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A coupled ordinates method for solution acceleration of rarefied gas dynamics simulations

Shankhadeep Das [a,b,*], Sanjay R. Mathur [a,b], Alina Alexeenko [a,c], Jayathi Y. Murthy [a,b]

[a] NNSA PRISM: Center for Prediction of Reliability, Integrity and Survivability of Microsystems, USA
[b] Department of Mechanical Engineering, The University of Texas at Austin, TX 78712, USA
[c] School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907, USA

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ABSTRACT

Non-equilibrium rarefied flows are frequently encountered in a wide range of applications, including atmospheric re-entry vehicles, vacuum technology, and microscale devices. Rarefied flows at the microscale can be effectively modeled using the ellipsoidal statistical Bhatnagar–Gross–Krook (ESBGK) form of the Boltzmann kinetic equation. Numerical solutions of these equations are often based on the finite volume method (FVM) in physical space and the discrete ordinates method in velocity space. However, existing solvers use a sequential solution procedure wherein the velocity distribution functions are implicitly coupled in physical space, but are solved sequentially in velocity space. This leads to explicit coupling of the distribution function values in velocity space and slows down convergence in systems with low Knudsen numbers. Furthermore, this also makes it difficult to solve multiscale problems or problems in which there is a large range of Knudsen numbers. In this paper, we extend the coupled ordinates method (COMET), previously developed to study participating radiative heat transfer, to solve the ESBGK equations. In this method, at each cell in the physical domain, distribution function values for all velocity ordinates are solved simultaneously. This coupled solution is used as a relaxation sweep in a geometric multigrid method in the spatial domain. Enhancements to COMET to account for the non-linearity of the ESBGK equations, as well as the coupled implementation of boundary conditions, are presented. The methodology works well with arbitrary convex polyhedral meshes, and is shown to give significantly faster solutions than the conventional sequential solution procedure. Acceleration factors of 5–9 are obtained for low to moderate Knudsen numbers on single processor platforms.

1. Introduction

A number of present day applications involve rarefied flows with a wide range of length scales. Such flows are frequently encountered in microsystems, hypersonic vehicles, and vacuum technology, amongst others. Over the years, a large number of studies have been performed on the aerothermodynamics of hypersonic systems [1,2]. On the other hand, non-equilibrium rarefied flows in microsystems have only recently begun to receive attention [3–5]. Examples of microscale rarefied flows

* Corresponding author at: Department of Mechanical Engineering, The University of Texas at Austin, TX 78712, USA. Tel.: +1 763 656 9271.
E-mail address: shankhadeep@utexas.edu (S. Das).

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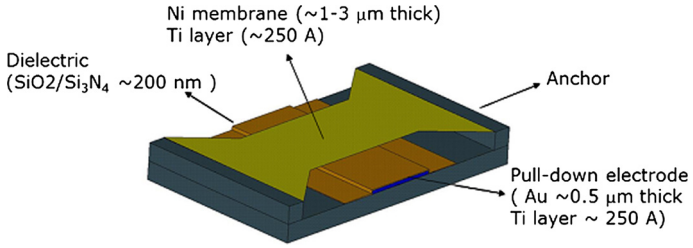

Fig. 1. RF MEMS switch showing nickel membrane, contact pads and anchors [6].

include those in resonators, radio-frequency micro-electromechanical systems (RF MEMS), and microturbines, amongst others. These flows are typically low-speed and incompressible, and thus are significantly different from compressible flows in hypersonic systems.

Furthermore, in many microsystem applications, dynamic transitions between continuum and rarefied regimes are frequently encountered, for example in the transient damping of MEMS switches [6] (see Fig. 1). Here, a metallic membrane makes periodic contact with a contact pad under the action of electrostatic forces induced by an applied voltage. In the open position, the gas-filled gap between the membrane and the contact pad is a few microns. The Knudsen number Kn ($=\lambda/g$, where λ is the molecular mean-free path and g is the gap height) is in the continuum regime. As the gap closes, the Knudsen number increases, and becomes arbitrarily large as contact is approached; the flow transitions periodically between the continuum and rarefied regimes as the switch opens and closes. In such a problem, hybrid approaches such as those in [7–9] become extremely complicated to implement, and assuring conservation of mass, momentum and energy over the switching cycle is very difficult. A unified treatment, with an efficient numerical scheme addressing the entire range of Knudsen numbers, is necessary.

One approach to modeling non-equilibrium rarefied flows is to solve the Boltzmann equation [10], which is valid over the entire range of Knudsen numbers, provided that distribution functions can be usefully defined. The Boltzmann equation is expressed as:

$$\frac{\partial f}{\partial t}+c_x\frac{\partial f}{\partial x}+c_y\frac{\partial f}{\partial y}+c_z\frac{\partial f}{\partial z}=\int_{-\infty}^{\infty}\int_{0}^{4\pi}\left(f^*f_1^*-ff_1\right)g\sigma\, d\Omega\, d\mathbf{c}_1 \tag{1}$$

where $f(\mathbf{x},t,\mathbf{c})$ is the distribution function for molecular velocity at location $\mathbf{x}$ and time t, and $\mathbf{c}$ ($=c_x i+c_y j+c_z k$) is the molecular velocity vector. The number of molecules with coordinates within infinitesimal element $d\mathbf{x}$ near $\mathbf{x}$ and velocities within velocity space element $d\mathbf{c}$ near $\mathbf{c}$ is given by $f d\mathbf{c} d\mathbf{x}$. The right hand side of the equation is the net result of two separate processes: collisions between molecules of velocities $\mathbf{c}$ and $\mathbf{c_1}$ leading to depletion in the number of molecules of velocity $\mathbf{c}$, and collisions between molecules of velocities $\mathbf{c}^*$ and $\mathbf{c}_1^*$ replenishing the molecules with velocities $\mathbf{c}$. Here g is the magnitude of the relative velocity, i.e. $g=|\mathbf{c}-\mathbf{c_1}|$, and σ represents the collision cross-section.

A commonly used particle-based approach for solving the Boltzmann equation is the Direct Simulation Monte Carlo (DSMC) method which solves it by stochastic simulations [10,11]. Even though DSMC was originally developed for hypersonic systems, in the subsequent years it has been extended to model micro-channel flows [12,13]. However, DSMC can become computationally very expensive for low-speed and unsteady flows. This is because a large number of samples are required to reduce noise-to-signal ratio in stochastic DSMC solutions. To solve this problem, an information preservation (IP) method, which preserves macroscopic flow information, has been developed for low speed micro-scale gas flows [14–16]. Over the years, hybrid continuum/particle methods have also been developed [7–9] for multi-scale system simulation. These methods solve Euler/Navier–Stokes equations in regions of near-equilibrium and DSMC in regions of non-equilibrium. A hybrid particle scheme was formulated in [17] where both continuum and rarefied regimes were modeled with particle-based methods. It modeled rarefied regions using DSMC, whereas it used a DSMC-based low diffusion particle method for inviscid flow simulation in the remaining regions of the flow.

As an alternative to stochastic solution techniques, deterministic approaches can also be used to solve the Boltzmann equation. These are noise-free and can be easily coupled to other deterministic solvers in multi-physics problems. For low-speed incompressible flows of the type encountered in microsystems, a relaxation approximation to the collision term is possible, and the Bhatnagar–Gross–Krook (BGK) form of the equation may be used [18]. In this model, the velocity distribution function $f(\mathbf{x},t,\mathbf{c})$ is given by:

$$\frac{\partial f}{\partial t}+c_x\frac{\partial f}{\partial x}+c_y\frac{\partial f}{\partial y}+c_z\frac{\partial f}{\partial z}=-\nu(f-f_\gamma) \tag{2}$$

where f_γ is a Maxwellian distribution function, and ν is the collision frequency. This model always gives non-negative production of entropy, and thus satisfies the Boltzmann H-theorem. Furthermore, it reproduces a Maxwellian distribution at equilibrium. However, the main shortcoming of the BGK equation is that the Prandtl number (Pr) is always unity instead of the correct value of around 2/3 for monatomic gases and 3/4 for diatomic gases. A variant of the BGK model