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Frequency-domain Monte Carlo method for linear oscillatory gas flows

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ABSTRACT

Gas flows generated by resonating nanoscale devices inherently occur in the non-continuum, low Mach number regime. Numerical simulations of such flows using the standard direct simulation Monte Carlo (DSMC) method are hindered by high statistical noise, which has motivated the development of several alternate Monte Carlo methods for low Mach number flows. Here, we present a frequency-domain low Mach number Monte Carlo method based on the Boltzmann–BGK equation, for the simulation of oscillatory gas flows. This circumvents the need for temporal simulations, as is currently required, and provides direct access to both amplitude and phase information using a pseudo-steady algorithm. The proposed method is validated for oscillatory Couette flow and the flow generated by an oscillating sphere. Good agreement is found with an existing time-domain method and accurate numerical solutions of the Boltzmann–BGK equation. Analysis of these simulations using a rigorous statistical approach shows that the frequency-domain method provides a significant improvement in computational speed.

1. Introduction

Advances in fabrication technology have led to the development of nanometer scale mechanical devices for a host of sensing applications, including ultra-small scale mass measurement [1–3], measurement of fluid properties [4,5], accurate sensing of environmental properties [6,7], and atomic scale imaging [8,9]. These devices are often driven at resonance in gas, e.g., air, which intrinsically generates oscillatory flows. Ability to model these flows is thus critical to proper device design and measurement interpretation. Unlike microscale devices, which often produce gas flows in the continuum regime, nanometer scale operation inherently generates non-continuum flows. This is because the device dimensions can be comparable to the molecular length scale, i.e., the gas mean free path, and/or the device oscillation frequency is similar to the molecular collision frequency.

The degree of gas rarefaction may be specified by the Knudsen number, which defines the ratio of the gas mean free path, λ, to the dominant length scale of the flow, L, i.e., $\mathrm{Kn} \equiv \lambda/L$. Another critical variable is $\theta \equiv \omega/\nu$, which is the ratio of the device frequency ω to the molecular collision frequency ν. In the continuum limit, $\mathrm{Kn} \to 0$ and $\theta \to 0$, gas flows are accurately modeled by the Navier–Stokes equations. These equations can be solved either analytically or computationally in many cases of practical interest. While there exists a plethora of simulation packages for this purpose, their utility

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at nanometer length scales is obviated by violation of the continuum hypothesis. Such flows consequently require more advanced treatments, such as those based on the Boltzmann equation.

One widely used technique for solving the Boltzmann equation is the direct simulation Monte Carlo (DSMC) method, originally proposed by Bird [10]. DSMC is a statistical method in which simulator particles are used to represent a much larger set of real particles/molecules, with collisions being determined probabilistically. Being fundamentally based on the temporal evolution of particle states, DSMC is naturally capable of modeling unsteady flows at arbitrary Kn and θ. However, in contrast to steady flows whose boundary conditions are time-invariant, extra computational considerations are required for unsteady flows [10]. A particular advantage of the DSMC method is its ability to easily accommodate a variety of molecular collision models. The most basic of these is the hard sphere (HS) model where particles collide elastically with no interaction prior to contact [10]. More sophisticated molecular interaction models can also be used, such as those that invoke an inverse power-law potential. While these provide a more realistic description, they introduce additional computational considerations [11]. A practical alternative is to use the variable hard sphere (VHS) model [11]. This model maintains the simple elastic scattering behavior of HS, but alters the collision cross section as a function of the relative velocity between particle pairs. Significantly, VHS gives values for the gas viscosity and heat conductivity that are consistent with those obtained using inverse power-law potentials, but it is more computationally efficient [11]. Another approach is to approximate the collision process with the Bhatnagar–Gross–Krook (BGK) relaxation model [12–14]. This models the collision of gas molecules by a single relaxation time process which mimics the behavior of a gas, eliminating the need to consider individual collisions. A well documented shortcoming of the BGK model is that the correct Prandtl number for a monatomic gas is not recovered [15,16]. Despite its limitations, the BGK approximation greatly simplifies analysis and has been widely applied to model gas flows both computationally and analytically [15,17].

Operation at low Mach number presents a significant challenge to statistically based simulation methods, such as DSMC. The overriding limitation is that the state of such flows deviates only slightly from the equilibrium state of the gas. As a result, the non-equilibrium properties of the flow are obscured by statistical noise, thus requiring considerable computational resources to generate accurate solutions. Even so, several studies using standard DSMC methods have been reported previously [18–21]. To overcome this shortcoming, several groups have proposed alternate Monte Carlo methods for low Mach number flows. Rather than solving for the complete distribution function of the gas, these approaches evaluate the deviation of its state away from a specified equilibrium. This dramatically reduces statistical noise and increases computational efficiency. Radtke, Hadjiconstanitinou and Wagner categorize these methods into two types [22]: (i) deviational, and (ii) weight-based methods. In the first type, the velocities of the simulator particles directly represent the deviation of the distribution function from equilibrium. In contrast, weight-based methods use a fixed equilibrium distribution function, and account for deviations from equilibrium through the allocation of weights as a function of molecular velocity. Both approaches have been implemented for HS [23–27] and BGK [28–31] models, with the deviational approach also being applied using VHS [22]. For simplicity, we refer collectively to these approaches and the original DSMC method of Bird [10] as 'Monte Carlo methods'.

Another approach for simulating gas flows is the lattice Boltzmann (LB) method, proposed by McNamara and Zanetti [32–34]. This method discretizes physical and velocity space on a fixed lattice, greatly simplifying numerical computation. It is based on a time-marching algorithm, and is thus suitable for both steady and unsteady flows. Similarly to the methods described above, linearization of the LB method facilitates evaluation at low Mach number [35]. Importantly, the LB method has been proved to be a weakly compressible formulation of the Navier–Stokes equations, in the continuum limit [36]. This has led to its wide spread use in a range of continuum flow problems, particularly those involving complicated boundaries [37–41]. Applicability of the LB method to non-continuum flows has also been explored [42–44], due to its foundation on the Boltzmann–BGK equation [45]. In such applications, it has been found to be most accurate in the near-continuum regime.

Recently a frequency-domain LB method, based on the linearized Boltzmann BGK equation, was proposed for oscillatory low Mach number flows [46,47]. This method maintains the time-marching algorithm of the original LB method through introduction of a 'virtual-time' variable. Thus, flow calculations at fixed frequency can proceed using the traditional algorithm of the LB method – steady solutions in virtual-time correspond to the required frequency-domain flows. This facilitates the evaluation of both amplitude and phase information of the flow while presenting some computational advantages. Here, we make use of this virtual-time concept to develop a frequency-domain low Mach number Monte Carlo method for linearized oscillatory flows, allowing for rigorous computation of gas flows at arbitrary degrees of rarefaction.

We begin with an overview of the linearized Boltzmann–BGK equation and then present the frequency-domain Monte Carlo method based on the BGK model. The particle weight method discussed above is used in this formulation.

The method is validated for two canonical flow problems: (i) oscillatory plane Couette flow, and (ii) flow generated by an oscillating sphere, for which good agreement with existing accurate numerical solutions of the Boltzmann–BGK equation [48] and time-domain Monte Carlo methods [31] is obtained. Finally, a rigorous assessment of the convergence properties of the frequency-domain method relative to the traditional time-domain Monte Carlo method is presented.

2. The frequency-domain Monte Carlo method

The frequency-domain Monte Carlo method combines the virtual-time concept proposed by Shi and Sader [46] with the time-domain low Mach number Monte Carlo algorithm of Ramanathan and Koch [31]. Both these approaches are based on