Low Variance Particle Simulations of the Boltzmann Transport Equation for the Variable Hard Sphere Collision Model

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Abstract. We present and validate a variance reduced deviational particle method for simulating the Boltzmann transport equation for the variable hard sphere (VHS) collision operator. In comparison with the direct simulation Monte Carlo (DSMC) method, the proposed method is more suitable for simulating transport in regimes where the departure from equilibrium is small, such as dilute gas flows in small-scale devices (MEMS, NEMS). In fact, the proposed method has a constant signal-to-noise ratio in the limit of small departure from equilibrium, and is thus able to simulate arbitrarily small deviations from equilibrium. The approach developed herein combines the variable hard sphere collision algorithm developed by Wagner [1] with an efficient advection routine based on Ref. [2]. The resulting method is stable and highly efficient, and results in dramatically reduced statistical noise in regimes typical of transport in small-scale devices.

Keywords: Variance reduction, Monte Carlo methods, Boltzmann equation, DSMC
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INTRODUCTION

Current applications of kinetic gas flows–where the Navier-Stokes description no longer applies–have focused on transport in small scale (MEMS and NEMS) devices. These devices typically operate in regimes with small deviation from equilibrium, characterized by low flow speeds and small temperature gradients. This situation is in stark contrast to earlier applications such as high speed aerodynamics, which operate in highly nonequilibrium regimes. This distinction is an important consideration when selecting appropriate numerical techniques to simulate transport in these modern applications.

The standard method for simulating kinetic flows is a particle method known as the direct simulation Monte Carlo (DSMC) method. Using equilibrium statistical mechanics, Hadjiconstantinou et. al. [3] derived expressions for the relative statistical error in the hydrodynamic properties for the DSMC and similar particle methods. For example, for small departures from equilibrium, the relative error in temperature in a monoatomic gas, is given by

$$\frac{\sigma_T}{\Delta T} = \frac{1}{\sqrt{MN}} \frac{\sqrt{2/3}}{\Delta T/T_0}; \tag{1}$$

In the above expression, σ_T is the standard deviation in temperature due to statistical fluctuations, M is the number of independent statistical ensembles, N is the number of particles per cell, ΔT is the temperature scale, and T_0 is the reference temperature. For small departure from equilibrium ($\Delta T/T_0 \ll 1$), very large values of MN are required to achieve low statistical uncertainty. Similar limitations exist for all hydrodynamic properties. Since computational cost scales with MN, DSMC and similar methods become unsuitable for simulations close to equilibrium conditions.

The inability of the DSMC method to efficiently simulate kinetic flows with small departure from equilibrium has led to the development of alternative particle methods exhibiting significantly reduced variance, leading to dramatically enhanced efficiency in these regimes. Deviational particle methods, including the method in this paper, achieve variance reduction by simulating only the difference between the velocity distribution and an underlying equilibrium distribution, resulting in a constant signal-to-noise ratio in the limit of small departure from equilibrium. This distribution can be chosen as a global (fixed), or a local (spatially-variable) equilibrium, and this choice influences the features of the resulting algorithm. This approach was first discussed by Baker and Hadjiconstantinou [4], and the resulting particle method [5, 6] was able to produce valid solutions to the Boltzmann transport equation, though requiring a particle cancellation scheme for stability.

The low-variance deviational particle Monte Carlo (LVDSMC) approach introduced by Homolle and Hadjiconstantinou [7, 8], achieved stability without resorting to a particle cancellation scheme by taking advantage of a special form of the collision integral. This first method [7, 8] simulated hard sphere collisions based on deviations from a spatially-variable equilibrium. Subsequent methods were developed for the Bhatnagar, Gross, and Krook (BGK) model including: a highly efficient linearized version based on deviation from a spatially variable equilibrium [2], as well as a simple nonlinear version [9] based on deviation from a fixed equilibrium. Recently, efficient computational algorithms for treating the more general variable hard sphere (VHS) collision operator were proposed by Wagner [1].

Different approaches for variance-reduced particle methods include the approach by Chun and Koch [10] which simulates linearized hard sphere collisions using weights; unfortunately, like the approach in Refs. [5, 6], this approach requireds a particle cancellation scheme for stability. More recently, the same approach was applied to the linearized BGK model [11], which does not require particle cancellation. A weight-based approach for variance reduction was recently introduced by Al-Mohssen and Hadjiconstantinou [12]; this formulation, known as VRDSMC, achieves variance reduction with minimal changes to the original DSMC algorithm.

In this paper, we combine the VHS collision algorithm developed by Wagner [1], with a highly efficient advection sampling routine based on ideas developed in Ref. [2]. The resulting method is stable and highly efficient, and results in dramatically reduced statistical noise in the typical transport regimes for small-scale devices. The paper is organized as follows: in the first section , the variance-reduced particle method is introduced; we consider the VHS collision and advection steps separately. In the second section, the method is validated using DSMC simulation results, and the computational efficiency is compared to DSMC for the case of heat transfer between parallel plates. Finally, the conclusion gives a summary and outlook.

VARIANCE-REDUCED PARTICLE METHOD

In this section, the LVDSMC method for simulating the VHS collision model [13] is developed, starting from the Boltzmann transport equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{c}\cdot\frac{\partial f}{\partial \boldsymbol{x}} + \boldsymbol{a}\cdot\frac{\partial f}{\partial \boldsymbol{c}} = \mathscr{Q}[f,f] \tag{2}$$

Here, f is the velocity distribution function, t is the time, $\boldsymbol{x}$ is the spatial coordinate, $\boldsymbol{c}$ is the particle velocity, and $\boldsymbol{a}$ is the body force per unit mass. The VHS collision operator is given by

$$\mathscr{Q}[f,g] = C_\beta \int_{\mathscr{S}^2} \mathrm{d}^2\boldsymbol{\Omega} \int_{\mathscr{R}^3} \mathrm{d}^3\boldsymbol{c}_* \, ||\boldsymbol{c}-\boldsymbol{c}_*||^\beta \left[f(\boldsymbol{c}')g(\boldsymbol{c}'_*) - f(\boldsymbol{c})g(\boldsymbol{c}_*)\right] \tag{3}$$

where $\boldsymbol{\Omega}$ is the spherical collision angle and primes denote post collision velocities. The constant prefactor is $C_\beta = \frac{1}{4} d_{\mathrm{ref}}^2 c_{\mathrm{r,ref}}^{2\omega-1}$ where $\omega = 1-\beta/2$ is the temperature coefficient of viscosity (i.e. $\mu \sim T^\omega$), d_{ref} is the reference diameter at the reference temperature T_{ref}, and $c_{\mathrm{r,ref}} = 4\sqrt{RT_{\mathrm{ref}}/\pi}$. The integration domains are the unit sphere ($\mathscr{S}^2$) and the entire velocity domain ($\mathscr{R}^3$) respectively.

In the deviational approach, we simulate only the deviation from equilibrium: $f^{\mathrm{d}} = f - f^0$. For this method, we have chosen a fixed equilibrium distribution parameterized by a constant number density n_0, velocity $\boldsymbol{u}_0$, and temperature T_0.

$$f^0 = \frac{n_0}{\pi^{3/2}c_0^3}\exp\left(-\frac{||\boldsymbol{c}-\boldsymbol{u}_0||^2}{c_0^2}\right), \qquad c_0 = \sqrt{2RT_0} \tag{4}$$

Typical of deviational particle methods, f^{d} is represented by deviational particles each having velocity, position, and sign $s \in \pm 1$.

$$f^d = W\sum_{k=1}^{N} s_k \delta^3(\boldsymbol{c}-\boldsymbol{c}_k)\delta^3(\boldsymbol{x}-\boldsymbol{x}_k) \tag{5}$$

Here, N is the total number of particles in the cell, and W is a (constant) weight, which is related to the number of simulated particles for every physical deviational particle in the cell.[1]

As with the DSMC method, the state of the gas is updated in separate collision and advection time steps (below), with characteristic time step Δt. This is followed by the calculation of cell-based hydrodynamic properties, which are evaluated from the current state of the gas by integrating the appropriate moments of f by using Eqn. (5).

VHS collision step

The key to the LVDSMC method is to take advantage of a special form of the collision operator in order to achieve stability by preventing uncontrolled growth in the number of simulated particles. By inserting $f = f^0 + f^{\mathrm{d}}$ into $\mathscr{Q}[f,f]$ (see Eq. (3)), we can split the collision operator into linear and nonlinear parts [14, 7, 8, 1], $\mathscr{Q}[f,f] = \mathscr{L}[f^{\mathrm{d}}] + \mathscr{Q}[f^{\mathrm{d}},f^{\mathrm{d}}]$, where $\mathscr{L}$ is the linear collision operator, which can be represented in terms of kernel functions $K_{1,2}$ and a particle deletion rate, as shown below [1].

$$\mathscr{L}[f^{\mathrm{d}}] = \int_{\mathscr{R}^3} \mathrm{d}^3\boldsymbol{c}_* [2K_1(\boldsymbol{c},\boldsymbol{c}_*) - K_2(\boldsymbol{c},\boldsymbol{c}_*)] f^{\mathrm{d}}(\boldsymbol{c}_*) - \nu f^{\mathrm{d}} \tag{6}$$

$$K_1(\boldsymbol{c},\boldsymbol{c}_*) = \frac{4C_\beta}{||\boldsymbol{c}-\boldsymbol{c}_*||} \int_{\Gamma_\perp(\boldsymbol{c}-\boldsymbol{c}_*)} \mathrm{d}^3\boldsymbol{\zeta}\, ||\boldsymbol{c}-\boldsymbol{c}_*-\boldsymbol{\zeta}||^{\beta-1} f^0(\boldsymbol{c}+\boldsymbol{\zeta}) \tag{7}$$

$$K_2(\boldsymbol{c},\boldsymbol{c}_*) = 4\pi C_\beta ||\boldsymbol{c}-\boldsymbol{c}_*||^\beta f^0 \tag{8}$$

$$\nu(\boldsymbol{c}) = 4\pi C_\beta \int_{\mathscr{R}^3} \mathrm{d}^3\boldsymbol{c}_* ||\boldsymbol{c}-\boldsymbol{c}_*||^\beta f^0(\boldsymbol{c}_*) \tag{9}$$

Here $\Gamma_\perp(\boldsymbol{c})$ is the plane normal to $\boldsymbol{c}$ passing through the origin. In the above formulation, the particle deletion step contributes to the stability of the LVDSMC approach by preventing an unchecked increase in the number of particles in the generation term. Sampling the entire particle creation step rather than processing the K_1 and K_2 terms seperately also contributes towards stability.

For the case of hard spheres ($\beta = 1$), the integrals K_1 and ν can be found analytically, leading to the LVDSMC approach for hard sphere collisions [7, 8, 1]. For VHS collisions, we follow the approach of Wagner [1], who simulates the linear collision operator as a series of Markov processes for particle creation and deletion. There exists a common bound on integrals of the kernel functions and the collision rate.

$$\int_{\mathscr{R}^3} \mathrm{d}^3\boldsymbol{c}\, K_{1,2}(\boldsymbol{c},\boldsymbol{c}_i) \le \psi(\boldsymbol{c}_i) \quad \text{and} \quad \nu(\boldsymbol{c}_i) \le \psi(\boldsymbol{c}_i) \tag{10}$$

$$\text{where} \quad \psi(\boldsymbol{c}_i) = 4\pi C_\beta c_0^\beta \left[(1-\beta) n_0 + \frac{\beta}{c_0} \int_{\mathscr{R}^3} \mathrm{d}^3\boldsymbol{c} ||\boldsymbol{c}-\boldsymbol{c}_i|| f^0(\boldsymbol{c}) \right] \tag{11}$$

The integral in Eq. (11) has a known analytical expression [1]. The collision events are processed as a series of random time steps sampled from an exponential distribution $\delta t \sim \lambda e^{-\lambda \delta t}$, until the overall time step Δt is exceeded; here, $\lambda = 4\sum_{i\in\mathscr{N}_j} \psi(\boldsymbol{c}_i)$ is the time step parameter and $\mathscr{N}_j$ is the set of particles contained in j^{th} cell.

For each random time step, trial events associated with the three terms of Eqn. (6) are processed: specifically, three events are considered: a creation event associated with the K_1 term occurs with probability $1/2$, a creation event associated with the K_2 term occurs with probability $1/4$, and a deletion event occurs with probability $1/4$. Each trial event is then accepted (by creating or deleting a particle) or rejected according to the appropriate criterion; the details can be found in [1]. This approach leads to a collision step with better time convergence properties than earlier LVDSMC approaches [7, 8].

The nonlinear part of the collision integral is sampled by performing collisions between deviational particles, as originally proposed by Baker and Hadjiconstantinou [5, 6]. This approach is identical to DSMC for collisions between

[1] The constant W is analogous to the number of simulated particles for every physical particle (N_{eff}) appearing in the DSMC formulation. Because there is a possibility of generating extraneous pairs of positive and negative particles in deviational particle methods which have no net effect on the state of the gas, W is not as precisely defined.

two positive particles, but for collisions involving negative particles it leads to a net increase of particles. As previously noted by Homolle and Hadjiconstantinou [7, 8], the resulting instability of the nonlinear part counteracts the stability of the linear part of the collision integral for large departures from equilibrium. However, for the linearized regime and the early nonlinear regime, the LVDSMC approach is significantly more efficient that the DSMC method.

Advection step

The advection step simulates the left hand side of the Boltzmann equation (2), where we neglect external forces ($\boldsymbol{a} = \mathbf{0}$) for simplicity. Inserting $f = f^0 + f^{\mathrm{d}}$ into (2) gives the advection equation, which shows that deviational particles advect identically to physical particles.

$$\frac{\partial f}{\partial t} + \boldsymbol{c} \cdot \frac{\partial f}{\partial \boldsymbol{x}} = \frac{\partial f^{\mathrm{d}}}{\partial t} + \boldsymbol{c} \cdot \frac{\partial f^{\mathrm{d}}}{\partial \boldsymbol{x}} = 0 \tag{12}$$

Thus particles are advected according to usual DSMC rule: $\{\boldsymbol{x}_k(t+\Delta t) = \boldsymbol{x}_k(t) + \boldsymbol{c}_k(t)\Delta t\}_{k \in \mathscr{N}}$ for each time step.

Boundary interactions, however, are processed differently than the DSMC method. In addition to reflecting escaping particles back into the simulation domain by sampling from the appropriate boundary distribution, additional particles must be generated at the boundary to account for the difference in fluxes between the equilibrium and boundary distributions [7, 8, 1]. Here, we will focus on diffuse reflections, although the more general Maxwell's accommodation model has been included in recent implementations [2, 9]. For diffuse reflections, the additional particle flux enforced by creating additional particles with velocities from a distribution proportional to $|F_{\mathrm{b}}(\boldsymbol{c})|$, with sign $\operatorname{sgn} F_{\mathrm{b}}(\boldsymbol{c})$, and advected back into the domain for the remainder of the time step. Here, $F_{\mathrm{b}}(\boldsymbol{c})$ is determined from the difference in flow per velocity element $\mathrm{d}^3\boldsymbol{c}$ on an element with normal surface area S_n.

$$S_n F_b \Delta t \, \mathrm{d}^3\boldsymbol{c} = S_n c_n \Delta t (f^{\mathrm{b}} - f^0) \, \mathrm{d}^3\boldsymbol{c}. \tag{13}$$

In Ref. [2], an efficient sampling method was developed for the linearized advection operator, based on the ratio-of-uniforms method [15]. In essence, this method samples from a transformed distribution $H(\boldsymbol{\xi})$ defined by $H = |F_{\mathrm{b}}|^{2/5}$ and $\boldsymbol{\xi} = H^{1/2}\boldsymbol{c}$. A key advantage of this approach is that all distributions are bounded: i.e.:

$$0 \le H \le a(f^0, f^{\mathrm{b}}) \tag{14}$$

$$|\xi_\ell| \le b_\ell(f^0, f^{\mathrm{b}}),\ \ell = 1,2,3. \tag{15}$$

Bounds were derived in Ref. [2] based on linearized conditions, which do not hold for nonlinear problems. We extend this approach by representing the bounds as $a(f^0, f^{\mathrm{b}}) = (1+\varepsilon)Aa^{\mathrm{L}}(f^0, f^{\mathrm{b}})$ and $b_\ell(f^0, f^{\mathrm{b}}) = (1+\varepsilon)B_\ell b_\ell^{\mathrm{L}}(f^0, f^{\mathrm{b}})$. Here $A \ge 1$ and $B_\ell \ge 1$ are parameters which track the ratio between current estimate of the ratios between nonlinear $\{a, b_\ell\}$ and linear $\{a^{\mathrm{L}}, b_\ell^{\mathrm{L}}\}$ bounds. The number $\varepsilon > 0$ causes the sampling routine to sample from an expanded domain (in $\{H, \boldsymbol{\xi}\}$), and when samples are accepted which exceed the estimated bounds $a(f^0, f^{\mathrm{b}}) = Aa^{\mathrm{L}}(f^0, f^{\mathrm{b}})$ and $b_\ell(f^0, f^{\mathrm{b}}) = B_\ell b_\ell^{\mathrm{L}}(f^0, f^{\mathrm{b}})$, factors A and B_ℓ are updated appropriately. This method will be documented in more detail in a future publication.

Time-splitting scheme

Higher order time convergence is achieved by using Strang's method for time integration, which introduces a symmetrized version of the ordinary DSMC algorithm. Specifically, for each time step there is an initial half advection step with time step $\Delta t/2$, a full collision step (Δt), another half advection step; after which the properties are sampled. This algorithm was shown to have second-order time convergence for the DSMC method in Ref. [16]. Since the LVDSMC method employs the same time splitting approach (between advection and collision steps) as the DSMC method, it was simple to implement Strang's method for the LVDSMC, as well as the DSMC method.

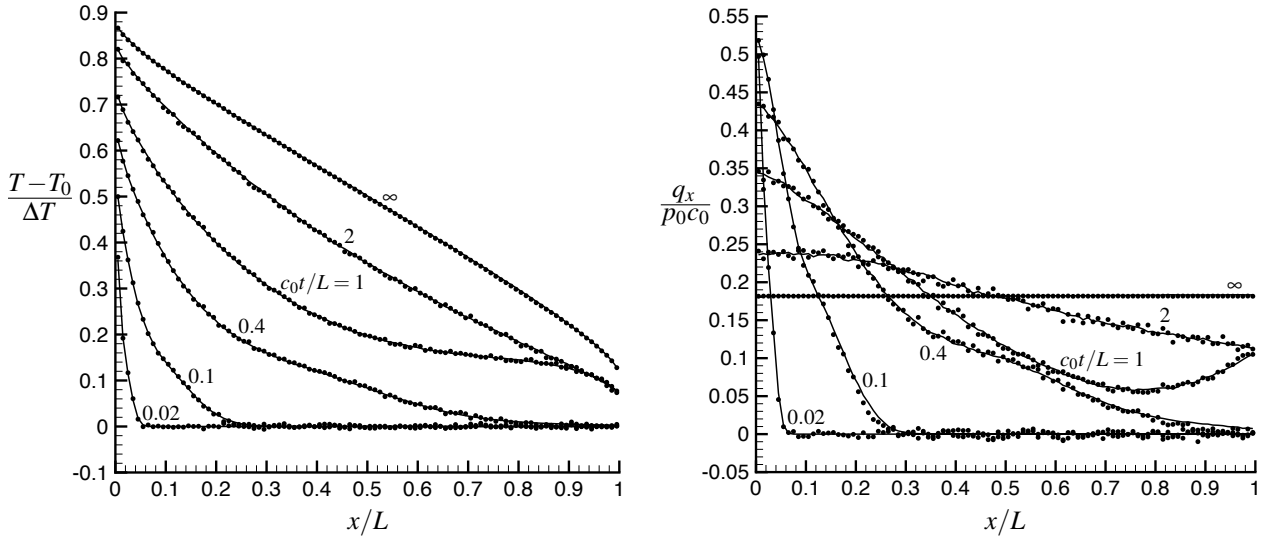

FIGURE 1. Transient temperature and heat flux profiles for $Kn = 0.1$, $\Delta T/T_0 = 0.1$.

VALIDATION

Validation was performed by comparing the results of the LVDSMC method with the standard DSMC method for the VHS collision operator. In this section, we show results from the heat transfer between two fully-accommodating parallel plates for argon gas ($\omega = 0.81$). The initial condition is a stationary gas at temperature T_0, and the boundary conditions are $T(x=0) = T_0$ and $T(x=L) = T_0 + \Delta T$. The transient response of the temperature and heat flux are shown in Figure 1 for $Kn = 0.1$, and $\Delta T/T_0 = 0.1$ for various time steps. Clearly, there is excellent agreement between the LVDSMC ($-$) and DSMC ($\bullet$) methods.

Variance reduction

Here, we compare the difference in efficiency between the two methods by comparing the square of their relative errors in temperature by measuring the variance of this quantity in two cells in the center of the simulation domain at steady state. Both methods used a single statistical ensemble and $N = 1000$ particles. Figure 2 plots $E^2_{\rm rel} = MN\sigma_T^2/\Delta T^2$ as a function of the departure from equilibrium $\Delta T/T_0$ for the DSMC method; simulations are shown as dots ($\bullet$) while the theoretical result (Eq. (1)) is shown in ($-$). Since the LVDSMC method involves added computational expense, we scale square of the relative statistical error by the ratio of the computational time taken to reach steady state for the LVDSMC method $t^{\rm CPU}_{\rm LVDSMC}$ to that for the DSMC method $t^{\rm CPU}_{\rm DSMC}$ at the same Kn. Thus, for the LVDSMC method we plot

$$E^2_{\rm rel} = MN \frac{t^{\rm CPU}_{\rm LVDSMC}}{t^{\rm CPU}_{\rm DSMC}} \frac{\sigma_T^2}{\Delta T^2} \tag{16}$$

for three different Knudsen numbers: $Kn = 0.1$ ($\blacklozenge$), $Kn = 1$ ($\blacktriangle$), and $Kn = 10$ ($\blacksquare$). This allows for a direct comparison of computatonal expense for both methods.

As is clear from Fig. 2, the LVDSMC method significantly outperforms the DSMC method for small deviations from equilibrium, with a constant level of statistical error in the limit of small deviation. In contrast, the DSMC method is very efficient in the highly nonlinear regime. Moreover, it can provide accurate solutions with significantly fewer particles per cell (e.g. $N = 100$). In contrast, the present LVDSMC algorithm is not strictly conservative. This can lead to random walks in the hydrodynamic variables when the number of particles per cell is low. A conservative LVDSMC algorithm is currently under development.

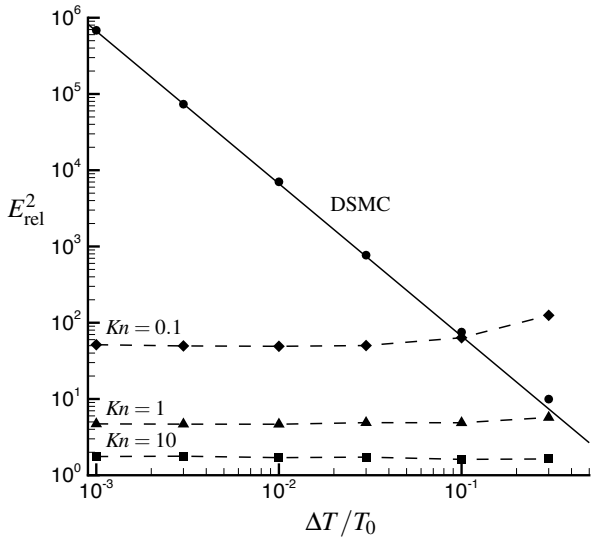

FIGURE 2. Efficiency of the LVDSMC method vs the DSMC method for the VHS collision operator.

CONCLUSION

We have presented an efficient, variance-reduced particle method capable of simulating the Boltzmann transport equation for VHS collisions with a significantly reduced level of statistical noise than the DSMC method for problems where the departure from equilibrium is small. This method combines the recently developed collision algorithms developed by Wagner [1] with an efficient advection routine which is a nonlinear version of the one introduced in Ref [2]. Development of this method is ongoing, and further details can be expected to appear in future publications.

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REFERENCES

1. W. Wagner, *Monte Carlo Methods Appl.* **14**, 191–268 (2008).
2. G. A. Radtke, and N. G. Hadjiconstantinou, *Phys. Rev. E* **79**, 056711 (2009).
3. N. G. Hadjiconstantinou, A. L. Garcia, M. Z. Bazant, and G. He, *J. Comp. Phys.* **187**, 274–297 (2003).
4. L. L. Baker, and N. G. Hadjiconstantinou, *Phys. Fluids* **17**, 051703 (2005).
5. L. L. Baker, and N. G. Hadjiconstantinou, "Variance reduction in particle methods for solving the Boltzmann equation," in *Proc.* 4^{th} *Intl. Conf. Nanochannels, Microchannels and Minichannels*, 2006, pp. 377–383.
6. L. L. Baker, and N. G. Hadjiconstantinou, *J. Comp. Theo. Nanoscience* **5**, 165–174 (2008).
7. T. M. M. Homolle, and N. G. Hadjiconstantinou, *Phys. Fluids* **19**, 041701 (2007).
8. T. M. M. Homolle, and N. G. Hadjiconstantinou, *J. Comp. Phys.* **226**, 2341–2358 (2007).
9. N. G. Hadjiconstantinou, G. A. Radtke, and L. L. Baker, *J. Heat Transfer* **accepted** (2010).
10. J. Chun, and D. L. Koch, *Phys. Fluids* **17**, 107107 (2005).
11. S. Ramanathan, and D. L. Koch, *Phys. Fluids* **21**, 033103 (2009).
12. H. A. Al-Mohssen, and N. G. Hadjiconstantinou, *Math. Model. Num. Anal.,* **in press** (2010).
13. G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Claredon Press, Oxford, 1994.
14. C. Cercignani, *The Boltzmann Equation and its Applications*, Springer Verlag, New York, 1988.
15. J. C. Wakefield, A. E. Gelfand, and A. F. M. Smith, *Stat. Comput.* **1**, 129–133 (1991).
16. D. J. Rader, M. A. Gallis, J. R. Torczynski, and W. Wagner, *Phys. Fluids* **18**, 077102 (2006).