A Practical Variance Reduced DSMC Method

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Abstract. The goal of this work is to develop a practical method for simulating low-signal kinetic (and small-scale) gaseous flows. These flows have recently received renewed attention in connection with the design, manufacturing, and optimization of MEMS/NEMS devices operating in gaseous environments; they are typically described using the Boltzmann equation which is most efficiently solved using the direct simulation Monte Carlo (DSMC) method. DSMC is a simple and versatile simulation method which is very efficient in producing samples of the single particle distribution function used for estimating hydrodynamic properties. Unfortunately, in the case of low-speed flows the computational cost associated with reducing the statistical uncertainty of simulation outputs becomes overwhelming. We will present a variance reduction approach for reducing the statistical uncertainty associated with low-signal flows making their simulation not only possible but also efficient. Variance reduction is achieved using a control variate approach based on the observation that low-signal flows are typically close to an equilibrium state. As with previous variance reduction methods, significant variance reduction is achieved making the simulation of arbitrarily small deviations from equilibrium possible. However, in contrast to previous variance-reduction methods, the method proposed, which we will refer to as the VRDSMC method, is able to reduce the variance with virtually no modification to the standard DSMC algorithm. This is achieved by introducing an auxiliary equilibrium simulation which, via an importance weight formulation, uses the same particle data as the non-equilibrium (DSMC) calculation; subtracting the equilibrium from the non-equilibrium hydrodynamic fields drastically reduces the statistical uncertainty of the latter because the two fields are correlated. By retaining the basic DSMC formulation, in contrast to previous approaches, the VRDSMC approach combines ease of implementation with computational efficiency and the ability to simulate all molecular interaction models available within the DSMC formulation. The work presented here represents a substantial improvement from the work presented in the previous symposium in two important ways. First, the kernel density estimation stabilization scheme has been further refined to allow substantially less bias without dramatically affecting stability. The second major improvement is the use of local cell reference states when performing particle collisions which results in a substantial reduction in the number of particles per cell required for stability, especially for small Knudsen numbers. Our validation tests show that the proposed VRDSMC method provides considerable variance reduction for only a small increase in computational cost and approximation error compared to equivalent DSMC simulations. In other words, by addressing the major weakness associated with DSMC, VRDSMC is well suited to the solution of low-signal kinetic problems of practical interest.

Keywords: DSMC, variance reduction, microscale gas flow
PACS: 02.70.Ns Molecular Dynamics and Particle Methods, 05.10.Ln Monte Carlo Methods, 47.45.Ab Kinetic theory of gases

INTRODUCTION

The objective of this work is the development of efficient simulation tools for modeling low-signal, small-scale gaseous flows. In this paper, we build on the framework that we previously introduced [3, 1, 2] towards a method that is able to practically resolve low-signal flows of engineering interest. The method (which we will refer to as VRDSMC) is based on the general idea of variance reduction [8] and the observation [5] that the statistical uncertainty of non-equilibrium hydrodynamic fields can be significantly reduced by formulating the desired result as the difference between the non-equilibrium DSMC [4] simulation of interest and a *correlated* simulation of equilibrium.

The problem of rigorously simulating kinetic flows that are close to equilibrium is of practical value in the design and analysis of MEMS/NEMS applications [12]. DSMC is the most commonly used method for simulating kinetic flows but requires an impractically large number of samples to resolve flows that are close to equilibrium [18]. Boltzmann solution methods that can treat low-signal flows can be broadly grouped into PDE-type and particle-based approaches. PDE-type approaches attempt to numerically solve the governing equation [16, 14]. Particle methods, on the other hand, simulate the problem of interest using particles. The most complete particle method for low-signal flows until now has been LVDSMC [9, 10, 13] although other approaches [19, 11] have also been proposed.

LVDSMC is a deviational particle method that uses the Hilbert form of the hard-sphere collision integral to stabilize the particle simulation. Other researchers [6, 20] have been able to extend LVDSMC to other collision models to allow, for example, the simulation of VHS gases [6]. The method discussed in this paper is an alternative low-signal kinetic simulation method that is substantially simpler than LVDSMC and easier to extend to more complex gas models.

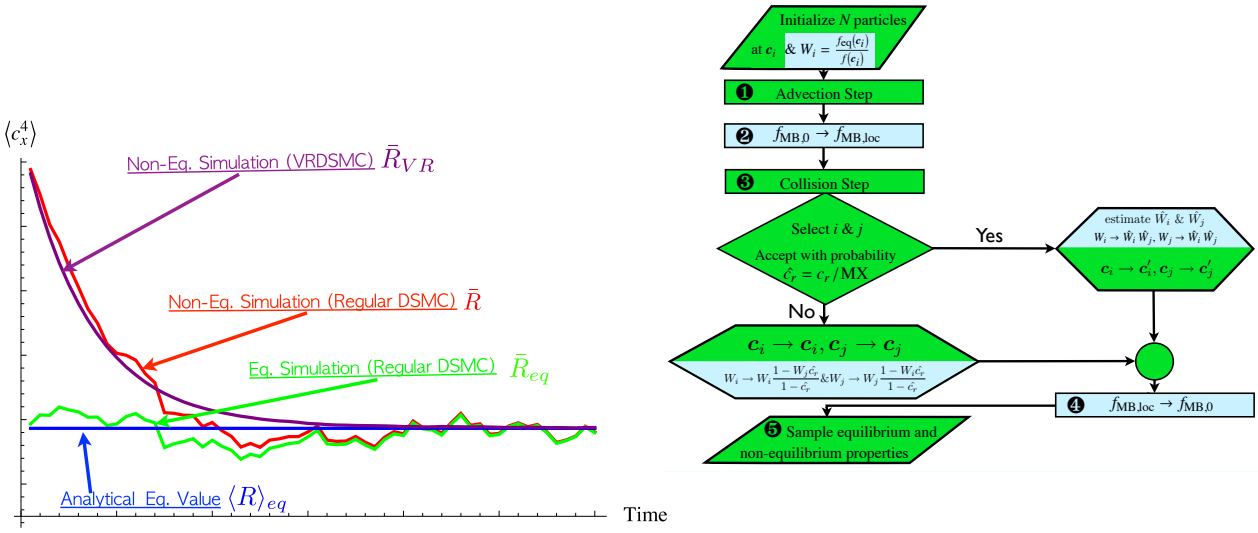

Figure 1. Left: a conceptual illustration of the VRDMSC approach to variance reduction. Right: the updated version of VRDSMC used in this paper and [1, 2].

In this paper we will present important updates on previous work [3, 1, 2] by introducing two important pieces that make VRDSMC substantially more robust. First, we will introduce the use of local reference states to reduce simulation bias and, secondly, we will present a more general method of deriving weight update rules. This updated version of VRDSMC still leaves DSMC *unaltered*, yet is able to practically resolve arbitrarily slow flows for a wide range of Knudsen numbers, making it attractive for many applications.

AN OVERVIEW OF VRDSMC

As introduced previously [1, 2, 3] and illustrated in Figure 1, VRDSMC achieves variance reduction with minimal modification to the original DSMC algorithm. The left side of the Figure shows the working principle: a variance reduced estimate of the property of interest $\bar{R}_{VR}$ is produced by replacing the equilibrium component of the property of interest $\bar{R}_{eq}$ (measured for the distribution $f_{eq}(c)$) with its expected value ($\langle R \rangle_{eq}$). Specifically, in VRDSMC the equilibrium property estimator is calculated using particle probability weight ratios W that describe the relative probability of an event happening in the equilibrium simulation (sampling distribution f_{eq}) given that it happened in the non-equilibrium simulation (sampling f). Specifically, for each particle i we have $W_i = f_{eq}(c_i)/f(c_i)$. If we take N samples of a property R the resulting estimator $\bar{R}_{VR} = \bar{R} - \bar{R}_{eq} + \langle R \rangle_{eq} = \frac{1}{N}\sum_{i=1}^{N}(1-W_i)R_i + \langle R \rangle_{eq}$ has substantially less variance than the regular DSMC estimator ($\bar{R} = \frac{1}{N}\sum_{i=1}^{N} R_i$) as long as the equilibrium and non-equilibrium simulations are correlated and $W_i - 1$ is small.

In order for the variance-reduced simulation to proceed, we need to devise a method of updating the probability ratio weights as the simulation proceeds. It was previously shown [3, 2] that starting directly from the collision term of the Boltzmann equation

$$\left[\frac{\partial f_{eq}}{\partial t}\right]_{\text{Coll}} = \frac{1}{2}\iiint (\delta_1' + \delta_2' - \delta_1 - \delta_2) W_1 W_2 f_1 f_2 c_r \sigma d\Omega dc_1 dc_2 \tag{1}$$

we can find that for collision candidates i and j the weight update rules are

Accepted Particles	Rejected Particles
$W_i \rightarrow W_i W_j$ and $W_j \rightarrow W_i W_j$	$W_i \rightarrow W_i \frac{1-W_j\hat{c}_r}{1-\hat{c}_r}$ and $W_j \rightarrow W_j \frac{1-W_i\hat{c}_r}{1-\hat{c}_r}$

where $\hat{c}_r = c_r/MX$ is the collision probability for some appropriately chosen upper bound MX. An alternative approach for deriving these evolution rules is discussed below.

As discussed previously, these relations are correct on average but produce numerically unstable simulations in the collision-dominated limit, a limitation that we were able to remove by using Kernel Density Estimation(KDE). We have found that weights reconstructed using KDE with kernels of width $\varepsilon c_0 = \varepsilon\sqrt{2kT_0/m}$ produce stable calculations but introduce bias in the simulation that is proportional to ε. From our experimentation we have found that applying the KDE step only to particles that are accepted for scattering provides the best trade-off between stability and bias.

In the end, due to the stability-bias tradeoff caused by KDE, stable *and* accurate simulations may require a larger number of particles in a cell (N_{cell}) than regular DSMC as $Kn \to 0$; here Kn is the Knudsen number, defined as the ratio of the molecular mean free path to the characteristic flow lengthscale. The final VRDSMC algorithm is summarized in the flow diagram on the right of Figure 1, including the change of reference state that is discussed below.

Bias Reduction using Local Reference States

Although it seems to be impossible to eliminate the bias introduced by KDE [17], this bias can be substantially reduced by judiciously choosing how the reconstruction is applied. Specifically, we found that induced bias can be substantially reduced by performing the collision step with weights referred to a local equilibrium reference state ($f_{MB,loc}$) instead of a global reference equilibrium state ($f_{eq,0}$) that is common across the computational domain.

Our approach is to temporarily modify the reference equilibrium state into a local (cell-based) Maxwell-Boltzmann distribution since the reminder of the formulation (e.g. boundary conditions and advection) is most easily dealt with based on the global state. To do this for each particle i, we can use the relations $W_i' = \gamma_i W_i$ and $W_i' = \gamma_i^{-1} W_i$ to switch between the $f_{MB,loc}$ and $f_{eq,0}$ reference states where $\gamma_i = \frac{f_{MB,loc}(c_i)}{f_{eq,0}(c_i)}$. The parameters that specify $f_{MB,loc}(c)$ are determined by the instantaneously measured density, velocity and temperature of each cell.

AN ALTERNATIVE APPROACH TO WEIGHT UPDATE RULES

We explore here an alternative approach to deriving the weight update rules based on conditional probability arguments. This approach is more general and allows the derivation of rules for other collision models and boundary conditions more directly and intuitively. To proceed, let us consider the simulation of two homogeneous systems with N_{cell} simulation particles; *both* start from the same initial conditions and obey the following dynamics:

1. Simulation A: each simulation particle represents N_{Eff} physical particles. After each timestep, the velocity of every particle i is updated from c_i to c_i' with probability $P_{A:c_i\to c_i'}$ and in general, c_i' may or may not be identical to c_i.
2. Simulation B: In contrast to Simulation A, each particle i represents $W_i N_{Eff}$ physical particles and $P_{B:c_i\to c_i'}$ is defined similarly to $P_{A:c_i\to c_i'}$, but captures the transition probabilities for Simulation B.

As discussed above, our variance reduction procedure requires that both simulations to stay correlated at all times. This can be done by integrating both simulations "synchronously"; updating the velocities of both simulations according to the transition probabilities of Simulation A but using weights that allow the representation of Simulation B. Consequently, at time t' the weights W_i' are modified to ensure that they are still representing Simulation B. Given there are N_{c_i} particles with velocity c_i in Simulation A at time=t, there will be $N_{Eff}P_{A:c_i\to c_i'}N_{c_i}$ actual particles landing at c_i' at time=t'. Likewise, in Simulation B the number of actual particles landing at c_i' should be $W_i N_{Eff} P_{B:c_i\to c_i'} N_{c_i}$ when time=t'. By taking $W_i' = W_i \frac{P_{B:c_i\to c_i'}}{P_{A:c_i\to c_i'}}$ we can keep both simulations in-step since this relation satisfies both Simulations A and B *on average*. This relation can be used as the primary relation for finding weight update rules used in a variety of physical phenomena, such as advection, particle collisions, wall interactions, etc. For the purposes of VRDSMC, identifying the non-equilibrium simulation with Simulation A and the equilibrium simulation with Simulation B yields

$$W_i' = W_i \frac{P_{eq:c_i\to c_i'}}{P_{c_i\to c_i'}} \tag{2}$$

where $P_{c_i \to c_i'}$ and $P_{eq:c_i \to c_i'}$ are the transition probabilities from c_i to c_i' for the non-equilibrium and equilibrium simulations, respectively. Particle-particle collisions are discussed in the next section; a discussion of advection and particle-wall interactions can be found in [2, 1].

Collision Transition Probabilities for Hard-Sphere Collisions

The collision step in DSMC is based on an acceptance-rejection procedure that selects a certain number of candidate particle pairs and either accepts them for scattering with probability $P_{c_i \to c_i} = \hat{c}_r$ or rejects them without modifying their velocities [4]. The scattering probability of the equilibrium simulation can be found by considering $N_{Eff} W_i$ real particles of class c_i in a cell and $N_{Eff} W_j$ particles of class c_j in the same cell. The average number of collisions between the two classes is $N_{Eff}^2 W_i W_j c_r \sigma \frac{\Delta t}{2V}$ and so *each simulation particle* of class c_i will have on average $N_{Eff} W_j c_r \sigma \frac{\Delta t}{2V}$ collisions. Keeping the same number of collision candidates as DSMC requires $N_{Eff} N_{cell} (N_{cell} - 1) MX \sigma \frac{\Delta t}{2V}$ candidates to sample the particle-particle collisions between all classes, and thus requires that the collision probability be $P_{eq:c_i \to c_i'} = \frac{W_j c_r}{MX}$ with $MX = \max_{i,j \in cell} W_i c_r$. Using this and (2), the update weight rule for accepted particles in hard-sphere VRDSMC is

$$W_i' = W_i \frac{P_{eq:c_i \to c_i'}}{P_{c_i \to c_i'}} = W_i W_j \tag{3}$$

while for the rejected particles

$$W_i' = W_i \frac{P_{eq:c_i \to c_i' = c_i}}{P_{c_i \to c_i' = c_i}} = W_i \frac{1 - P_{eq:c_i \to c_i'}}{1 - P_{c_i \to c_i'}} = W_i \frac{1 - W_j c_r / MX}{1 - c_r / MX} \tag{4}$$

as shown above.

The key advantage of this formulation compared to the previously presented one is that it can be extended to many other collision models since it does not explicitly use the analytical form of the hard-sphere collision integral.

VRDSMC ALGORITHM

In summary, the VRDSMC algorithm can be summarized as follows:

1. **Advection Step:** positions of particles are updated normally. ie. $x_i \to x_i + \Delta t c_i$. Wall interactions are handled identically as DSMC but with particle weights assigned based on the reference global equilibrium distribution $W_i = \frac{f_{eq,0}(c_i)}{f(c_i)}$.
2. **Weight Adjustment to local Reference State:** weights are updated so that they refer to the local reference distribution $f_{MB,loc}$.
3. **Collision Step:** candidates are chosen and accepted in a manner that is identical to DSMC but for
   (a) Accepted particles: KDE is used to estimate the local particles weights $\hat{W}_i$ and $\hat{W}_j$ before scattering, weights are then updated using (3).
   (b) Rejected particles: weights are updated according to (4) with particle velocities kept unchanged.
4. **Weight Adjustment to Global Reference State:** reverse of Step 2.
5. **Sampling:** sample cell properties using the modified variance reduced estimators [2, 1].

VRDSMC VERIFICATION AND PERFORMANCE

VRDSMC has been extensively verified over a large number of 1D kinetic flow problems in both transient and steady state cases and shown to be able to resolve arbitrarily low-signal flows over a large range of Knudsen numbers [2, 1]. As discussed before, more stable calculations require a larger number of particles per cell (N_{cell}) for a fixed KDE averaging radius ε; at the same time, bias only disappears as $\varepsilon \to 0$. The introduction of local reference states can

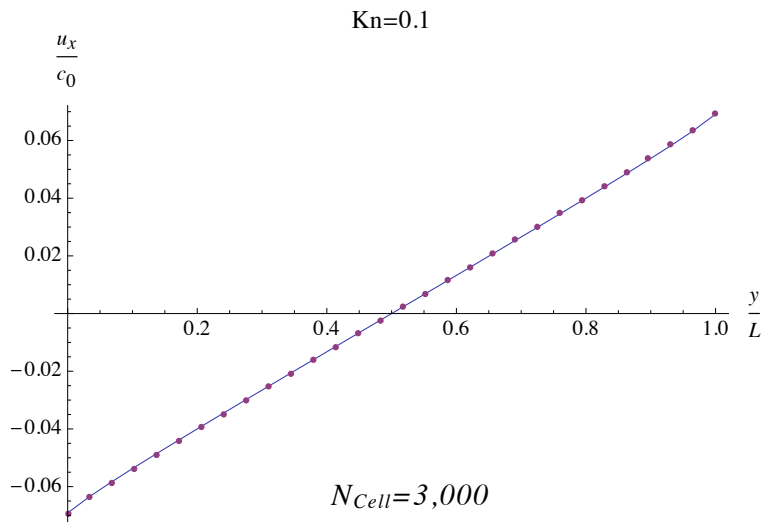

Figure 2. VRDSMC simulation of 1D Couette flow (solid line) compared to DSMC (points). The difference is less than 1% with $3,000$ particles per cell; in contrast, $\sim 50,000$ particles per cell are needed if we use a single global reference state.

substantially reduce N_{cell} required for a stable and accurate calculation, especially for small Kn, as illustrated in Figure 2 for the case of a 1D Couette flow with $Kn = 0.1$.

Figure 3 shows excellent agreement between VRDSMC and DSMC for the case of a transient simulation of a 1D gas layer whose boundaries' temperatures are suddenly changed.

SUMMARY AND CONCLUSIONS

In this paper we discussed VRDSMC, a practical variance-reduced method that is based on DSMC and is able to resolve arbitrary low-signal kinetic flows. There are three main ingredients to this method: The first is the use of particle weights to relate the DSMC simulation to a correlated simulation of equilibrium that is used to produce a variance reduced property estimator. The second ingredient is the use of KDE to stabilize the particle weights making it practical to use the method for steady state problems. The final ingredient of the method is the use of local equilibrium reference states which dramatically improves the method's efficiency, especially at low Knudsen numbers. We also presented an alternative approach to weight update rules that allows us to extend the method in a simple manner to more complex boundary conditions and collision models [1, 21].

Since the method is directly based on DSMC, we expect it to be accurate for a wide range of flow configurations, including transient flows, different initial conditions, etc. This has been confirmed by our tests in which VRDSMC has been shown to be able to reproduce DSMC results within engineering accuracy without substantially changing how the method scales with the number of particles. In fact, the only time VRDSMC may have a disadvantage compared to other VR methods is in extremely low Knudsen number flows where the large N_{cell} for a large number of cells may be a limitation. In conclusion, we recommend VRDSMC (along with LVDSMC) be considered seriously for any engineering-type, low-signal calculation.

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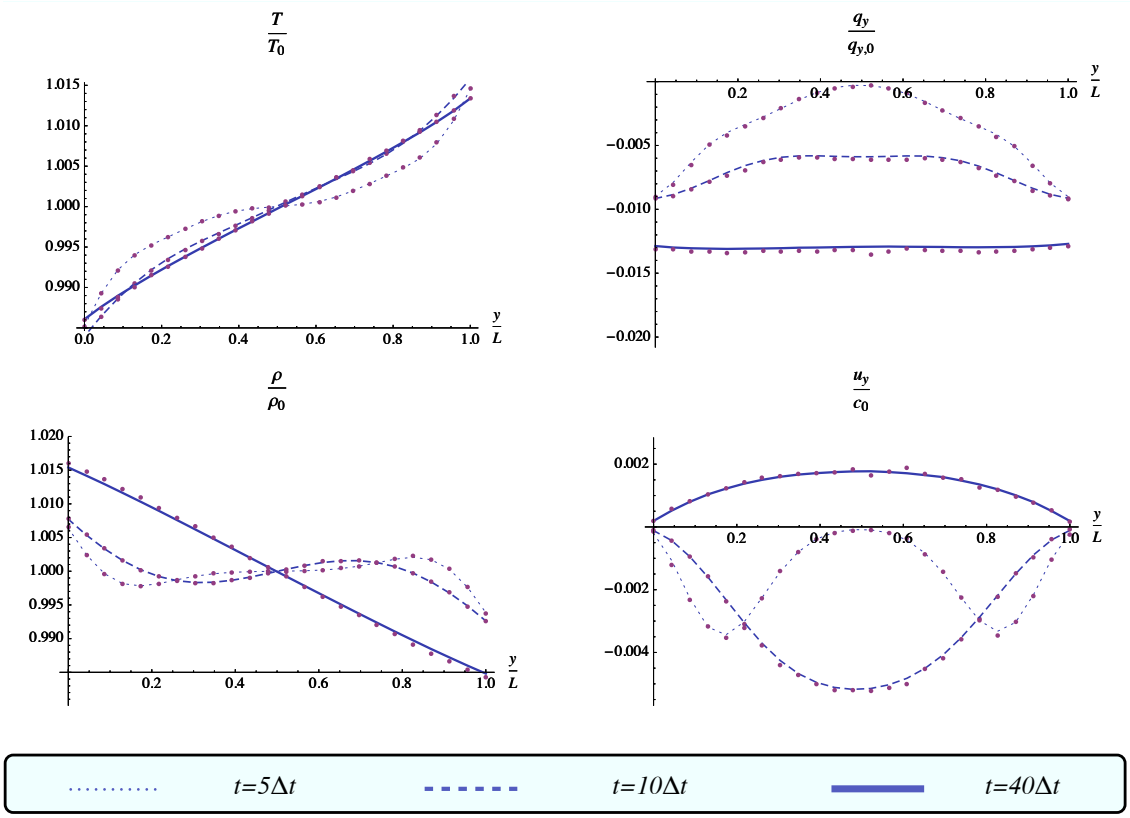

Figure 3. Transient results for an impulsive boundary temperature change problem for $Kn = 1.0$. Solid lines denote VRDSMC results with $N_{cell} = 500$; DSMC results are shown in dots. The snapshots shown correspond to $t = \{5, 10, 40\}\Delta t$ where $\Delta t = \frac{1}{24}\sqrt{\pi}\lambda/(2c_0)$.

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