, particles must be drawn from an analytically defined distribution: to generate the initial conditions, to update after wall collision, and to update after particle-particle collisions. Aside from particle velocities normal to the wall after a wall collision, particle velocities are drawn from Gaussian distributions. This process relies on knowledge of the standard deviation, $\sigma$, of the distribution and its mean, $\mu$. If $N(0,1)$ is a standard normal random deviate, a random deviate velocity, $c_i$, from a gaussian with mean $\mu$ and standard deviation of $\sigma$ can be generated by noting that

$$c_i \sim \sigma N(0,1) + \mu = N(\mu_i, \sigma^2).$$  \hspace{1cm} (A.1)

For the velocity normal to the wall after a wall collision, the distribution is given by $\frac{2}{T_{\text{wall}}} c_\perp \exp \left( - \frac{c_\perp^2}{T_{\text{wall}}} \right)$; velocities from these distributions are generated using the following analytical transformation [4].

$$c_i \sim -T_{\text{wall}} \log (1 - U),$$  \hspace{1cm} (A.2)
where $U$ is a uniformly distributed random deviate.

### A.2 Biased Estimators

For the collision step in a particle simulation of the BGK collision operator, the collided particles are redrawn from a Maxwell-Boltzmann distribution with the same moments as the particles in that region. These are $M^0$, $M^1_0$, $M^1_1$, $M^2_1$, and $M^2$. Let the sample variance (the variance measured from the particle distribution) be defined as

$$S^2 = \frac{1}{3}(M^2_i - M^1_1 M^1_i), \quad (A.3)$$

where summation over $i$ is implied. The collided particle is then redrawn from a Maxwell-Boltzmann distribution with those properties.

$$c_i^{(j)} \sim SN(0, 1) + M^1_i \quad (A.4)$$

The sample variance of the velocities of the particles drawn from such a distribution can be found beginning with the definition of the variance

$$\text{var}(c_i) = \sigma^2 = E[(c_i)^2] - E[c_i]^2 \quad (A.5)$$

For an unbiased estimator, the expected value of the sample variance would be equal to the true variance. In this case, it will be seen that $S$ is not an unbiased estimator. First rewrite (A.3) in terms of the velocities $c$ and $u$ and take the expected value as

$$E[S^2] = \frac{1}{3} \left( \frac{1}{N} E \left[ \sum_{j=1}^{N} (c_i^{(j)})^2 \right] - E[u_i^2] \right). \quad (A.6)$$

By linearity of expectation and considering each particle as an independent random variable, the summation is eliminated.

$$E[S^2] = \frac{1}{3} \left( E[c_i^2] - E[u_i^2] \right) \quad (A.7)$$
Using the definition of the variance.

\[ E[S^2] = \frac{1}{3} \left( \text{var}(c_i) + E[c_i]^2 - \text{var}(u_i) - E[u_i]^2 \right) \]  \hspace{1cm} (A.8)

The two expectation terms \( E[c_i]^2 \) and \( E[u_i]^2 \) are equal, and by the central limit theorem \( \text{var}(u_i) = \frac{1}{N} \text{var}(c_i) \).

\[ E[S^2] = \frac{1}{3} \left( \text{var}(c_i) - \frac{1}{N} \text{var}(c_i) \right) = \frac{N - 1}{N} \sigma^2 \]  \hspace{1cm} (A.9)

So when measuring the variance use the corrected formula

\[ S^2 = \frac{N}{N - 1} S^2 \]  \hspace{1cm} (A.10)

However, this only applies when using the standard estimator for properties (no variance reduction). Variance reduction makes the variance of the mean velocity \( u_i \) vanishingly small and the variance (or temperature, or shear, etc.) is, to a good approximation, an unbiased estimator.
Bibliography


