

# Simulation of Plane Poiseuille Flow of a Rarefied Gas with an Extended Lattice Boltzmann Method

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**Abstract.** Several algorithmic extensions to the Lattice Boltzmann method (LBM) that permits its application to rarefied gas flows are presented. The accuracy of the new method is first demonstrated by validating the desired power-law viscosity-temperature relationship over the range of power-law exponents typically found in single component fluids. Next, the plane Poiseuille flow scenario is simulated for a series of Knudsen numbers,  $Kn$ , ranging from the continuum to the transition regimes, using a single computational framework. The reduced flow rate with the new approach is found to agree well with previously reported results for  $Kn < 1$ .

## INTRODUCTION

This paper presents several algorithmic extensions of the Lattice Boltzmann method (LBM) that permits its application to rarefied gas flows. The most general current method for modeling such flows is known as Direct Simulation Monte Carlo (DSMC) [1,2] which evolves the dynamics of a statistically representative number of particles underlying the macroscopic flow. While demonstrably accurate over a wide range of flow scenarios, the DSMC becomes prohibitively expensive computationally for practical flows that approach continuum conditions [1]. This is a pervasively common scenario for subsonic rarefied gas flows such as found in microfluidic devices [1,3]. The LBM is a relatively recently developed alternative kinetic-based approach to simulating fluid dynamics that solves the Boltzmann equation using a discrete velocity representation and a simplified collision model, such as the standard BGK model [4,5]. Previously, its main application areas have tended to involve continuum flows containing complex physics and geometry where the main priority has been to minimize the fluid viscosity in order to progress towards large Reynolds numbers typical of such flows [6]. The standard LBM does not accurately simulate flows with non-vanishing Knudsen number due to its use of a single parameter BGK model that is equivalent to the molecular Maxwell model (i.e. linear relationship between viscosity and fluid temperature [2]) and its use of a physically inappropriate “bounce-back” boundary condition at solid surfaces.

We have extended the collision model used in the LBM to allow for a general power-law relationship between the viscosity and temperature as found in the Variable Hard Sphere (VHS) molecular model typically used in DSMC [2]. We have also extended the gas-surface interaction model to include Maxwell’s scattering kernel to allow for a combination of specular and diffuse reflection via an accommodation coefficient [7]. This scattering kernel was achieved through the use of flux-based boundary conditions [8] that allow for a surface generally oriented with respect to the underlying regular Cartesian grid.

As well as the extended LBM approach described above, another hybrid technique has been developed. This approach solves the same discrete kinetic Boltzmann equation used in the LBM but incorporates a discrete Monte Carlo collision model with several extensions that accelerates its computational capability relative to DSMC, particularly in the near-continuum regime, and permits its application to rarefied gas dynamics. Specifically, efficiency advantages are a consequence of: a reduction in the number of degrees of freedom that must be evolved (phase-space is discrete rather than continuous); a reduction in the overhead of selecting and then finding particles in memory to collide (they are all collocated at the same discrete lattice site, e.g. indices in memory); a reduction in the length of time or number of ensembles that must be averaged to achieve a clean signal by allowing “multiple” collisions at once; and finally, the ability to achieve larger time steps due to an implicit implementation of the collision process. This new method is called Lattice Boltzmann-Monte Carlo (LBMC) to reflect its underlying discreteness and its use of a stochastic collision process.

The key to the proposed LBMC model is the determination of an “adequately” sampled discrete-velocity model. The chosen discrete system not only possesses the requisite symmetry to erase the underlying discrete lattice structure at the macroscopic level, but also possesses several number theoretic properties that assures its collisional “completeness” at the microscopic level [9], which is critical for achieving statistical equivalence with the continuous DSMC model and avoiding spurious invariant quantities. This is in contrast to typical discrete-velocity models applied to the Boltzmann equation that commonly suffer from insufficient collisional variation to produce

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realistic dynamics [10]. However, despite these sources of acceleration, it was found that the efficiency of this new LBMC approach was still inferior compared to the extended LBM approach described above. Thus, due to space limitations in this paper, we focus on the latter method and reserve a detailed description of the LBMC for a subsequent paper although we do include some results of this method here for comparison purposes.

In this paper, the performance of the extended LBM is first demonstrated by validating the desired viscosity-temperature relationship over the range of allowed temperature and power-law exponents typically found in single-component fluids. Next, reduced flow rate results for the plane Poiseuille scenario are presented for a series of Knudsen numbers,  $Kn$ , ranging from the continuum ( $Kn < 0.01$ ) to the transition ( $0.1 < Kn < 10$ ) regimes for subsonic flow conditions within a single computational framework. Good agreement is found between the new method and previously reported results using other techniques.

In the following sections, the general LBM method used here is described as are the extensions required for application to rarefied gas flows. Subsequently, computational results of the two flow scenarios described above using a MATLAB-based prototype code are presented and discussed. The paper concludes with a summary of the main results as well as directions for future work.

## LATTICE BOLTZMANN METHOD

In this section we briefly summarize the analysis of the discrete form of the update process used to evolve the fluid status in this work. The origin of this process is the continuous Boltzmann equation which is discretized not only in space and time, but also in the microscopic velocity. The discrete Boltzmann update process investigated had the following general form

$$N_{ij}(\mathbf{x} + \mathbf{c}_{ij}\Delta t, t + \Delta t) = A(Kn)N_{ij}(\mathbf{x}, t) + B(Kn)\Omega_{ij}(\{N_{ij}\}) + C(Kn)N_{ij}^{eq}(\mathbf{x}, t) \quad (1)$$

where the discrete velocity notation of [9] has been used, indicating the presence of multiple energy particles ( $j, i$  designate the allowable discrete energy and discrete velocity within a given energy, respectively, of the allowed discrete velocity vectors  $\mathbf{c}_{ij}$ ). The quantity on the left-hand side represents the updated particle density after the advection and collision process. The update process on the right-hand side is a combination of three elements: first, the old free-streamed distribution,  $N_{ij}$ , secondly, the output of an explicit collision process,  $\Omega_{ij}$ , and thirdly, an equilibrium distribution, designed to have the same macroscopic collisional invariants as the pre-collision distribution, specifically mass, momentum and energy [MME]. They are linearly combined according to the three update coefficients  $A, B, C$ , which may be functions of the local Knudsen number. This representation encompasses a broad variety of specific models [17].

A discrete form of kinetic theory is applied to (1) by expanding about a given point in space and time (but maintaining the microscopic velocity discretization) and forming discrete moments of the distribution function and its evolution equation. The general form of the conservation equations, formed by taking appropriate moments of (1), indicates that in order for the MME to be collisionally invariant the update coefficients must sum to unity,  $A+B+C = 1$ .

The analysis continues by computing higher-order moments leading to the momentum flux tensor,  $\mathbf{S}$ , and energy flux vector,  $\mathbf{Q}$  and then substituting them into the conservation relations. This leads to a system of macroscopic equations that require additional closure relations for these higher order moments, as in the continuous microscopic velocity case. A discrete form of the Chapman-Enskog closure analysis is performed, which requires specification of the equilibrium distribution and the specific velocity field discretization used.

For the results presented in this work, we have used a three-speed system based on the four-dimensional,  $D=4$ , face-centered hypercube (FCHC) structure (see [9,12,17] for specification of direction vectors). This system permits three-dimensional, coupled, artifact-free simulation of subsonic near-isothermal flows [9,12]. The total number of directions is 34 for an implicit three-dimensional projection of the system. Key ingredients of this discrete velocity system are its symmetry properties, supported by number theoretic analysis of the system [9,12], and its ‘‘collisional variety’’ whereby any discrete pre-collision binary combination of states may be transferred to a number of potential out-states while preserving local MME within the discrete system [9]. This is a necessary property to avoid spurious invariants in methods that employ an explicit collision process, such as the LBMC approach described above. In the future, we will explore the use of reduced discrete velocity sets in order to further improve computational efficiency.

Further background details on the application and results of the Chapman-Enskog analysis leading to the recovery of the Navier-Stokes equations for this system may be found in [11], which may be straightforwardly extended for the generalized LBM system (1) used here.

## ALGORITHMIC EXTENSIONS FOR RAREFIED FLOWS

The LBM system described above was extended in order to facilitate its application to rarefied gas flows. Extensions were developed and implemented in two areas: i) the discrete BGK collision model was extended to permit a general power-law relationship between the fluid dynamic viscosity and its temperature and ii) gas-surface interactions were extended to include Maxwell's scattering kernel for a general surface orientation. These developments are briefly described in this section.

### Collision Model For Rarefied Flows

The goal of initial efforts in this area was to adapt Bird's "No Time Counter" [2] explicit collision process to the discrete velocity case within the LBMC framework. This required implementation of an appropriate collisional cross-section model and the commonly used Variable Hard Sphere (VHS) [2] technique was selected to accomplish this. This model achieves a realistic power-law relationship between the dynamic viscosity of the fluid,  $\mu$ , and fluid temperature,  $T$ . This relationship is considered one of the most critical physical properties to capture in order to achieve accurate rarefied gas flow simulation [2].

Implementation of the VHS model into the LBMC required appropriate specification of the collision operator. Within the LBM framework, ( $\{A,B,C\}=\{1-\lambda,0,\lambda\}$  in (1)) this can be accomplished by setting the single-time relaxation parameter,  $\lambda$ , as follows

$$\frac{\mu}{\rho} = \left( \frac{1}{\lambda} - \frac{1}{2} \right) \tilde{T} = \alpha \tilde{T}^\omega \Rightarrow \lambda = \frac{2}{2\alpha \tilde{T}^{\omega-1} + 1} \quad (2)$$

where  $\tilde{T} \equiv RT$  is the temperature,  $T$ , multiplied by the gas constant,  $R$ . The proportionality factor,  $\alpha$ , is dependent on the particular molecule being simulated and may be readily computed from tabulated data or simple models [2]. Values of the exponent,  $\omega$ , range from unity for so-called Maxwell molecules (the standard model used in the LBM) to  $\omega=1/2$  for the hard-sphere model with typical gases being somewhere in between. Locally setting the BGK collision parameter consistent with (2) permits the desired viscosity power-law relation to be achieved consistent with the VHS cross-section model. A similar approach is employed for implementations of the BGK model within the continuous Boltzmann equation (see Section 2.5.1 of [13]).

### Gas-Surface Interactions Models

The inclusion of gas-surface interaction models into the LBMC/LBM was accomplished in two steps. First, a general technique for achieving boundary conditions on a generally oriented surface using a previously developed flux-based method [8] in conjunction with a discrete velocity system was implemented. Secondly, techniques for achieving diffuse and specular reflection, the two components of Maxwell's model of gas-surface interaction [10], were developed within this framework. It is noted that the general boundary interaction capability developed here will also allow more sophisticated interaction models, such as the Cercignani-Lampis model [7], to be incorporated into the approach in the future.

Theoretical and implementation details of the flux-based boundary condition method may be found in [8]. Briefly, a general surface overlaying the underlying regular lattice is discretized into a series of point-wise continuous linear elements and at each surface element fluxes of particles are collected from all discrete directions and volumes that reach that element in a single time-step. Particles are considered to be spread evenly throughout a lattice cell to perform this calculation. These fluxes, from a half-sided distribution, are altered so that the out-going flux produces a desired net change of a fluid property at the surface in order to achieve the desired boundary condition (e.g. velocity, temperature). The use of partial volumes and fluxes, rather than a one-to-one scattering process for each discrete velocity direction, permits boundary conditions to be applied independent of the position and orientation of this surface with respect to the underlying discrete lattice.

Consistent with existing theories on gas-surface interaction models in rarefied systems (e.g. [10]), we require that the out-going flux,  $\Gamma_{\chi,i}^{out}$ , in a given direction,  $i$ , from a given surface element,  $\chi$ , with outwards pointing normal,  $\mathbf{n}$ , be computed from the in-coming flux according to a the scattering kernel,  $R(\mathbf{c}'_{ij} \rightarrow \mathbf{c}_{ij})$  using

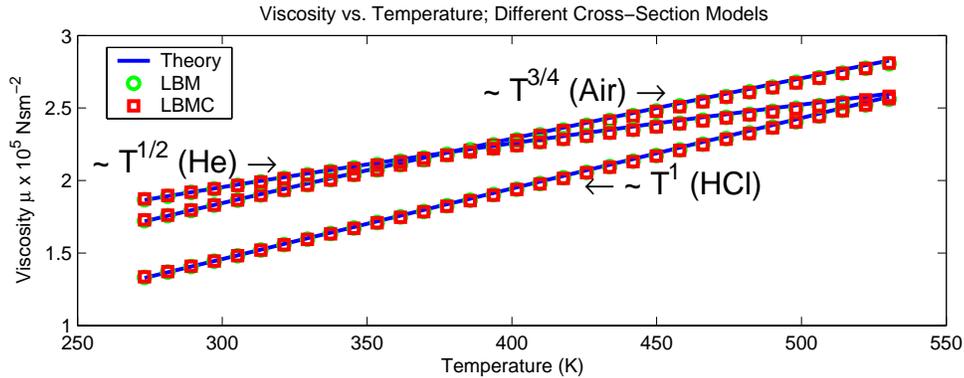
$$\Gamma_{\chi,i}^{out} = \sum_{\mathbf{c}'_{ij} \cdot \mathbf{n} < 0} R(\mathbf{c}'_{ij} \rightarrow \mathbf{c}_{ij}) \Gamma_{\chi,i'}^{in} = (1 - \sigma_v) \Gamma_{\chi,i}^{out,spec} + \sigma_v \Gamma_{\chi,i}^{out,diffuse} \quad (3)$$

where a specific implementation resulting in Maxwell's model [10] is indicated. This model results in contributions from both specular and diffuse reflection as controlled by the single accommodation coefficient,  $\sigma_v$ .

Algorithms for achieving both of these types of boundary interaction have been developed but, for space limitation reasons, are presented elsewhere [17]. We note that a no-slip boundary condition, as would be achieved in continuum flows, may also be implemented via the use of a “bounce-back” boundary condition where  $\Gamma_{\chi,i}^{out} = \Gamma_{\chi,i}^{in}$  and  $\mathbf{c}_{ij} = -\mathbf{c}_{ij}$  [8]. For the case of stationary walls, this will achieve a “zero-velocity” boundary condition. Thus we see that boundary conditions involving a general combination of diffuse, specular and bounce-back reflections may be incorporated into the extended LBM/LBMC technique via the developed algorithms.

## SIMULATION RESULTS

The extensions described in the previous section were implemented into a MATLAB-based prototype code and applied to two basic “building-block” flow scenarios: fluid-only shear decay and plane-Poiseuille flow. The purpose of the first simulation was to validate the desired viscosity-temperature relationship over the allowed temperature range and power-law exponents typically found in single-component fluids. An initial sinusoidal velocity shear is prescribed in a fluid-only system and allowed to decay over time. The rate of decay indicates the viscosity of the fluid, see [9] for details. Figure 1 presents simulated dynamic viscosity vs. temperature results for both the LBMC (incorporating a direct collision process) and the extended LBM (with the new collision model) for three different molecules (i.e. three different power-law relationships): HCl, Air and Helium. Results are presented in physical units after conversion from “lattice” units and the proportionality constant,  $\alpha$ , in (2) was chosen to match experimental results for each molecule (from Appendix A of [2]). There is excellent agreement between the two developed approaches and semi-empirical theory for all molecules over the allowed temperature range (nominally a factor of two in absolute units for this three-speed discrete system [9,11]). This validated the implementation of the VHS model within this new discrete computational framework. It is noted that the results of this simulation are insensitive to the difference in internal energy degrees of freedom between an actual polyatomic gas (e.g. Air, HCl) and the simulated monatomic gas (which has only translational degrees of freedom).



**FIGURE 1** : Dynamic viscosity as a function of temperature in physical units for three different molecules with differing viscosity-temperature power-law exponents. Simulated results using both the extended LBM and LBMC approaches in comparison with semi-empirical theory shown.

Next, a series of pressure-driven Poiseuille flow simulations were performed at Knudsen numbers that varied from the continuum ( $Kn < 0.01$ ) to the transition flow regimes ( $Kn \sim 1$ ). The same channel geometry was used for all cases, specifically 150 x 50 cells, (the parallel solid walls were oriented horizontally). All simulations were begun with the same initial no-flow conditions within the geometry. Inlet and outlet boundary conditions were implemented via a specification of the particle distribution with the desired flow properties in buffer cells situated immediately upstream and downstream of the simulated volume. For a prescribed pressure gradient, the inlet density, pressure and temperature (via the ideal gas equation of state,  $p = \rho \tilde{T}$ ) were specified and the velocity was allowed to float self-consistently assuming zero-gradient at the inlet. At the outlet, the pressure and temperature were specified and the density and velocity were allowed to float consistent with a zero-gradient assumption. Similar boundary conditions were used for DSMC in [14]. The accuracy of these inlet-outlet boundary conditions was verified using a continuum flow scenario where analytical results are available (not shown). Future work will extend the flux-based boundary condition method used at the solid walls to the inlet-outlet boundaries as well.

The Knudsen number for the pressure-driven flow was set by adjusting the mean-free path of collisions via the fluid viscosity. The characteristic length scale used to compute  $Kn$  was the height of the channel,  $H=50$ , so that

$$Kn = \frac{\lambda_{mfp}}{H} = \sqrt{\frac{\gamma\pi}{2}} \frac{Ma}{Re} = \alpha \sqrt{\frac{\pi}{2}} \frac{\tilde{T}^{\omega-0.5}}{H} \quad (4)$$

where the VHS model was used to set the viscosity,  $\gamma$  is the ratio of specific heats, and  $Ma$  and  $Re$  are the Mach and Reynolds numbers respectively. The initial bulk fluid temperature was set equal to the wall temperature, which was kept constant for all cases. The hard sphere molecular model,  $\omega = 0.5$ , was used throughout. Consequently, the Knudsen number was adjusted through the viscosity coefficient parameter,  $\alpha$ . The values of Knudsen number examined covered from the continuum through the slip flow and well into the transition flow regime ( $0.1 < Kn < 10$ ). The results presented here focus on this latter regime.

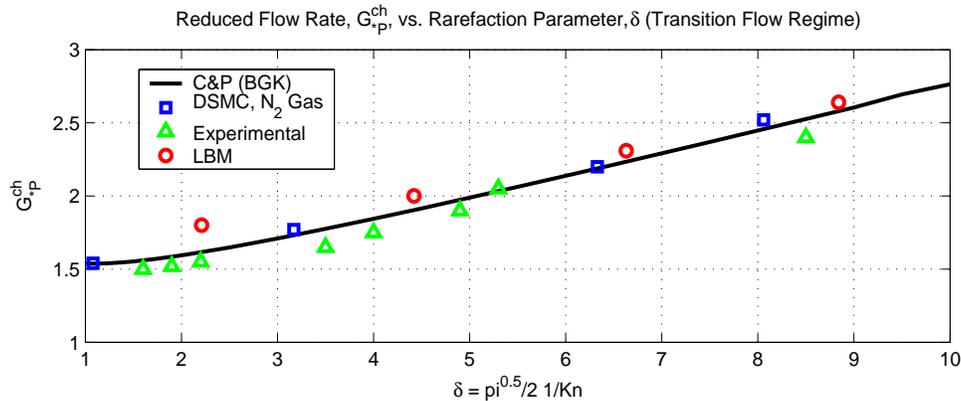
Profiles of longitudinal velocity, pressure and temperature as a function of both the cross-wise and longitudinal coordinate for these  $Kn$  with the fully diffuse wall boundary condition,  $\sigma_v = 1.0$  have been examined (not shown) and found to exhibit qualitatively similar trends as found in a recent study using DSMC for the same geometry with similar  $Kn$  [14]. Moreover, the curvature of the cross-stream pressure profile increased as  $Kn$  increased and was found to qualitatively agree with the DSMC results (i.e. concave with a maximum near the walls) [14], both of which were in the opposite direction to that produced by the slip-enhanced Navier-Stokes equations [14].

Quantitatively, we have compared the simulated reduced flow rate in the channel,  $G_{sp}^{ch}$ , as a function of Knudsen number with previously published results using other approaches including DSMC [3], Boltzmann-BGK using a variational approach [15], and experiment [16]. The reduced flow rate is defined

$$G_{sp}^{ch} = \frac{-\dot{M}}{\beta H^2 dP_s/dx} \quad (5)$$

where  $H$  is the channel height,  $\dot{M}$  is the local mass flow rate,  $dP_s/dx$  is the local pressure gradient at a central point far from the ends of the channel and  $\beta = (2\tilde{T})^{-0.5}$ . It is assumed that temperature gradient effects are negligible.

Figure 2 presents this comparison focusing on the transition flow regime in terms of the rarefaction parameter,  $\delta = \sqrt{\pi}/(2Kn)$ , at an accommodation coefficient of  $\sigma_v = 1.0$ , i.e. the fully diffuse boundary condition. The agreement between all of the methods is quite good, indicating the accuracy of the extended LBM in this important rarefied flow regime. Figure 3 presents simulated results at four values of the accommodation coefficient,  $\sigma_v = \{0.50, 0.80, 0.92, 1.00\}$ , for the developed approach in comparison with the variational Boltzmann-BGK results reported in [15]. The agreement between the two approaches for all investigated values of  $\sigma_v$  is quite good. This further illustrates the accuracy of the Maxwell gas-surface interaction model scattering kernel implemented within the discrete velocity framework that has been developed here.

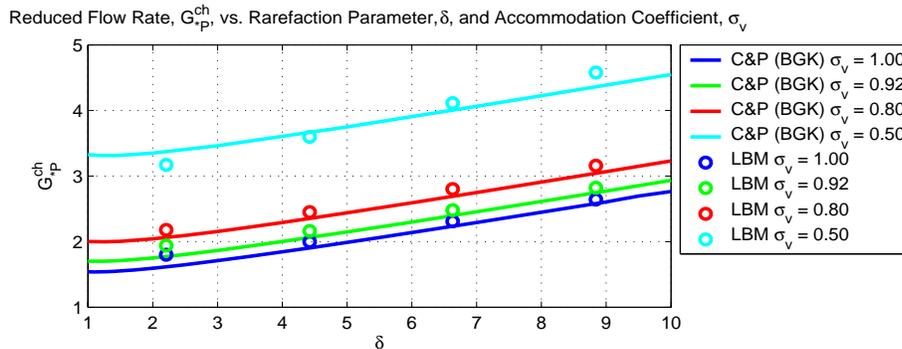


**FIGURE 2 :** Reduced flow rate,  $G_{sp}^{ch}$ , as a function of the rarefaction parameter,  $\delta$ , in the transition flow regime. The legend indicates the source of the results. Good agreement between the extended LBM and the other results was found.

## CONCLUSIONS

This paper presents two new approaches for simulating rarefied gas flows using a discrete velocity system. The extended LBM incorporates two developments that i) extends the standard lattice-Boltzmann BGK collision model to allow for a general power-law relationship between the viscosity and temperature as found in the VHS molecular

model, and ii) extends a previously developed flux-based boundary condition approach for discrete Boltzmann systems to include the two elements of the Maxwell scattering kernel, specular and diffuse reflection, the contribution of which may be adjusted by a single accommodation coefficient. The second developed approach, denoted LBMC, incorporates the above two extensions but does so within the context of a discrete Monte Carlo collision process. The two developed approaches are shown to give equally accurate viscosity measurements over the range of the VHS power-law relationship but focus is placed on the extended LBM approach due to its improved computational efficiency in comparison with the LBMC.



**FIGURE 3** : Reduced flow rate,  $G_p^{ch}$ , as a function of the rarefaction parameter,  $\delta$ , and accommodation coefficient,  $\sigma_v$ , in the transition regime. Comparison of extended LBM and BGK results from [15] shown.

Pressure-driven plane Poiseuille flow results demonstrate qualitatively accurate flow (i.e. velocity, temperature, pressure) profiles in both the longitudinal and cross-wise directions consistent with reported DSMC results, including the capturing of the appropriate curvature of the crosswise pressure profile that is incorrectly captured with the slip-enhanced Navier-Stokes approach. Quantitatively, the reduced flow rate as a function of Knudsen number with the extended LBM was found to be consistent with previously reported results from the continuum up to  $Kn \sim 1$  (i.e. the transition regime) for the series of accommodation coefficients investigated. This was accomplished using a single computational framework and the same geometry resolution for all cases.

Future analysis will focus on performance at  $Kn > 1$ . Initial results demonstrate the qualitative capturing of Knudsen's minimum for Poiseuille flow and will be reported in the future. Extended LBMs with a reduced number of discrete velocities, which will improve computational efficiency, will also be investigated. The combination of a single computational framework for a large  $Kn$  range, the use of a discrete velocity update process, and applicability to general flow geometry makes the new LBM-based technique an efficient and accurate analytical tool for subsonic rarefied gas scenarios such as found in microfluidic applications.

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