

## NONLOCAL BOUNDARY CONDITIONS FOR THE NAVIER–STOKES EQUATIONS \*

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In this paper nonlocal boundary conditions for the Navier–Stokes equations are derived, starting from the Boltzmann equation in the hydrodynamic limit. Basing on phenomenological arguments, two scattering kernels which model non–local interactions between the gas molecules and the wall boundary are proposed. They 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 new class of nonlocal boundary conditions.

### 1. Introduction

In many practical cases, like geophysical models or turbulence modelling, the no–slip boundary conditions usually imposed for the Navier–Stokes Equations (NSE) fail to correctly describe the interactions between the fluid and a solid boundary and the problem of finding appropriate boundary conditions is a major one.

In the framework of turbulence modelling, the approach known as Large Eddy Simulation (LES) seeks to predict local spatial averages of the fluid’s velocity above a preassigned length scale. The mathematical problem of finding appropriate boundary conditions in LES has been tackled in<sup>4,5</sup>. The nonlocal boundary condition for the coarse grained Navier–Stokes that have been proposed for the averaged flow  $\bar{\mathbf{u}}$  are<sup>5</sup>:

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

where  $\bar{\mathbf{u}}$  represents the velocity averaged with a gaussian filter,  $\mathbf{n}$  and  $\boldsymbol{\tau}$  are

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the wall normal and tangential unit vectors, respectively,  $Re$  is the Reynolds number and  $\mathbb{D}_{ij}(\mathbf{u}) = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})$  is the velocity deformation tensor. Conditions (1) are the Robin boundary conditions for the averaged velocity. Recently<sup>1</sup> a mean field approach to the Boltzmann equation, filtering out subgrid scales, led to a subgrid turbulence model. It was shown<sup>1</sup> that, as for the Navier–Stokes equations, the Smagorinsky subgrid model enjoys a consistent derivation from the kinetic theory.

Motivated by the above considerations, in this paper we want to derive Robin–type boundary conditions for the macroscopic variables taking into account the effect of nonlocal interactions at the wall, starting from a kinetic description. We shall investigate the steady behavior of a fluid on the basis of the Boltzmann equation on a 3-dimensional half space. Two simple models are introduced whose corresponding scattering kernels generalize the Maxwell gas–surface interaction law. The first model describes a situation in which particles can penetrate the wall (thought as a lattice) and can experience a specular reflection from the inner layers of the wall. In the hydrodynamical limit this model leads to BC for the NS equations weakly non local; in the sense that the heat flux at the boundary is driven from (besides the classical term expressing the temperature difference between the fluid and the wall) the divergence of the velocity at the wall. In the second model (from which, in the hydrodynamical limit, we derive (1)) large structures (in the Fourier sense) of the fluid are specularly reflected, while small structures penetrate the wall, get in thermal equilibrium with it and are re–emitted through a Maxwellian. The proposed kernels are shown to satisfy a nonlocal mass conservation and a generalized reciprocity relation.

## 2. Notations

We shall consider a fluid confined to the 3– $D$  half space  $\mathbb{D} = \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}$ , the  $\mathbf{x} = x_i (i = 1, 2, 3)$  are 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 distribution function of the fluid molecules;  $\hat{\rho}$  is the dimensionless density,  $u_i$  the dimensionless fluid velocity,  $\hat{T}$ ,  $\hat{p}$  are the dimensionless temperature and the pressure of the fluid,  $\hat{T}_w$ ,  $\hat{\rho}_w$ ,  $\hat{p}_w$ ,  $u_{iw}$  are the dimensionless wall temperature, density, pressure and velocity, respectively and  $R$  is the fluid constant per unit mass. We also introduce the Maxwellian  $f_0$  with  $v_i = 0, p = p_0$  and  $T = T_0$ :

$$f_0 = \frac{\rho_0}{(2\pi RT_0)} E(\zeta); \quad E(\zeta) = \frac{1}{\pi} \exp(-\zeta^2), \quad \zeta = (\zeta_i^2)^{1/2} = |\zeta|. \quad (2)$$

In what follows we shall consider the state of the gas close to the Maxwellian distribution function  $f_0$  given by Eq. (2). The nondimensional perturbed variables are given by:

$$\begin{aligned} \phi &= \hat{f}/E - 1, & \omega &= \hat{\rho} - 1, & \tau &= \hat{T} - 1, & P &= \hat{p} - 1, \\ \tau_w &= \hat{T}_w - 1, & \omega_w &= \hat{\rho}_w - 1, & P_w &= \hat{p}_w - 1. \end{aligned} \quad (3)$$

The steady Boltzmann equation in dimensionless form reads:

$$\zeta_i \frac{\partial \phi}{\partial x_i} \frac{1}{\varepsilon} [\mathcal{L}(\phi) + \mathcal{J}(\phi, \phi)], \quad \varepsilon = \frac{\sqrt{\pi}}{2} \text{Kn} \quad (4)$$

where  $\mathcal{J}(\phi)$  and  $\mathcal{L}(\phi)$  are the collision integral and the linearized collision integral respectively, and Kn is the Knudsen number<sup>6</sup>. The relations between the nondimensional macroscopic variables and the nondimensional velocity distribution function  $\phi$  are:

$$\begin{aligned} \omega &= \int \phi E d\zeta, & (1 + \omega)u_i &= \int \zeta_i \phi E d\zeta, \\ (1 + \omega)\tau &= \int (\zeta_i^2 - 1) \phi E d\zeta - (1 + \omega)u_i^2, & P &= \omega + \tau + \omega\tau. \end{aligned} \quad (5)$$

Let us consider a particle hitting the wall: let  $\zeta' = (\zeta'_1, \zeta'_2, \zeta'_3)$  and  $\zeta = (\zeta_1, \zeta_2, \zeta_3)$  be the velocity of the impinging and of the outgoing particle. For a simple boundary one usually assumes a fluid particle-surface interaction law of the following form: for  $x_1 = 0, \zeta \cdot \mathbf{n} > 0$

$$|\zeta \cdot \mathbf{n}| E(\zeta) (1 + \phi(\mathbf{y}, \zeta)) = \int_{\zeta' \cdot \mathbf{n} < 0} |\zeta' \cdot \mathbf{n}| R(\zeta' \rightarrow \zeta; \mathbf{y}) E(\zeta') (1 + \phi(\mathbf{y}, \zeta')) d\zeta', \quad (6)$$

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

The scattering kernel has to satisfy the positivity condition, the conservation of mass and the Reciprocity relation<sup>3</sup>. A widely used scattering kernel is the one proposed by Maxwell:

$$R(\zeta' \rightarrow \zeta, \mathbf{y}) = (1 - \alpha) \delta(\zeta_1 + \zeta'_1) \delta(\zeta_2 - \zeta'_2) + \alpha \frac{2}{\sqrt{\pi} (\hat{T}_w)^{3/2}} \zeta_1 \exp \left[ -\frac{(\zeta_i - u_{iw})^2}{\hat{T}_w} \right],$$

where  $\zeta'_1 < 0, \zeta_1 > 0$  and  $u_{iw}$  is the wall velocity. The above model prescribes that an  $1 - \alpha$  fraction of the molecules is specularly reflected at the surface of the wall, while the remaining  $\alpha$  fraction of the molecules is in thermal equilibrium with the wall. All the interactions are local in space.

### 3. The nonlocal scattering kernel I

In this section we want to propose a different model of the interaction between the gas and the wall. We suppose that, other than being reflected

at the surface, the molecule can pass some layers of the wall without experiencing any impact and then can be specularly reflected by some inner molecule of the wall lattice. This introduces a nonlocality effect into the scattering kernel: in fact if the molecule hits the wall at point  $\mathbf{y}'$  on the wall  $x_1 = 0$ , it will travel for some distance inside the wall, will hit the lattice and will come out at a different point  $\mathbf{y}$ . Since it is specularly reflected, the impact will take place half-way between  $\mathbf{y}'$  and  $\mathbf{y}$ . Let  $\mathbf{y} = (x_2, x_3)$ ,

$$\mathbf{y} - \mathbf{y}' = \rho_y \begin{pmatrix} \cos \alpha_y \\ \sin \alpha_y \end{pmatrix}; \zeta_y = (\zeta_2, \zeta_3) = \rho_\zeta \begin{pmatrix} \cos \alpha_\zeta \\ \sin \alpha_\zeta \end{pmatrix}; \zeta'_y = (\zeta'_2, \zeta'_3) = \rho'_\zeta \begin{pmatrix} \cos \alpha'_\zeta \\ \sin \alpha'_\zeta \end{pmatrix} \quad (7)$$

where  $(\rho_y, \alpha_y)$  are the polar coordinates on the plane  $(x_2, x_3)$  centered in  $\mathbf{y}'$ , and  $(\rho_\zeta, \alpha_\zeta)$  are the polar coordinates on the plane  $(\zeta_2, \zeta_3)$ . Let  $\zeta'_y$  be the tangential velocity of the incident particle. The probability of the above process taking place is the product of three different probabilities: the probability of the particle travelling for a distance  $\rho_y/2 = (|\mathbf{y} - \mathbf{y}'|)/2$  without hitting any other molecule; the probability of having an impact between  $\rho_y/2$  and  $\rho_y/2 + d\rho_y$  and the probability of travelling again for  $\rho_y/2$  without impacts. We shall assume each process to be governed by a Poisson distribution function with  $\frac{1}{\varepsilon}$  as mean value. Moreover the tangential part of the incident velocity  $\zeta'_y$  has to be parallel (with the same sign) to the vector  $\mathbf{y} - \mathbf{y}'$ , which will introduce the term  $\delta(\alpha_y - \alpha'_\zeta)$ . Then one has:

$$\begin{aligned} &\text{Probability} \\ &\text{of having only one} \quad \simeq \frac{\rho_y}{\varepsilon^2} \exp -\frac{\rho_y}{\varepsilon} \delta(\alpha_y - \alpha'_\zeta) d\rho_y d\alpha_y \\ &\text{impact at } \mathbf{y}' + \frac{\rho_y}{2} \end{aligned} \quad (8)$$

This term will affect the specular reflection part of the scattering kernel.

On the other hand, we suppose that the molecules which experience multiple scattering inside the solid will obey the diffusive reflection law at the boundary. Hence the nonlocal scattering kernel which takes into account both the nonlocal specular reflection and the diffusive reflection is:

$$\begin{aligned} R(\zeta' \rightarrow \zeta, \mathbf{y}' \rightarrow \mathbf{y}) &= (1 - \varepsilon\beta) \delta(\zeta_1 + \zeta'_1) \delta(\zeta_y - \zeta'_y) \frac{1}{\varepsilon^2} e^{-\frac{|\mathbf{y}-\mathbf{y}'|}{\varepsilon}} \delta(\alpha_y - \alpha'_\zeta) \\ &+ \varepsilon\beta \frac{2}{\pi(1 + \tau_w)^2} \zeta_1 \exp -\frac{(\zeta_i - u_{iw})^2}{1 + \tau_w} \delta(\mathbf{y} - \mathbf{y}'), \quad \text{for } \zeta'_1 < 0, \zeta_1 > 0 \end{aligned} \quad (9)$$

The above scattering kernel satisfies the positivity condition. Moreover it satisfies a nonlocal mass conservation law and the reciprocity relation in a nonlocal form<sup>2</sup>. The asymptotic procedure to derive the Navier–Stokes equations and the corresponding boundary conditions for the fluid dynamic variables is standard<sup>6</sup>. To first order in  $\varepsilon$  we get<sup>2</sup> the following BC:

$$u_1 = 0, \quad (10)$$

$$\sqrt{\pi} \gamma_1 \frac{\partial u_i}{\partial x_1} - 8\beta (u_i - u_{iw}) = 0, \quad (i = 2, 3) \quad (11)$$

$$4\sqrt{\pi} \gamma_2 \frac{\partial \tau}{\partial x_1} - 5\beta (\tau - \tau_w) - \sqrt{\pi} \left( \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) = 0, \quad (12)$$

Equations (10), (11) and (12) are the boundary conditions for the fluid dynamic equations: Eq. (10) is the usual no-flux boundary condition. Eq. (11) are the Robin boundary conditions for the tangential component of the velocity. Eq. (12) is the usual Robin BC for the temperature plus an extra term which is proportional to the *tangential* divergence of the velocity.

Introducing the Fourier transform with respect to  $\mathbf{y}$ , denoting by  $\boldsymbol{\omega} = (\omega_2, \omega_3)$  the dual variable of  $\mathbf{y}$ , namely:  $\hat{f}(\boldsymbol{\zeta}, \boldsymbol{\omega}) = \mathcal{F}(f(\boldsymbol{\zeta}, \mathbf{y}))$ , and denoting with  $K$  the specular reflection part of the scattering kernel (9), one easily verifies that:

$$\hat{K}(\boldsymbol{\zeta}' \rightarrow \boldsymbol{\zeta}, \boldsymbol{\omega}) \equiv \mathcal{F}(K(\boldsymbol{\zeta}' \rightarrow \boldsymbol{\zeta}, \mathbf{y})) = (1 - \varepsilon\beta) \frac{\delta(\zeta_1 + \zeta'_1) \delta(\zeta_2 - \zeta'_2) \delta(\zeta_3 - \zeta'_3)}{(1 + \varepsilon^2 |\boldsymbol{\omega}|^2)^{3/2}}, \quad (13)$$

where  $|\boldsymbol{\omega}|^2 = \omega_2^2 + \omega_3^2$ . Therefore the kernel can be interpreted as a low-pass filter: it allows large structures (small  $\boldsymbol{\omega}$ ) to pass the filter and hence to 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). It is with this interpretation in mind that, in the next section, we shall suggest a different scattering kernel.

#### 4. The nonlocal scattering kernel II

In this section we pursue the idea of constructing a nonlocal scattering kernel that can act as low-pass filter. Instead of a power-law low-pass filter, as the one in Eq. (13), we propose a Gaussian filter, as it is common in turbulence modelling. Namely, for  $\zeta_1 > 0$ , and with  $\beta > \gamma$ :

$$\begin{aligned} R(\boldsymbol{\zeta}' \rightarrow \boldsymbol{\zeta}, \mathbf{y}' \rightarrow \mathbf{y}) &= (1 - \varepsilon\beta) \delta(\zeta_1 + \zeta'_1) \delta(\zeta_2 - \zeta'_2) \delta(\zeta_3 - \zeta'_3) \delta(\mathbf{y} - \mathbf{y}') \\ &+ \varepsilon\gamma \delta(\zeta_1 + \zeta'_1) \delta(\zeta_2 - \zeta'_2) \delta(\zeta_3 - \zeta'_3) \frac{e^{-\frac{(x_2 - x'_2)^2 + (x_3 - x'_3)^2}{4\lambda^2}}}{4\lambda^2 \pi} \\ &+ \frac{2\varepsilon(\beta - \gamma)}{\pi(1 + \tau_w)^2} \delta(\mathbf{y} - \mathbf{y}') \zeta_1 e^{-\frac{(\zeta_i - u_{wi})^2}{1 + \tau_w}}. \quad (14) \end{aligned}$$

The first and the third term on the right hand side of (14) are 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  $\mathbf{y}'$  are reflected from a inner layer of wall molecules and exit at  $\mathbf{y}$  with Gaussian probability.

The scattering kernel given by (14) acts as a Gaussian low-pass filter, whose filter width is  $\lambda$ . The above scattering kernel satisfies the positivity condition, the conservation of mass and the reciprocity relation.

We now consider the limit  $\varepsilon \rightarrow 0$ . Following the same lines as in Sec.3, one finds the following boundary conditions for the fluid dynamic variables:

$$u_1 = 0, \quad (15)$$

$$4\sqrt{\pi} \gamma_1 \frac{\partial u_i}{\partial x_1} - \beta (u_i - u_{iw}) - \gamma [u_{iw} - G(\lambda, x_2, x_3) * u_i] = 0 \quad (i = 2, 3) \quad (16)$$

$$10\sqrt{\pi} \gamma_2 \frac{\partial \tau}{\partial x_1} + 8\beta (\tau_{w1} - \tau) - 9\gamma [\tau - G(\lambda, x_2, x_3) * \tau] = 0 \quad (17)$$

where with  $G(\lambda, x_2, x_3)$  we have denoted the 2D Gaussian with standard deviation  $\lambda$ , while  $*$  denotes the convolution in  $\mathbb{R}^2$ . Equations (15)-(16)-(17) are the boundary conditions for the Navier-Stokes equations: (16) 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 Eq. (16) with the gaussian kernel, one obtains the same boundary conditions of the near wall model<sup>5</sup>. Analogously, Eq. (17), prescribes a Robin condition for the temperature plus a nonlocal extra term. It is interesting to notice that, to second order, one gets the following BC for the mass flux:

$$u_1^{(2)} = \frac{\gamma}{4\sqrt{\pi}} [\tau - G(\lambda, x_2, x_3) * \tau] \quad (18)$$

The above condition prescribes (locally) a non zero mass flux at the boundary. This effect is due to the penetrative BC for the Boltzmann equation. If one integrates (18) on the whole boundary one gets that the total mass flux is zero.

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