Asymptotic Analysis of a Slightly Rarefied Gas with Nonlocal Boundary Conditions

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Abstract In this paper nonlocal boundary conditions for the Navier–Stokes equations are derived, starting from the Boltzmann equation in the limit for the Knudsen number being vanishingly small. In the same spirit of (Lombardo et al. in J. Stat. Phys. 130:69–82, 2008) where a nonlocal Poisson scattering kernel was introduced, a gaussian scattering kernel which models nonlocal interactions between the gas molecules and the wall boundary is proposed. It is proved to satisfy the global mass conservation and a generalized reciprocity relation. The asymptotic expansion of the boundary-value problem for the Boltzmann equation, provides, in the continuum limit, the Navier–Stokes equations associated with a class of nonlocal boundary conditions of the type used in turbulence modeling.

Keywords Nonlocal boundary conditions · Boltzmann equation · Fluid dynamic limit

1 Introduction

In this paper we introduce a nonlocal gaussian scattering kernel for a structured solid boundary and derive, in the fluid dynamic limit, the set of corresponding boundary conditions for the fluid dynamic variables.

During the last years there has been a growing interest on gas-surface interaction and on gas flows close to solid boundaries. In fact, in many instances, the validity domain of the fluid dynamic equations can be extended up to higher Knudsen numbers if these equations

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are complemented with the correct boundary conditions. This is for instance the case of moderately rarefied gas flows, turbulence modeling and microflows in microelectromechanical systems (MEMS) where surface effects play a preponderant role in the calculation of flow properties. Solving these problems requires to investigate the complicated processes of interaction between the gas and the solid surface. In fact the issue of establishing the right boundary conditions related to gas-surface interaction is still open and the results obtained so far are far from being satisfactory.

From a microscopic level description, the interaction law linking the distribution function of the reflected and incoming particles at the wall is given by the scattering kernel, which provides the boundary conditions to be used for the kinetic equations. Performing the asymptotic expansion of the boundary-value problem for the Boltzmann equations gives, in the limit of vanishingly small Knudsen number, the set of fluid dynamic equations and the corresponding boundary conditions for the macroscopic variables (see, for instance, [5, 10, 20, 21, 24]).

In a previous paper [14], we have introduced a new form of scattering kernel which takes into account nonlocal interactions of the impinging particles with the wall lattice: a portion of the particles, in fact, is allowed to penetrate the boundary being reflected by inner layers with a penetration probability ruled by the Poisson distribution. The remaining portion of particles thermalizes with the wall, as in the classical Maxwell scattering kernel. The boundary conditions for the fluid dynamic variables derived in the hydro-dynamic limit are of the Robin type and do not contain nonlocal terms.

In this paper we want to propose a form of scattering kernel which gives, in the fluid dynamic limit, the nonlocal boundary condition of the type used in turbulence modeling. In fact a promising approach in turbulence modeling is Large Eddy Simulation (LES), which seeks to predict local spatial averages of the fluid velocity above a preassigned length scale. There are essentially two ways to treat boundary conditions in LES [15]. The first is to decrease the filter width to zero at the boundary (Near Wall Resolution), which has high computational costs. In the second, which is referred to as Near Wall Modeling, the discretization near boundary remain coarse and the boundary conditions are developed with the aid of physical modeling such as ensuring conditions in LES is addressed in [12, 13]. In [13] nonlocal boundary condition for the coarse grained Navier–Stokes are constructed, where the velocity is convolved with a gaussian filter. The boundary conditions proposed in [13] for the averaged (in the sense that it is obtained from the velocity **u** convolving with a gaussian filter) flow $\bar{\mathbf{u}}$ are:

$$\bar{\mathbf{u}} \cdot \mathbf{n} = 0$$
 and $\beta \bar{\mathbf{u}} \cdot \boldsymbol{\tau} + 2Re^{-1}\mathbf{n} \cdot \mathbb{D}(\bar{\mathbf{u}}) \cdot \boldsymbol{\tau} = 0,$ (1.1)

where **n** and τ are the wall normal and tangential unit vectors, respectively, *Re* is the Reynolds number and $\mathbb{D}_{ij}(\mathbf{u}) = 1/2 (\partial u_i/\partial x_j + \partial u_j/\partial x_i)$ is the velocity deformation tensor. (1.1) are the Robin boundary conditions for the averaged velocity.

Recently, Ansumali, Karlin and Succi [2] applied a mean field approach to the Boltzmann equation, filtering out subgrid scales, in order to derive a subgrid turbulence model based on kinetic theory. They show that, similar to the Navier–Stokes equations, the Smagorinsky subgrid model [19] enjoys the consistent derivation from the kinetic theory. They do not tackle the boundary-value problem.

Here we propose a new form of scattering kernel which models the interaction of the impinging particles with the solid boundary. It is a nonlocal generalization of the classical Maxwell scattering kernel: a small portion of particles is allowed to be nonlocally reflected

from an inner layer of the boundary thought as a lattice. The nonlocal scattering probability is ruled by the gaussian distribution. The remaining part of the particles are specularly reflected as in the classical Maxwell kernel.

This model provides, in the hydrodynamical limit, the Robin boundary conditions for the tangential velocity plus a nonlocal term which is the convolution of the velocity with a gaussian kernel. If one takes the average of the obtained condition with a gaussian filter, the same boundary condition as in the near wall model [13] are obtained. Therefore this paper can be considered a first step in tackling the problem of boundary conditions in the kinetic theory of turbulence modeling.

The plan of the paper is the following: in Sect. 2 some basic notation is introduced and the physical conditions required in the scattering kernel theory are recalled. In Sect. 3 the Poisson scattering kernel introduced in [14] is briefly presented. Its nonlocal part is shown to behave as a low pass filter which wipes out small structures and allows large structures to be nonlocally reflected. In Sect. 4 the nonlocal gaussian kernel is derived. In Sect. 5 the asymptotic limit when the mean free path of the gas molecules is small compared with the characteristic length of the system (small Knudsen number) is performed and the boundary conditions for the fluid-dynamic variables derived. Finally, for the reader's convenience, Appendices A and B are inserted. In Appendix A the definition and the basic properties of the collision integral are given. In Appendix B the asymptotic analysis usually adopted to derive the fluid-dynamic equations is outlined.

2 Basic Equations and Scattering Kernel Properties

We shall investigate the steady behavior of a gas confined to the 3 - D half space $\Omega = \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}$ on the basis of the Boltzmann equation. Let the $\mathbf{x} = x_i$ (i = 1, 2, 3) be the dimensionless Cartesian coordinates of the physical space, \hat{x}_1 is the unit vector normal to the boundary wall, $\mathbf{y} = (x_2, x_3)$ is the position of a point on the plane $x_1 = 0$, $\boldsymbol{\zeta} = (\zeta_1, \zeta_2, \zeta_3)$ is the dimensionless molecular velocity; $\hat{f}(\mathbf{x}, \boldsymbol{\zeta})$ is the dimensionless velocity distribution function of the gas molecules; $\hat{\rho}$ is the dimensionless temperature, \hat{p} is the dimensionless gas velocity, \hat{T} is the dimensionless temperature, \hat{p} is the dimensionless pressure of the gas, R is the gas constant per unit mass and \hat{T}_w , $\hat{\rho}_w$, \hat{p}_w and u_{iw} are the dimensionless wall temperature, density, pressure and velocity, respectively.

In what follows we shall consider the state of the gas close to an equilibrium state at rest, so that the reference state is the dimensionless Maxwellian distribution function \hat{f}_0 with $u_i = 0$:

$$\hat{f}_0 = \frac{1}{\pi^{3/2}} \exp(-\zeta^2), \quad \zeta = (\zeta_i^2)^{1/2} = |\zeta_i|.$$
 (2.1)

We shall also use the following notation:

$$E(\zeta) = \frac{1}{\pi^{3/2}} \exp(-\zeta^2).$$
 (2.2)

It is convenient to choose the variables expressing the perturbation from the equilibrium state so that the nondimensional perturbed variables are given by:

$$\phi = \hat{f} / E - 1, \qquad \omega = \hat{\rho} - 1, \qquad \tau = \hat{T} - 1,$$

$$P = \hat{p} - 1, \qquad \tau_w = \hat{T}_w - 1.$$

$$(2.3)$$

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Then the steady Boltzmann equation in dimensionless form reads:

$$\zeta_i \frac{\partial \phi}{\partial x_i} = \frac{1}{k} [\mathcal{L}(\phi) + \mathcal{J}(\phi, \phi)], \qquad (2.4)$$

where $\mathcal{J}(\phi)$ and $\mathcal{L}(\phi)$ are the collision integral and the linearized collision integral, respectively, whose explicit expressions are given in Appendix A, see (A.1a) and (A.3); moreover:

$$k = \frac{\sqrt{\pi}}{2} \frac{\lambda}{L} = \frac{\sqrt{\pi}}{2} Kn, \qquad (2.5)$$

where L is a typical length of the system, λ is the mean free path of the gas molecules, and Kn is the Knudsen number.

Throughout the rest of this paper we shall make use of the following notation for the local Maxwellian distribution in the nondimensional perturbed form:

$$E\phi_e(\omega, u_i, \tau) = \frac{1+\omega}{\pi^{3/2}(1+\tau)^{3/2}} \exp\left(-\frac{(\zeta_i - u_i)^2}{1+\tau}\right) - E,$$
(2.6)

which satisfies:

$$\mathcal{L}(\phi_e) + \mathcal{J}(\phi_e, \phi_e) = 0. \tag{2.7}$$

The relation of the nondimensional macroscopic variables and the nondimensional velocity distribution function ϕ are:

$$\begin{cases}
\omega = \int \phi E d\boldsymbol{\zeta}, \\
(1+\omega)u_i = \int \zeta_i \phi E d\boldsymbol{\zeta}, \\
\frac{3}{2}(1+\omega)\tau = \int (\zeta_i^2 - \frac{3}{2})\phi E d\boldsymbol{\zeta} - (1+\omega)u_i^2, \\
P = \omega + \tau + \omega\tau.
\end{cases}$$
(2.8)

We shall restrict our discussion to the case where the mass flux through the wall is zero. Let the boundary wall be at $x_1 = 0$, let $\boldsymbol{\zeta}' = (\zeta'_1, \zeta'_2, \zeta'_3)$ be the velocity of the impinging particle referred to the wall and $\boldsymbol{\zeta} = (\zeta_1, \zeta_2, \zeta_3)$ the velocity of the reflected particle.

The interaction law between the surface layers of the wall and the gas molecules is assumed of the following general form:

$$|\boldsymbol{\zeta} \cdot \mathbf{n}| E(\boldsymbol{\zeta})(1 + \boldsymbol{\phi}(\boldsymbol{y}, \boldsymbol{\zeta}))$$

=
$$\int_{\boldsymbol{\zeta}' \cdot \mathbf{n} < 0} |\boldsymbol{\zeta}' \cdot \mathbf{n}| R(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}; \boldsymbol{y}) E(\boldsymbol{\zeta}')(1 + \boldsymbol{\phi}(\boldsymbol{y}, \boldsymbol{\zeta}')) d\boldsymbol{\zeta}' \quad (x_1 = 0, \ \boldsymbol{\zeta} \cdot \mathbf{n} > 0), \qquad (2.9)$$

where **n** is the unit vector normal to the boundary pointing into the gas, and $R(\zeta' \rightarrow \zeta; \mathbf{x})$ is the scattering kernel, i.e. the probability that a molecule impinging on the wall at point \mathbf{y} with velocity ζ' is scattered with velocity between ζ and $\zeta + d\zeta$.

The scattering kernel obeys the nonnegativity condition:

$$R(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}; \boldsymbol{y}) \ge 0. \tag{2.10}$$

The conservation of the mass at the wall (nonabsorbing and nonporous) is expressed by the following normalization relation:

$$\int_{\boldsymbol{\zeta} \cdot \mathbf{n} > 0} R(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}; \, \boldsymbol{y}) d\boldsymbol{\zeta} = 1 \quad (\boldsymbol{\zeta}' \cdot \mathbf{n} < 0).$$
(2.11)

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The last condition to be satisfied by the scattering kernel is the reciprocity relation:

$$|\boldsymbol{\zeta}' \cdot \mathbf{n}| E[1 + \phi_e(\boldsymbol{\zeta}')] R(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}; \boldsymbol{y}) = |\boldsymbol{\zeta} \cdot \mathbf{n}| E[1 + \phi_e(-\boldsymbol{\zeta})] R(-\boldsymbol{\zeta} \to -\boldsymbol{\zeta}'; \boldsymbol{y}), \quad (2.12)$$

where ϕ_e is the Maxwellian given by (2.6).

A widely used scattering kernel is the one proposed by Maxwell:

$$R(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \boldsymbol{y}) = (1 - \alpha)\delta(\zeta_1 + \zeta_1')\delta(\zeta_2 - \zeta_2')\delta(\zeta_3 - \zeta_3') + \alpha \frac{2}{\pi (1 + \tau_w)^2} \zeta_1 \exp\left[-\frac{(\zeta_i - u_{iw})^2}{1 + \tau_w}\right] \quad \text{(for } \zeta_1' < 0, \ \zeta_1 > 0\text{)}, \qquad (2.13)$$

where u_{iw} is the wall velocity. This physically means that the α part of particles is reflected diffusely: it is absorbed and re-emitted after a multiple-collision interaction with the molecules of the wall lattice getting in thermal equilibrium with the wall. The rest part $1 - \alpha$ is reflected specularly. We stress the fact that all the interactions are local in space: the particle hitting at point y of the wall is re-emitted at the same position.

3 The Nonlocal Poisson Scattering Kernel

In [14] a generalization of the Maxwell scattering kernel which takes into account the effect of the nonlocal interactions at the wall was introduced. The wall is thought as a lattice which the particles can penetrate, experiencing specular reflection from the inner layers of the wall. If the molecule hits the wall at point y' on the wall $x_1 = 0$, it will travel for some distance inside the wall, will strike the lattice and will come out at a different point y. Since it is specularly reflected, the impact will take place half-way between y' and y. Considering the one-impact nonlocal interactions gas-wall governed by the Poisson distribution function with $1/\eta$ as mean value (η is a parameter measuring the rarefaction of the wall) and accounting for the multiple scattering in the diffuse reflection law, the following scattering kernel is proposed:

$$R(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \boldsymbol{y}' \to \boldsymbol{y})$$

$$= (1 - \alpha)K(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \boldsymbol{y}' \to \boldsymbol{y})$$

$$+ \alpha \frac{2}{\pi (1 + \tau_w)^2} \zeta_1 \exp\left[-\frac{(\zeta_i - u_{iw})^2}{1 + \tau_w}\right] \delta(\boldsymbol{y} - \boldsymbol{y}') \quad (\text{for } \zeta_1' < 0, \ \zeta_1 > 0) \quad (3.1a)$$

where

$$K(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \, \boldsymbol{y}' \to \boldsymbol{y}) = \delta(\zeta_1 + \zeta_1')\delta(\boldsymbol{\zeta}_y - \boldsymbol{\zeta}_y')\frac{1}{\eta}\exp\left(-\frac{|\boldsymbol{y} - \boldsymbol{y}'|}{\eta}\right)\frac{\delta(\theta_y - \theta_\zeta')}{\rho_y}.$$
 (3.1b)

In the above expressions ζ'_y and ζ_y are the tangential velocity of the incident and reflected particle respectively, (ρ_y, θ_y) are the polar coordinates in the plane (x_2, x_3) centered in y = y' and θ_{ζ} is the angular variable of the polar coordinates in the plane (ζ_2, ζ_3) . In the above model a $1 - \alpha$ fraction of the molecules is specularly nonlocally reflected at the surface of the wall with a Poisson distribution function if y - y' is parallel to ζ'_y (which introduces the term $\delta(\theta_y - \theta'_{\zeta})$), while the remaining α fraction experiences multiple scattering inside the wall, thus getting into equilibrium with the wall. The above scattering kernel satisfies the following nonlocal normalization condition:

$$\int_{\mathbb{R}^2} d\mathbf{y} \int_{\zeta_1 > 0} R(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}; \, \mathbf{y}' \to \mathbf{y}) d\boldsymbol{\zeta} = 1 \quad (\zeta_1' < 0).$$
(3.2)

Notice that the above condition (3.2) is the nonlocal analog of (2.11): the latter expresses a pointwise conservation of the mass while the former requires the overall mass flux to be conserved. Moreover the reciprocity relation (2.12) is satisfied in the following form:

$$|\zeta_1'|E(\zeta')[1+\phi_e(\zeta')]R(\zeta'\to\zeta;\,y\to' y) = |\zeta_1|E(\zeta)[1+\phi_e(-\zeta)]R(-\zeta\to-\zeta';\,y\to y'),$$
(3.3)

where ϕ_e is the Maxwellian given by (2.6).

The boundary condition for the distribution function ϕ at the wall are then found by imposing the nonlocal analog of (2.9), namely:

$$\begin{aligned} |\zeta_{1}|E[1+\phi(\mathbf{y},\boldsymbol{\zeta})] \\ &= \int d\mathbf{y}' \int_{\zeta_{1}'<0} |\zeta_{1}'|R(\boldsymbol{\zeta}'\rightarrow\boldsymbol{\zeta};\,\mathbf{y}'\rightarrow\mathbf{y})E[1+\phi(\mathbf{y}',\boldsymbol{\zeta}')]d\boldsymbol{\zeta}' \quad (x_{1}=0,\,\,\boldsymbol{\zeta}\cdot\mathbf{n}>0). \end{aligned}$$

$$(3.4)$$

In [14] a systematic asymptotic analysis for vanishingly small Knudsen number was performed which provided a new class of weakly nonlocal boundary conditions for the fluid dynamic variables.

3.1 The Low-Pass Filter

Let us consider the nonlocal part of the scattering kernel given in (3.1a)-(3.1b):

$$K(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \boldsymbol{y}) = \delta(\boldsymbol{\zeta}_1 + \boldsymbol{\zeta}_1')\delta(\boldsymbol{\zeta}_y - \boldsymbol{\zeta}_y')\frac{\delta(\theta_y - \theta_{\boldsymbol{\zeta}}')}{\rho_y}\frac{1}{\eta}\left(-\frac{|\boldsymbol{y}|}{\eta}\right).$$
(3.5)

The action of the nonlocal term $K(\zeta' \to \zeta, y)$ on the boundary conditions for ϕ is represented by the spatial convolution of $K(\zeta' \to \zeta, y)$ with the distribution function, as it can be seen by applying (3.4). Therefore, introducing the Fourier transform with respect to y and denoting by $\xi = (\xi_2, \xi_3)$ the dual variable of y, namely:

$$f(\boldsymbol{\zeta}, \boldsymbol{\xi}) = \mathcal{F}(f(\boldsymbol{\zeta}, \boldsymbol{y})), \tag{3.6}$$

then

$$\hat{K}(\boldsymbol{\xi}' \to \boldsymbol{\zeta}, \boldsymbol{\xi}) \equiv \mathcal{F}(K(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \boldsymbol{y})) = \frac{1}{2\pi} \frac{\delta(\zeta_1 + \zeta_1')\delta(\boldsymbol{\zeta}_y - \boldsymbol{\zeta}_y')}{-1 + i\eta(\xi_2 \cos\theta_{\boldsymbol{\zeta}}' + \xi_3 \sin\theta_{\boldsymbol{\zeta}}')}$$
$$= \frac{1}{2\pi} \frac{\delta(\zeta_1 + \zeta_1')\delta(\boldsymbol{\zeta}_y - \boldsymbol{\zeta}_y')}{-1 + i\eta\boldsymbol{\xi} \cdot \hat{\boldsymbol{\zeta}}_y'}, \qquad (3.7)$$

where $\hat{\boldsymbol{\zeta}}'_{y}$ is the unit vector in the direction of $\boldsymbol{\zeta}'_{y}$. Therefore the kernel can be interpreted as a low-pass filter: it allows large structures (small $\boldsymbol{\xi}$) to pass the filter and hence experience specular reflection. On the other hand, small structures are cut-offed, do not experience specular reflection and finally get in thermal equilibrium with the wall (that is, they enter in the

count of the Maxwellian part of the scattering kernel). Hence the model describes a structured boundary wall: the large structures in the incident particle flux resolve the wall lattice and are reflected nonlocally, while the small structures penetrate the wall and thermalize.

4 The Nonlocal Gaussian Scattering Kernel

In this section, pursuing the idea of constructing a nonlocal scattering kernel that can act as low-pass filter, we want to propose a different model of the interaction between the gas and the wall. We propose a gaussian filter, that is common in turbulence modeling and that describes the particle diffusion inside the wall. Having in mind the idea of performing the asymptotic limit of the Boltzmann boundary-value problem for vanishingly small Knudsen number, let

$$\varepsilon = \frac{\sqrt{\pi}}{2} Kn \ (=k) \ll 1. \tag{4.1}$$

Let us consider the following scattering kernel:

$$R(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \boldsymbol{y}' \to \boldsymbol{y}) = (1 - \varepsilon\beta)\delta(\boldsymbol{\zeta}_{1} + \boldsymbol{\zeta}_{1}')\delta(\boldsymbol{\zeta}_{y} - \boldsymbol{\zeta}_{y}')\delta(\boldsymbol{y} - \boldsymbol{y}') + \varepsilon\gamma K(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \boldsymbol{y}' \to \boldsymbol{y}) + \frac{2\varepsilon(\beta - \gamma)}{\pi(1 + \tau_{w})^{2}}\delta(\boldsymbol{y} - \boldsymbol{y}')\boldsymbol{\zeta}_{1}\exp\left[-\frac{(\boldsymbol{\zeta}_{i} - \boldsymbol{u}_{wi})^{2}}{1 + \tau_{w}}\right] \quad (\boldsymbol{\zeta}_{1} > 0).$$
(4.2a)

where

$$K(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \boldsymbol{y}' \to \boldsymbol{y}) = \delta(\zeta_1 + \zeta_1')\delta(\boldsymbol{\zeta}_y - \boldsymbol{\zeta}_y')\frac{1}{2\pi\mu^2} \left[-\frac{(\boldsymbol{y} - \boldsymbol{y}')^2}{2\mu^2}\right].$$
(4.2b)

The meaning of the above kernel is the following: the first term on the right hand side of (4.2a) is just the same as in the Maxwell kernel. The second term accounts for a small ($O(\varepsilon)$) fraction of molecules which are nonlocally specularly reflected: particles that hit the wall at y' are reflected from an inner layer of wall molecules and exit at y with exponentially decaying probability $\exp[-(y - y')^2/(2\mu^2)]/(2\pi\mu^2)$, where μ is a positive constant. Finally the third term accounts for the ε fraction of molecules which are absorbed and re-emitted by the wall: namely, it is the usual term of the Maxwell scattering kernel.

It is obvious that the above scattering kernel satisfies the positivity condition (2.10). Moreover the constants are chosen so as to satisfy the nonlocal mass conservation law (3.2). Finally, it is straightforward to prove that the reciprocity relation is satisfied in the form given by (3.3).

Using the same notation as in the previous section, the nonlocal part of the scattering kernel (4.2a), is given by (4.2b), and has Fourier transform:

$$\hat{K}(\boldsymbol{\zeta}' \to \boldsymbol{\zeta}, \boldsymbol{\xi}) = \delta(\zeta_1 + \zeta_1')\delta(\boldsymbol{\zeta}_y - \boldsymbol{\zeta}_y')\exp\left(-\mu^2 \boldsymbol{\xi}^2\right), \tag{4.3}$$

which is the low-pass filter, where μ is the filter width.

4.1 Boundary Conditions for the Distribution Function

We want to find the boundary condition for ϕ at the wall with the scattering kernel $R(\zeta' \rightarrow \zeta; y' \rightarrow y)$ given by (4.2a)–(4.2b). We impose a nonlocal analog of (2.9), namely we require at the wall (3.4) to hold.

Using the explicit expression for $R(\zeta' \to \zeta, y' \to y)$ given by (4.2a)–(4.2b), the following boundary condition in $x_1 = 0$ is obtained:

$$\phi(\boldsymbol{\zeta}, \boldsymbol{y}) = (1 - \varepsilon \beta)\phi(\boldsymbol{\zeta}_{R}, \boldsymbol{y}) + \varepsilon \gamma \frac{1}{2\pi\mu^{2}} \int_{\mathbb{R}^{2}} \exp\left[-\frac{(\boldsymbol{y} - \boldsymbol{y}')^{2}}{2\mu^{2}}\right] \phi(\boldsymbol{\zeta}_{R}, \boldsymbol{y}') d\boldsymbol{y}' + \varepsilon(\beta - \gamma)\phi_{e} \quad (\text{for } \zeta_{1} > 0),$$
(4.4a)

where $\boldsymbol{\zeta}_R = (-\zeta_1, \zeta_2, \zeta_3)$ and $\phi_e(\check{\sigma}_w, u_w, \tau_w)$ is defined by:

$$E\phi_e(\check{\sigma}_w, u_w, \tau_w) = \frac{1 + \check{\sigma}_w}{\pi^{3/2}(1 + \tau_w)^{3/2}} \exp\left[-\frac{(\zeta_i - u_{iw})^2}{1 + \tau_w}\right] - E,$$
(4.4b)

being $\check{\sigma}_w$ given by:

$$\check{\sigma}_w = -2\left(\frac{\pi}{1+\tau_w}\right)^{1/2} \int_{\zeta_1'<0} \zeta_1' E(\zeta') \phi(\zeta_i', \mathbf{y}) d\boldsymbol{\zeta}' + \left(\frac{1}{1+\tau_w}\right)^{1/2} - 1.$$
(4.4c)

5 Fluid-Dynamic Type Equations

We shall now study the limit $Kn \rightarrow 0$ for the flow of a rarefied gas with finite Reynolds number starting from the kinetic description given by (2.6) with the boundary conditions (4.4a)–(4.4c). Our concern is to get a new set of boundary conditions for the fluid dynamic variables which generalize the Robin-type boundary conditions.

The asymptotic analysis of the boundary-value problem (2.6) and (4.4a)–(4.4c) will give, in the leading order, the set of Navier–Stokes equations and its appropriate boundary conditions. We stress the fact that we are considering the case of the accommodation coefficient $O(\varepsilon)$, which will give Robin-type boundary conditions for the macroscopic variables. The case $\alpha = O(\varepsilon)$, was first considered in [1], where, on the basis of the linearized BKW equation with an arbitrary but smooth shaped boundary, the Stokes system with mixed-type boundary conditions was derived. Recently the small accommodation coefficient case was analyzed in [3], where the authors studied the cylindrical Couette flow of a rarefied gas using the nonlinear Boltzmann equation.

We now carry out the procedure to derive the fluid dynamic equations following [22]. Since this procedure is described in great detail in the books of Sone (see also [23]), we shall only briefly outline the main steps.

We shall investigate the asymptotic behavior of the solution of the boundary-value problem (2.6) and (4.4a)–(4.4c) when $Kn \rightarrow 0$. We want to describe the case of finite Reynolds number, namely Re = O(1). According to the Von Karmann relation $Ma \propto ReKn$, the Mach number (Ma) (which is one of the scales that indicate the deviation of the system from a uniform equilibrium state at rest) has to be of the same order as Kn. Thus we shall consider the case where the velocity distribution function is a global Maxwellian plus a deviation that is of the order of the Knudsen number. This accounts to choose $\phi = O(\varepsilon)$. In terms of the macroscopic parameters, the assumption on the velocity distribution function requires that the nondimensional temperature and density variation are $O(\varepsilon)$.

First, putting aside the boundary condition (4.4a)-(4.4c), we look for a moderately varying solution of (2.6), whose length scale of variation is of the order of the characteristic length *L* of the system in a power series of ε : (i.e. the velocity distribution function

does not vary appreciably over a distance of the order of mean free part which implies $\partial \phi / \partial x_i = O(\phi)$:

$$\phi_S = \phi_{S1}\varepsilon + \phi_{S2}\varepsilon^2 + \cdots, \tag{5.1}$$

where the series starts from the first order in ε since ϕ is assumed to be $O(\varepsilon)$, and the component function ϕ_{Sm} is a quantity of order of unity. This solution will be called the *S* solution.

The relation between the macroscopic variables and the distribution function is the same as (2.8), except for the subscript *S*.

Corresponding to the expansion (5.1), the macroscopic variables ω_S , u_{iS} , τ_S , ... are also expanded in ε :

$$h_S = h_{S1}\varepsilon + h_{S2}\varepsilon^2 + \cdots, \tag{5.2}$$

where *h* represents ω , u_i , τ , *P* and the component function h_{Sm} is a quantity of the order of unity. The relation between the component function h_{Sm} of the macroscopic variable h_S and the component function ϕ_{Sr} is obtained by substituting in (2.8), (5.1) and (5.2) and by equating the coefficients of the same power of ε .

Substituting the expansion (5.1) into the Boltzmann equation (2.6) and arranging the same order quantities in ε , we obtain the following series of integral equations for ϕ_{Sm} :

$$\mathcal{L}(\phi_{S1}) = 0, \tag{5.3}$$

$$\mathcal{L}(\phi_{Sm}) = \zeta_i \frac{\partial \phi_{Sm-1}}{\partial x_i} - \sum_{r=1}^{m-1} \mathcal{J}(\phi_{Sm-r}, \phi_{Sr}) \quad (m = 2, 3, \ldots).$$
(5.4)

The solution ϕ_{S1} of (5.3) is given by:

$$\phi_{S1} = \omega_{S1} + 2\zeta_i u_{iS1} + \left(\zeta_i^2 - \frac{3}{2}\right) \tau_{S1}.$$
(5.5)

This is the first term of the expansion of the perturbed Maxwellian $\phi_e(\omega_S, u_{iS}, \tau_S)$ (= ϕ_{eS}) in terms of ε , which means that ϕ_{S1} is a local Maxwellian distribution.

As for the inhomogeneous Boltzmann equation (5.4), it is a linear integral equation containing the linearized collision integral \mathcal{L} , with inhomogeneous terms consisting of the earlier terms of the expansion. The corresponding homogeneous equation, namely $\mathcal{L}(\phi_{Sm}) = 0$, has five independent solutions $1, \zeta_i, \zeta_i^2$. This implies that, for the inhomogeneous equation to have a solution, its inhomogeneous term should satisfy the solvability condition:

$$\int g\zeta_i \frac{\partial \phi_{Sm-1}}{\partial x_i} E d\zeta = 0, \tag{5.6}$$

where $g = 1, \zeta_i$, or ζ_i^2 . The application of this condition to $\phi_{S1}, \phi_{S2}, ...$ in the solution process of the sequence of the integral equations (5.4) from the lower order, leads to the fluid dynamic equations for h_m in (5.2).

Rearranging the equations obtained from the series of the solvability conditions (5.6), in a set of equations that determine the component functions of the expansion of the macroscopic variables:

$$\frac{\partial P_{S1}}{\partial x_i} = 0, \tag{5.7}$$

$$\frac{\partial u_{iS1}}{\partial x_i} = 0, \tag{5.8}$$

$$u_{jS1}\frac{\partial u_{iS1}}{\partial x_j} = -\frac{1}{2}\frac{\partial P_{S2}}{\partial x_i} + \frac{\gamma_1}{2}\frac{\partial^2 u_{iS1}}{\partial x_i^2},\tag{5.9}$$

$$u_{iS1}\frac{\partial\tau_{S1}}{\partial x_i} = \frac{\gamma_2}{2}\frac{\partial^2\tau_{S1}}{\partial x_i^2}$$
(5.10)

where i, j = 1, 2, 3, and the expressions of γ_1 and γ_2 are given in Appendix B. Equation (5.7) is the momentum equation at the order ε and imposes P_{S1} to be a constant. The pressure variation at order ε must vanish for a flow field with Mach number of order ε to be established.

The next (5.8)–(5.10), which determine ω_{S1} , u_{iS1} , τ_{S1} and P_{S2} are the Navier–Stokes equations for an incompressible fluid, with γ_1 and γ_2 as the nondimensional viscosity and thermal conductivity.

The explicit expressions of ϕ_{S1} and ϕ_{S2} are given in Appendix **B**.

We remark that the velocity distribution function ϕ_{S1} at the order of ε is Maxwellian and that the functions ω_{S1} , u_{iS1} and τ_{S1} determining the Maxwellian ϕ_{S1} are governed by the incompressible Navier–Stokes equations (see e.g. [4, 11]).

5.1 Boundary Conditions for the Fluid Dynamic Variables

We now take into account the boundary conditions (4.4a)–(4.4b) that were not considered in the previous section where the distribution function ϕ_S was derived. Since ϕ_{S1} is a local Maxwellian given by (5.5), it can be made so as to satisfy the boundary conditions (4.4a)–(4.4c) at order ε . In other words, provided that

$$u_{1S1} = u_{1w1} = 0, \tag{5.11}$$

 ϕ_{S1} satisfies the boundary conditions in the leading order, i.e.

$$\phi_{S1}(\boldsymbol{\zeta}, \boldsymbol{y}) = \phi_{S1}(\boldsymbol{\zeta}_R, \boldsymbol{y}). \tag{5.12}$$

However the next order term ϕ_{S2} , is no longer a Maxwellian (see (B.2)), so that, as in the usual situation, it cannot satisfy the boundary conditions at order ε^2 . This is not surprising as the Boltzmann equation (2.6) is of singular type. To obtain the solution of the boundary-value problem we need to introduce a correction close to the boundary, the so-called Knudsen layer. We shall put the solution in the form:

$$\phi = \phi_S + \phi_K, \tag{5.13}$$

where

$$\phi_K = \varepsilon^2 \phi_{K2} + \varepsilon^3 \phi_{K3} + \cdots, \tag{5.14}$$

is the Knudsen solution, which varies appreciably in a thin layer of thickness $O(\varepsilon)$ adjacent to the boundary $(\varepsilon \partial \phi_K / \partial x_1 = O(\varepsilon))$. We stress the fact that the expansion starts form order ε^2 because ϕ_{S1} could satisfy the boundary conditions at order ε . Introducing the normal stretched variable $\eta = x_1/\varepsilon$, so that $\phi_K = \phi_K(\zeta, \eta, y)$ and substituting (5.13) into (2.4) with (5.1) and (5.14), one gets the equation for ϕ_{K2} :

$$\zeta_1 \frac{\partial \phi_{K2}}{\partial \eta} = \mathcal{L}(\phi_{K2}). \tag{5.15}$$

In order to get the boundary condition for ϕ_{K2} we need to write explicitly the boundary condition for the distribution function ϕ , (4.4a)–(4.4c), at order $O(\varepsilon^2)$.

The quantity $\check{\sigma}_w$ (defined in (4.4c)) has the following expansion in powers of ε :

$$\check{\sigma}_{w} = \varepsilon \left[-2\sqrt{\pi} \int_{\zeta_{1}'<0} \zeta_{1}' E(\zeta') \phi_{S1}(\zeta_{i}', \mathbf{y}) d\boldsymbol{\zeta}' - \frac{1}{2} \tau_{w1}(x_{2}) \right] + O(\varepsilon^{2})$$
$$= \varepsilon \left[\omega_{S1} + \frac{1}{2} (\tau_{S1} - \tau_{w1}) \right] + O(\varepsilon^{2}), \tag{5.16}$$

where, in passing from the first to the second line, we have used the explicit expression of ϕ_{S1} .

Therefore, using (5.16), the ε -expansion of ϕ_e is:

$$\phi_e = \varepsilon \left[\omega_{S1} + \frac{1}{2} (\tau_{S1} - \tau_{w1}) + 2\zeta_i u_{iw1} + \left(\zeta^2 - \frac{3}{2} \right) \tau_{w1} \right] + O(\varepsilon^2), \quad (5.17)$$

so that the boundary condition for ϕ expressed by (4.4a), at order ε^2 , writes as:

$$\begin{split} \phi_{K2}(\boldsymbol{\zeta},\,\boldsymbol{y}) &= -\phi_{S2}(\boldsymbol{\zeta},\,\boldsymbol{y}) + \phi_{S2}(\boldsymbol{\zeta}_{R},\,\boldsymbol{y}) + \phi_{K2}(\boldsymbol{\zeta}_{R},\,\boldsymbol{y}) - \beta\phi_{S1}(\boldsymbol{\zeta}_{R},\,\boldsymbol{y}) \\ &+ \gamma \frac{1}{2\pi\mu^{2}} \int_{\mathbb{R}^{2}} \exp\left[-\frac{(\boldsymbol{y}-\boldsymbol{y}')^{2}}{2\mu^{2}}\right] \phi_{S1}(\boldsymbol{\zeta}_{R},\,\boldsymbol{y}') d\,\boldsymbol{y}' \\ &+ (\beta - \gamma) \left[\omega_{S1}(\boldsymbol{y}) + \frac{1}{2}(\tau_{S1} - \tau_{w1})(\boldsymbol{y}) + 2\zeta_{i}u_{iw1}(\boldsymbol{y}) + \left(\zeta^{2} - \frac{3}{2}\right)\tau_{w1}(\boldsymbol{y})\right] \\ \text{for } \zeta_{1} > 0, \text{ at } \eta = 0. \end{split}$$
(5.18)

We notice that the first and the last line in (5.18) are the usual terms of the Maxwell boundary condition, while the second row is the effect of the nonlocality of the scattering kernel.

In all the above procedure we are considering the steady case. In the unsteady case one cannot ignore the fact that the particle, entering at location y' would get out at y with a time delay. If one would consider this effect, then, in the asymptotic expansion (4.4a)–(4.4b), one would get the time derivative of the ϕ .

To get the boundary conditions for the fluid dynamic variables (following the procedure of [3]) we shall use the orthogonality condition (the analog of (5.6)) for ϕ_{K2} :

$$\frac{\partial}{\partial \eta} \int g\zeta_1 \phi_{K2} E d\zeta = 0, \quad \text{for } \eta \ge 0, \tag{5.19}$$

at the boundary $\eta = 0$, so that ϕ_{K2} is given by (5.18), and the explicit expressions of ϕ_{S1} and ϕ_{S2} given in the Appendix B are used. We recall that $g = 1, \zeta_i$, or ζ_i^2 are the collision invariants.

When we evaluate (5.19) for g = 1, we get the following condition:

$$u_{1S2} = \frac{\gamma}{4\sqrt{\pi}} \bigg[\tau_{S1} - \frac{1}{2\pi\mu^2} \int_{\mathbb{R}^2} \exp\bigg[-\frac{(\mathbf{y} - \mathbf{y}')^2}{2\mu^2} \bigg] \tau_{S1}(\mathbf{y}') d\mathbf{y}' \bigg],$$
(5.20)

which expresses the nonlocal conservation mass flux: in fact on integration of the above relation (5.20) over the \mathbb{R}^2 -plane, global zero mass flux is obtained.

When we evaluate (5.19) for $g = \zeta_i$ (i = 2, 3), the following boundary condition for the velocity u_{iS1} is obtained:

$$4\sqrt{\pi}\gamma_{1}\frac{\partial u_{iS1}}{\partial x_{1}} - \beta(u_{iS1} - u_{iw1}) -\gamma\left\{u_{iw1} - \frac{1}{2\pi\mu^{2}}\int_{\mathbb{R}^{2}}\exp\left[-\frac{(\mathbf{y} - \mathbf{y}')^{2}}{2\mu^{2}}\right]u_{iS1}(\mathbf{y}')d\mathbf{y}'\right\} = 0.$$
(5.21)

Finally, evaluating (5.19) for $g = \zeta^2$, one obtains the following boundary condition for the temperature:

$$10\sqrt{\pi}\gamma_{2}\frac{\partial\tau_{S1}}{\partial x_{1}} + 8\beta(\tau_{w1} - \tau_{S1}) - 9\gamma\left\{\tau_{S1} - \frac{1}{2\pi\mu^{2}}\int_{\mathbb{R}^{2}}\exp\left[-\frac{(\mathbf{y} - \mathbf{y}')^{2}}{2\mu^{2}}\right]\tau_{S1}(\mathbf{y}')d\mathbf{y}'\right\} = 0.$$
(5.22)

Equations (5.20)–(5.22) are the boundary conditions for the Navier–Stokes equations (5.8)–(5.10).

Equation (5.21) is the Robin boundary condition for the tangential component of the velocity plus an additive term, which is proportional to the difference between the wall velocity and a filtered flow. Notice that, if one takes the convolution of (5.21) with the gaussian kernel, one obtains (in the particular case $\mathbf{u}_w = 0$) the second boundary condition in (1.1) of the near wall model [13]. Analogously, the boundary condition for the temperature field, (5.22), prescribes a Robin condition plus a nonlocal extra term.

6 Concluding Remarks

In this paper, starting from the kinetic theory, nonlocal boundary conditions for the Navier– Stokes equations have been derived in the hydrodynamic limit. The motivation of this work comes from the need of generating nonlocal boundary conditions of the type used in turbulence modeling, from more fundamental principles. The gas-surface interaction we proposed generalize the Maxwell scattering kernel introducing nonlocal effects. The nonlocal part of the scattering kernel was chosen to behave as a low-pass filter, so as to describe nonlocal specular reflection of the small structures in the incoming flux and cut-off of the large structures. Our description provides, in the continuum limit, a new class of boundary conditions for the fluid-dynamic variables.

A similar analysis with a nonlocal Poisson scattering kernel was performed in [14] where weakly nonlocal boundary conditions for the Navier–Stokes equations were found.

A similar analysis starting from more realistic gas-surface interaction models could also be of interest. In fact, the criticisms opposed to the Maxwell scattering kernel [6, 16–18] suggest to take into account the case when more than one accommodation coefficient is present (see the Cercignani–Lampis model [6–8], and the anisotropic scattering kernel [9]). This will be the subject of a subsequent work.

Appendix A: The Collision Integral

The collision integral $\mathcal{J}(\phi, \psi)$ is given by:

$$\mathcal{J}(\phi,\psi) = \frac{1}{2} \int E_*(\phi'\psi'_* + \phi'_*\psi' - \phi\psi_* - \phi_*\psi)\hat{B}d\Omega(\alpha)d\xi_*,$$
(A.1a)

$$\phi = \phi(\zeta_i), \quad \phi_* = \phi(\zeta_{i*}), \quad \phi' = \phi(\zeta'_i), \quad \phi'_* = \phi(\zeta'_{i*}), \quad (A.1b)$$

where ζ_i' and ζ_{i*}' are related to ζ_i and ζ_{i*} by

$$\zeta_i' = \zeta_i + \alpha_i \alpha_j (\zeta_{j*} - \zeta_j), \qquad \zeta_{i*}' = \zeta_i + \alpha_{i*} \alpha_j (\zeta_{j*} - \zeta_j), \tag{A.1c}$$

 α_i is a unit vector expressing the variation of the direction of the molecular velocity owing to an intermolecular collision, $d\Omega(\alpha)$ is the solid-angle element in the direction of α_i and $\hat{B} = \hat{B}(|\alpha_i(\zeta_{i*} - \zeta_i)|/|(\zeta_{k*} - \zeta_k)|, |(\zeta_{i*} - \zeta_i)|)$, generally depends on T_0 as well as on the intermolecular potential. For hard-sphere gas

$$\hat{B} = \frac{|\alpha_i(\zeta_{i*} - \zeta_i)|}{4(2\pi)^{1/2}};$$
(A.2)

 $d\zeta_* = d\zeta_{*1}d\zeta_{*2}$; the domain of integration in (A.1a) is all directions of α and the whole space of $d\zeta_*$ (see Sect. 2.9 in [22]).

The linear part of the collision integral, called the linearized collision integral $\mathcal{L}(\phi)$ is given by:

$$\mathcal{L}(\phi) = \int E_*(\phi' + \phi'_* - \phi - \phi_*) \hat{B} d\Omega(\alpha) d\boldsymbol{\zeta}_*.$$
(A.3)

The operator \mathcal{J} is related to \mathcal{L} in the following way:

$$2\mathcal{J}(1,\phi) = \mathcal{L}(\phi). \tag{A.4}$$

Moreover the operator \mathcal{L} satisfies the following relations:

$$\int E\psi(\boldsymbol{\zeta})\mathcal{L}(\phi)d\boldsymbol{\zeta} = \frac{1}{4}\int EE_*(\psi + \psi_* - \psi' - \psi'_*)(\phi' + \phi'_* - \phi - \phi_*)\hat{B}d\Omega(\boldsymbol{\alpha})d\boldsymbol{\zeta}_*d\boldsymbol{\zeta},$$

for any ϕ and ψ , (A.5)

$$\int g(\boldsymbol{\zeta}) \mathcal{L}(\phi) E d\boldsymbol{\zeta} = 0 \quad \text{for any } \phi, \tag{A.6}$$

$$\mathcal{L}(g(\boldsymbol{\zeta})) = 0, \tag{A.7}$$

where $g(\boldsymbol{\zeta})$ is one of the collision invariants 1, ζ_i , or ζ_i^2 . Moreover, from (A.5), it follows that the operator \mathcal{L} is selfadjoint. Finally:

$$\int g(\boldsymbol{\zeta}) \mathcal{J}(\phi, \psi) E d\boldsymbol{\zeta} = 0 \quad \text{for any } \phi \text{ and } \psi, \qquad (A.8a)$$

$$\int g(\boldsymbol{\zeta}) \mathcal{L}(\phi) E d\boldsymbol{\zeta} = 0 \quad \text{for any } \phi .$$
 (A.8b)

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Appendix B: Explicit Expressions of ϕ_{S1} and ϕ_{S2}

The first-order S-solution ϕ_{S1} is given by:

$$\phi_{S1} = \omega_{S1} + 2\zeta_i u_{iS1} + \left(\zeta_i^2 - \frac{3}{2}\right) \tau_{S1}.$$
(B.1)

This is the first term of the expansion of the perturbed Maxwellian $\phi_e(\omega_S, u_{iS}, \tau_S) (= \phi_{eS})$ in terms of ε .

The second-order S-solution ϕ_{S2} is given by:

$$\phi_{S2} = \phi_{eS2} - \zeta_i \zeta_j B(\zeta) \frac{\partial u_{iS1}}{\partial x_j} - \zeta_i A(\zeta) \frac{\partial \tau_{S1}}{\partial x_i}, \tag{B.2}$$

where ϕ_{eS2} is the second term of the expansion of the perturbed Maxwellian ϕ_{eS} and the functions $A(\zeta)$ and $B(\zeta)$ are the solutions of the following integral equations:

$$\begin{cases} \mathcal{L}[\zeta_i A(\zeta)] = -\zeta_i (\zeta_j^2 - \frac{5}{2}), \\ \text{subsidiary condition } \int_0^\infty \zeta^4 A(\zeta) \exp(-\zeta^2) d\zeta = 0, \\ \mathcal{L}\left[\left(\zeta_i \zeta_j - \frac{1}{3} \zeta_k^2 \delta_{ij} \right) B(\zeta) \right] = -2 \left(\zeta_i \zeta_j - \frac{1}{3} \zeta_k^2 \delta_{ij} \right). \end{cases}$$
(B.3)

The coefficients γ_1 and γ_2 occurring in the Navier–Stokes equations (5.7)–(5.10) are given by:

$$\gamma_1 = I_6(B), \qquad \gamma_2 = 2I_6(A), \quad I_n(Z) = \frac{8}{15\sqrt{\pi}} \int_0^\infty \zeta^n Z(\zeta) \exp(-\zeta^2) d\zeta.$$
 (B.4)

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