Variance-Reduced Direct Simulation Monte Carlo with the Bhatnagar-Gross-Krook Collision Operator

C. D. Landon and N. G. Hadjiconstantinou

Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, 02139, USA

Abstract. Direct Simulation Monte Carlo (DSMC) is perhaps the most prevalent stochastic method for simulating rarefied gas flows. High-signal flows (e.g. Mach number greater than 0.1) are efficiently resolved using DSMC; but low-signal flows require drastically increased statistical sampling. To address this limitation, Al-Mohssen and Hadjiconstantinou [1] presented a variance-reduced DSMC algorithm that dramatically improves the signal-to-noise ratio of low-signal flows. This variance reduction is achieved by exploiting a nearby, analytically-known equilibrium using importance weights. The weights are updated according to rules derived from the Boltzmann equation.

The Bhatnagar-Gross-Krook (BGK) collision operator is a simplistic approximation of the collision term in the Boltzmann equation that is useful in a number of fields involving particle-mediated transport. In this work, we show that the BGK collision operator lends itself naturally to the application of variance reduction using weights by allowing the derivation of weight-update rules from first principles. This feature removes the instabilities introduced by more complex collision rules and produces a stable variance-reduced particle method. We validate the method by comparing to analytic solutions and numerical results from other BGK particle methods.

Keywords: Variance reduction, Monte Carlo methods, Boltzmann equation, DSMC, BGK Operator
PACS: 05.10.Ln, 51.10.+y, 47.45.-n

INTRODUCTION

Over the past forty years, direct simulation Monte Carlo (DSMC) has been used to simulate the Boltzmann transport equation for dilute gases. DSMC efficiently generates samples of the velocity distribution function from which properties are statistically sampled. Typical of Monte Carlo methods, DSMC property estimators have variance, σ^2, that is inversely proportional to the number of samples.

Fractional error (standard deviation over signal strength) is a more direct measure of the signal-obscuring noise in the simulation. Hadjiconstantinou et al [2] showed that fractional error scales inversely with the signal strength and the square root of the number of samples. For example, the fractional error in flow velocity is given by $E_u \propto \left(\sqrt{MN}Ma\right)^{-1}$, where N is the number of particles, and M is the number of ensembles. As the Mach number, Ma, decreases, the number of samples must increase drastically to maintain an acceptable signal-to-noise ratio. This scaling requirement is particularly detrimental when considering flows in small-scale devices that are inherently low-signal.

Variance reduction methods have been developed to address this problematic scaling requirement [1, 3, 4, 5]. These methods exploit a nearby equilibrium to concentrate computational effort on the deviation from equilibrium. Of these methods, only the Al-Mohssen and Hadjiconstantinou approach (VR DSMC) [1] achieves variance reduction without altering the DSMC code. The key to this minimally invasive method is to simulate the reference equilibrium using importance weights. These weights are updated according to rules derived from the Boltzmann equation and require relatively few lines of code to implement. Unfortunately, VR DSMC has a numerical instability, similar to the other variance-reduced methods for dilute gases [3, 4]; fortunately, in the VR DSMC method this can be overcome [1] using kernel density estimation. The other alternative is to use the stable LVDSMC method of Homolle and Hadjiconstantinou [5, 6], which has recently been extended to the VHS model in [7].

An alternative approach that eliminates the problematic instability of VR DSMC is to utilize a simpler collision operator such as the Bhatnagar-Gross-Krook (BGK) approximation [8]. The BGK operator approximates the effect of collisions on the particle distribution function, $f(\mathbf{x},\mathbf{c},t)$, as a relaxation towards the local equilibrium distribution function, $f^{\mathrm{loc}}(\mathbf{x},\mathbf{c},t)$. This form of the collision operator has also been exploited to improve the numerical behavior of

other variance-reduced rarefied gas simulations [6, 9], albeit at the cost of an incorrect Prandtl number.[1]

This work presents a direct simulation Monte Carlo method for simulating the BGK-Boltzmann equation that incorporates the Al-Mohssen and Hadjiconstantinou [1] variance reduction methodology of importance weights. The new method, $(\mathrm{VR})^2$-BGK-DSMC, is stable and virtually eliminates random walks present in previous BGK particle formulations [12, 13, 14] due to statistical noise.

DIRECT SIMULATION OF THE BOLTZMANN EQUATION WITH THE BGK OPERATOR

Direct Monte Carlo simulation of the BGK operator has been the subject of a number of previous papers [12, 13, 14]. Although our own version, BGK-DSMC, is less complete than the BGK methods referenced (it does not directly address conservation problems associated with particle BGK methods), when coupled with variance reduction, it vastly outperforms its non-variance-reduced predecessors.

The Boltzmann equation that is simulated by these methods (with the BGK operator) is given by [10]:

$$\frac{\partial f}{\partial t}+\mathbf{c}\cdot\frac{\partial f}{\partial \mathbf{x}}+\mathbf{F}\cdot\frac{\partial f}{\partial \mathbf{c}}=\nu\Big(f^{\mathrm{loc}}(\mathbf{x},\mathbf{c},t)-f(\mathbf{x},\mathbf{c},t)\Big), \tag{1}$$

where ν is the collision frequency. The local equilibrium distribution, f^{loc}, is a Maxwell-Boltzmann distribution,

$$f^{\mathrm{MB}}(\mathbf{c};n,\mathbf{u},T)=\frac{n}{(2\pi RT)^{3/2}}\exp\left(-\frac{||\mathbf{c}-\mathbf{u}||^2}{2RT}\right), \tag{2}$$

with properties $n(\mathbf{x},t)$, $\mathbf{u}(\mathbf{x},t)$, and $T(\mathbf{x},t)$ defined by the local average number density, flow velocity, and temperature, respectively, in the region around $\mathbf{x}$ at time t. The gas constant R is given by the ratio of the Boltzmann constant and the molecular mass, $R=k_{\mathrm{B}}/M_{\mathrm{m}}$.

In a particle simulation, the distribution function is represented with appropriately distributed computational particles. To recover flow properties (e.g. density, flow velocity, and temperature), moments of the distribution function are approximated by summing over all of the computational particles. Statistically sampling properties in this manner gives rise to the uncertainty associated with DSMC and all Monte Carlo methods.

CONTROL VARIATE VARIANCE REDUCTION IN BGK-DSMC

The method of control variates can significantly reduce the uncertainty associated with statistical sampling. In this method, two correlated simulations (one that simulates an analytically known distribution and one that simulates an unknown distribution) are run simultaneously. The statistically sampled properties of the known distribution can then be subtracted from the statistically sampled properties of the (non-equilibrium) distribution of interest, thereby removing much of the statistical noise. A low-variance estimate of a property is then constructed by adding back the analytical contribution of the known distribution.

For a DSMC-like simulation, the known distribution is chosen to be an equilibrium distribution, f^{eq}, which is usually a Maxwellian with properties n_0, $\mathbf{u}=\mathbf{0}$, and T_0. Using $\langle ...\rangle$ to denote an analytically evaluated integral, and $\bar{...}$ to indicate a statistically sampled value, a variance-reduced estimator of some arbitrary property, A, can be obtained [15] from

$$\bar{A}^{\mathrm{VR}}=\bar{A}-\beta(\bar{A}^{\mathrm{eq}}-\langle A\rangle^{\mathrm{eq}}), \tag{3}$$

where the parameter $\beta=\frac{cov(A,A^{\mathrm{eq}})}{var(A^{\mathrm{eq}})}$ optimizes the amount variance reduction and may be evaluated from the simulation data[2]. Typically, for small deviations from equilibrium, $\beta\approx 1$, and in such cases it is inefficient to calculate a more exact value [11].

---

[1] Methods exist to capture the correct Prandtl number dependence [10], and their application to the variance-reduced method presented hereafter is discussed elsewhere [11].

[2] These variance measures may be evaluated from the same particle samples, A_i, used to evaluate the average value $\bar{A}$.

Following Al-Mohssen and Hadjiconstantinou [1], the correlated equilibrium in DSMC can be simulated efficiently using importance weights, $W = W(\mathbf{x}, \mathbf{c}, t)$. In other words, instead of performing two separate simulations, we perform one simulation (non-equilibrium) and use a set of weights (one for each particle) to describe the equilibrium simulation. The weights are defined by

$$W = \frac{f^{\mathrm{eq}}}{f}, \tag{4}$$

which leads to estimators of the form

$$\bar{A}^{\mathrm{VR}} = \sum_i (1 - W_i) A_i + \langle A \rangle^{\mathrm{eq}}. \tag{5}$$

Standard DSMC methods evolve particle positions and velocities according to the Boltzmann equation. The variance-reduced algorithm proceeds identically, but also requires a prescription for the evolution of these particle weights. When the distribution of interest, f, and the equilibrium distribution are known analytically (i.e. the initial condition), the weights can be evaluated from Equation (4). Below we describe the evolution dynamics for the weights when the distribution is not known analytically.

BGK-DSMC AND (VR)^2-BGK-DSMC ALGORITHMS

Like DSMC, BGK-DSMC splits the evolution of the Boltzmann equation in two parts: advection and collision. The variance-reduced algorithm, (VR)^2-BGK-DSMC, leaves BGK-DSMC unaltered, and adds relatively few additional lines of code.

Advection

The advection step is defined by simple ballistic particle motion as governed by the left-hand side of the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{x}} + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{c}} = 0. \tag{6}$$

The well-known numerical integration of (6) is given by $\mathbf{c}' = \mathbf{c}(t + \delta t) = \mathbf{c}(t) + \mathbf{F}\delta t$, and $\mathbf{x}' = \mathbf{x}(t + \delta t) = \mathbf{x}(t) + \mathbf{c}(t)\,\delta t + \frac{1}{2}\mathbf{F}\delta t^2$. By considering the advection equation for an equilibrium distribution and $f^{\mathrm{eq}} = Wf$ we obtain

$$\frac{\partial Wf}{\partial t} + \mathbf{c}\frac{\partial Wf}{\partial \mathbf{x}} = 0, \tag{7}$$

from which it can be shown [11] that the weights must update according to

$$W' = W(\mathbf{x}, \mathbf{c}, t + \delta t) = \frac{f^{\mathrm{eq}}(\mathbf{c} + \mathbf{F}\delta t)}{f^{\mathrm{eq}}(\mathbf{c})} W(\mathbf{x}, \mathbf{c}, t). \tag{8}$$

In the absence of a body force, according to (8), the weights remain unchanged by the advection step.

Specular or toroidal boundaries also require no weight update. However, if a particle collides with a diffuse boundary, its velocity is redrawn from the flux distribution at the wall and again advected for the remainder of the time step (for details see [16]). In this case, the equilibrium and non-equilibrium distribution functions at the walls may be different. Applying conservation of mass at the wall and using (4) the weight of a particle after a wall collision can be shown [1] to be

$$W' = \left(\frac{T_{\mathrm{wall}}}{T_0}\right)^{\frac{1}{2}} \frac{f^{\mathrm{eq}}(\mathbf{c}')}{\tilde{f}^{\mathrm{wall}}(\mathbf{c}')} \frac{\sum W}{N}, \tag{9}$$

where $\tilde{f}(\mathbf{c}')$ is the normalized distribution function of particles emitted from the boundary (see for example [17]). The summation, $\sum W$, of pre-wall-collision weights is performed over the N particles that collide with the wall (or an area element of the wall). This term is calculated as a multiplicative constant that is applied at the end of the advection step. While other forms of the wall collision rules are available [1], Equation (9) is preferable for its generality and stability.

Collision

During the collision step, the non-equilibrium simulation integrates

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} = \nu\left(f^{\text{loc}} - f\right), \tag{10}$$

while the equilibrium simulation integrates

$$\left[\frac{\partial f^{\text{eq}}}{\partial t}\right]_{\text{coll}} = 0. \tag{11}$$

The solution of (10) shows that in a time step, δt, a fraction of the distribution function, f, is replaced by the local equilibrium, f^{loc}. This can be implemented by selecting the appropriate fraction of particles from the N_{cell} particles in the cell,

$$N_{\text{coll}} = N_{\text{cell}}\left(1 - \exp\left(-\delta t \nu\right)\right), \tag{12}$$

and by then redrawing their velocities from the local equilibrium distribution function.

Using Equations (4), (10), (11), and the chain rule, we obtain a differential equation for the weights

$$\left[\frac{\partial W}{\partial t}\right]_{\text{coll}} = \nu\left(1 - \frac{f^{\text{loc}}}{f}\right)W. \tag{13}$$

With a little algebra, (13) gives an equation that can be easily interpreted in a particle sense.

$$\left[\frac{\partial W}{\partial t}\right]_{\text{coll}} = \frac{f^{\text{loc}}}{f}\nu\left(\frac{f^{\text{eq}}}{f^{\text{loc}}} - W\right). \tag{14}$$

For small deviations from equilibrium, $\frac{f^{\text{loc}}}{f}$ is approximately unity and can be ignored. In this limit, (14) prescribes replacing a weight, W, with a new weight $\frac{f^{\text{eq}}}{f^{\text{loc}}}$ with rate ν. This can be conveniently implemented by assigning a new weight to each particle that is selected to undergo a "collision" (i.e. being redrawn from the local velocity distribution function)

$$W(\mathbf{c}') = W' = \frac{f^{\text{eq}}(\mathbf{c}')}{f^{\text{loc}}(\mathbf{c}')}. \tag{15}$$

Since both distribution functions (f^{eq} and f^{loc}) are known analytically, the weight is also calculated analytically. Particles that are not selected for collision require no update. This simple and intuitive procedure entirely eliminates the stability concerns that burden VR DSMC (the collision rules in VR DSMC magnify the statistical noise in the weights whereas these collision rules eliminate it).

When measuring the properties for the local equilibrium distribution, f^{loc}, it is convenient to use the variance-reduced properties (5). Using variance-reduced properties to drive the relaxation imparts an additional level of variance reduction which led to the name of the method, $(\text{VR})^2$-BGK-DSMC. Additionally, BGK-DSMC is not conservative due to random walks in local property estimators that arise from statistical noise. By reducing the statistical noise in the estimators, we also mitigate the random walk and the subsequent loss of conservation. The remaining noise in the variance-reduced estimators still may cause loss of conservation at long times, but typically for low-signal flows in the transitional regime, noticeable errors only occur well after steady state and do not interfere with the variance-reduced simulation.

RESULTS

Like related variance-reduced methods, $(\text{VR})^2$-BGK-DSMC vastly outperforms its non-variance-reduced counterpart, particularly in the limit of weak signals. Figure 1 shows the fractional variance (variance over signal strength squared) vs. the dimensionless signal for a simple shear flow. Both methods (BGK-DSMC and $(\text{VR})^2$-BGK-DSMC) were run with the same number of samples, which was chosen to be sufficiently large to avoid conservation concerns in BGK-DSMC. The additional computation per sample for the variance-reduced method is small (i.e. $\mathcal{O}(1)$), so Figure 1 corresponds to the computational cost for a fixed level of fractional variance. As can be seen from Figure

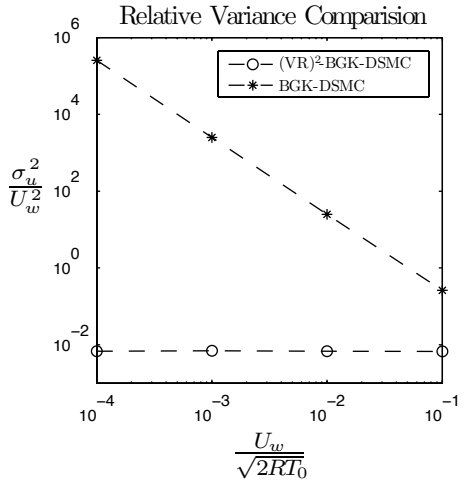

FIGURE 1. Comparison of relative variance for a constant number of samples. The computational cost per sample is essentially constant across methods, so this plot directly corresponds to computational cost for a fixed uncertainty. The variance-reduced method efficiently simulates flows with arbitrarily small signals.

1, the computational cost of the variance-reduced method is independent of signal strength, which enables efficient simulation of arbitrarily low signal flows. BGK-DSMC becomes extremely inefficient in the same regime.

Figure 2 shows results from two simple validation problems: a linearized, pressure-driven flow between parallel plates, and a temperature jump across a channel. (VR)^2-BGK-DSMC shows good agreement with tabulated exact solutions [18] and with results from a related variance-reduced method [19].

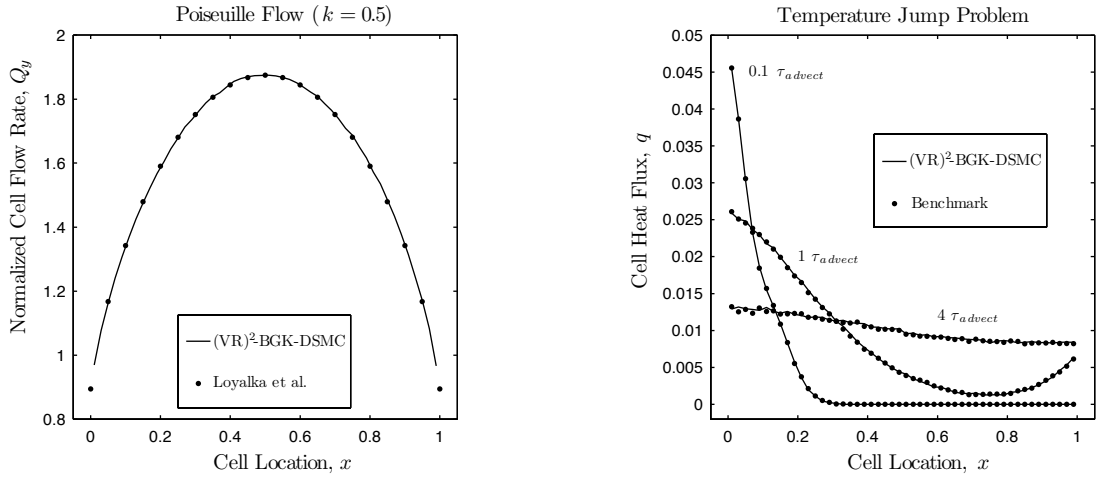

FIGURE 2. (VR)^2-BGK-DSMC is validated against known benchmarks. For a pressure driven flow at Knudsen number, $k = \frac{\sqrt{\pi}}{2} Kn = .5$ (left), the normalized flow rate, $Q_y = \frac{2u_y}{\kappa}$, is compared to tabulated exact results [18]; for a temperature jump problem (right) the benchmark is a related variance-reduced code [19]. In both cases, (VR)^2-BGK-DSMC agrees well with the benchmark.

CONCLUSION

A new variance-reduced method for simulating the Boltzmann equation with the BGK collision operator, (VR)^2-BGK-DSMC, is presented. The variance reduction makes this method capable of efficiently resolving flows with arbitrarily

small deviations from equilibrium. Use of the BGK approximation results in an unconditionally stable formulation, with no special treatment. Perhaps most appealing, the $(VR)^2$-BGK-DSMC method is based on the Al-Mohssen and Hadjiconstantinou [1] variance reduction method, so it preserves the underlying non-variance-reduced code and can be easily incorporated into existing code with minimal additions. This feature should be particularly appealing when extending the method to particle mediated transport problems that use the relaxation time approximation for electron, phonon, and radiative transport.

ACKNOWLEDGMENTS

Colin Landon gratefully acknowledges support from a DoD, Air Force Office of Scientific Research, National Defense Science and Engineering Graduate (NDSEG) Fellowship, 32 CFR 168a.

REFERENCES

1. H. A. Al-Mohssen, and N. G. Hadjiconstantinou, *Math. Model. Num. Anal.,* **44**, 1069–1083 (2010).
2. N. G. Hadjiconstantinou, A. L. Garcia, M. Z. Bazant, and G. He, *J. Comp. Phys.* **187**, 274–297 (2003).
3. L. L. Baker, and N. G. Hadjiconstantinou, *J. Comp. Theo. Nanoscience* **5**, 165–174 (2008).
4. J. Chun, and D. L. Koch, *Phys. Fluids* **17**, 107107 (2005).
5. T. M. M. Homolle, and N. G. Hadjiconstantinou, *J. Comp. Phys.* **226**, 2341–2358 (2007).
6. G. A. Radtke, and N. G. Hadjiconstantinou, *Phys. Rev. E* **79**, 056711 (2009).
7. G. A. Radtke, N. G. Hadjiconstantinou, and W. Wagner, "Low Variance Particle Simulations of the Boltzmann Transport Equation for the Variable Hard Sphere Collision Model," in *Proc.* 27^{th} *Intl. Symp. Rarefied Gas Dynamics*, AIP, Pacific Grove, Ca, 2010, in press.
8. P. L. Bhatnagar, E. P. Gross, and M. Krook, *Phys. Rev.* **94**, 511–525 (1954).
9. S. Ramanathan, and D. L. Koch, *Phys. Fluids* **21**, 033103 (2009).
10. C. Cercignani, *The Boltzmann Equation and its Applications*, Springer Verlag, New York, 1988.
11. C. D. Landon, *Weighted Particle Variance Reduction of Direct Simulation Monte Carlo for the Bhatnagar-Gross-Krook Collision Operator*, Master's thesis, Massachusetts Institute of Technology, Cambridge, Massachusetts (2010).
12. M. Lee, J. W. Dufty, J. M. Montanero, A. Santos, and J. F. Lutsko, *Phys. Rev. Lett.* **76**, 2702 (1996).
13. M. A. Gallis, and J. R. Torczynski, "The Application of the BGK Model in Particle Simulations," in *Proc.* 34^{th} *AIAA Thermophysics Conf.*, AIAA, Denver, CO, 2000.
14. M. N. Macrossan, "A particle simulation method for the BGK equation," in *Proc.* 22^{nd} *Intl. Symp. Rarefied Gas Dynamics*, edited by T. J. Bartel, and M. A. Gallis, AIP, Sydney, Australia, 2001, pp. 426–433.
15. S. Asmussen, and P. W. Glynn, *Stochastic Simulation: Algorithms and Analysis*, Springer, New York, 2007.
16. F. J. Alexander, and A. L. Garcia, *Comput. Phys.* **11**, 588–593 (1997).
17. Y. Sone, *Molecular Gas Dynamics: Theory, Techniques, and Applications*, Birkhauser, Boston, 2007.
18. S. K. Loyalka, N. Petrellis, and T. S. Storvick, *Zeitschrift Angewandte Mathematik und Physik* **30**, 514–521 (1979).
19. N. G. Hadjiconstantinou, G. A. Radtke, and L. L. Baker, *J. Heat Transfer* **132**, 112401 (2010).