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Technical Notes

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Capturing the Knudsen Layer in Continuum-Fluid Models of Nonequilibrium Gas Flows

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Introduction

THE Knudsen layer is the region of local nonequilibrium extending one or two molecular mean free paths from the wall in any gas flow near a surface. In most hypersonic and microflow applications, it is the momentum and energy fluxes from the region of the Knudsen layer to the boundaries that are of most interest to designers. A correct description of the Knudsen layer, therefore, is critical when modeling practical applications of such flows.

Although the Knudsen layer's characteristics have been investigated extensively using kinetic theory,[1–3] the ability to capture it within a continuum-fluid formulation (in conjunction with slip boundary conditions) suitable for engineering applications would offer distinct and practical computational advantages. The Navier–Stokes constitutive relations cannot, however, model the nonlinear stress/strain-rate behavior within the Knudsen layer. Although higher-order continuum equations, such as the Burnett equations, can provide an alternative, Kogan[1] has shown that the Chapman–Enskog series (from which the Burnett and super-Burnett equations are derived) does not provide a solution to the Boltzmann equation in the Knudsen layer. Furthermore, higher-order continuum equations require additional boundary conditions to ensure a unique solution: without using results from other simulations or experiments, it is not a straightforward matter to choose these. Within continuum-fluid formulations for locally nonequilibrium gas flows, a phenomenological approach could therefore be a practical way of capturing the essential Knudsen-layer structure. It is, after all, accepted and commonplace for phenomenological methods to be applied at wall boundaries. (Maxwell's velocity slip and the classical nonslip boundary condition are partly phenomenological.)

When the Navier–Stokes equations are used to model a slightly rarefied gas flow, the most common approach is to account for (rather than model) the Knudsen layer by employing "fictitious" or "macro" slip boundary conditions u^*_{slip} (in Fig. 1). If the "actual" or "micro" velocity slip u_{slip} is applied at the boundary, the prediction of the velocity both inside and outside the Knudsen layer is poor (the dash-dot line in Fig. 1). Prescribing a fictitious velocity slip does, at least, provide an accurate solution outside the Knudsen layer (the dashed line in Fig. 1). Kogan,[1] Cercignani,[2] and Sone[3] all proposed such slip boundary conditions. (Here we note that the condition proposed by Sone was intended to be used in conjunction with a tabulated Knudsen-layer correction. This approach will be discussed later.)

The drawback with employing fictitious slip boundary conditions, however, is that some part of the flowfield is then necessarily fictitious. For flows with higher global Knudsen numbers, the physical extent of the Knudsen layer increases, and the fictitious element of a Navier–Stokes solution to the flowfield therefore occupies a significant proportion of the entire flow. The error that this generates near the boundary is unacceptable because, in the majority of applications (from hypersonics and microfluidics), it is the accurate prediction of surface properties that is of paramount importance. Higher-order slip boundary conditions[4–6] cannot remedy this problem because the error arises not from an inaccuracy in the slip model at the boundary, but from within the Navier–Stokes equations themselves (i.e., from the linearity of these constitutive relations).

Another current approach is to apply the Navier–Stokes equations with fictitious slip boundary conditions, as described in the preceding two paragraphs, and then make a kinetic theory-based correction to either the resulting velocity field by using precalculated values[3] or to an averaged property of interest, such as mass flow rate.[4] In both approaches the Navier–Stokes calculation of the flowfield is treated separately from the Knudsen-layer correction; consequently, the presence of the Knudsen layer does not directly affect the flow solution. Furthermore, because in these cases the

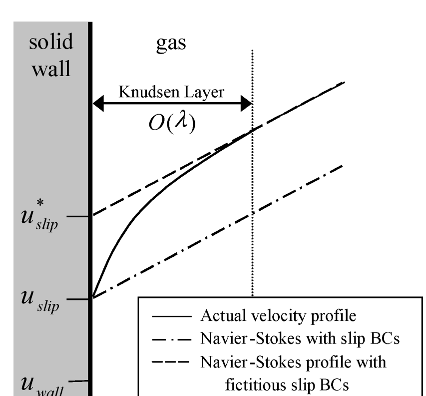

Fig. 1 Schematic of the velocity structure of the Knudsen layer near a wall in a shear flow, with a comparison of the two types of slip boundary condition.

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Navier–Stokes solution uses fictitious boundary conditions, some properties of the entire flow solution are likely to remain partially in error even after the Knudsen-layer corrections.

Wall-Function Approach

In this Note we do not present a physical model for the Knudsen layer, but rather a wall-function technique, akin to that used in turbulent boundary-layer modeling, which can capture its essential features in computational fluid dynamics. We use a solution to the linearized Boltzmann equation for a wall-bounded shear flow of a monatomic gas as a basis for a new scaling law for the gas effective viscosity as a function of normal wall distance. Although the Knudsen layer also affects the relationship between heat flux and temperature gradient, at this stage we restrict our attention to its effect on the stress/strain-rate relationship (noting that the variation of viscosity will also cause the thermal conductivity to vary).

For a planar wall (with diffuse molecular reflection) bounding a monatomic gas flow subject to a uniform shear stress, Cercignani showed[2] that the linearized Boltzmann equation predicts a velocity profile u through the Knudsen layer of the form

$$u = -(\tau/\mu)[x + \zeta - \lambda I(x/\lambda)] \tag{1}$$

where x is the normal distance from the planar wall, τ is the uniform shear stress, μ is the viscosity, λ is the mean free path, and ζ is a constant. For convenience, we propose a curve-fitted approximation to the velocity correction function $I(x/\lambda)$ (evaluated by Cassell and Williams[7]) as follows:

$$I(x/\lambda) \approx (7/20)\,(1 + x/\lambda)^{-2} \tag{2}$$

with a mean free path given by

$$\lambda = \mu\sqrt{\pi/2p\rho} \tag{3}$$

where ρ is the gas density and p its pressure.

On differentiating Eq. (1), a correction to the constitutive relations of the Navier–Stokes equations that is appropriate throughout the Knudsen layer can be obtained:

$$\frac{\mathrm{d}u}{\mathrm{d}x} = -\frac{\tau}{\mu}\Psi\left(\frac{x}{\lambda}\right) \tag{4}$$

where the wall function $\Psi(x/\lambda)$ is given by

$$\Psi\left(\frac{x}{\lambda}\right) = 1 - \lambda\frac{\mathrm{d}I(x/\lambda)}{\mathrm{d}x} \approx 1 + \frac{7}{10}\left(1 + \frac{x}{\lambda}\right)^{-3} \tag{5}$$

For a given shear stress, this wall function generates a strain rate at the wall that departs some 70% from the Navier–Stokes predictions, decreasing to roughly 10% difference a distance of one mean free path into the gas. The wall function can be very simply implemented within a Navier–Stokes solver by substituting the real-gas viscosity μ with an effective viscosity $\mu\Psi^{-1}$ calculated in accordance with Eq. (5). A consequence of this scaling of the gas viscosity is that the normal strain rate is affected similarly to the shear strain rate.

Because this wall function is based on Cercignani's linearized Boltzmann solution for a uniform shear stress over a planar surface, strictly our model should only be applicable to low-Mach-number, low-Knudsen-number flows over planar surfaces for diffuse reflection at solid boundaries. However, our main heuristic premise is that this wall function is a practical way of improving predictions in general flow configurations with negligible computational time penalty. This is no less, and no more, justifiable than the common practice of using fictitious boundary conditions in situations other than those for which they were originally derived. This is a preliminary investigation into developing straightforward techniques for incorporating Knudsen-layer structure within conventional fluid-dynamics simulations—a general wall function approach cannot be expected to obtain predictions comparable with the accuracy of modern kinetic theory.

With the wall function given by Eq. (4), Maxwell's general slip condition[8] should also be used:

$$u_{\mathrm{slip}} = -A_1[(2-\sigma)/\sigma]\lambda(\tau/\mu) \tag{6}$$

where A_1 is the slip coefficient and σ is the momentum accommodation coefficient (equal to one for perfectly diffuse molecular reflection and zero for purely specular reflection). Kinetic theory and molecular simulations indicate that Maxwell's slip coefficient ($A_1 = 1$) significantly overestimates the amount of actual velocity slip. Consequently, there is a large amount of fictitious slip incorporated within Maxwell's formulation, and this fortuitously improves its predictive capabilities when used with Navier–Stokes models. So here we use, instead, the actual (micro) slip, obtained by evaluating Eq. (1) at the wall:

$$A_1 = \sqrt{2/\pi} \approx 0.8 \tag{7}$$

Results and Discussion

To test our proposed wall-function approach, we first use a simple centered finite difference numerical scheme to solve the Navier–Stokes equations for monatomic gas flow in benchmark one-dimensional planar Couette and Poiseuille systems. Figures 2 and 3 show a comparison of solutions obtained by using the direct simulation Monte Carlo (DSMC) method and the Navier–Stokes equations by using both the wall-function approach just described and conventional fictitious slip boundary conditions with $A_1 = 1.146$ as proposed by Cercignani.[2] (This value provides a significantly better prediction of the absolute velocity than that obtained by using Maxwell's value of $A_1 = 1$.) In both cases the Knudsen number is defined as the ratio of the mean free path to half the channel height L. Although the differences are fairly minor for these particular benchmark cases, results over a range of Mach numbers M show that the

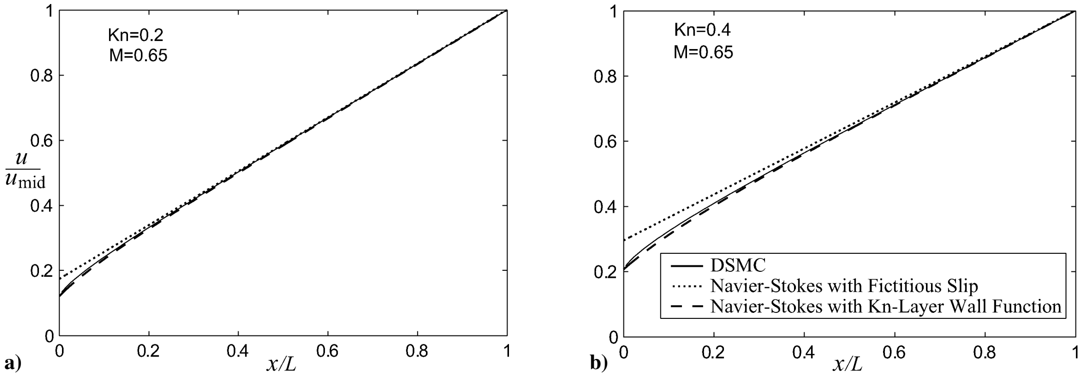

Fig. 2 Normalised velocity profiles in rarefied Couette flow: ——, DSMC results; . . . ., Navier–Stokes solution with fictitious slip; and – – –, Navier–Stokes solution with the Knudsen-layer wall function. The wall at $x/L = 0$ is stationary, and that at $x/L = 2$ is moving at Mach 0.65 with Knudsen numbers Kn = a) 0.2 and b) 0.4.

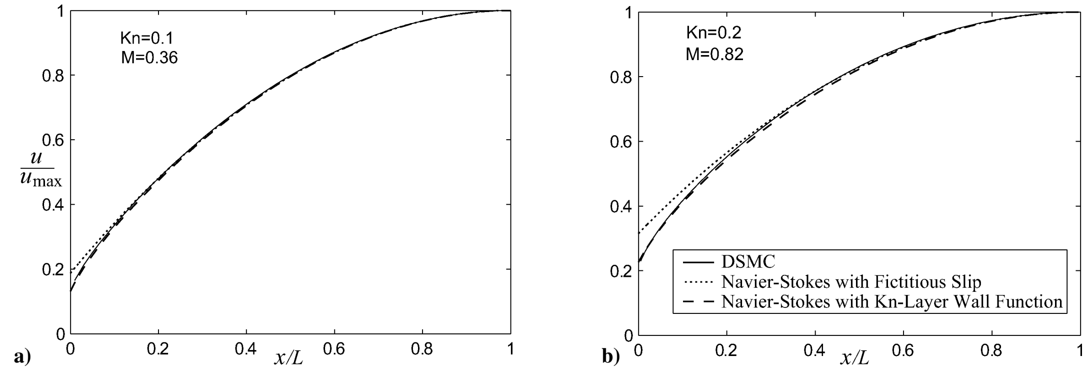

Fig. 3 Normalized velocity profiles in rarefied Poiseuille flow: ——, DSMC results; . . . ., Navier–Stokes solution with fictitious slip; and – – –, Navier–Stokes solution with the Knudsen-layer wall function where a) $Kn = 0.1$, $M = 0.36$ and b) $Kn = 0.2$, $M = 0.82$.

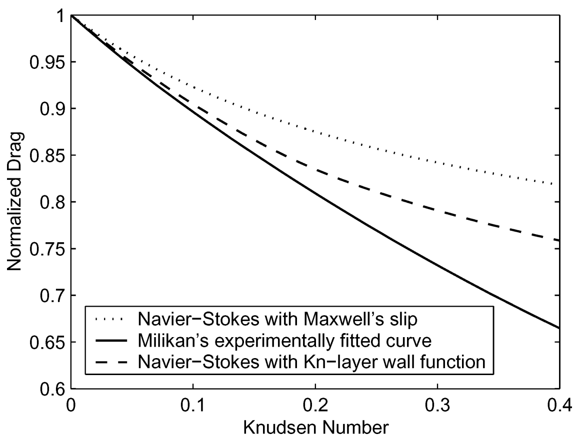

Fig. 4 Normalized drag of an unconfined sphere over a range of Knudsen numbers: ——, experimentally fitted curve[9]; . . . , Navier–Stokes solution with Maxwell's slip; and – – –, Navier–Stokes solution with the Knudsen-layer wall function. The characteristic length used to define the Knudsen number is the sphere radius.

Knudsen-layer wall-function approach produces better agreement with the DSMC data than conventional fictitious slip solutions do.

For each case in Figs. 2 and 3, the shear-stress profile throughout the channel is identical for the three methods of simulation shown (i.e., the shear stress is not affected by our wall function). Two further points to note are 1) both the wall function and the fictitious slip approaches are based on the same kinetic theory, and corresponding assumptions, and are comparably easy to implement numerically; and 2) the Mach numbers considered here are reasonably high, and slight viscous heating is exhibited in the DSMC data. To ensure a fair comparison with the isothermal continuum solutions, the mild variation of actual viscosity is extracted from the DSMC data and accounted for within the Navier–Stokes calculations. In practice this only marginally affects the results.

We now investigate a nonplanar case: low-Reynolds-number (monatomic gas) flow past an unconfined sphere. Figure 4 compares the total drag (normalized by the Stokes drag, the limiting case as the Knudsen number tends to zero) of Milikan's experimentally-fitted curve for air[9] with Navier–Stokes results using the Knudsen-layer wall function and conventional slip-flow analysis (equivalent to a Navier–Stokes solution with slip coefficient $A_1 = 1$). Even though our wall function is derived from a planar Knudsen-layer solution, this method gives improved predictions of drag, particularly up to $Kn \approx 0.1$ (which is the upper end of the Navier–Stokes slip flow regime). The gradient of the curve is also captured at low Knudsen numbers.

Conclusions

In this Note we have proposed a wall function to scale the constitutive relations so that both the velocity slip and Knudsen-layer structure can be captured within a continuum-fluid formulation for locally nonequilibrium gas flows. This wall function is based on a simple Knudsen-layer solution of the Boltzmann equation and improves the predictive capabilities of the Navier–Stokes equations for a variety of flow configurations of engineering interest. This method could be used as a simple and practical technique for incorporating the Knudsen-layer structure within conventional fluid-dynamic simulations, although it is not comparable in either accuracy or complexity to the results from modern kinetic theory.

The technique could be used in conjunction with higher-order constitutive relations evaluated outside the Knudsen layer and would circumvent the need to provide additional boundary conditions for a unique solution. Future work includes implementing a more general Knudsen-layer correction (such as that proposed by Sone[3]) using the wall-function approach and investigating empirical Knudsen-layer wall-functions for specific flow configurations at higher Knudsen numbers.

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