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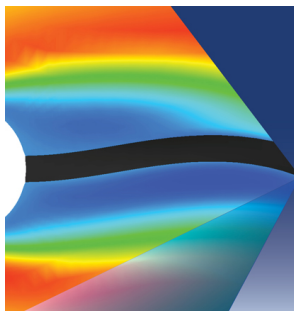
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ABSTRACT

A gas flow in a square cavity driven by a lid sliding in the direction of its line of contact with the cavity wall is considered. The steady behavior of the gas is numerically investigated based on the linearized Bhatnagar–Gross–Krook kinetic equation and the diffuse reflection boundary condition. When one applies the Stokes equation and the no-slip boundary condition to the system considered here, the flow velocity becomes multivalued at the corner between the lid and the cavity wall, and the shear stress diverges at the corner inversely proportionally to the distance from there, which is known as the so-called corner singularity. In the present work, the behavior of the gas near the corner is examined based on numerical results obtained from the kinetic theory. Although the range of the flow velocity value in the kinetic solution is limited due to the significant velocity slip near the corner, the flow velocity is, nevertheless, multivalued at the corner. The shear stress varies inversely proportionally to the distance from the corner up to the position that is a few tens of mean free paths away from there. The increase in the stress is suppressed at positions closer to the corner and its magnitude remains bounded. Thus, the total forces acting on the lid and the side cavity walls are bounded as well. Due to the distinctive behavior of the stress near the corner, the resulting nondimensional total forces behave with an unconventional rate $\text{Kn} \ln \text{Kn}$ for small Knudsen numbers Kn .

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I. INTRODUCTION

A flow in a cavity driven by the motion of its lid is a fundamental problem in fluid mechanics. In particular, a case where the cavity is an infinitely long rectangular one and the lid slides in the direction perpendicular to its line of contact with the cavity walls is often considered. This is the so-called two-dimensional lid-driven cavity flow. It has been intensively studied for various purposes, such as studying eddy structures, obtaining insight into related engineering applications, and validating numerical schemes for incompressible fluid flows (see, e.g., Refs. 1–9).

As is widely known, the solution becomes singular due to the requirement of no-slip boundary condition at the contact point of the moving lid and the resting cavity walls,¹⁰ which we simply call the corner hereafter. The flow velocity changes significantly within arbitrarily small distance near the corner, and it becomes multivalued there although it is bounded. Some components of the stress tensor diverge in approaching the corner inversely proportionally to the distance r from there. This divergence rate is a nonintegrable one, which leads to the divergence of the total forces acting on the lid and the cavity walls.

The divergence of fundamental physical quantities, such as the stress and the force acting on body surfaces implies that, at least locally, there are difficulties in the description of the lid-driven cavity flow in terms of conventional fluid mechanics.

Let us estimate from how much distance from the corner the fluid-dynamic description becomes unreliable. Hereafter, we consider solely a monatomic gas as a fluid. To begin with, the following property can be found in the literature: the pressure as well as the stress diverge to infinity with the aforementioned rate for the case of lid-driven cavity flow and the related Taylor's scraping flow,^{10,11} namely, $p - p_{\text{ref}} \propto \pm \mu U/r$. Here, p and p_{ref} are, respectively, the local and the reference pressure, μ is the viscosity, and U is the lid speed. The plus (or minus) sign is taken if the lid goes toward (or away from) the corner under consideration when viewed from the gas region. Nondimensionalizing the expression, we obtain the relation $[(p/p_{\text{ref}}) - 1]/\text{Ma} \propto \ell/r$. Here, the proportionality constant is $O(1)$; Ma is the Mach number defined in terms of the speed U and the sound speed corresponding to the temperature of the cavity walls; and ℓ is the mean free path of gas molecules in the equilibrium

state at rest with pressure p_{ref} and temperature of the cavity walls. In the nondimensionalization, the relation between the viscosity μ and the mean free path ℓ is taken into account. The obtained relation implies that it is inside the region within $O(\ell)$ from the corner ($r \leq \ell$) that the conventional fluid mechanics would fail to describe the behavior correctly. Generally, phenomena with a characteristic length scale comparable to the mean free path are well described if we resort to the kinetic theory of gases. Thus, it may give a reliable result also for the situation under consideration.

There are several studies investigating the lid-driven flow in a rectangular cavity on the basis of the kinetic theory. Structures of eddies and the total force acting on the lid are reported in Ref. 12. References 13–15 focus on heat transfer associated with the comparatively high-speed shear such that the viscous heating is nonnegligible. Unsteady flows driven by a lid oscillating harmonically are investigated in Refs. 16 and 17. The cavity flow problem is utilized to validate the proposed numerical methods in Refs. 18–23. These works commonly focus on nonequilibrium effects (or non-fluid-dynamic effects) occurring in the bulk region whose magnitude is characterized by the Knudsen number, which is defined as the ratio of the mean free path to the size of the cavity. Thus, gas flows for a wide range of the Knudsen number are analyzed by solving boundary-value problems of kinetic equations in these works.

However, investigation of the behavior of the gas near the corner, or the problem of corner singularity, based on the kinetic theory seems not to be reported yet, despite the expected advantage of the theory in its description. Given this circumstance, we aim to shed light on the understanding of the behavior of the flow velocity and the stress fields near the corner from the viewpoint of the kinetic theory. In the present work, the slow steady flow in a square cavity is considered. We consider the case where the lid slides in the direction of its line of contact with the cavity wall. The corner singularity problem arises in whichever direction the lid moves, and the setting allows more accurate and direct observation of the behavior of the gas near the corner compared to the usual lid-driven cavity flow problem because of its simplicity.

The paper is organized as follows. In Sec. II, the problem is stated and formulated as a boundary-value problem of a kinetic equation. Before proceeding to the numerical analysis of the problem, the Stokes solution and the solution in the free molecular limit, where in the latter the effect of intermolecular collision is neglected, are given in Sec. III. We explicitly confirm the multivaluedness of the flow velocity and the divergence of the stress in the former and it is compared to the latter where the kinetic effect becomes pronounced. Then, the numerical method is briefly explained in Sec. IV. Section V presents the numerical results. As the main interest lies in the fluid-dynamic circumstances, predominantly the results for small Knudsen numbers are given.²⁴ As a result, it is demonstrated that the shear stress and accordingly the force acting on the lid and the cavity walls are bounded and that the flow velocity is still multivalued at the corner for the kinetic solution. The dependence of the total force on the Knudsen number is also discussed. Section VI concludes the paper.

II. FORMULATION

A. Problem and assumptions

Consider a gas in a cavity with a square cross section $-L/2 < X_1 < L/2$, $-L/2 < X_2 < L/2$ (see Fig. 1 and X_i are the Cartesian coordinates). The cavity is infinitely long in the X_3 direction. The upper part

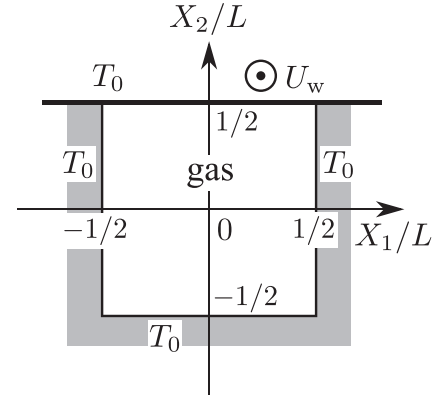


FIG. 1. Sketch of the problem.

of the cavity ($X_2 = L/2$) is closed by a planar lid moving at a constant speed U_w in the X_3 direction. The cavity walls and the lid are kept at a common uniform temperature T_0 . The average density of the gas over the cross section is given by ρ_0 . There is no external force acting on the gas. We will investigate the steady behavior of the gas under the assumptions that (i) the behavior of the gas is described by the Bhatnagar–Gross–Krook (BGK) equation,^{25,26} (ii) the gas molecules are diffusely reflected on the surface of the cavity walls and the lid; and (iii) the lid speed U_w is so small compared with the most probable speed $(2RT_0)^{1/2}$ of gas molecules that the equation and the boundary condition can be linearized around a uniform equilibrium state at rest with density ρ_0 and temperature T_0 (R is the specific gas constant).

B. Basic equation and boundary condition

Let us denote by Lx_i ($i = 1, 2, 3$) the position, by $(2RT_0)^{1/2}\zeta$ [or $(2RT_0)^{1/2}\zeta_i$] the molecular velocity, by $\rho_0(2RT_0)^{-3/2}E(\zeta)[1 + \phi(x_1, x_2, \zeta)]$ the velocity distribution function (VDF) of gas molecules, and by $U_w = (2RT_0)^{1/2}u_w$ the lid speed, where $E(\zeta) = \pi^{-3/2}e^{-\zeta^2}$ and $\zeta = |\zeta|$. Furthermore, we denote by $\rho_0[1 + \omega(x_1, x_2)]$ the density of the gas, by $(2RT_0)^{1/2}u_i(x_1, x_2)$ the flow velocity, by $T_0[1 + \tau(x_1, x_2)]$ the temperature, by $p_0[1 + P(x_1, x_2)]$ the pressure, and by $p_0[\delta_{ij} + P_{ij}(x_1, x_2)]$ the stress tensor, respectively. Here, $p_0 = \rho_0 RT_0$ is the reference pressure and δ_{ij} is the Kronecker delta.

From assumptions (i)–(iii) in Sec. II A, the behavior of the gas is described by a boundary-value problem of the linearized BGK equation for the VDF ϕ . The equation is given by

$$\zeta_1 \frac{\partial \phi}{\partial x_1} + \zeta_2 \frac{\partial \phi}{\partial x_2} = \frac{1}{k} \left[\omega + 2\zeta_j u_j + \tau \left(\zeta^2 - \frac{3}{2} \right) - \phi \right] \quad \left(|x_1| < \frac{1}{2}, |x_2| < \frac{1}{2} \right), \quad (1a)$$

$$\omega = \int \phi E d\zeta, \quad (1b)$$

$$u_j = \int \zeta_j \phi E d\zeta, \quad (1c)$$

$$\tau = \frac{2}{3} \int \left(\zeta^2 - \frac{3}{2} \right) \phi E d\zeta, \quad (1d)$$

$$k = \frac{\sqrt{\pi}}{2} \text{Kn}, \quad \text{Kn} = \frac{\ell_0}{L}, \quad \ell_0 = \frac{(8RT_0/\pi)^{1/2}}{A_c \rho_0}. \quad (1e)$$

Here, $A_c \rho_0$ and ℓ_0 are the collision frequency and the mean free path of gas molecules for the BGK model in the equilibrium state at rest with density ρ_0 and temperature T_0 (A_c : constant), and Kn is the Knudsen number. The integration in (1b)–(1d) and (3a)–(3b) appearing later is carried out over the whole space of the molecular velocity ζ . The boundary conditions for ϕ are written as

$$\phi = 2\sqrt{\pi} \int_{\zeta_2 > 0} \zeta_2 \phi E d\zeta + 2\zeta_3 u_w \left(x_2 = \frac{1}{2}, |x_1| < \frac{1}{2}, \zeta_2 < 0 \right), \quad (2a)$$

$$\phi = -2\sqrt{\pi} \int_{\zeta_2 < 0} \zeta_2 \phi E d\zeta \left(x_2 = -\frac{1}{2}, |x_1| < \frac{1}{2}, \zeta_2 > 0 \right), \quad (2b)$$

$$\phi = \pm 2\sqrt{\pi} \int_{\zeta_1 \geq 0} \zeta_1 \phi E d\zeta \left(x_1 = \pm \frac{1}{2}, |x_2| < \frac{1}{2}, \zeta_1 \leq 0 \right). \quad (2c)$$

Equations (1b)–(1d) are the definitions of perturbations of the density, flow velocity, and temperature. Similarly, the perturbations of pressure and stress tensor are defined as the following moments of the VDF ϕ :

$$P = \omega + \tau = \frac{2}{3} \int \zeta^2 \phi E d\zeta, \quad (3a)$$

$$P_{ij} = 2 \int \zeta_i \zeta_j \phi E d\zeta. \quad (3b)$$

The first equality in (3a) represents the linearized equation of state.

We can assume without any inconsistency that the solution $\phi(x_1, x_2, \zeta_1, \zeta_2, \zeta_3)$ of the boundary-value problem, (1) and (2), is odd in the molecular velocity component ζ_3 . Then, the moments ω , u_1 , u_2 , and τ in Eq. (1a) and the integrals in the right-hand sides of (2a)–(2c) can be put zero. Consequently, (1a) is rewritten as

$$\zeta_1 \frac{\partial \phi}{\partial x_1} + \zeta_2 \frac{\partial \phi}{\partial x_2} = \frac{1}{k} (2\zeta_3 u_3 - \phi) \quad \left(|x_1| < \frac{1}{2}, |x_2| < \frac{1}{2} \right). \quad (4)$$

The boundary conditions (2) are rewritten as

$$\phi = 2\zeta_3 u_w \left(x_2 = \frac{1}{2}, |x_1| < \frac{1}{2}, \zeta_2 < 0 \right), \quad (5a)$$

$$\phi = 0 \quad \left(x_2 = -\frac{1}{2}, |x_1| < \frac{1}{2}, \zeta_2 > 0 \right), \quad (5b)$$

$$\phi = 0 \quad \left(x_1 = \pm \frac{1}{2}, |x_2| < \frac{1}{2}, \zeta_1 \leq 0 \right). \quad (5c)$$

As expected from the geometry and the direction of the lid motion (see also Fig. 1), ϕ can be considered to be symmetric with respect to $x_1 = 0$ in the following sense:

$$\phi(x_1, x_2, \zeta_1, \zeta_2, \zeta_3) = \phi(-x_1, x_2, -\zeta_1, \zeta_2, \zeta_3). \quad (6)$$

The flow velocity component u_3 and the stress components P_{13} and P_{23} are determined by (1c) and (3b), respectively. Owing to (6), they have the following properties:

$$u_3(x_1, x_2) = u_3(-x_1, x_2), \quad (7a)$$

$$P_{13}(x_1, x_2) = -P_{13}(-x_1, x_2), \quad (7b)$$

$$P_{23}(x_1, x_2) = P_{23}(-x_1, x_2). \quad (7c)$$

Since ϕ is odd in ζ_3 (see the beginning of the present paragraph), the other macroscopic quantities, including the aforementioned ones ω , u_1 , u_2 , and τ , vanish:

$$h(x_1, x_2) = 0 \quad (h = \omega, u_1, u_2, \tau, P, P_{11}, P_{22}, P_{33}, P_{12}). \quad (8)$$

C. Integral equation

In the problem, (4) and (5), the VDF $\phi(x_1, x_2, \zeta_1, \zeta_2, \zeta_3)$ is discontinuous for $\zeta_1 \leq 0$, $\zeta_2 < 0$ at the upper corners $(x_1, x_2) = (\pm 1/2, 1/2)$ due to the mismatch between the boundary conditions (5a) and (5c). This discontinuity propagates into the gas along the characteristic lines of (4) passing through the corners $(\pm 1/2, 1/2)$. This would complicate the numerical analysis of the problem. However, in the case of the linearized BGK equation under the diffuse reflection boundary condition, this difficulty can be bypassed by reducing the system to the system of linear integral equations for the macroscopic quantities (see, e.g., Refs. 27–30). We first express ϕ in terms of u_3 by integrating Eq. (4) along its characteristics under the boundary conditions (5a)–(5c). Then, substitute the result into (1c) ($j = 3$) to eliminate ϕ . The integral equation for the flow velocity field $u_3(x)$ obtained by the procedure is given by

$$u_3(x) - A[u_3](x) = u_w b(x). \quad (9)$$

Here,

$$A[u_3](x) = \frac{1}{k\pi} \int_{\Omega} G^{(u_3)}(x_* - x) u_3(x_*) dx_* \\ = \frac{1}{k\pi} \int_{\Omega_R} \left[G^{(u_3)}(x_* - x) + G^{(u_3)}(x_* - \bar{x}) \right] u_3(x_*) dx_*, \quad (10)$$

$$G^{(u_3)}(z) = \frac{1}{|z|} J_0 \left(\frac{|z|}{k} \right), \quad (11)$$

$$b(x) = \frac{1}{\pi} \int_{-1/2}^{1/2} \frac{(1/2 - x_2)}{|x_*^{(U)} - x|^2} J_1 \left(\frac{|x_*^{(U)} - x|}{k} \right) dx_{1*}. \quad (12)$$

The positions $x = (x_1, x_2)$ and $\bar{x} = (-x_1, x_2)$, the integration variable $x_* = (x_{1*}, x_{2*})$, and the position $x_*^{(U)} = (x_{1*}, 1/2)$ on the lid are the two-dimensional vectors in the $x_1 x_2$ plane. In (10), $dx_* = dx_{1*} dx_{2*}$. The domains Ω and Ω_R , appearing in the linear integral operator $A[\cdot]$ given by (10), are, respectively, the cross section of the cavity $-\frac{1}{2} < x_{1*} < \frac{1}{2}$, $-\frac{1}{2} < x_{2*} < \frac{1}{2}$ and its right half $0 < x_{1*} < \frac{1}{2}$, $-\frac{1}{2} < x_{2*} < \frac{1}{2}$. The second equality in (10) is due to the evenness (7a) of u_3 with respect to x_1 . The source term $u_w b(x)$ is given as the integral over the lid surface $x_{2*} = 1/2$ [see (9) and (12)]. The functions J_0 , J_1 , and J_2 appearing, respectively, in (11), (12), and (15) shown later are the Abramowitz functions defined by

$$J_n(\xi) = \int_0^\infty t^n \exp\left(-t^2 - \frac{\xi}{t}\right) dt \quad (\xi \geq 0). \quad (13)$$

Since the range of integration in $A[u_3]$ is limited to Ω_R [see the most right-hand side of (10)], the right half of the cavity cross section, the integral equation (9) can be solved in Ω_R . In (9), the VDF and the molecular velocity ζ are eliminated, and accordingly the discontinuity of the VDF explained at the beginning of this subsection does not enter this equation directly. Thus, (9) is advantageous for carrying out an accurate numerical analysis.

It should be noted that the function $b(\mathbf{x})$ in (9) is multivalued at the upper corner $(x_1, x_2) = (1/2, 1/2)$. Namely, the limiting value of $b(\mathbf{x})$ depends on the direction from which the corner is approached, which can be actually confirmed based on its expression (12). As anticipated from the structure of Eq. (9), the flow velocity component $u_3(\mathbf{x})$ can also be multivalued at the corner. To handle this property associated with the corner appropriately, we introduce the following plane polar coordinates with their origin at corners, say (σ_+, φ_+) and (σ_-, φ_-) as follows (see Fig. 2):

$$x_1 = \frac{1}{2} - \sigma_{\pm} \cos \varphi_{\pm}, \quad x_2 = \pm \frac{1}{2} + \sigma_{\pm} \sin \varphi_{\pm} \quad (0 \leq \varphi_{\pm} \leq \pi/2). \quad (14)$$

Here, $\sigma_{\pm}$ is the distance from the top or bottom corner on the right side $(1/2, \pm 1/2) \equiv \mathbf{x}_c^{\pm}$ to the point $\mathbf{x}$, and $\varphi_{\pm}$ is an angle of the vector $\mathbf{x} - \mathbf{x}_c^{\pm}$ measured from $x_2 = \pm 1/2$ to $x_1 = 1/2$. Using these coordinates, e.g., the values of $u_3(\mathbf{x})$ at the upper right corner are expressed as $u_3(\mathbf{x}(\sigma_+ = 0, \varphi_+))$. Thus, its possible multivaluedness can be appropriately taken into account as its dependence on the angle φ_+ .

Substituting the expression of the VDF ϕ in terms of u_3 that is mentioned in the part before (9) into (3b), we obtain the following expression of the stress components P_{13} and P_{23} in terms of u_3 :

$$\begin{aligned} \begin{bmatrix} P_{13}(\mathbf{x}) \\ P_{23}(\mathbf{x}) \end{bmatrix} &= \frac{1}{k\pi} \int_{\Omega_R} \begin{bmatrix} G^{(P_{13})}(\mathbf{x}_* - \mathbf{x}) + G^{(P_{13})}(\mathbf{x}_* - \bar{\mathbf{x}}) \\ G^{(P_{23})}(\mathbf{x}_* - \mathbf{x}) + G^{(P_{23})}(\mathbf{x}_* - \bar{\mathbf{x}}) \end{bmatrix} u_3(\mathbf{x}_*) d\mathbf{x}_* \\ &\quad - \frac{2u_w}{\pi} \int_{-1/2}^{1/2} \frac{(1/2 - x_2)}{|\mathbf{x}_*^{(U)} - \mathbf{x}|^2} \\ &\quad \times \begin{bmatrix} (x_{1*} - x_1) |\mathbf{x}_*^{(U)} - \mathbf{x}|^{-1} J_2(|\mathbf{x}_*^{(U)} - \mathbf{x}|/k) \\ (1/2 - x_2) |\mathbf{x}_*^{(U)} - \mathbf{x}|^{-1} J_2(|\mathbf{x}_*^{(U)} - \mathbf{x}|/k) \end{bmatrix} dx_{1*}. \end{aligned} \quad (15)$$

Here,

$$G^{(P_{i3})}(\mathbf{z}) = -\frac{2z_i}{|\mathbf{z}|} J_1\left(\frac{|\mathbf{z}|}{k}\right) \quad (i = 1, 2). \quad (16)$$

Once the flow velocity field u_3 is obtained by solving (9), P_{13} and P_{23} can be obtained immediately by (15).

III. STOKES AND FREE MOLECULAR SOLUTIONS

Before proceeding to numerical analysis of the integral equation (9), we give the Stokes solution and the solution in the free molecular

limit ($k \rightarrow \infty$). Note that the qualitative behavior of the stress near the corner for the Stokes solution is same as that in Taylor's scraping flow.^{10,11} However, we need more information, namely, an accurate quantitative solution not only near the corner but also in the bulk region, as we will extensively use it later in Sec. V. Unfortunately, the simple series solution, which can be obtained by a standard way, thanks to the simplicity of the Stokes equation and the geometry, is not available for our purpose due to its disadvantages near the boundaries. The remaining option to have satisfactory results is extracting the singularity in the solution near the corner successfully and obtaining the remainder of solution numerically. The former is achieved by introducing suitable functions [(20) and (22) appearing later]. After the explanation of the procedure, we explicitly confirm the multivaluedness of the flow velocity and the divergence of the stress in the Stokes solution (Sec. III A). In the free molecular solution, while the flow velocity is still multivalued, the shear stress and accordingly the forces acting on the bodies are bounded (Sec. III B).

A. Stokes solution

The Stokes solution in the present problem can be sought under the assumption that the flow is unidirectional and there is no pressure gradient. Thus, the Stokes equation reduces to the Laplace's equation for the flow velocity u_3 ,

$$\Delta u_3 = 0 \quad \left(|x_1| < \frac{1}{2}, |x_2| < \frac{1}{2} \right). \quad (17)$$

Here, Δ is the Laplacian, i.e., $\Delta = \partial_{x_1}^2 + \partial_{x_2}^2$. The no-slip boundary conditions are given by

$$u_3 = u_w \quad \left(x_2 = \frac{1}{2}, |x_1| < \frac{1}{2} \right), \quad (18a)$$

$$u_3 = 0 \quad \left(x_2 = -\frac{1}{2}, |x_1| < \frac{1}{2} \right), \quad (18b)$$

$$u_3 = 0 \quad \left(x_1 = \pm \frac{1}{2}, |x_2| < \frac{1}{2} \right). \quad (18c)$$

The stress components P_{13} and P_{23} are given in terms of u_3 based on the Newton's law and the expression of the viscosity for the BGK model:

$$P_{13}(x_1, x_2) = -k \frac{\partial u_3}{\partial x_1}, \quad P_{23}(x_1, x_2) = -k \frac{\partial u_3}{\partial x_2}. \quad (19)$$

Note that k is defined in (1e).

For the system, (17) and (18), defined in the square domain, a series solution can be easily obtained by the separation of variables. However, this series converges slowly near the corner due to the mismatch between the boundary conditions (18a) and (18c) at the upper corners $(x_1, x_2) = (\pm 1/2, 1/2)$. Moreover, it is convergent but not absolutely convergent on the lid (including its part near the corner), and the series corresponding to the stress obtained by term-by-term differentiation is not convergent on the lid. Incidentally, corresponding properties of a series solution are pointed out in Ref. 31 for the paintbrush problem whose setting is similar to the present one and is given by replacing the square cavity considered here with an infinitely deep rectangular cavity. The simple series solution is not suitable for the present work that focuses on the behavior of the gas near the corner.

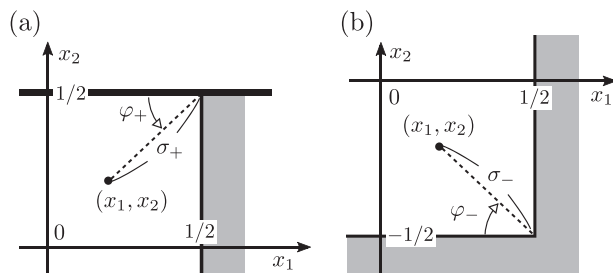


FIG. 2. Plane polar coordinates with its origin at a corner. (a) (σ_+, φ_+) and (b) (σ_-, φ_-) .

Hence, we will construct the solution in a different way as explained below.

To start with, note that the Laplacian is given as $\Delta = \partial_{\sigma_+}^2 + \sigma_+^{-1} \partial_{\sigma_+} + \sigma_+^{-2} \partial_{\varphi_+}^2$ when we use the polar coordinates with its origin at the upper right corner, σ_+ and φ_+ [see Fig. 2(a) and (14)]. Thus, in terms of a simple linear function,

$$B(\varphi_+(\mathbf{x})) = \frac{2}{\pi} \left(\frac{\pi}{2} - \varphi_+(\mathbf{x}) \right), \quad (20)$$

it is easily seen that $u_w B(\varphi_+(\mathbf{x}))$ satisfies Eq. (17) in the domain Ω_R ($x_1 \geq 0$), the condition (18a) on the lid ($\varphi_+ = 0$), and the condition (18c) on the sidewall ($\varphi_+ = \pi/2$). [It does not satisfy the condition (18b) on the bottom wall.] Assuming that the function $u_w B$ well represents the behavior of the flow velocity field u_3 near the corner, we decompose u_3 into the following known part $u_3^\dagger$ and unknown part $u_3^\#$:

$$u_3(\mathbf{x}) = u_3^\dagger(\mathbf{x}) + u_3^\#(\mathbf{x}). \quad (21)$$

Here, the known part $u_3^\dagger(\mathbf{x})$ is defined by

$$u_3^\dagger(\mathbf{x}) = u_w B(\varphi_+(\mathbf{x})) S(\sigma_+(\mathbf{x})) \quad (x_1 \geq 0), \quad (22a)$$

$$S(z) = \begin{cases} \frac{e^{-1/(1-2z)}}{e^{-(1/2z)} + e^{-1/(1-2z)}} & \left(z < \frac{1}{2} \right), \\ 0 & \left(z \geq \frac{1}{2} \right), \end{cases} \quad (22b)$$

$$u_3^\dagger(x_1, x_2) = u_3^\dagger(-x_1, x_2) \quad (x_1 < 0). \quad (22c)$$

The radial function S chosen here is a smooth function decreasing from unity to zero on $0 \leq \sigma_+ \leq 1/2$ (see also Fig. 3). Note that the approximation, $u_3^\dagger$, agrees well with $u_w B$ near the corner. The unknown part $u_3^\#$ satisfies the following Poisson's equation, which is derived by substituting (21) into (17):

$$\Delta u_3^\# = -\Delta u_3^\dagger \quad \left(|x_1| < \frac{1}{2}, |x_2| < \frac{1}{2} \right). \quad (23)$$

The boundary conditions for $u_3^\#$ are derived similarly from (18), (21), and (22a):

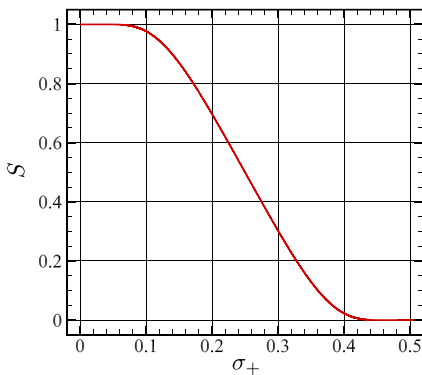


FIG. 3. The radial function $S(\sigma_+)$ given by (22b).

$$u_3^\# = u_w \left[1 - S\left(\frac{1}{2} - |x_1|\right) \right] \quad \left(x_2 = \frac{1}{2}, |x_1| < \frac{1}{2} \right), \quad (24a)$$

$$u_3^\# = 0 \quad \left(x_2 = -\frac{1}{2}, |x_1| < \frac{1}{2} \right), \quad (24b)$$

$$u_3^\# = 0 \quad \left(x_1 = \pm \frac{1}{2}, |x_2| < \frac{1}{2} \right). \quad (24c)$$

Note that (23) and (24) are the problem determining the unknown part $u_3^\#$.

Thanks to the present choice of B and S [see (20) and (22b)], the resulting problem for the remainder $u_3^\#$, (23) and (24), can be safely handled without singular factors.³² Indeed, $u_3^\#$ and the magnitude of its gradient $\nabla u_3^\#$ are both bounded, which is seen in Fig. 4. In the figure, the result numerically obtained by a standard second-order central finite difference scheme with a uniform grid consisting of 800×800 points is shown.³³

It can be confirmed from the numerical result that $u_3^\#$ approaches 0 as the corner is approached ($\sigma_+ \rightarrow +0$). In the meantime, $u_3^\dagger|_{\sigma_+=0} = u_w B(\varphi_+)$ depends on the angle φ_+ . Thus, $u_3 (= u_3^\dagger + u_3^\#)$ is multi-valued. Now, let us introduce the following circumferential component $P_{\varphi 3}$ of the stress:

$$P_{\varphi 3} = P_{13} \sin \varphi_+ - P_{23} \cos \varphi_+ = -\frac{k}{\sigma_+} \frac{\partial u_3}{\partial \varphi_+}. \quad (25)$$

Here, the differentiation with respect to φ_+ in the most right-hand side is carried out with σ_+ being fixed. From (25) and the decomposition (21) of the flow velocity field u_3 , $P_{\varphi 3}$ can be decomposed as

$$P_{\varphi 3} = P_{\varphi 3}^\dagger + P_{\varphi 3}^\#. \quad (26)$$

Here,

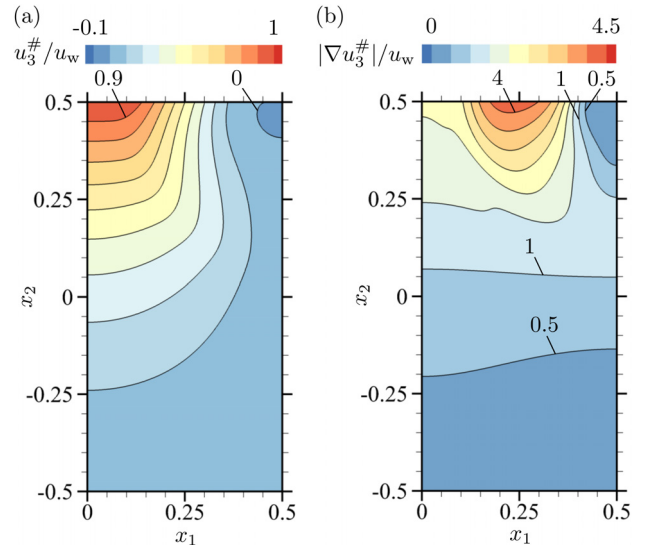


FIG. 4. Contour plots of the remainder part $u_3^\#$ for the Stokes solution and the magnitude of its gradient. (a) $u_3^\#/u_w$ and (b) $|\nabla u_3^\#|/u_w$. Since $u_3^\#$ and $|\nabla u_3^\#|$ are even in x_1 , their plots over $x_1 \geq 0$ is shown. In (a) and (b), the curves are drawn with intervals 0.1 and 0.5, respectively.

$$P_{\varphi 3}^{\dagger} = -\frac{k}{\sigma_+} \frac{\partial u_3^{\dagger}}{\partial \varphi_+}, \quad (27a)$$

$$P_{\varphi 3}^{\#} = P_{13}^{\#} \sin \varphi_+ - P_{23}^{\#} \cos \varphi_+, \quad (27b)$$

and $P_{13}^{\#}$ and $P_{23}^{\#}$ are defined by (19) with u_3 being replaced by $u_3^{\#}$. Since $\nabla u_3^{\#}$ is bounded [Fig. 4(b)], so is $P_{\varphi 3}^{\#}$. Meanwhile, since substituting (22a) into (27a) leads to the following relation:

$$P_{\varphi 3}^{\dagger} = \frac{2k}{\pi \sigma_+} S(\sigma_+) u_w \quad (28)$$

and $S \rightarrow 1$ as $\sigma_+ \rightarrow +0$, $P_{\varphi 3}^{\dagger}$ and accordingly $P_{\varphi 3} (= P_{\varphi 3}^{\dagger} + P_{\varphi 3}^{\#})$ diverge with the rate σ_+^{-1} as $\sigma_+ \rightarrow +0$. This inversely proportional rate is the same as that for the pressure field in the Taylor's scraping flow^{10,11} mentioned in the third paragraph of Sec. I.

The cavity has a corner also on the bottom ($x_1 = 1/2$, $x_2 = -1/2$). The aforementioned singular properties do not appear at this corner ($1/2, -1/2$) and the solution is smooth including there.³⁴ The difference in the effect of the corner on the behavior of the gas between top and bottom sides comes from that the velocity of the boundaries is discontinuous at the top corner while it is continuous at the bottom one.

Note that the divergence of the shear stress at the corner according to (28) occurs in exactly the same way when the generalized slip-flow theory,^{30,35–37} which is based on the asymptotic analysis of the Boltzmann system for small Knudsen numbers and enables the fluid-dynamic description of the behavior of a slightly rarefied gas for various physical situations, is applied to the present problem. This is because in the theory the steady behavior of the gas at the leading order of the Knudsen number expansion is described by the Stokes system under the no-slip conditions within the linearized regime, which is nothing but (17) and (18) for the present problem.³⁸ As the generalized slip-flow theory assumes that both the boundary shape and the boundary data are smooth, which is not true for the present problem, an extension of the theory to the case where these assumptions are not made is required to avoid the difficulty within its framework. Note that such kind of analysis is carried out in Refs. 39 and 40 for the problem of a gas flow between two parallel plates with a discontinuous wall temperature. In the references, it is shown that the conventional generalized slip-flow theory breaks down near the point where the surface temperature is discontinuous, and how it can be extended is illustrated.

We close the present subsection by providing a summary of its key points. To obtain the Stokes solution, we introduced its decomposition as $u_3 = u_3^{\dagger} + u_3^{\#}$ [see (21)]. The singular behavior near the upper corner was well represented by the part $u_3^{\dagger}$, which was constructed by combining the functions representing its angular and radial dependence [see (20) and (22)]. The remainder $u_3^{\#}$ was obtained numerically without any difficulty. The results for the total flow velocity field $u_3 = u_3^{\dagger} + u_3^{\#}$ and the corresponding shear stress field $P_{\varphi 3} = P_{\varphi 3}^{\dagger} + P_{\varphi 3}^{\#}$ shall be used later in Sec. V. The divergence of the stress was confirmed based on the behavior of $P_{\varphi 3}^{\dagger}$ [see (28)].

B. Free molecular solution

In the free molecular limit ($k \rightarrow \infty$), the VDF ϕ obeys the simple equation given by (4) with its right-hand side being dropped. This can be easily solved under the boundary conditions (5a)–(5c) to yield

$$\frac{\phi(\mathbf{x}, \zeta)}{u_w} = \begin{cases} 2\zeta_3 & [\theta_R(\mathbf{x}) \leq \theta_{\zeta} \leq \theta_L(\mathbf{x})] \\ 0 & (\text{otherwise}) \end{cases}, \quad (29a)$$

$$\frac{u_3(\mathbf{x})}{u_w} = \frac{1}{2\pi} [\theta_L(\mathbf{x}) - \theta_R(\mathbf{x})], \quad (29b)$$

$$\frac{P_{13}(\mathbf{x})}{u_w} = -\frac{1}{2\sqrt{\pi}} [\sin \theta_L(\mathbf{x}) - \sin \theta_R(\mathbf{x})], \quad (29c)$$

$$\frac{P_{23}(\mathbf{x})}{u_w} = \frac{1}{2\sqrt{\pi}} [\cos \theta_L(\mathbf{x}) - \cos \theta_R(\mathbf{x})]. \quad (29d)$$

Here, θ_{ζ} is the angle of the vector $(-\zeta_1, -\zeta_2)$ and $\theta_R(\mathbf{x})$ and $\theta_L(\mathbf{x})$ are those of the vectors $(1/2 - x_1, 1/2 - x_2)$ and $(-1/2 - x_1, 1/2 - x_2)$, respectively, which start at $\mathbf{x}$ and terminate at right upper and left upper corners (see also Fig. 5). These angles are measured counter-clockwise from the x_1 direction. Note that $\theta_R(\mathbf{x}) = \varphi_+(\mathbf{x})$ [see also Fig. 2(a)]. In the right-hand side of (29a), the upper row represents the contribution of the molecules coming from the moving lid surface ($x_2 = 1/2$), and the lower row represents that of the molecules coming from the resting cavity wall surfaces. From this and (29b), we see that the value of $u_3(\mathbf{x})/u_w$ is equal to the proportion of the contribution from the former over the whole molecules, when measured by the range of the angle θ_{ζ} .

As is seen from the expressions (29c) and (29d), the stress is bounded in the case of the free molecular limit, which contrasts with its divergence in the Stokes solution. Since $\theta_R(\mathbf{x}) = \varphi_+(\mathbf{x})$ and $\theta_L(\mathbf{x}) \rightarrow \pi$ as $\sigma_+ \rightarrow +0$, from (29b), we have

$$\frac{u_3(\mathbf{x})}{u_w} \rightarrow \frac{1}{2\pi} [\pi - \varphi_+(\mathbf{x})] \quad \text{as } \sigma_+ \rightarrow +0. \quad (30)$$

Thus, the flow velocity u_3 is multivalued at the corner also in the free molecular solution. Taking (29a) and its explanation in the previous paragraph into account as well, we see that the multivaluedness occurs because u_3 is determined by the proportion of the contribution of the molecules coming from the lid that depends on the azimuthal angle φ_+ , and this feature remains the same when the corner is approached ($\sigma_+ \rightarrow +0$). The φ_+ component of the gradient of u_3 , i.e., $\sigma_+^{-1} \partial_{\varphi_+} u_3$, diverges as $\sigma_+ \rightarrow +0$. Note that this divergence does not contradict the boundedness of the stress since the stress is not expressed by the velocity gradient in the kinetic framework. Incidentally, as in the case of the Stokes solution, u_3 is not multivalued at the bottom right corner. Indeed, as $(x_1, x_2) \rightarrow (1/2, -1/2)$, $\theta_L(\mathbf{x}) \rightarrow 3\pi/4$ and $\theta_R(\mathbf{x}) \rightarrow \pi/2$, accordingly $u_3/u_w \rightarrow 1/8$.

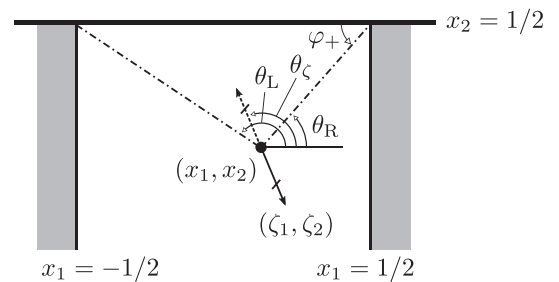


FIG. 5. The angles θ_{ζ} , θ_R , and θ_L occurring in Eq. (29). Note that $\theta_R = \varphi_+$.

IV. NUMERICAL METHOD

The integral equation (9) for the flow velocity field $u_3(\mathbf{x})$ can be solved by the method of successive approximation. Namely, starting from some initial guess $u_3^0(\mathbf{x})$, we construct a sequence $\{u_3^n\}$ by the following recurrence formula:

$$u_3^n(\mathbf{x}) = A[u_3^{n-1}](\mathbf{x}) + u_w b(\mathbf{x}) \quad (n = 1, 2, \dots) \quad (31)$$

corresponding to (9). The solution of (9) is obtained as the limit of the sequence. The actual computation is carried out by following Refs. 27–29.

A. Discretization and some details of computation

In the present work, we aim to accurately capture the variation of the solution including near the corner and to appropriately take the possible multivaluedness of the quantities there into account. For this purpose, we use a hybrid grid system consisting of the Cartesian grid system and the polar grid system near the corner based on the coordinates (14).

We divide the region Ω_R (or $0 \leq x_1 \leq 1/2, -1/2 \leq x_2 \leq 1/2$) by $2N_1 + 1$ straight lines $x_1 = \chi_1^{(i)}$ ($i = 0, 1, \dots, 2N_1$) and $4N_2 + 1$ straight lines $x_2 = \chi_2^{(j)}$ ($j = -2N_2, -2N_2 + 1, \dots, 2N_2$). We also consider the circular sector regions with its center at the corners $(1/2, \pm 1/2)$ and given radius $\sigma_{\max}$, $0 \leq \sigma_{\pm} \leq \sigma_{\max}$, $0 \leq \varphi_{\pm} \leq \pi/2$ (hereafter denoted by $F_{\pm}$). We divide them by $2N_{\sigma}$ arcs $\sigma_{\pm} = \sigma^{(k)}$ ($k = 1, \dots, 2N_{\sigma}$) and $4N_{\varphi} + 1$ radial lines $\varphi_{\pm} = \varphi^{(\ell)}$ ($\ell = -2N_{\varphi}, -2N_{\varphi} + 1, \dots, 2N_{\varphi}$) (see also Fig. 6). Here, $\{\chi_1^{(i)}\}$, $\{\chi_2^{(j)}\}$, $\{\sigma^{(k)}\}$, and $\{\varphi^{(\ell)}\}$ are numerical sequences such that

$$0 = \chi_1^{(0)} < \chi_1^{(1)} < \dots < \chi_1^{(2N_1)} = \frac{1}{2}, \quad (32a)$$

$$0 = \chi_2^{(0)} < \chi_2^{(1)} < \dots < \chi_2^{(2N_2)} = \frac{1}{2}, \quad (32b)$$

$$\chi_2^{(j)} = -\chi_2^{(-j)} \quad (j = -2N_2, \dots, -1),$$

$$0 = \sigma^{(0)} < \sigma^{(1)} < \dots < \sigma^{(2N_{\sigma})} = \sigma_{\max}, \quad (32c)$$

$$0 = \varphi^{(-2N_{\varphi})} < \varphi^{(-2N_{\varphi}+1)} < \dots < \varphi^{(2N_{\varphi})} = \frac{\pi}{2}. \quad (32d)$$

The value $\sigma^{(0)} = 0$ corresponding to the corners is added to the sequence $\{\sigma^{(k)}\}$. The region Ω_R can be divided in units of the rectangular cell consisting of 3×3 points inside the Cartesian mesh $\chi_1^{(2\alpha-2)} \leq x_1 \leq \chi_1^{(2\alpha)}, \chi_2^{(2\beta-2)} \leq x_2 \leq \chi_2^{(2\beta)}$ ($\alpha = 1, 2, \dots, N_1; \beta = -N_2 + 1, -N_2 + 2, \dots, N_2$). We denote by G the set of all cells such that the intersection of them and the exteriors of $F_{\pm}$ is not empty. A part of the boundary of G has a stepwise shape and is included in $F_{\pm}$. By gathering the Cartesian grid points in the region G and the polar grid points in the regions F_+ and F_- and by assigning numbers to them, we have the grid points $\mathbf{x}^{(I)}$ used in computation ($I = 1, 2, \dots, N$; N : total number of grid points). By distinguishing and storing the values of quantities at $\sigma_{\pm} = \sigma^{(0)} = 0$, $\varphi_{\pm} = \varphi^{(\ell)}$ ($\ell = -2N_{\varphi}, -2N_{\varphi} + 1, \dots, 2N_{\varphi}$), computation can be carried out with the aforementioned multivaluedness at the corners being properly taken into account.

To carry out the iteration corresponding to (31), we need to do the numerical integration to compute the integral $A[u_3^{n-1}](\mathbf{x}^{(I)})$ from the known data of u_3^{n-1} on the grid points. For this purpose, first, we split the computational domain Ω_R into the circular sector regions F_+ and F_- and the rest $[\Omega_R = F_+ \cup F_- \cup (F_+ \cup F_-)^c]$. Then, given the

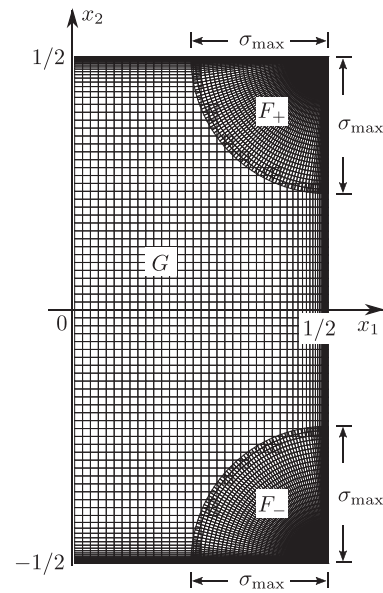


FIG. 6. Sketch of the grid system.

data $\{u_3^{n-1}(\mathbf{x}^{(I)})\}$, $u_3^{n-1}(\mathbf{x}_*)$ is approximated piecewise quadratically with respect to variables σ_+ and φ_+ (or σ_- and φ_-) on F_+ (or F_-) and with respect to variables x_1 and x_2 on $(F_+ \cup F_-)^c$. Respective domains F_+ , F_- , and $(F_+ \cup F_-)^c$ are further divided in units of polar or rectangular grid cells consisting of 3×3 points.⁴¹ To get rid of the singularity $|\mathbf{x}_* - \mathbf{x}|^{-1}$ contained in the integrand in $A[u_3]$ [see also (10) and (11)], we take another polar coordinate variables (denoted by $\hat{r}$ and ϑ) with its origin at the focused point $\mathbf{x}^{(I)}$. This enables accurate calculation on each divided region. The interval of $\hat{r}$ is further divided at the radial positions where a circle $\hat{r} = \text{const.}$ passes through the vertices or is tangent to the sides of each divided region. The each interval of $\hat{r}$ is finally divided equally into $K_{\hat{r}}$ subintervals. On each small domains so prepared, the integrations with respect to $\hat{r}$ and ϑ are carried out numerically by applying the $M_{\hat{r}}$ - and M_{ϑ} -points Gauss-Legendre rules. The results can be stored as a coefficient matrix (denoted by $\mathcal{A}_{I,J}$) beforehand. Then, the required integral $A[u_3^{n-1}](\mathbf{x}^{(I)})$ can be obtained by computing the weighted sum: $A[u_3^{n-1}](\mathbf{x}^{(I)}) \simeq \sum_{J=1}^N \mathcal{A}_{I,J} u_3^{n-1}(\mathbf{x}^{(J)})$.

Based on the plan and the way to compute $A[u_3^{n-1}]$ explained, respectively, at the beginning of Sec. IV and the previous paragraph, we carry out the actual computation as follows. First, normalize the solution by u_w and set its initial value $\{u_3^0(\mathbf{x}^{(I)})/u_w\}$. Then, compute $u_3^n(\mathbf{x}^{(I)})/u_w$ ($I = 1, 2, \dots, N$) successively by the following equation [see also (31)]:

$$\frac{u_3^n(\mathbf{x}^{(I)})}{u_w} = \sum_{J=1}^N \mathcal{A}_{I,J} \frac{u_3^{n-1}(\mathbf{x}^{(J)})}{u_w} + b(\mathbf{x}^{(I)}) \quad (n = 1, 2, \dots). \quad (33)$$

The stress components P_{13} and P_{23} are obtained by carrying out the numerical integration corresponding to (15) in the same way as in the previous paragraph after the numerical solution of u_3 is obtained.

Information on the values of parameters and accuracy is briefly given in the Appendix.

V. NUMERICAL RESULTS AND DISCUSSION

First, we show the profiles of macroscopic quantities for representative Knudsen numbers to grasp the overall behavior of the gas in Sec. V A. Then, we proceed to examine the behavior near the corner for small Knudsen numbers and the forces acting on the lid and the cavity walls in Secs. V B and V C, which are the main parts of the present paper.

A. Macroscopic quantities in whole cavity

In Fig. 7, we show the contour plots of the flow velocity component u_3/u_w for $k = 0.01, 1$, and 10 in the whole right half of the cavity [note that $k = (\sqrt{\pi}/2)\text{Kn}$ as defined in (1e) and we shall use the parameter k instead of the Knudsen number Kn]. As the figure implies, a flow is induced in the direction of lid motion. For all cases shown in the figure, the flow speed is faster near the lid ($x_2 \rightarrow +1/2$) with the horizontal position x_1 being fixed and faster at the central part of the cavity ($x_1 \rightarrow 0$) with the vertical position x_2 being fixed. The velocity slip on the lid, namely, the difference between the velocity of the gas and the lid, is larger for larger Knudsen numbers.

While the shear stress is spatially uniform in one-dimensional slow Couette flow between two parallel walls, in this time, naturally spatial variation of the stress is observed because of the presence of sidewalls (see Figs. 8 and 9). For all cases shown in the figure, the magnitude of the stress is larger near the boundary. The magnitudes of P_{13} and P_{23} are particularly large on the sidewall and on the lid, respectively [see, e.g., Figs. 8(c) and 9(c)]. For the case of small Knudsen number ($k = 0.01$), the magnitude of the shear stress in the bulk region away from the boundary is smaller than those for the larger Knudsen numbers ($k = 1$ and 10). According to Figs. 8(a) and 9(a), the magnitudes of P_{13}/u_w and P_{23}/u_w in the bulk region are, respectively, less than 0.05 and 0.06 . They can be regarded as $O(k)$, which is plausible since the magnitude of the stress obtained from the Newton's law and a smooth velocity field is also $O(k)$ [see (19)].

B. Macroscopic quantities near corner for small Knudsen numbers and its comparison with Stokes solution

As clearly indicated in Figs. 7–9, all the macroscopic quantities vary steeply near the corner between the lid and the sidewall. This tendency is significant for smaller Knudsen numbers [for example, compare Figs. 7(c), 7(b), and 7(a)]. Thus, we focus on the case for $k = 0.01$ and try to understand the behavior of the gas near the corner in more detail. Simultaneously, the result is compared to the Stokes solution in Sec. III A. Figure 10 shows the contour plots of the macroscopic quantities u_3/u_w , P_{13}/u_w , P_{23}/u_w in the region $0.45 \leq x_{1,2} \leq 0.5$ for both the Stokes and the BGK solutions.⁴²

For the Stokes solution, the contour lines of u_3/u_w are emitted radially from the corner [Fig. 10(a)]. There is no contour line impinging to the lid $x_2 = 1/2$ and the sidewall $x_1 = 1/2$ since the solution is constant along the surfaces owing to the no-slip condition. On the other hand, for the BGK solution [Fig. 10(d)] some contour lines impinge to the boundaries. Although the Knudsen number considered is fairly small ($k = 0.01$), the results imply that the kinetic theory gives a significantly different result compared to the Stokes solution. The magnitude of velocity slip is larger than 0.2 over part of the lid ($0.49 \leq x_1 \leq 0.5$, $x_2 = 1/2$) and the sidewall ($0.49 \leq x_2 \leq 0.5$, $x_1 = 1/2$). This is evidently larger than the magnitude of the velocity slip observed over positions away from the corner, which is $O(k)$ [see, e.g., the plots over $\sigma_+ \geq 0.2$ in Figs. 11(a) and 11(b) appearing later]. The large slip is one of the features of the behavior of the gas near the corner. The related things are further examined later in Figs. 11 and 12.

In Figs. 10(b) and 10(c), we show the stress components for the Stokes solution. The contour lines that are the closest to the corner are the ones with the maximum magnitude level among the drawn lines (the corresponding values are $P_{13}/u_w = 0.45$, $P_{23}/u_w = -0.6$). In the regions enclosed by these lines and the boundaries, the magnitude of P_{13} and P_{23} does not saturate but increases infinitely as the corner is

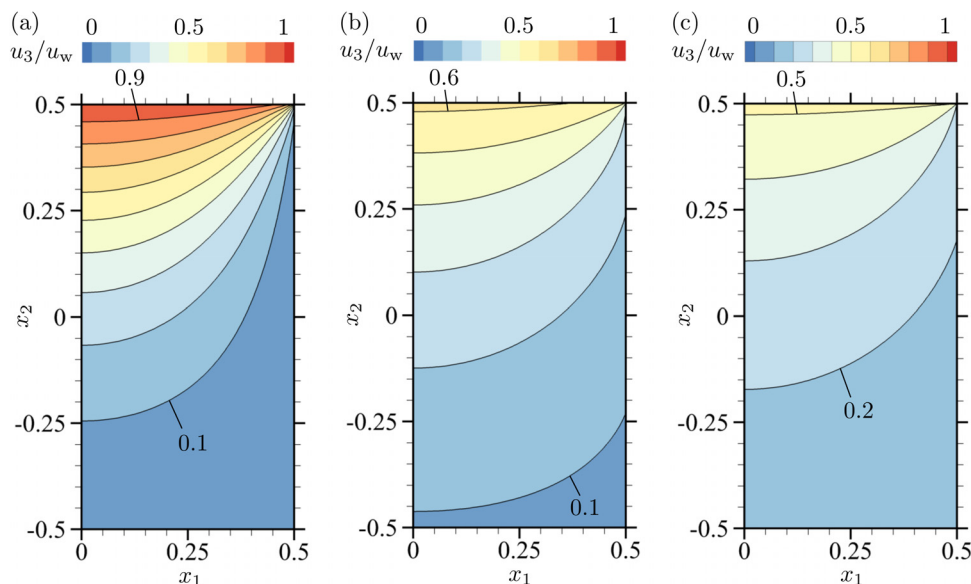


FIG. 7. Contour plots of the flow velocity component u_3/u_w on the x_1x_2 plane. The curves are drawn with intervals of 0.1 . (a) $k = 0.01$, (b) $k = 1$, and (c) $k = 10$.

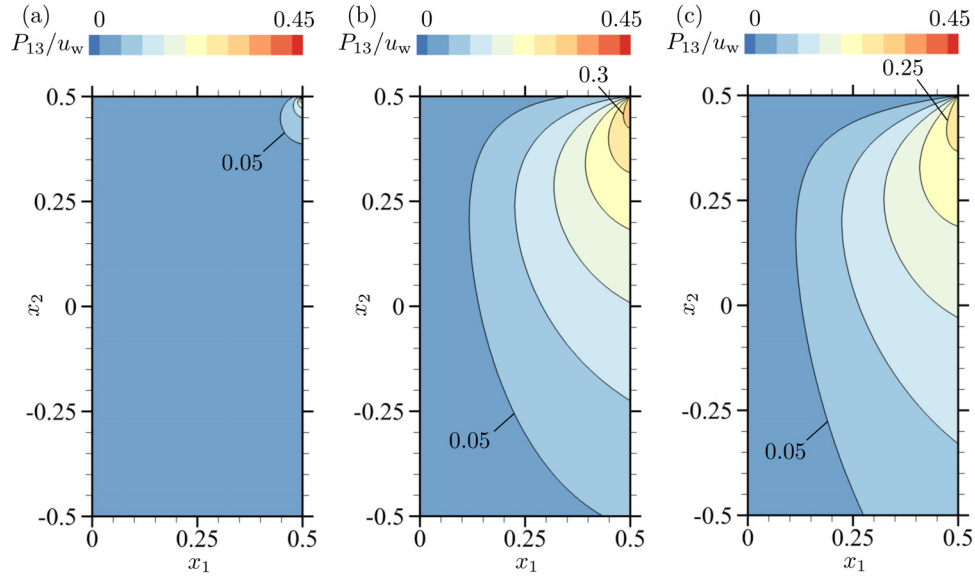


FIG. 8. Contour plots of the stress component P_{13}/u_w on the x_1x_2 plane. The curves are drawn with intervals of 0.05. (a) $k = 0.01$, (b) $k = 1$, and (c) $k = 10$.

approached as explained in the paragraph including (28) in Sec. III A. In contrast to this, in the case of BGK solution, P_{13} and P_{23} are bounded [see Figs. 10(e) and 10(f)] as in the case of the free molecular limit in Sec. III B. The magnitudes of P_{13}/u_w and P_{23}/u_w are both less than 0.445 in the whole region including the corner. Thus, although what we examine here is the result for only one specific case $k = 0.01$, it implies that the problem of stress divergence exhibited by the Stokes solution is resolved in the description based on the kinetic theory. The relevant results for smaller Knudsen numbers are shown later in

Figs. 11 and 12. The magnitude of P_{13}/u_w and P_{23}/u_w shown in Figs. 10(e) and 10(f) is significantly larger than $O(k)$ expected from the Newton's law [see, e.g., the plots over $\sigma_+ \geq 0.2$ in Figs. 11(c) and 11(d) appearing later]. This is also a feature of the behavior of the gas near the corner compared to that away from there.

In Fig. 11, the profiles of the flow velocity and the stress for $k = 0.1, 0.01$, and 0.001 along the direction of the angle $\varphi_+ = 0$ and $\pi/2$, which correspond to the lid surface and the sidewall, respectively [see also Fig. 2(a)], are shown as functions of the distance σ_+ . As for

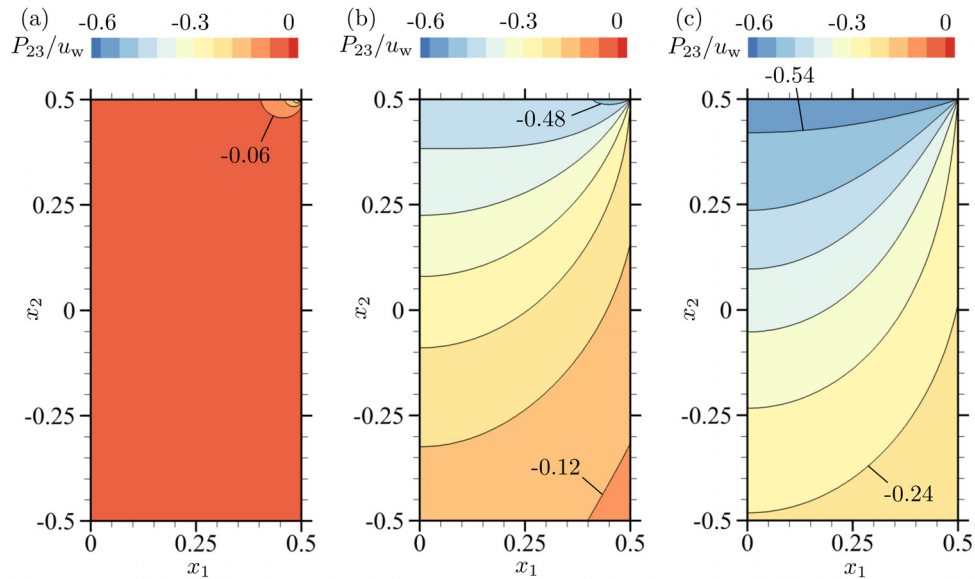


FIG. 9. Contour plots of the stress component P_{23}/u_w on the x_1x_2 plane. The curves are drawn with intervals of 0.06. (a) $k = 0.01$, (b) $k = 1$, and (c) $k = 10$.

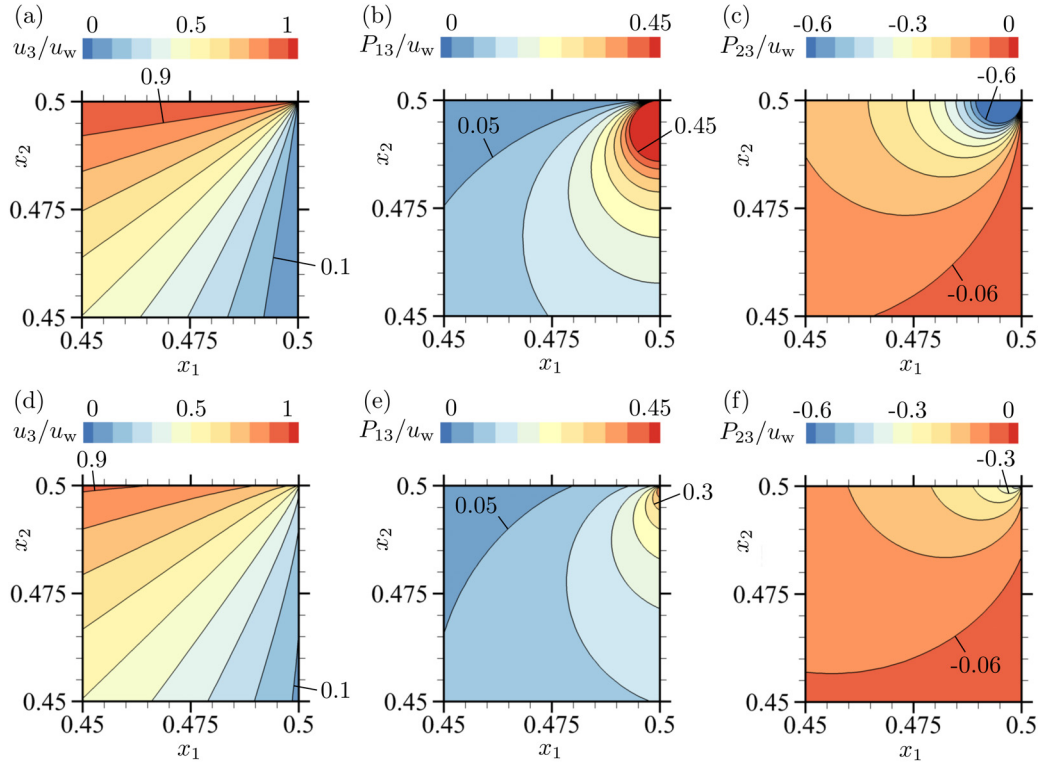


FIG. 10. Contour plots of the macroscopic quantities near the corner $(1/2, 1/2)$ for the Stokes and BGK solutions with $k=0.01$. (a) u_3/u_w (Stokes), (b) P_{13}/u_w (Stokes), (c) P_{23}/u_w (Stokes), (d) u_3/u_w (BGK), (e) P_{13}/u_w (BGK), and (f) P_{23}/u_w (BGK). The curves are drawn with intervals 0.1, 0.05, and 0.06 in (a) and (d), (b) and (e), and (c) and (f), respectively.

the stress, its circumferential component $P_{\phi 3}$ associated with the coordinates (σ_+, φ_+) is plotted [see also (25) and $P_{\phi 3} = -P_{23}(\varphi_+ = 0)$, $P_{\phi 3} = P_{13}(\varphi_+ = \pi/2)$]. From Fig. 11(a) [or Fig. 11(b)], it is seen that, while u_3/u_w for $\varphi_+ = 0$ (or $\varphi_+ = \pi/2$) approaches toward the value unity (or zero) of the Stokes solution specified by the no-slip condition in overall region as k decreases, it approaches to the value 0.625... (or 0.375...) near $\sigma_+ = 0$ for the cases with any k shown in the figures. While the stress $P_{\phi 3}/u_w$ is $O(k)$ for large σ_+ and also agrees well with the Stokes solution for $k=0.01$ and 0.001 [Figs. 11(c) and 11(d)], the BGK solution approaches an $O(1)$ value 0.443... near $\sigma_+ = 0$ for the cases with any k shown in the figures. The results imply that the magnitude of velocity slip and stress remains $O(1)$ near the corner irrespective of k .

The spatial variations of the macroscopic quantities observed in Fig. 11 can be understood clearer by changing a length scale used in plot from the cavity size to a length of the order of the mean free path. With such a length scale, we show the plots of u_3/u_w and $P_{\phi 3}/u_w$ with the angle being fixed at $\varphi_+ = 0$ (corresponding to the lid surface) in Figs. 12(a) and 12(b) and their contour plots in Figs. 12(c) and 12(d). The plot curves for various k converge to a common one. This demonstrates the emergence of a characteristic region near the corner with its size of the order of the mean free path when the Knudsen number is small.

Before ending this subsection, to examine whether the macroscopic quantities are multivalued or not, we show u_3/u_w and $P_{\phi 3}/u_w$

for $k=0.01$ as functions of the angle φ_+ with the distance σ_+ being fixed at several values. Although the slope of curves for the BGK solution is small due to the velocity slip compared to the case of the Stokes solution, the plot curves for the former also converge to the nonconstant profile as $\sigma \rightarrow +0$ in Fig. 13(a). This means that the flow velocity is multivalued not only in the Stokes solution but also in the kinetic solution. The multivaluedness is observed also for the stress field [Fig. 13(b)].

The origin of the multivaluedness is in fact similar to that in the case of the free molecular solution, which was explained in the last paragraph in Sec. III B. Let us explain the reason below, starting from (9). The flow velocity component consists of $A[u_3]$ and $u_w b$: $u_3(\mathbf{x}) = A[u_3](\mathbf{x}) + u_w b(\mathbf{x})$. At the corner $(x_1, x_2) = (1/2, 1/2)$, $A[u_3](\mathbf{x})$ is not multivalued,⁴³ which can also be confirmed from the numerical results. On the other hand, as for $b(\mathbf{x})$ [see (12)], introducing the change of variable from x_{1*} to ψ defined by $x_{1*} - x_1 = (1/2 - x_2)/\tan \psi$, we have

$$\begin{aligned} b(\mathbf{x}) &= \frac{1}{\pi} \int_{\theta_R(\mathbf{x})}^{\theta_L(\mathbf{x})} J_1 \left(\frac{1/2 - x_2}{k \sin \psi} \right) d\psi \\ &= \frac{1}{\pi} \int_{\varphi_+}^{\theta_L(\mathbf{x})} J_1 \left(\frac{\sigma_+ \sin \varphi_+}{k \sin \psi} \right) d\psi \\ &\rightarrow \frac{1}{\pi} \int_{\varphi_+}^{\pi} J_1(0) d\psi = \frac{\pi - \varphi_+(\mathbf{x})}{2\pi} \quad (\text{as } \sigma_+ \rightarrow +0). \end{aligned} \quad (34)$$

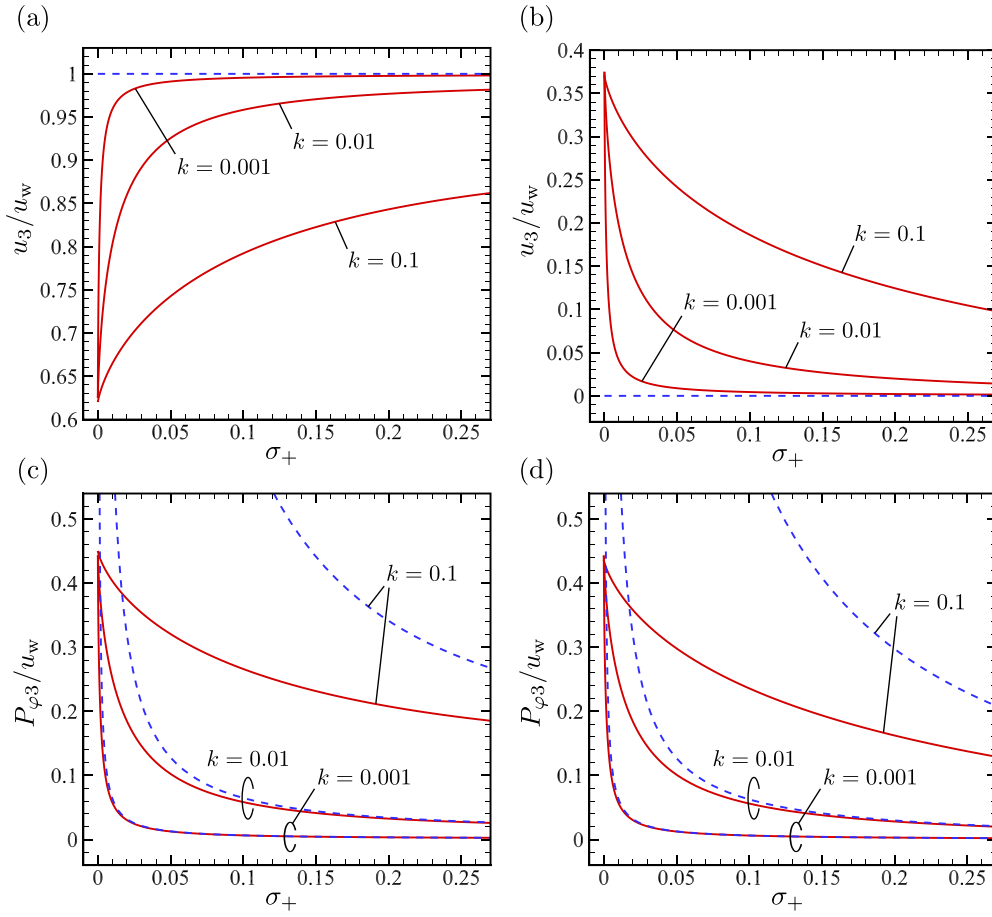


FIG. 11. Profiles of flow velocity and shear stress near the corner (1/2, 1/2) for $k=0.1, 0.01$, and 0.001 . (a) u_3/u_w for $\varphi_+ = 0$, (b) u_3/u_w for $\varphi_+ = \pi/2$, (c) $P_{\varphi 3}/u_w$ for $\varphi_+ = 0$, and (d) $P_{\varphi 3}/u_w$ for $\varphi_+ = \pi/2$. The solid and dashed lines indicate the BGK and Stokes solutions, respectively. The quantities are plotted as functions of σ_+ , the distance from the corner.

Here, we have used that $\theta_l(\mathbf{x}) \rightarrow \pi$ in taking the limit⁴⁴ $\sigma_+ \rightarrow +0$ and that $J_1(0) = 1/2$. From the most right-hand side of (34), we see that $b(\mathbf{x})$ at the corner is equal to the expression (30) for the free molecular solution. It can be confirmed, also, that the part of the VDF corresponding to $b(\mathbf{x})$ at the corner is given by the right-hand side of (29a) for the free molecular solution.⁴⁵ This corresponds to the situation that the molecules coming from the lid to the corner do not experience intermolecular collisions since their flight distance is zero (when $\sigma_+ \rightarrow +0$, the points on the lid where the molecules are scattered degenerate to the corner, the focused point $\mathbf{x}$ itself) and, thus, their behavior is free molecular.

C. Total forces acting on lid and cavity walls and local stress profile

Let us denote by $p_0 u_w L F_U$, $p_0 u_w L F_B$, and $p_0 u_w L F_R$ the total forces in the X_3 direction per unit length in X_3 acting on the lid, the bottom wall, and the right sidewall, respectively. Then, F_U , F_B , and F_R are given by

$$F_U = \int_{-1/2}^{1/2} \frac{P_{23}(x_1, 1/2)}{u_w} dx_1, \quad (35a)$$

$$F_B = - \int_{-1/2}^{1/2} \frac{P_{23}(x_1, -1/2)}{u_w} dx_1, \quad (35b)$$

$$F_R = \int_{-1/2}^{1/2} \frac{P_{13}(1/2, x_2)}{u_w} dx_2. \quad (35c)$$

Figure 14(a) shows F_U , F_B , and F_R as functions of k . All of them increase monotonically with k (or the Knudsen number Kn). The force acting on the sidewall is larger than that acting on the bottom wall for k smaller than about 2. For larger k , the latter becomes bigger than the former.

To provide the information of the magnitude of the forces for small Knudsen numbers, again F_U , F_B , and F_R are shown as functions of k in Fig. 14(b), but as a log-log plot. The force F_B acting on the bottom wall is practically proportional to k . Actually, the following relation:

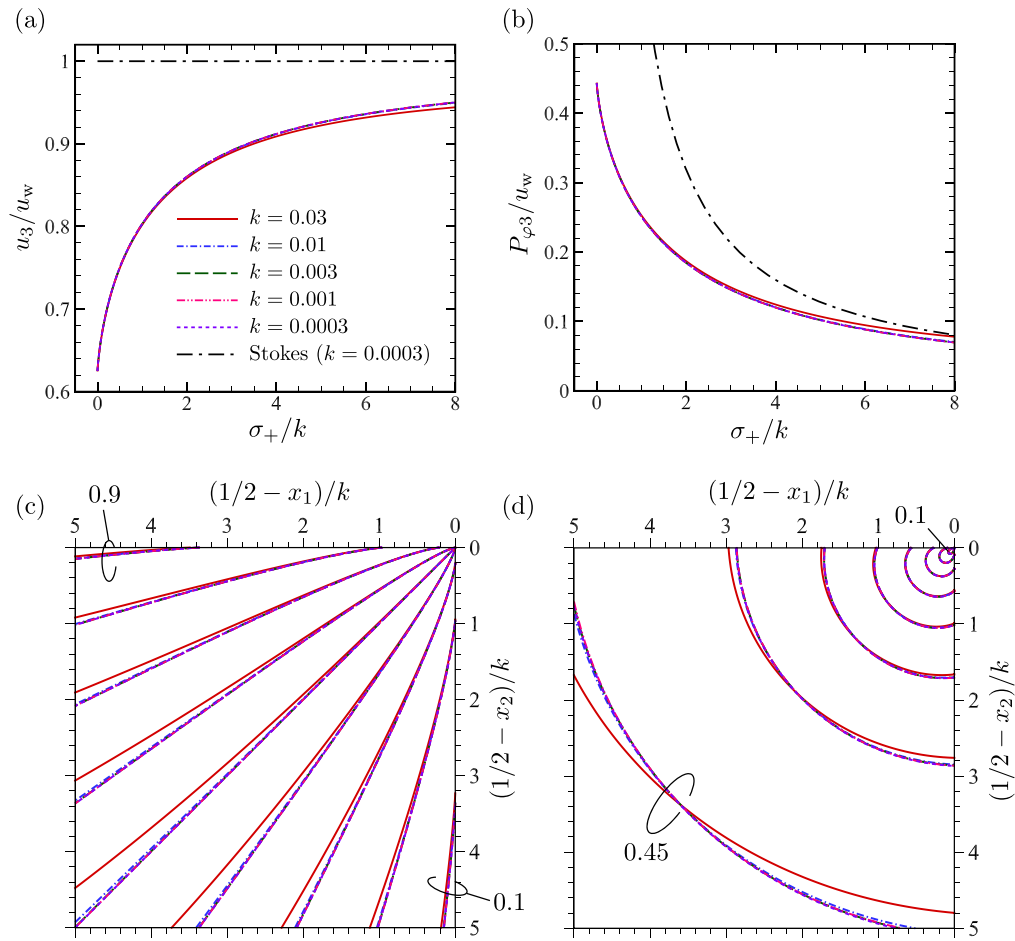


FIG. 12. Plots of macroscopic quantities for $k = 0.03, 0.01, 0.003, 0.001$, and 0.0003 . In (a) and (b), u_3/u_w and $P_{\phi 3}/u_w$ on the lid ($\varphi_+ = 0$) are plotted, respectively, as functions of σ_+/k , the rescaled distance from the corner $(1/2, 1/2)$. In (c) and (d), contour plots of u_3/u_w and $P_{\phi 3}/u_w$ vs $((1/2 - x_1)/k, (1/2 - x_2)/k)$, the position relative to the corner rescaled by k , are shown with the curves being drawn with intervals 0.1 and 0.05 , respectively. The types of lines used are common in (a)–(d) and see the line legend in (a). The Stokes solution is shown only in (a) and (b).

$$F_B \simeq 0.22k \quad (k \ll 1) \quad (36)$$

can be deduced based on the numerical results for $0.0002 \leq k \leq 0.01$.⁴⁶ This relation (36) can be also recovered by the Stokes solution in Sec. III A including the value 0.22 of the proportionality constant. Thus, the Stokes equation under the no-slip condition (and accordingly the conventional generalized slip-flow theory) can predict well the force acting on the bottom wall although the bottom wall meets corners between it and the sidewalls. This is consistent with that the effect of corners on the behavior of the gas is rather weak on the bottom side (see also the third last paragraph in Sec. III A). The good agreement between the BGK and the Stokes solutions at the bottom wall is observed also at the level of the local stress profile (see the plot curves for $k = 0.01$ and 0.001 in Fig. 15).

On the other hand, by closer examination of Fig. 14(b), we see that F_U and F_R are not simply proportional to k . To find how F_U and F_R depend on k , we show another plot in Fig. 14(c). We divide the quantity in the vertical axis of the original plot (here, $F_{U,B,R}$) by one

in the horizontal axis (here, k) and choose a semilog plot by following Ref. 47, where this type of plot is shown to examine spatial singularities of macroscopic quantities in boundary-value problems of a rarefied gas. The $-F_U/k$ and F_R/k increase as k decreases, and the symbols are almost on the straight lines in the plot. This implies that F_U and F_R behave like $k \ln k$ for small k . The dashed and dashed-dotted lines are the fitting curves determined by the method of least squares using the numerical results for k smaller than 0.01 . According to them

$$F_U \simeq 1.267k \ln k + 0.948k, \quad (37a)$$

$$F_R \simeq -0.634k \ln k - 0.584k. \quad (37b)$$

It should be noted that the factor $k \ln k$ in the solution cannot be actually recovered by the conventional generalized slip-flow theory based on the power series expansion in k , which implies its breakdown for the present problem (if it is applied, instead F_U and F_R diverge to infinity, see also the second last paragraph of Sec. III A).

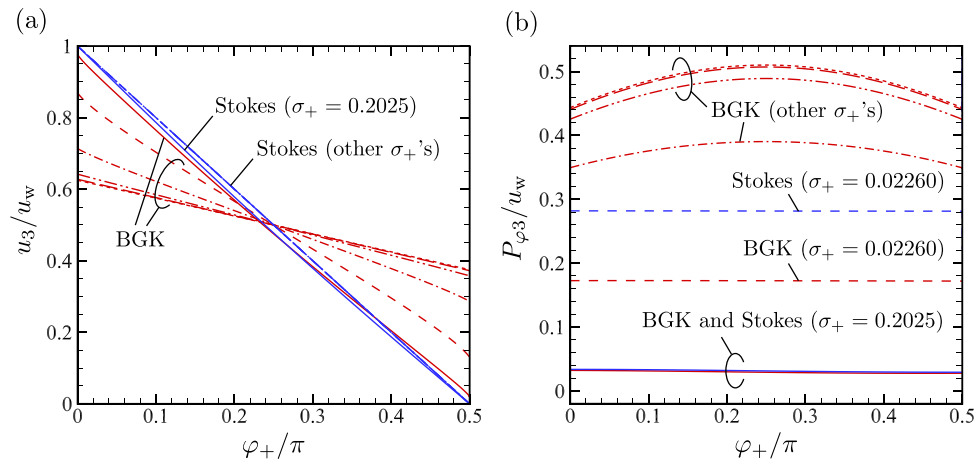


FIG. 13. Profiles of flow velocity and shear stress for the BGK and Stokes solutions with $k = 0.01$. (a) u_3/u_w and (b) $P_{\varphi 3}/u_w$. The quantities are plotted as functions of the azimuthal angle φ_+ with σ_+ , the distance from the corner $(1/2, 1/2)$, being fixed. The solid, dashed, dashed-dotted, dashed-double-dotted, long-dashed, and dotted lines indicate the results for $\sigma_+ = 0.2025, 0.02260, 2.771 \times 10^{-3}, 2.770 \times 10^{-4}, 2.778 \times 10^{-5}$, and 0, respectively.

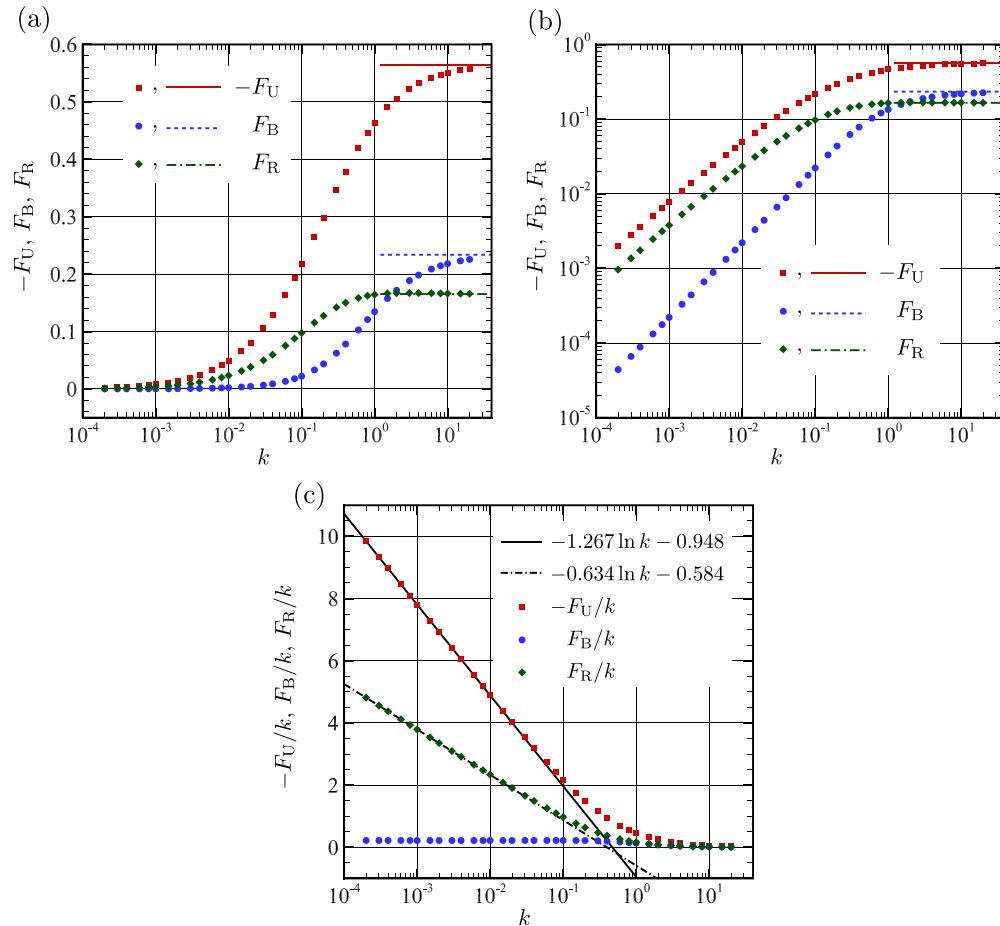


FIG. 14. The forces acting on the lid and the cavity walls. Plots related to F_U , F_B , and F_R as functions of k . (a) $(-F_U, F_B, F_R)$ in the semilog plot, (b) $(-F_U, F_B, F_R)$ in the log-log plot, and (c) $(-F_U/k, F_B/k, F_R/k)$ in the semilog plot. Horizontal lines in (a) and (b) indicate the free molecular solution, $(-F_U, F_B, F_R)|_{k \rightarrow \infty} = (1, \sqrt{2} - 1, 1 - 1/\sqrt{2})/\sqrt{\pi}$, which is obtained from (29c) and (29d).

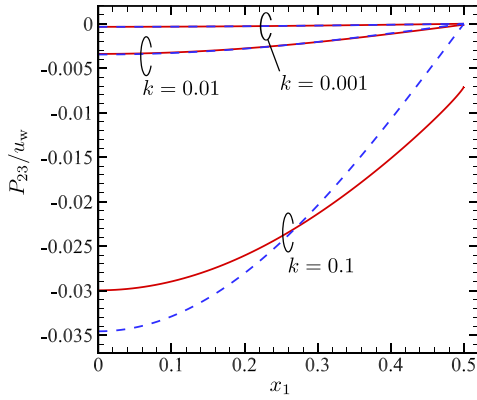


FIG. 15. Profiles of shear stress on the bottom cavity wall ($x_2 = -1/2$) for $k = 0.1$, 0.01 , and 0.001 . x_1 vs P_{23}/u_w . The solid and dashed lines indicate the BGK and Stokes solutions, respectively.

Let us consider next the reason why the factor $k \ln k$ appears in the forces F_U and F_R . For this purpose, the profiles of the stress on the lid are shown as a log–log plot in Fig. 16(a). The results for $k = 0.1$, 0.01 , 0.001 , and 0.0003 are shown as functions of the distance σ_+ from the corner. For small k (or the Knudsen number Kn), the magnitude of the stress increases inversely proportionally to σ_+ over a wide range from the position with $\sigma_+ = 0.1 \sim 0.2$ to the neighborhood of the corner. This corresponds to the fluid-dynamic behavior of the stress confirmed in the paragraph including (28) in Sec. III A. We show another plot with the distance σ_+ being rescaled by k in Fig. 16(b). It is seen from the figure that the BGK-solution curves overlap well up to larger σ_+/k as k becomes smaller and that the Stokes solution agrees well with the BGK solution up to $\sigma_+/k = 10$ or 20 . To summarize, Figs. 16(a) and 16(b) imply that the BGK solution practically increases inversely proportionally to the distance from the corner over the range from comparatively far position to the position that is a few tens of mean free paths away from there (for example, $\sigma_+ = ck$ with $c = 10$ or 20). Now, consider the integral of a function k/σ_+ on the interval deduced from the above-mentioned observations,

i.e., on $ck < \sigma_+ < x_0$ (x_0 : constant such as 0.1 or 0.2). Then, the factor $k \ln k$ appears since $\int_{ck}^{x_0} (k/\sigma_+) d\sigma_+ = -k \ln(ck) + k \ln(x_0)$. Thus, it is implied that the factor $k \ln k$ occurs because of the continuation of the above-mentioned fluid-dynamic stress increase up to the position that is only a few tens of mean free paths away from the corner and of the subsequent transition to another bounded profile at positions closer to the corner. Incidentally, although we have focused here on the stress profile and the total force on the lid, the corresponding property can be confirmed for the sidewall as well.

Finally, motivated by the fact that the local shear stress is larger near the corner compared to the part away from there [see, e.g., Figs. 11(c) and 12(b)], let us consider the proportion of the contribution from the stress over the neighborhood of the corner to the total force. For this purpose, we introduce the contribution from the stress over the part within distance $k\eta$ from the corner by

$$\mathcal{P}^U(k; \eta) = \int_{1/2-k\eta}^{1/2} P_{23}\left(z, \frac{1}{2}\right) dz, \quad (38)$$

where η is a fixed constant. For example, with η being fixed at 1 , 3 , 5 , and 10 , $\mathcal{P}^U$ can be confirmed to be practically proportional to k by checking the value of $\mathcal{P}^U/u_w k$ for the cases with k smaller than 0.01 ,

$$\frac{\mathcal{P}^U(k; \eta)}{u_w} \simeq -a_\eta k \quad (k \ll 1, \eta = 1, 3, 5, 10). \quad (39)$$

Here, $a_1 = 0.32$, $a_3 = 0.70$, $a_5 = 0.94$, and $a_{10} = 1.32$. Thus, taking (39) and (37a) into account, the proportion of the contribution from the stress over the part within distance $k\eta$ from the corner to the total force acting on the lid, namely, $\int_{1/2-k\eta}^{1/2} P_{23}(z, \frac{1}{2}) dz / \int_0^{1/2} P_{23}(z, \frac{1}{2}) dz = 2\mathcal{P}^U/u_w F_U$, is well expressed by

$$\frac{2\mathcal{P}^U}{u_w F_U} \simeq \frac{-2a_\eta}{1.267 \ln k + 0.948} \quad (k \ll 1, \eta = 1, 3, 5, 10). \quad (40)$$

This proportion decreases with the decrease in k . However, its rate is very slow. For example, (40) with $\eta = 5$ implies that about 10% of the total force comes from the localized range within about 4.4 times the

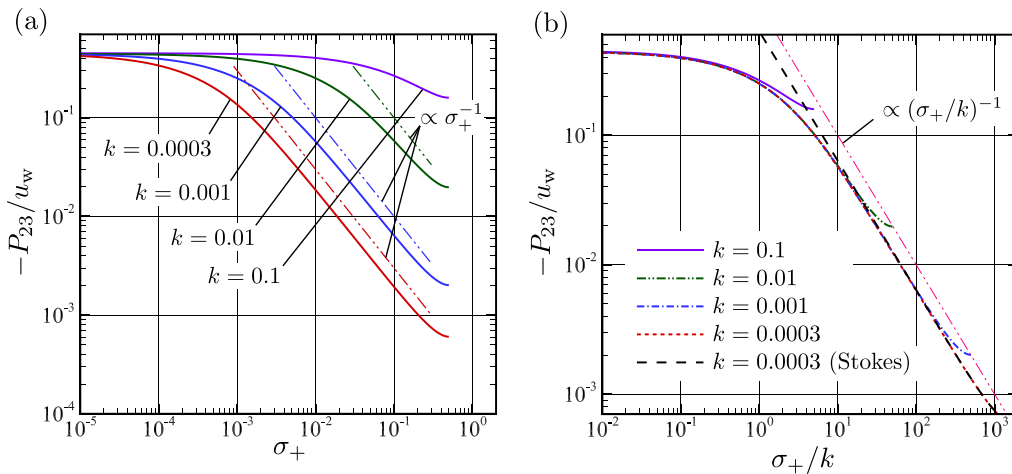


FIG. 16. Profiles of shear stress on the lid. In (a) and (b), they are shown as a function of σ_+ and σ_+/k , the distance from the corner and the rescaled one, respectively.

mean free path ℓ_0 from the corner even when $k = 10^{-7}$. (This corresponds to the situation where a gas at the atmospheric condition occupies the cavity with the size of several tens of centimeters.) Note that a corresponding property can be confirmed for the sidewall as well.

VI. CONCLUSION

In the present paper, motivated by the problem of corner singularity in fluid mechanics, we considered a gas flow in a square cavity driven by a lid sliding in the direction of its line of contact with the cavity walls. The problem was formulated as the boundary-value problem of the linearized BGK equation under the diffuse reflection boundary condition and it was reduced to the integral equation for the flow velocity field that is suitable for an accurate analysis. As confirmed explicitly in Sec. III A before the numerical analysis, applying the Stokes equation and the no-slip boundary condition leads to the fact that the flow velocity becomes multivalued at the corner between the lid and the cavity wall and the shear stress diverges there inversely proportionally to the distance from the corner. In the case of the free molecular solution, first despite the significant slip at the corner the flow velocity is still multivalued. The multivalueness occurs because the flow velocity is determined by the proportion of the contribution of the molecules coming from the lid over that of the whole molecules that depends on the azimuthal angle measured from the corner, and this feature remains the same when the corner is approached. Second, the shear stress and accordingly the forces acting on the lid and the cavity walls are bounded. The two properties were common in the numerical results for the small Knudsen numbers, which correspond to the ordinary fluid-dynamic circumstances, presented in Sec. V. The second property means that the difficulty associated with the description in terms of the Stokes equation is resolved by using the kinetic approach. The shear stresses given by the Stokes solution and the BGK one for small Knudsen numbers agree well with each other up to the position that is a few tens of mean free paths away from the corner. Within the region, the shear stress varies inversely proportionally to the distance from the corner. At positions closer to the corner, the increase in the stress is suppressed and its magnitude remains bounded for the BGK solution. According to these behavior of the shear stress, the total forces acting on the lid and the side cavity wall behave as $k \ln k$ ($k \ll 1$), where $k = (\sqrt{\pi}/2) \text{Kn}$ is a parameter corresponding to the Knudsen number Kn . The proportion of the contribution from the positions within a few mean free paths from the corner to the total force acting on the lid and the side cavity wall is given as $C/(A + B \ln k)$ [A, B, C : constants of $O(1)$] and is nonnegligible even for small Knudsen numbers.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Masanari Hattori: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

APPENDIX: INFORMATION OF COMPUTATIONS

In this Appendix, we briefly provide the information of computations. The results shown in Sec. V are obtained with the parameters $\sigma_{\max} = 0.27$, $N_1 = N_2 = N_\sigma = N_\varphi = 62$, $K_f = 5$, $M_f = 6$, and $M_\theta = 6$. For x_1 (or x_2), the minimum lattice interval is 2.2122×10^{-6} around $x_1 = 1/2$ (or $x_2 = \pm 1/2$), while the maximum interval is 7.8125×10^{-3} around $x_1 = 0$ (or $x_2 = 0$). For $\sigma_\pm$, the minimum lattice interval is 1.1946×10^{-6} around $\sigma_\pm = 0$, while the maximum interval is 4.2188×10^{-3} around $\sigma_\pm = \sigma_{\max} = 0.27$. For $\varphi_\pm$, the minimum lattice interval is $1.1061\pi \times 10^{-6}$ around $\varphi_\pm = 0$ and $\pi/2$, while the maximum interval is $3.9062\pi \times 10^{-3}$ around $\varphi_\pm = \pi/4$. For the results shown in Figs. 7–11, 13, and 15 and the plots for $k \geq 0.001$ shown in Figs. 12, 14, and 16, numerical convergence has been judged within the error invisible in the figures through the comparison with the results obtained with other parameters corresponding to coarser discretization compared to the aforementioned set of parameters. The balance between the total forces acting on the lid and the cavity walls provides another measure of accuracy including the cases for $0.0002 \leq k \leq 0.0008$ shown in Figs. 12, 14, and 16. Namely, $F_U + F_B + 2F_R = 0$ should hold theoretically owing to the momentum conservation in the x_3 direction, and numerically the following are confirmed for representative values of k :

$$(|F_U + F_B + 2F_R|, |F_U|) = \begin{cases} (2.6 \times 10^{-13}, 0.5505) & (k = 10), \\ (4.1 \times 10^{-11}, 0.4631) & (k = 1), \\ (9.4 \times 10^{-10}, 0.2173) & (k = 0.1), \\ (8.1 \times 10^{-9}, 0.0489) & (k = 0.01), \\ (1.8 \times 10^{-7}, 0.0078) & (k = 0.001), \\ (2.2 \times 10^{-7}, 0.0020) & (k = 0.0002). \end{cases} \quad (\text{A1})$$

REFERENCES

- ¹P. N. Shankar and M. D. Deshpande, "Fluid mechanics in the driven cavity," *Annu. Rev. Fluid Mech.* **32**, 93–136 (2000).
- ²H. K. Moffatt, "Viscous and resistive eddies near a sharp corner," *J. Fluid Mech.* **18**, 1–18 (1964).
- ³O. R. Burggraf, "Analytical and numerical studies of the structure of steady separated flows," *J. Fluid Mech.* **24**, 113–151 (1966).
- ⁴F. Pan and A. Acrivos, "Steady flows in rectangular cavities," *J. Fluid Mech.* **28**, 643–655 (1967).
- ⁵P. N. Shankar, "The eddy structure in Stokes flow in a cavity," *J. Fluid Mech.* **250**, 371–383 (1993).
- ⁶R. Srinivasan, "Accurate solutions for steady plane flow in the driven cavity. I. Stokes flow," *Z. Angew. Math. Phys.* **46**, 524–545 (1995).

- ⁷U. Ghia, K. N. Ghia, and C. T. Shin, "High-Re solutions for incompressible flow using the Navier–Stokes equations and a multigrid method," *J. Comput. Phys.* **48**, 387–411 (1982).
- ⁸O. Botella and R. Peyret, "Benchmark spectral results on the lid-driven cavity flow," *Comput. Fluids* **27**, 421–433 (1998).
- ⁹F. Auteri, N. Parolini, and L. Quartapelle, "Numerical investigation on the stability of singular driven cavity flow," *J. Comput. Phys.* **183**, 1–25 (2002).
- ¹⁰H. K. Moffatt, "Singularities in fluid dynamics and their resolution," in *Lectures on Topological Fluid Mechanics*, edited by R. L. Ricca (Springer, Berlin, Heidelberg, 2009), pp. 157–166.
- ¹¹G. I. Taylor, "On scraping viscous fluid from a plane surface," in *The Scientific Papers of Sir Geoffrey Ingram Taylor*, edited by G. K. Batchelor (Cambridge University Press, Cambridge, 1962), pp. 410–413.
- ¹²S. Naris and D. Valougeorgis, "The driven cavity flow over the whole range of the Knudsen number," *Phys. Fluids* **17**, 097106 (2005).
- ¹³B. John, X.-J. Gu, and D. R. Emerson, "Investigation of heat and mass transfer in a lid-driven cavity under nonequilibrium flow conditions," *Num. Heat Transfer B* **58**, 287–303 (2010).
- ¹⁴B. John, X.-J. Gu, and D. R. Emerson, "Effects of incomplete surface accommodation on non-equilibrium heat transfer in cavity flow: A parallel DSMC study," *Comput. Fluids* **45**, 197–201 (2011).
- ¹⁵A. Mohammadzadeh, E. Roohi, H. Niazmand, S. Stefanov, and R. S. Myong, "Thermal and second-law analysis of a micro- or nanocavity using direct-simulation Monte Carlo," *Phys. Rev. E* **85**, 056310 (2012).
- ¹⁶L. Wu, J. M. Reese, and Y. Zhang, "Oscillatory rarefied gas flow inside rectangular cavities," *J. Fluid Mech.* **748**, 350–367 (2014).
- ¹⁷P. Wang, W. Su, L. Zhu, and Y. Zhang, "Heat and mass transfer of oscillatory lid-driven cavity flow in the continuum, transition and free molecular flow regimes," *Int. J. Heat Mass Transfer* **131**, 291–300 (2019).
- ¹⁸Y. Y. Kloss, P. V. Shuvalov, and F. G. Tcheremissine, "Solving Boltzmann equation on GPU," *Procedia Comput. Sci.* **1**, 1083–1091 (2010).
- ¹⁹A. Frezzotti, G. P. Ghiroldi, and L. Gibelli, "Solving the Boltzmann equation on GPUs," *Comput. Phys. Commun.* **182**, 2445–2453 (2011).
- ²⁰Z. Guo, K. Xu, and R. Wang, "Discrete unified gas kinetic scheme for all Knudsen number flows: Low-speed isothermal case," *Phys. Rev. E* **88**, 033305 (2013).
- ²¹G. P. Ghiroldi and L. Gibelli, "A direct method for the Boltzmann equation based on a pseudo-spectral velocity space discretization," *J. Comput. Phys.* **258**, 568–584 (2014).
- ²²M. T. Ho, J. Li, L. Wu, J. M. Reese, and Y. Zhang, "A comparative study of the DSBGK and DVM methods for low-speed rarefied gas flows," *Comput. Fluids* **181**, 143–159 (2019).
- ²³L. Zhang, W. Ma, Q. Lou, and J. Zhang, "Simulation of rarefied gas flows using physics-informed neural network combined with discrete velocity method," *Phys. Fluids* **35**, 077124 (2023).
- ²⁴Motivation of the present work comes from the corner singularity problem in fluid mechanics, where the gas of ordinary pressure occupying the cavity of ordinary size is considered. In such a case, the Knudsen number is small.
- ²⁵P. L. Bhatnagar, E. P. Gross, and M. Krook, "A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems," *Phys. Rev.* **94**, 511–525 (1954).
- ²⁶P. Welander, "On the temperature jump in a rarefied gas," *Ark. Fys.* **7**, 507–553 (1954).
- ²⁷M. Hasegawa and Y. Sone, "Poiseuille and thermal transpiration flows of a rarefied gas for various pipes," *J. Vac. Soc. Jpn.* **31**, 416–419 (1988).
- ²⁸K. Aoki, Y. Sone, and T. Yano, "Numerical analysis of a flow induced in a rarefied gas between noncoaxial circular cylinders with different temperatures for the entire range of the Knudsen number," *Phys. Fluids A* **1**, 409–419 (1989).
- ²⁹S. Taguchi and P. Charrier, "Rarefied gas flow over an in-line array of circular cylinders," *Phys. Fluids* **20**, 067103 (2008).
- ³⁰Y. Sone, *Molecular Gas Dynamics* (Birkhäuser, Boston, 2007), supplementary Notes and Errata are available from Kyoto University Research Information Repository. <http://hdl.handle.net/2433/66098>.
- ³¹G. K. Batchelor, *An Introduction to Fluid Dynamics* (Cambridge University Press, Cambridge, 2000), pp. 183–185.
- ³²In equation (23) the source term $-\Delta u_3^+$ behaves nicely near the corner $[(x_1, x_2) = (\pm 1/2, 1/2) \text{ or } \sigma_+ = 0]$ since $u_3^+ = u_w BS$, $\Delta B = 0$, and the variation of $S(\sigma_+)$ near $\sigma_+ = 0$ is small. Furthermore, two boundary conditions (24a) and (24c) exhibit no mismatch at the corner, thanks to $S(1/2 - |x_1|) \rightarrow 1$ as $x_1 \rightarrow 1/2$.
- ³³The computation is carried out also with fewer lattice points and a good convergence of the results is confirmed.
- ³⁴Indeed, since $\sigma_+ > 1/2$, and thus, $u_3^+ = 0$ near the corner, the regular $u_3^{\#}$ shown in Fig. 4 is none other than the solution there.
- ³⁵Y. Sone, "Asymptotic theory of flow of rarefied gas over a smooth boundary I," in *Rarefied Gas Dynamics*, Vol. 1, edited by L. Trilling and H. Y. Wachman (Academic Press, New York, 1969), pp. 243–253.
- ³⁶Y. Sone, "Asymptotic theory of flow of rarefied gas over a smooth boundary II," in *Rarefied Gas Dynamics*, Vol. 2, edited by D. Dini (Editrice Tecnica Scientifica, Pisa, 1971), pp. 737–749.
- ³⁷Y. Sone, *Kinetic Theory and Fluid Dynamics* (Birkhäuser, Boston, 2002), supplementary Notes and Errata are available from Kyoto University Research Information Repository. <http://hdl.handle.net/2433/66099>.
- ³⁸The rarefaction effects for finite Knudsen numbers included in the theory, which constitute the differences from the results given by the conventional fluid mechanics, appear only from higher orders of the expansion.
- ³⁹S. Taguchi and T. Tsuji, "On the motion of slightly rarefied gas induced by a discontinuous surface temperature," *J. Fluid Mech.* **897**, A16 (2020).
- ⁴⁰S. Taguchi and T. Tsuji, "A generalized slip-flow theory for a slightly rarefied gas flow induced by discontinuous wall temperature," in *Recent Advances in Kinetic Equations and Applications*, Springer INdAM Series, Vol. 48, edited by F. Salvarani (Springer, Cham, 2021), pp. 327–344.
- ⁴¹Note that for part of the rectangular cells, the intersection of them and $F_{\pm}$ (the region where the Cartesian and polar grids overlap in Fig. 6) is cut off.
- ⁴²Note that if the Stokes solutions in the whole region are plotted with the same scale as in Figs. 7–9, then it is found that the Stokes and BGK solutions agree well with each other in the scale, except near the corner. The corresponding figure is omitted here.
- ⁴³The quantity $A[u_3]$ does not depend on φ_+ in the limit $\sigma_+ \rightarrow +0$ since it is given as a surface integral and $\mathbf{x}$ appears there only through the distance $|\mathbf{x}_+ - \mathbf{x}|$.
- ⁴⁴Since both the denominator $k \sin \psi$ and the numerator $\sigma_+ \sin \varphi_+$ of the argument of J_1 tend to 0 as $\sigma_+ \rightarrow +0$ and $\psi \rightarrow \theta_L(\mathbf{x})$, care should be taken in taking the limit $\sigma_+ \rightarrow +0$. Fortunately, the result in (34) can be justified, for example, as follows. To begin with, $\theta_L(\mathbf{x})$ can be expressed as $\theta_L = \pi - \alpha$ with $\alpha = \tan^{-1}(\sigma_+ \sin \varphi_+ / (1 - \sigma_+ \cos \varphi_+))$. We can take another angle $\beta = \tan^{-1}(\sqrt{\sigma_+} \sin \varphi_+ / (1 - \sigma_+ \cos \varphi_+))$, which is larger than α and tends to 0 as $\sigma_+ \rightarrow +0$. Then, we may split the integral as $b(\mathbf{x}) = \pi^{-1} \int_{\varphi_+}^{\pi-\alpha} J_1 d\psi = \pi^{-1} \int_{\varphi_+}^{\pi-\beta} J_1 d\psi + \pi^{-1} \int_{\pi-\beta}^{\pi-\alpha} J_1 d\psi$. Thanks to the choice of β , in the first integral, where $\varphi_+ < \psi < \pi - \beta$, the argument of J_1 approaches 0 uniformly as $\sigma_+ \rightarrow +0$. Thus, it approaches the result in (34). On the other hand, we see that the second integral tends to 0 because its magnitude is bounded from above by $\pi^{-1} J_1(0)(\beta - \alpha)$ [$J_1(0)$ is the maximum of the function J_1] and $\alpha, \beta \rightarrow 0$ as $\sigma_+ \rightarrow +0$.
- ⁴⁵The expression of the VDF, including the part corresponding to $A[u_3]$, at any point not limited to the corner, can be obtained by applying the discussion in Sec. A.4.2 of Ref. 30 to the present problem. Here, it is omitted.
- ⁴⁶The value of F_B/k for each k in the range is larger than 0.22026 and less than 0.22072.
- ⁴⁷S. Takata and S. Taguchi, "Gradient divergence of fluid-dynamic quantities in rarefied gases on smooth boundaries," *J. Stat. Phys.* **168**, 1319–1352 (2017).