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► **To cite this version:**

I. Ginzbourg, P. Adler. Boundary flow condition analysis for the three-dimensional lattice Boltzmann model. *Journal de Physique II*, 1994, 4 (2), pp.191-214. 10.1051/jp2:1994123 . jpa-00247955

HAL Id: jpa-00247955

<https://hal.science/jpa-00247955>

Submitted on 4 Feb 2008

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Classification
Physics Abstracts
47.11 — 47.55M

Boundary flow condition analysis for the three-dimensional lattice Boltzmann model

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(Received 10 May 1993, revised 17 September 1993, accepted 22 October 1993)

Abstract. — In the continuum limit, the velocity of a Newtonian fluid should vanish at a solid wall. This condition is studied for the FHC lattice Boltzmann model with rest particles. This goal is achieved by expanding the mean populations up to the second order in terms of the ratio ε between the lattice unit and a characteristic overall size of the medium. This expansion is applied to two extreme flow situations. In Poiseuille flow, the second eigenvalue of the collision matrix can be chosen so that velocity vanishes at the solid walls with errors smaller than ε^2 ; however the choice depends on the angle between the channel walls and the axes of the lattice. In a plane stagnation flow, the tangential and normal velocities do not vanish at the same point, except for particular choices of the parameters of the model; this point does not coincide with the solid wall. It is concluded that the boundary conditions are as a matter of fact imposed with errors of second order.

1. Introduction.

Lattice-gas and lattice Boltzmann models have been recently introduced (see [1] as some of the first contributions to the topic) to simulate macroscopic fluid mechanics. The particular application we have in mind in using these methods is porous media which are characterized by complex and random shapes [2]. In such an application, it is crucial to be able to discretize the porous medium by a numerical mesh as large as possible and to impose the usual no slip condition for velocity at the solid walls.

The major purpose of this work is to study this no slip condition both from a numerical and a theoretical standpoint in simple geometries. At lattice nodes close to the surface, bounce back conditions are usually used (and sometimes specular reflections). Problems on the location of the solid boundaries were already apparent in earlier papers [3, 4], but they were directly addressed in a recent publication [5].

This paper is organized as follows. Section 2 is devoted to a general exposition of the face centered hypercubic (hereafter referred to as FHC) lattice Boltzmann model with rest particles on which our numerical computations are based. It does not provide any new feature since it was already developed [6], but it provides all the necessary background for future developments. However, it should be mentioned that we could determine all the eigenvalues and eigenvectors of the collision matrix analytically. The classical bounce back condition is used at nodes close to the solid wall.

The general analytical method that we use is the following. The lattice unit is assumed to be very small when compared to the characteristic overall size of the porous medium. This enables us to introduce the small parameter ε which is the ratio between these two quantities. The mean populations can then be expanded in terms of ε . Constitutive relations are necessary to express the populations of various orders as linear functions of the main macroscopic quantities and of their derivatives. Finally, the Boltzmann equation is used to calculate the coefficients of these constitutive relations.

In section 3, the first order terms are addressed. They can be decomposed into two parts. The latter depends upon the external force and the former does not. This latter term induces a modification in the determination of the macroscopic velocity.

Section 4 is devoted to the second order terms which were not addressed before to the best of our knowledge. The form of these terms is obtained from invariance considerations. The coefficients of the constitutive relations are expressed as functions of the eigenvalues of the collision matrix.

These developments are applied to the analysis of flow close to solid boundaries and in particular to the classical no slip condition on velocity. Plane Poiseuille flow provides the simplest example of a flow field and it is analysed in section 5. Two situations were investigated ; in the first one, the solid walls are perpendicular to one of the axes of the FCHC lattice ; in the second situation, they make an angle of 45° with it. In both cases, it can be shown that up to the second order in ε , the velocity vanishes exactly in the middle between two lattice points for a particular choice of the second eigenvalue of the collision matrix. However, this value depends on the angle.

The more difficult case of a stagnation flow is dealt with in section 6. The same condition as previously is obtained for the velocity component parallel to the wall, a result which might have been expected on physical basis only. This is also true for the normal velocity component when density fluctuations are negligible. When these fluctuations are not negligible, it is shown how the model parameters are to be taken into account so that it is true.

However, these developments do not hold in general. In the final section, some perspectives are given on the use of mixed bounce back and specular reflections at the boundary in order that the no slip condition is fulfilled at the same point for all the velocity components.

2. General.

Let us briefly present the FCHC lattice Boltzmann model with rest particles on which are based our numerical simulations. This model has also been developed by Gustensen and Rothman [6]. A similar model with B_r rest particles of different masses has been introduced by d'Humières and Lallemand [7]. This section starts by the basic equations and conditions which govern the collisions. The mean populations are then expressed in terms of the density ρ and the velocity \mathbf{u} . The Navier-Stokes equations are derived by an expansion in the small parameter ε . Finally a Boltzmann model with a linear collision operator is presented.

BASIC EQUATIONS. — Consider a FCHC lattice in a space of $D = 4$ dimensions. b_m particles of unit mass per node are moving with velocities \mathbf{c}_i ($i = 1, \dots, b_m$). The component α ($\alpha = 1, \dots, D$) of these velocities is denoted by $c_{i\alpha}$. The norm $\|\mathbf{c}\|$ is denoted by c .

M_c particles of unit mass and with zero velocity are also present at each node of the FCHC lattice. The number M_c is arbitrary.

Let $N_i(\mathbf{r}, t)$ ($i = 1, \dots, b_m$) denote the mean population of moving particles at the node \mathbf{r} and time t . The mean population of each rest particle is denoted by $N_0(\mathbf{r}, t)$; its index i is thus

equal to 0. These particles move and collide on the lattice. This process can be expressed formally by the equation

$$N_i(\mathbf{r} + \mathbf{c}_i, t + 1) = \\ = N_i(\mathbf{r}, t) + \Delta_i^B [N_1(\mathbf{r}, t), \dots, N_{b_m}(\mathbf{r}, t), M_c N_0(\mathbf{r}, t)], \quad i = 0, 1, \dots, b_m. \quad (1)$$

This relation enables us to calculate the mean populations as time $t + 1$, provided that the functions Δ_i^B are known.

These functions are restricted by the physical conditions that the mass and the momentum must be conserved at each node for any time

$$\sum_{i=1}^{b_m} N_i(\mathbf{r} + \mathbf{c}_i, t + 1) + M_c N_0(\mathbf{r}, t + 1) = \sum_{i=1}^{b_m} N_i(\mathbf{r}, t) + M_c N_0(\mathbf{r}, t) \quad (2a)$$

$$\sum_{i=1}^{b_m} N_i(\mathbf{r} + \mathbf{c}_i, t + 1) \mathbf{c}_i = \sum_{i=1}^{b_m} N_i(\mathbf{r}, t) \mathbf{c}_i. \quad (2b)$$

Macroscopic quantities such as the density ρ and the momentum $\rho \mathbf{u}$ are related to these mean populations by the relations

$$\rho(\mathbf{r}, t) = \sum_{i=1}^{b_m} N_i(\mathbf{r}, t) + M_c N_0(\mathbf{r}, t) \quad (3a)$$

$$\rho \mathbf{u}(\mathbf{r}, t) = \sum_{i=1}^{b_m} N_i(\mathbf{r}, t) \mathbf{c}_i. \quad (3b)$$

At equilibrium, it can be shown that the mean populations are given by a Fermi Dirac distribution [9]

$$N_i^0(\mathbf{r}, t) = [1 + \exp(h + \mathbf{q} \cdot \mathbf{c}_i)]^{-1} \quad (4)$$

where the superscript ⁰ refers to equilibrium. The functions h and \mathbf{q} depend upon ρ and \mathbf{u} .

EXPANSIONS OF THE MEAN POPULATIONS IN TERMS OF DENSITY AND VELOCITY. — The mean populations can be expressed in terms of ρ and \mathbf{u} for small values of \mathbf{u} in the following way. The unknown functions h and \mathbf{q} can be expanded as a Taylor series around $\mathbf{u} = 0$. The coefficients of this series are unknown and depend upon ρ . It is a simple matter to expand (4) in terms of \mathbf{u} . Finally, these various expressions of N_i^0 must verify the relations (3). These conditions enable us to determine the unknown coefficients.

The results obtained in our situation with rest particles of unit mass is a trivial modification of the ones derived by d'Humières and Lallemand [7] and have been already derived by Noullez [8]

$$N_i^0(\mathbf{r}, t) = d + d' \rho \mathbf{u} \cdot \mathbf{c}_i + dG(\rho) \mathbf{u}^1 \cdot \{ \mathbf{Q}_i + (c^2/D - c_s^2) \mathbf{I} \} \cdot \mathbf{u}, \quad i = 1, \dots, b_m \\ N_0^0(\mathbf{r}, t) = d [1 - c_s^2 G(\rho) \mathbf{u} \cdot \mathbf{u}], \quad (5)$$

where

$$d = \rho/b, \quad b = b_m + M_c, \quad d' = D/(b_m c^2), \quad c_s^2 = [d' b]^{-1}, \\ G(\rho) = (1 - 2d) [2(1 - d) c^2 c_s^2]^{-1}, \quad \mathbf{Q}_i = \mathbf{c}_i \mathbf{c}_i - \mathbf{I} c^2/D. \quad (6)$$

EXPANSIONS OF THE MEAN POPULATIONS IN TERMS OF ε . — The usual last step in these models consists in the derivation of the macrodynamic equations, in other words of the Navier-Stokes equations. In the previous step, the velocity was assumed to be small ; here the size 1 of the unit cell is assumed to be very small when compared to the size L of the whole fluid domain. Let ε be the value of this ratio

$$\varepsilon = 1/L \ll 1. \quad (7)$$

One would like to derive the macroscopic equations which govern the macroscopic quantities ρ and \mathbf{u} . This operation, which is an upscaling from the lattice unit to the macroscopic scales can be performed in the following way. Macroscopic variables denoted by a prime are introduced

$$\mathbf{r}' = \varepsilon \mathbf{r}, \quad t'_1 = \varepsilon t, \quad t'_2 = \varepsilon^2 t. \quad (8)$$

The scaling of the space variable is clear. The two times t'_1 and t'_2 correspond to the propagation of density perturbations and to diffusive effects, respectively. They are introduced by the standard Chapman-Enskog procedure which is used to derive the macrodynamical equations from the microscopical ones.

The derivation operators can be written as [8]

$$\partial_t = \varepsilon \partial_{t'_1} + \varepsilon^2 \partial_{t'_2}; \quad \nabla_{\mathbf{r}} = \varepsilon \nabla_{\mathbf{r}'}. \quad (9)$$

The mean population $N_i(\mathbf{r}, t)$ can be expanded in terms of this small parameter ε

$$N_i(\mathbf{r}, t) = N_i^0(\mathbf{r}, t) + \varepsilon N_i^1(\mathbf{r}, t) + \varepsilon^2 N_i^2(\mathbf{r}, t) + \dots \quad (10)$$

Note that the term of order zero N_i^0 corresponds to the equilibrium term given in (5).

The macrodynamic equations are obtained by using the differential operators (9) in the expression of the mean populations $N_i(\mathbf{r} + \mathbf{c}_i, t + 1)$. The corresponding relations are then introduced into the equations (2) and the usual macrodynamic equations are readily derived. An expansion to order $O(\varepsilon^2)$ combined with the results to order ε yields

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (11a)$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot \mathbf{P} = \nabla \cdot [\nu(\rho) \nabla(\rho \mathbf{u})] + \nabla \cdot \{ \nu(\rho) (D - 2)/D + \xi \} \nabla \cdot (\rho \mathbf{u}) \quad (11b)$$

where the momentum flux \mathbf{P} is expressed as

$$\mathbf{P} = \rho c_s^2 \{ 1 - g(\rho) u^2/c^2 [1 + 0.5(D - c^2/c_s^2)] \mathbf{I} \} + g(\rho) \rho \mathbf{u} \cdot \mathbf{u}. \quad (12)$$

The so-called Galilean factor is given by

$$g(\rho) = [Db(1 - 2d)] / [(D + 2)h_m(1 - d)]. \quad (13a)$$

The kinematic shear viscosity ν and the bulk viscosity ξ may be written as

$$\nu = -\frac{b_m c^2}{D(D + 2)} \psi - \frac{c^2}{2(D + 2)} \quad (13b)$$

$$\xi = -\frac{b_m c^2}{D} \chi - \frac{1}{2} \left(\frac{c^2}{D} - c_s^2 \right). \quad (13c)$$

The coefficients ψ and χ are in principle derived from the expression of the functions Δ_i^B (cf. (1)) once the collision rules are established, and their derivation will be detailed in section 4.

BOLTZMANN MODEL WITH A LINEAR COLLISION OPERATOR. — It should be emphasized that the previous developments are perfectly general and apply whatever the precise collision model is. Let us now present a Boltzmann model with a linear collision operator A . In other words, it means that the general relation (1) is replaced by the linearized equation

$$N_i(\mathbf{r} + \mathbf{c}_i, t + 1) = N_i(\mathbf{r}, t) + \sum_{j=0}^{b_m} A_{ij}(N_j(\mathbf{r}, t) - N_j^0(\mathbf{r}, t)) W_j ; \quad i = 0, 1, \dots, b_m$$

$$W_j = \begin{cases} 1, & j \neq 0 \\ M_c, & j = 0 \end{cases} \quad (14)$$

Such a simplified model with rest particles has been studied previously [6].

The collision matrix A may be decomposed as follows

$$(A_{ij}) = \begin{pmatrix} c^0 & b^0 & b^0 & b^0 & b^0 \\ b^0 & & & & \\ b^0 & & A'_{ij} & & \\ \dots & & & & \\ b^0 & & & & \end{pmatrix}. \quad (15)$$

The matrix A' corresponds to collisions between moving particles. The unknown coefficients b^0 and c^0 correspond to collisions between moving/rest particles and rest/rest particles, respectively.

Because space is isotropic, the coefficients of A can only depend on the angle between the two velocity vectors \mathbf{c}_i and \mathbf{c}_j . On an FCHC lattice, it is easy to show that only 5 angles are possible ; hence A' and A only depend on 5 coefficients which are unknown

$$a_0, a_{60}, a_{90}, a_{120}, a_{180}. \quad (16)$$

The subscript corresponds to the angle expressed in degrees between the two velocity vectors. To these five unknowns the two additional unknowns b^0, c^0 should be added.

Because of the linear character of the collision operator, many progress can be made analytically. The coefficients of A should be such that the mass and momentum conservation equation (2) are verified. The eigenvalues and the eigenvectors of A can be calculated. For sake of clarity, all these usefull relations are gathered in Appendix A. It should be emphasized that seven unknown coefficients appear in A ; their choice is discussed in Appendix A [10].

BOUNDARY CONDITION AT A SOLID WALL. — It should be noticed that the lattice nodes are staggered with respect to the solid walls, i.e. that the minimal distance between a lattice node and a solid wall is approximately half a lattice unit. This is illustrated in figure 1 in the simple case of a Poiseuille flow.

Consider a node \mathbf{r}_0 which is located in the gas phase, but which is close to a solid wall. More precisely, assume that the node $\mathbf{r}_0 + \mathbf{c}_{i+}$ is located inside the solid phase ; \mathbf{c}_{i+} denotes one of the 24 elementary velocities \mathbf{c}_i .

The population $N_{i+}(\mathbf{r}_0 + \mathbf{c}_{i+}, t + 1)$ left the node \mathbf{r}_0 at time t with velocity \mathbf{c}_{i+} and would arrive at the node $\mathbf{r}_0 + \mathbf{c}_{i+}$ at time $t + 1$ if $\mathbf{r}_0 + \mathbf{c}_{i+}$ were located in the gas phase. This population $N_{i+}(\mathbf{r}_0 + \mathbf{c}_{i+}, t + 1)$ is assumed to bounce back to the node \mathbf{r}_0 with a reverse velocity $\mathbf{c}_{i-} = -\mathbf{c}_{i+}$.

This condition, which is called the bounce back condition, may be summarized by the relations

$$N_{i-}(\mathbf{r}_0, t + 1) = N_{i+}(\mathbf{r}_0 + \mathbf{c}_{i+}, t + 1)$$

$$\mathbf{c}_{i-} = -\mathbf{c}_{i+}. \quad (17)$$

3. Addition of a body force and first-order expansion of the mean populations.

For Boltzmann models, it was proposed [10] to implement a body force \mathbf{F} by adding to the mean population $N_i(\mathbf{r}, t)$ at each time step the quantity

$$\Delta N_i = d' \rho \mathbf{F} \cdot \mathbf{c}_i, \quad i = 1, \dots, b_m. \quad (18)$$

The mass conservation equation (2.a) is not modified by this addition. However, the momentum conservation equation (2.b) is now modified as

$$\sum_{i=1}^{b_m} N_i(\mathbf{r} + \mathbf{c}_i, t + 1) \mathbf{c}_i = \sum_{i=1}^{b_m} N_i(\mathbf{r}, t) \mathbf{c}_i + \rho \mathbf{F} \quad (19)$$

where the following identity has been used

$$\sum_{i=1}^{b_m} \mathbf{c}_i \mathbf{c}_i = d'^{-1} \mathbf{I}. \quad (20)$$

We shall now derive the macrodynamical equations when such terms are included. Inter alia, it will be shown that the expansion of the mean populations is modified by these terms. This section follows closely the derivation of the macrodynamical equations by Frisch *et al.* [9] (their Sect. 5).

First the body force \mathbf{F} is assumed to be of order ε

$$\mathbf{F} = \varepsilon \mathbf{f}. \quad (21)$$

Hence the addition of this force does not disturb the equilibrium populations, i.e. the zeroth order terms $N^0(\mathbf{r}, t)$.

The mean populations $N_i(\mathbf{r}, t)$ can be expanded in terms of ε (cf. (10)). The first order term $N_i^1(\mathbf{r}, t)$ can be split into two parts, the former for a zero external force, the latter for an external force \mathbf{f} . It seems natural to assume that this last term is proportional to \mathbf{f} . This can be expressed by

$$\begin{aligned} N_i^1(\mathbf{r}, t) &= N_i^{10}(\mathbf{r}, t) + N_i^{1f}(\mathbf{r}, t), \quad i = 0, \dots, b_m, \\ N_i^{1f}(\mathbf{r}, t) &= K_i \rho \mathbf{f}. \end{aligned} \quad (22)$$

Following Frisch *et al.* [9] the first order term N_i^{10} should not contribute to the local values of density and momentum (cf. (3)); hence,

$$\sum_{i=1}^{b_m} N_i^{10}(\mathbf{r}, t) + M_c N_0^{10}(\mathbf{r}, t) = 0, \quad \sum_{i=1}^{b_m} N_i^{10}(\mathbf{r}, t) \mathbf{c}_i = 0. \quad (23)$$

The terms $K_i \rho \mathbf{f}$ have a different effect; they do not modify the density, but the momentum balance

$$\sum_{i=1}^{b_m} N_i^{1f}(\mathbf{r}, t) + M_c N_0^{1f}(\mathbf{r}, t) = 0, \quad \sum_{i=1}^{b_m} N_i^{1f}(\mathbf{r}, t) \mathbf{c}_i = -\Theta \rho \mathbf{f}. \quad (24)$$

The momentum change is proportional to \mathbf{f} , Θ being an unknown constant.

The derivation of the macrodynamical equations parallels the work of Frisch *et al.* [9] summarized in section 2 after equation (7). Expansion of the mass conservation (2a) implies

two equations. The first one to order ε is the usual continuity equation

$$\partial_{t_1} \rho + \nabla' \cdot (\rho \mathbf{u}^0) = 0 \quad (25a)$$

where ∇' stands for ∇_r and (see (3b))

$$\rho \mathbf{u}^0 = \sum_{i=1}^{b_m} N_i^0(\mathbf{r}, t) \mathbf{c}_i \quad (25b)$$

The second equation to ε^2 contains extra terms due to the body force \mathbf{f}

$$\partial_{t_2} \rho = (\Theta - 0.5) \nabla' \cdot (\rho \mathbf{f}) \quad (26)$$

where an anticipated use of (28a) is made. In order to avoid artificial creation or destruction of mass, it is legitimate to choose

$$\Theta = 0.5 \quad (27)$$

Expansion of the modified momentum equation (19) yields terms of order ε

$$\partial_{t_1} (\rho \mathbf{u}^0) + \nabla' \cdot \mathbf{P} = \rho \mathbf{f} \quad (28a)$$

where the leading order approximation of the momentum flux tensor is

$$\mathbf{P} = \sum_{i=1}^{b_m} N_i^0(\mathbf{r}, t) \mathbf{c}_i \mathbf{c}_i \quad (28b)$$

The expansion of equation (19) to order ε^2 can be made along the same lines as [9]. The terms N^{10} (cf. (22)) are linear functions of the gradients $\nabla \rho$ and $\nabla(\rho \mathbf{u}^0)$; since these functions are invariant under the isometry group L of the lattice, this relation should be of the form

$$N_i^{10}(\mathbf{r}, t) = (\Psi \mathbf{Q}_i + \chi \mathbf{I}) : \nabla'(\rho \mathbf{u}^0), \quad i = 1, \dots, b_m \quad (29)$$

The constants ψ and χ will be computed in the next section by means of the collision matrix \mathbf{A} .

The same property of invariance will be requested for the terms $N_i^{1f}(\mathbf{r}, t)$ in (22). Since any set of i -dependent vectors is of the form $\lambda \mathbf{c}_i$ (cf. property P2 in [9]), one may assume

$$N_i^{1f}(\mathbf{r}, t) = \lambda \rho \mathbf{f} \cdot \mathbf{c}_i, \quad i = 1, \dots, b_m \quad (30)$$

The constant λ is determined by means of (24) and (27); hence, the first order correction to the mean populations can be expressed as

$$N_i^{1f}(\mathbf{r}, t) = -0.5 d' \rho \mathbf{f} \cdot \mathbf{c}_i, \quad i = 1, \dots, b_m \quad (31)$$

The corresponding corrections for the rest particles N_0^{10} and N_0^{1f} can be derived from the mass conservation (23) and (24)

$$N_0^{10}(\mathbf{r}, t) = -b_m/M_c \chi \nabla' \cdot (\rho \mathbf{u}^0), \quad N_0^{1f}(\mathbf{r}, t) = 0 \quad (32)$$

With these preliminary relations, it is not difficult to expand the momentum equation to order ε^2 . The results of the expansion to order ε and ε^2 must be combined to yield the full set of

macrodynamical equations [9], including the dissipation term

$$\partial_t \rho = \nabla \cdot (\rho \mathbf{u}^0) = (\Theta - 0.5) \nabla \cdot (\rho \mathbf{F}) \quad (33a)$$

$$\begin{aligned} \partial_t (\rho \mathbf{u}^0) + \nabla \cdot \mathbf{P} = \rho \mathbf{F} + \nabla \cdot [\nu(\rho) \nabla (\rho \mathbf{u}^0)] + \\ + \nabla [\{\nu(\rho) (D - 2)/D + \xi\} \nabla \cdot (\rho \mathbf{u}^0)] \\ - \varepsilon \partial_{t_i} (\rho \mathbf{F}) (\Theta - 0.5) - \varepsilon^2 \nabla' \cdot \left(\sum_{i=1}^{b_m} N_i^{1f}(\mathbf{r}, t) \mathbf{c}_i \right). \end{aligned} \quad (33b)$$

Except for the inclusion of the external force, these equations reduce to equations (11) because of the values of Θ and N_i^{1f} ; hence they may be written as

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}^0) = 0 \quad (34a)$$

$$\partial_t (\rho \mathbf{u}^0) + \nabla \cdot \mathbf{P} = \rho \mathbf{F} + \nabla \cdot [\nu(\rho) \nabla (\rho \mathbf{u}^0)] + \nabla [\{\nu(\rho) (D - 2)/D + \xi\} \nabla \cdot (\rho \mathbf{u}^0)] \quad (34b)$$

4. Second-order expansion of the Boltzmann equation.

The purpose of this section is twofold. First we want to derive the previous relations by a different route. Second we want to extend the previous results to second-order as indicated by the expansion (10).

BASIC EQUATION. — The basic equation is obtained in the following way. The expansion (10) is inserted in the Boltzmann equation (14). The left hand side of equation (14), i.e. $N_i(\mathbf{r} + \mathbf{c}_i, t + 1)$ is expanded in a Taylor series. In a straightforward manner, one obtains with the addition (18) to the mean population

$$\begin{aligned} \varepsilon (\partial_{t_i} N_i^0 + \mathbf{c}_i \cdot \nabla' N_i^0) + \\ + \varepsilon^2 (\partial_{t_i^2} N_i^0 + 0.5 \partial_{t_i} \partial_{t_i} N_i^0 + 0.5 \mathbf{c}_i \mathbf{c}_i : \nabla' \nabla' N_i^0 \\ + \mathbf{c}_i \cdot \nabla^1 \partial_{t_i} N_i^0 + \partial_{t_i} N_i^1 + \mathbf{c}_i \cdot \nabla' N_i^1) \\ = \sum_{j=0}^{b_m} \{ \varepsilon A_{ij} N_j^1(\mathbf{r}, t) + \varepsilon^2 A_{ij} N_j^2(\mathbf{r}, t) \} W_j + \varepsilon d' \rho \mathbf{f} \cdot \mathbf{c}_i, \quad i = 0, \dots, b_m. \end{aligned} \quad (35)$$

This compact equation can be discussed as follows. All the N_i^j are taken at point \mathbf{r} and time t . The last term on the right-hand side is not included in the equation $i = 0$ by using the convention $\mathbf{c}_0 = 0$.

FIRST-ORDER EQUATION. — Let us consider the terms of order ε in (35) in order to verify the consistency of the developments made in the previous section. They should verify

$$\partial_{t_i} N_i^0 + \mathbf{c}_i \cdot \nabla' N_i^0 = \sum_{j=0}^{b_m} A_{ij} N_j^1(\mathbf{r}, t) W_j + d' \rho \mathbf{f} \cdot \mathbf{c}_i, \quad i = 1, \dots, b_m \quad (36a)$$

$$\partial_{t_1} N_0^0 = \sum_{j=0}^{b_m} A_{0j} N_j^1(\mathbf{r}, t) W_j = c^0 M_c N_0^1(\mathbf{r}, t) + b^0 \sum_{j=1}^{b_m} N_j^1(\mathbf{r}, t). \quad (36b)$$

The second equation is modified as follows. The left hand side is evaluated with the help of (5) and (25a). The right-hand side is calculated with (29) and (30). One obtains

$$-b^{-1} \nabla' \cdot (\rho \mathbf{u}^0) = b^0 b_m \chi (1 + b_m/M_c) \nabla' \cdot (\rho \mathbf{u}^0) \quad (37)$$

from which the value of χ easily follows when flow is compressible (i.e. $\nabla_1 \cdot (\rho \mathbf{u}^0) \neq 0$)

$$\chi = -M_c [b^2 b^0 b_m]^{-1} \quad (38)$$

The equation (36a) can be handled in very much the same way. The various quantities can be expressed with the help of the previous developments. Finally, one obtains

$$M_c [b_m b]^{-1} \nabla' (\rho \mathbf{u}^0) + d' \mathbf{Q}_i : \nabla' (\rho \mathbf{u}^0) = \sum_{j=0}^{b_m} A_{ij} N_j^1(\mathbf{r}, t) W_j, \quad i = 1, \dots, b_m.$$

The expressions (29), (31), (32), (38) are used to evaluate the right-hand side of this equation. When one takes into account the fact that \mathbf{Q}_i is an eigenvector of \mathbf{A} , the previous relation is verified provided that ψ is related to the eigenvalue λ_ψ by the relation (A.4b).

SECOND-ORDER EQUATION. — The second-order terms can be readily derived from (35) and they may be expressed as

$$\begin{aligned} \partial_{t_2}^2 N_i^0 + 0.5 \partial_{t_1} \partial_{t_1} N_i^0 + 0.5 \mathbf{c}_i \cdot \mathbf{c}_i : \nabla' \nabla' N_i^0 + \mathbf{c}_i \cdot \nabla^1 \partial_{t_1} N_i^0 + \partial_{t_1} N_i^1 + \mathbf{c}_i \cdot \nabla' N_i^1 = \\ = \sum_{j=0}^{b_m} A_{ij} N_j^2(\mathbf{r}, t) W_j, \quad i = 0, \dots, b_m. \end{aligned} \quad (39)$$

The second-order corrections N_j^2 are so far unknown. However, these terms are not expected to contribute to the local values of density and momentum (cf. the same argument (23) as for the first-order terms) : hence,

$$\sum_{i=0}^{b_m} N_i^2(\mathbf{r}, t) W_i = 0, \quad \sum_{i=1}^{b_m} N_i^2(\mathbf{r}, t) \mathbf{c}_i = 0. \quad (40)$$

One can now proceed in two ways since the N_j^2 are unknown. The first method consists of the expansion of the left hand side of (39) ; from the terms which appear in this expansion, one can guess the general form of the unknown corrections N_j^2 in the right hand side of (39) ; note that since \mathbf{A} is not invertible, N_j^2 is not uniquely defined. The second method consists in making an *a priori* guess on the general form of N_i^2 as it was done for N_i^1 (cf. (29) and (30)). This is the one which will be used here. It seems natural to demand that N_i^2 be a linear function of the higher order gradients $\nabla' \nabla' \rho$, $\nabla' \nabla' (\rho \mathbf{u})$ and $\nabla' (\rho \mathbf{f})$ as a straightforward extension of (29) and (30). Hence, one should have

$$\begin{aligned} N_i^2(\mathbf{r}, t) = \sigma_1 \mathbf{S}_i : \nabla' \nabla' \rho + \sigma_2 \mathbf{S}_i : \nabla' (\rho \mathbf{f}) + \tau \mathbf{T}_i : \nabla' \nabla' (\rho \mathbf{u}), \quad i = 1, \dots, b_m \\ N_0^2(\mathbf{r}, t) = \sigma_1^0 \mathbf{S}_0 \cdot \nabla' \nabla' \rho + \sigma_2^0 \mathbf{S}_0 \cdot \nabla' (\rho \mathbf{f}) + \tau^0 \mathbf{T}_0 : \nabla' \nabla' (\rho \mathbf{u}) \end{aligned} \quad (41)$$

where the tensors \mathbf{S} and \mathbf{T} are second- and third-order tensors, respectively. These tensors should be invariant under the isometry group L of the lattice and verify the conservation conditions (40) ; they are given in Appendix B within a multiplicative constant (cf. (B.1) and (B.4)).

The coefficients $\sigma_1, \sigma_1^0, \sigma_2, \sigma_2^0$ and τ, τ^0 are obtained by inserting the relations (41) into the second order equation (39). They are given by (B.6).

APPLICATION TO PARTICULAR FLOW FIELDS. — The theoretical material is now ready to be applied to various flow fields. Essentially, the second order expansion (41) will be used in conjunction with the bounce back condition (17) and the solution for velocity deduced from the Navier-Stokes equations. The exact location where the velocity vanishes will be derived for Poiseuille and stagnation flows.

5. Localization of boundaries for Poiseuille flow.

Poiseuille flow is the simplest possible physical situation and it is addressed in this section. Detailed calculations are given when the solid boundaries are parallel to the (x, y) -plane of the FCHC lattice ; an extension to inclined solid boundaries is proposed and discussed. These two cases are called horizontal and inclined channels, respectively.

BASIC EQUATIONS FOR AN HORIZONTAL CHANNEL. — Consider a Poiseuille flow in a plane channel where the two walls are separated by a distance $2h$. The flow is along the x -direction triggered by the action of a constant external force $\mathbf{f} = (f_x, 0, 0)$ which plays the role of a constant pressure gradient. The physical situation is depicted in figure 1a.

The Navier-Stokes equations (of the general form (28a)) reduce to the following simple form because the flow is along straight lines parallel to the x -axis

$$0 = f_x + \nu \nabla^2 u_x^0, \quad -h \leq z \leq h \tag{42}$$

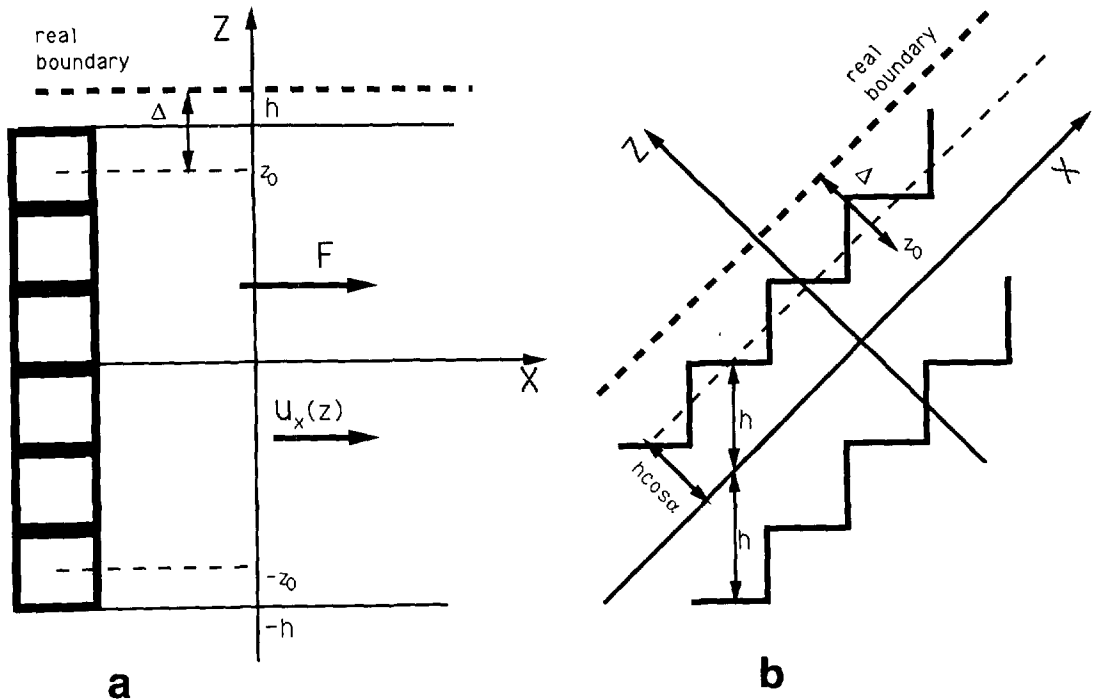


Fig. 1. — Poiseuille flow. a) horizontal channel ; the solid walls are located at $z = \pm h$; b) inclined channel.

whose solution is

$$u_x^0(z) = u_0(z^2 - h^2), \quad u_0 = -0.5 f_x / \nu. \quad (43)$$

When the lattice Boltzmann model is used to calculate the flow, the calculations take place at the nodes of the staggered mesh which was described in section 2. Let $\pm z_0$ be the z -coordinate of the nodes close to the solid wall.

For the steady state, because inertial terms vanish identically independently of the Galilean factor $g(\rho)$ (cf. (13a)), it is not necessary to take into account rest particles in the Boltzmann model. Therefore, when (42) is used in the expressions (5), (29), (30) and (B.5) for the various terms of the mean populations, one obtains

$$N_i(\mathbf{r}, t) = N_i^0(\mathbf{r}, t) + d' \rho \left\{ \lambda_\psi^{-1} Q_{i,xz} \partial_z u_x^0 - 0.5 f_x c_{i,x} + \nu \lambda_2^{-1} \partial_x \partial_x u_x^0 (c_{i,x} - 3 c_{i,x} c_{i,z}^2) \right\}. \quad (44)$$

This expression is introduced into the bounce back condition (17) at $z = \pm z_0$; hence when (42) is used, one has for $\mathbf{c}_{i,+} = -\mathbf{c}_{i,-}$

$$u_x^0 c_{i,-x} + \lambda_\psi^{-1} Q_{i,-xz} \partial_z u_x^0 - 0.5 f_x c_{i,-x} - \lambda_2^{-1} f_x (c_{i,-x} - 3 c_{i,-x} c_{i,-z}^2) = \\ = u_x^0 c_{i,+x} + \lambda_\psi^{-1} Q_{i,+xz} \partial_z u_x^0 - 0.5 f_x c_{i,+x} - \lambda_2^{-1} f_x (c_{i,+x} - 3 c_{i,+x} c_{i,+z}^2). \quad (45)$$

Let us restrict ourselves to the upper plane and assume that the velocity vanishes at $z = z_0 + \Delta$; this amounts to replace (43) by

$$u_x^0(z) = u_0 \{ z^2 - (z_0 + \Delta)^2 \}. \quad (46)$$

This expression is substituted into (45) and Δ is a solution of the equation

$$(z_0 + \Delta)^2 = z_0^2 + z_0 + 0.5 + \nu + \lambda_\psi^{-1} - 4 \nu \lambda_2^{-1} \quad (47)$$

When z_0 is assumed to be large, the solution to this equation can be approximated by

$$\Delta = 0.5 \left\{ 1 + z_0^{-1} [0.25 + \nu + \lambda_\psi^{-1} - 4 \nu \lambda_2^{-1}] + \dots \right\}. \quad (48)$$

This equation is very important for several reasons. First, it shows the importance of the second-order terms. Even in the simplest case of a Poiseuille flow, the second derivatives of the velocity displace the point where velocity vanishes. This is an extension of previous results [5]. Second, the error which is made, is of the order $1/z_0$ i.e. of order ϵ if the eigenvalues of the matrix are chosen without any particular care as described after the relations (A.4).

However, the error can be reduced if λ_2 is chosen in such a way as to cancel the second-order term in (48). The expression (A.4b) of the viscosity can be used (together with $c^2/(D+2) = 1/3$ for the FCHC lattice). Some elementary algebra yields the critical value λ_{2c}

$$\lambda_{2c} = -8(\lambda_\psi + 2)/(\lambda_\psi + 8), \quad (49)$$

$$\Delta \equiv 0.5 \quad \text{if} \quad \lambda_2 = \lambda_{2c}.$$

It is interesting to note that when λ_ψ varies in the allowed interval $(-2, 0)$, λ_{2c} varies also from 0 to -2 . Hence, no extra condition is imposed by the interval of variation. Whatever λ_ψ , λ_2 can be chosen in such a way as to cancel the second-order term in (48).

NUMERICAL TEST FOR A HORIZONTAL CHANNEL. — Numerical calculations were done for Poiseuille flow in order to check the predictions of equations (48) and (49). The routine corresponds to the one described at the end of section 2 ; it is based on the linearized Boltzmann equation (14) and the bounce back conditions (17). There is no rest particle. The numerical parameters of the routine are the following

$$\begin{aligned} \lambda_\psi &= -0.5 \Rightarrow \nu = 0.5 \\ 2h = 3, 4, 16 &\Rightarrow z_0 = 1, 1.5, 7.5 \\ f_x &= 2 \times 10^{-6}, \quad \lambda_1 = -1. \end{aligned} \tag{50}$$

The eigenvalue λ_2 varies between -2 and -0.2 . According to (49), the critical value λ_{2c} is equal to

$$\lambda_{2c} = -8/5. \tag{51}$$

Two kinds of comparisons were made. First, overall comparisons were made between the computed profiles and parabolic profiles such as (46) where Δ is given by equation (47). Some comparisons are reported in figure 2 and the agreement is seen to be excellent.

The second comparison was done close to the solid walls. One can interpolate the numerical velocities in order to calculate the exact location $z_0 + \delta$ where the velocity vanishes and compare it to the analytical prediction $z_0 + \Delta$ where Δ is given by (47). The interpretation is made by means of a Taylor expansion around the point z_0 . δ is given by the equation

$$u_x^0(z_0) + \delta \partial_z u_x^0(z_0) + 0.5 \delta^2 \partial_z^2 u_x^0 = 0 \tag{52a}$$

where the two first derivatives are deduced from the numerical results within errors of order $1/z_0^2$ as

$$\partial_z u_x^0(z_0) = 0.5 [3 u_x^0(z_0) - 4 u_x^0(z_0 - 1) + u_x^0(z_0 - 2)] \tag{52b}$$

$$\partial_z^2 u_x^0 = u_x^0(z_0) - 2 u_x^0(z_0 - 1) + u_x^0(z_0 - 2). \tag{52c}$$

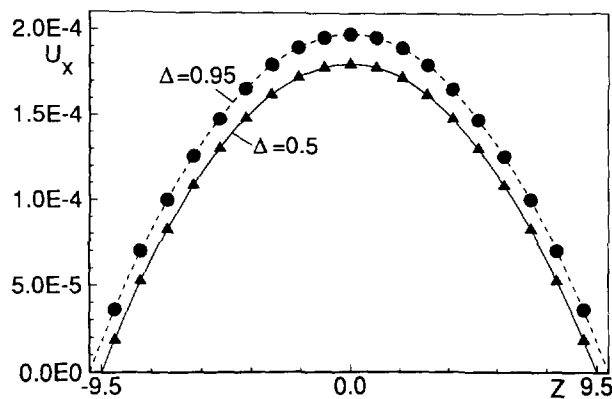


Fig. 2. — Comparison between computed (\blacktriangle , \bullet) and analytical (-----, — — —) parabolic profiles. Data are for : (-----), \blacktriangle ($2h = 19$, $\lambda_\psi = -0.5$, $\lambda_2 = -1.6$, $\Delta = 0.5$), (— — —) \bullet ($2h = 19$, $\lambda_\psi = -0.5$, $\lambda_2 = -0.2$, $\Delta = 0.949874$).

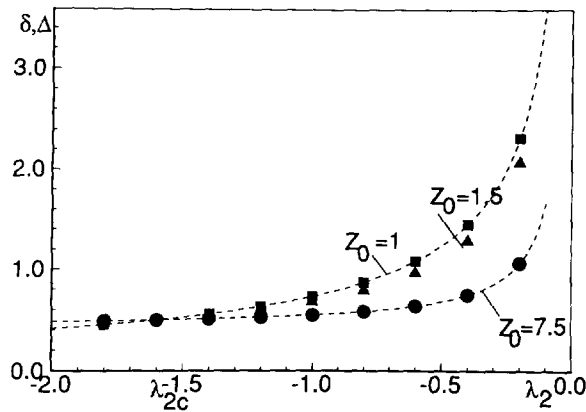


Fig. 3. — Numerical (x) and analytical (broken lines) predictions of the location of the solid boundary in a Poiseuille flow as a function of the eigenvalue λ_2 . Data are for: ($2h = 3$), . . . ($2h = 4$), — — — ($2h = 16$).

δ can be determined from the equations (52) for various values of the parameters λ_2 and z_0 . In figure 3, δ is compared to the analytical predictions (47). The agreement between δ and Δ is seen to be excellent even for very low values of z_0 . The critical value λ_{2c} is extremely well verified.

Hence, there is a complete agreement between analytical and numerical predictions.

EXTENSION TO INCLINED CHANNELS. — The same calculations can be performed for inclined channels, when the solid walls are not parallel to the (x, y) -plane of the FCHC lattice (cf. Fig. 1b). This inclination, measured by the angle α , does not change the continuum analysis with the Navier-Stokes equations and the parabolic profile (43) is still obtained.

The analytical calculations can be easily made when the angle α is equal to 45° since all the nodes close to the wall play the same role. For sake of brevity, only the results are given here. Consider a channel whose characteristic vertical dimension is given by $2h$ (Fig. 1b); its width in the usual sense is equal to $2h \cos \alpha$. It can be shown that the distance Δ' between the last lattice node z'_0 and the plane where the velocity vanishes is given by the relation (cf. Fig. 1b)

$$\Delta' = -z'_0 + z'_0 \left[1 + \frac{1}{\sqrt{2} Z'_0} - \frac{\nu}{2 Z_0'^2} \left(1 + \frac{2}{\lambda_2} \right) \right]^{\frac{1}{2}} \tag{53}$$

where

$$z' = -x \sin \alpha + z \cos \alpha .$$

The actual width of the channel is thus $2h \cos \alpha$ if

$$\Delta' = \sqrt{2}/4 .$$

According to (53), this condition implies that

$$\frac{\nu}{2} \left(1 + \frac{2}{\lambda_{2c}} \right) = -\frac{1}{8} \tag{54a}$$

or, equivalently

$$\lambda'_{2c} = -4(\lambda_\psi + 2)/(4 - \lambda_\psi). \quad (54b)$$

This new value of the second eigenvalue of A differs from the value (49) obtained for horizontal channels except when λ_ψ is equal to -2 . It is interesting to notice that λ'_{2c} varies in the interval $(-2, 0)$ when λ_ψ varies also from 0 to -2 . Needless to say, the results (53), (54b) were confirmed by the numerical solutions in the inclined channels with $\alpha = 45^\circ$.

In view of this result, it can be expected that the right choice of λ_2 is a function of the inclination angle α . It is equivalent to say that for a given value of λ_2 , the location of the plane where the actual velocity vanishes depends on α .

6. Localization of boundaries in stagnation flow.

BASIC EQUATIONS. — Stagnation flow can be considered in some sense as the exact opposite to Poiseuille flow. In the former case, the flow is as perpendicular as possible to the wall, while in the latter it is parallel to it.

The physical situation is depicted in figure 4. The flow is assumed to be two-dimensional ; a plane potential flow arrives along the y -axis and impinges on a flat wall placed at $y = 0$; the flow divides into two streams on the wall. One wishes to study the region close to the wall where flow separation occurs, i.e. close to the origin. The solution was first devised by Hiemenz (cf. [11]). The solution is supposed to be of the form

$$u = xf'(y), \quad v = -f(y), \quad p_0 - p = 0.5 \rho a^2 [x^2 + F(y)] \quad (55)$$

p_0 denotes the stagnation pressure, a is a constant. The unknown functions f and F must satisfy the Navier-Stokes equations. More precisely, when the calculations are made by means of the lattice gas, one has to verify the equations (11)

$$g(\rho_0) [f'^2 - ff''] = a^2 + \nu f''' \quad (56a)$$

$$g(\rho_0) ff' = 0.5 a^2 F' - \nu f'' \quad (56b)$$

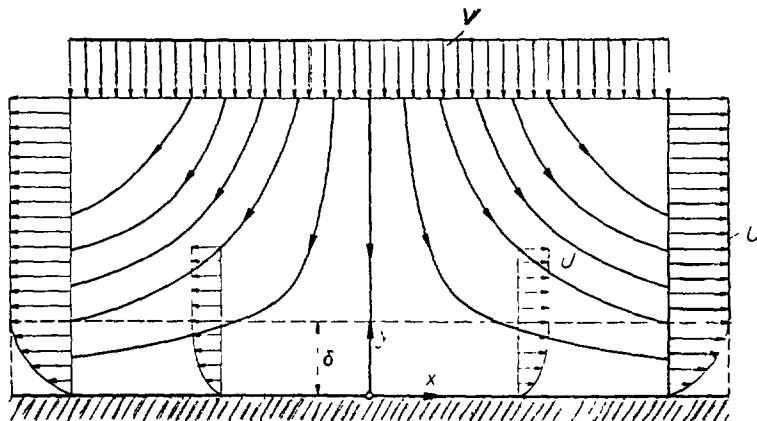


Fig. 4. — Stagnation in plane flow (cf. [11]).

where $g(\rho_0)$ is the Galilean factor (13a) and ρ_0 denotes the density at the stagnation point.

The no slip condition at the wall implies that

$$f(0) = f'(0) = 0 ; \tag{57a}$$

$$F(0) = 0 . \tag{57b}$$

Far away from the wall, the flow is frictionless and the velocity should be of the form $u = ax$; hence

$$f' = a , \quad y = \infty . \tag{57c}$$

Finally, it is assumed that the fluid can be considered as incompressible, i.e. the velocity of the fluid is very small when compared to the speed of sound c_s .

DETERMINATION OF THE POINTS OF ZERO VELOCITY. — The same development as for Poiseuille flow applies, except that rest particles are included in the model in order to have a Galilean factor equal to 1. Detailed calculations are given in Appendix C, and only the major steps and final results are given below.

First the mean population $N_i(\mathbf{r})$ is evaluated up to the second order in ε . Before this expansion is used in the bounce back conditions, it is worth considering a node of ordinate y_0 close to a wall in the FCHC lattice (cf. Fig. 5) ; it turns out that it is more efficient to write down the bounce back conditions in linear combinations of populations such as $N_{+1} - N_{+2}$ and $N_{+1} + N_{+2}$. The 6 conditions, which can be written for the 6 virtual nodes located in the solid, are equivalent to three independent relations (cf. (C.5)). These equations are linear functions of the three first derivatives of f at the point y_0 , namely $f'(y_0)$, $f''(y_0)$, $f'''(y_0)$. This linear system can be easily solved and one obtains the explicit expressions (C.10) for $f'(y_0)$, $f''(y_0)$ and $f'''(y_0)$. Finally, it is a simple matter to express the two no slip conditions (57a) on the components u and v by means of a Taylor expansion around y_0 . These conditions read as

$$0 = 3(1 + \xi - P_{vy}) + (1 - P_{xv}) y_0/k + 0.5 A_z y_0^2/k^2 \tag{58a}$$

$$0 = 1 - 3(1 + \xi - P_{rv}) y_0 - 0.5(1 - P_{rv}) y_0^2/k - A_z y_0^3/(6 k^2) \tag{58b}$$

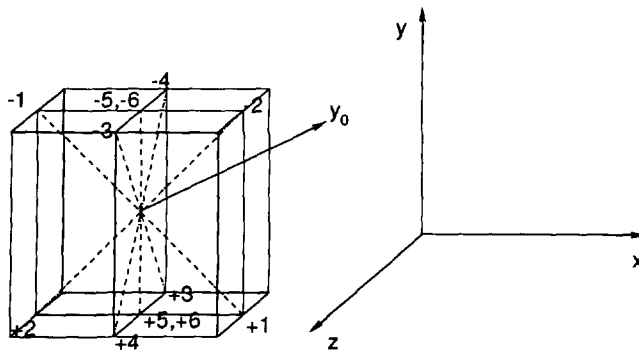


Fig. 5. — A node y_0 of the FCHC lattice close to the solid surface W . The coordinate system is the one of the stagnation flow. The virtual nodes + 1 to + 6 belong to the solid. The nodes ± 5 and ± 6 have a nonzero component in the fourth dimension.

where

$$\xi = \nu a^2 / f(y_0), \quad P_{xy} = P_{xy}^0 / [2 f(y_0)], \quad A_- = (6k + 1)(1 - P_{xy}) + 6k\xi \quad (59)$$

P_{xy}^0 and k are given by (C.7) and (C.8), respectively.

Let us first consider the condition (58a) which is relative to the component u . This quadratic equation in y_0 can easily be solved. Hence, the continuous solution y_{0u} where u is equal to zero may be expressed by

$$y_{0u}(k, \xi, P_{xy}) = A_z^{-1} \left\{ -k(1 - P_{xy}) + \sqrt{[(k^2(1 - P_{xy})^2 - 6k^2(1 + \xi - P_{xy})A_z)]} \right\}. \quad (60)$$

One can see that

$$y_{0u} = 0.5 \quad \text{if} \quad k = -0.25 \quad (61)$$

for any P_{xy}, ξ ; consequently, λ_2 has the value λ_{2c} given by (49).

This remarkable property of the solution to the equation (58a) is a consequence of the following relations: if the second derivative $g''(y_0)$ of some function $g(y)$ can be obtained from the equation

$$2\tilde{g}(y_0) - \tilde{g}'(y_0) - k\tilde{g}''(y_0) = 0 \quad (62)$$

(cf. (C.5a) for stagnation flow, (45) for Poiseuille flow), then the Taylor expansion around y_0

$$\tilde{g}(y_0) - \tilde{g}'(y_0)y_0 + 0.5\tilde{g}''(y_0)y_0^2 = 0 \quad (63)$$

has a solution $y_0 = 0.5$ if $k = -0.25$, independently of the value $\tilde{g}'(y_0)/\tilde{g}(y_0)$.

Moreover, it is quite natural that the no slip condition for the velocity component parallel to the wall is obtained for the same value as in horizontal Poiseuille flow.

Let us now look at the no slip condition $v = 0$. The solution y_{0v} to (58b) up to $O(y_0^2)$ with the relations (C.5a), (C.5b) is the same as for Poiseuille flow (61) only if

$$P_{xy}^0 = 0, \quad a^2 = 0.$$

Thus, when the density fluctuations (C.6) are taken into account, one should look for the common solution y_0^{st} to the equations (58b), (60)

$$y_0^{st} = y_{0u} = y_{0v}. \quad (64a)$$

This means that for each fixed value of P_{xy} one can look for pairs (k, ξ) which satisfy the equations (58b), (60); equivalently, since (58b) is a cubic equation in y_0 , it is easier to look for the numerical solution

$$\xi = \xi^{st}(k, P_{xy}). \quad (64b)$$

Such a solution numerically exists only if k obeys to the condition

$$k < k_0(P_{xy}).$$

The functions $y_0^{st}[k, P_{xy}, \xi = \xi^{st}(k, P_{xy})]$, $\xi^{st}(k, P_{xy})$ are represented in figures 6 and 7. It will be shown later (cf. (65)-(67)) that when the physical parameters a^2 and ν are given, one

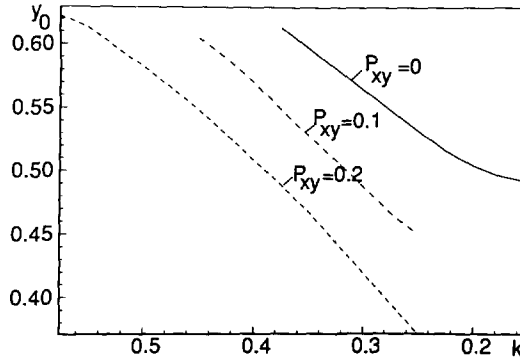


Fig. 6. — Common solution y_0^{st} to the two no slip conditions for stagnation flows as a function of the parameters $k, P_{xy}, \xi = \xi^{st}(k, P_{xy})$.

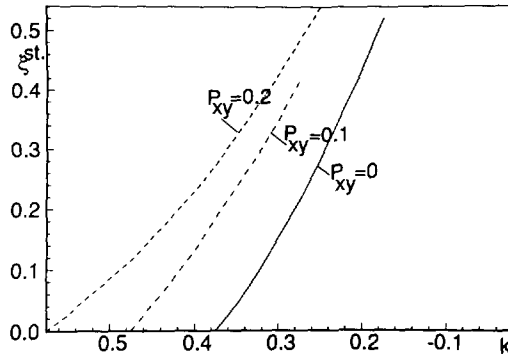


Fig. 7. — Solution ξ^{st} as a function of the parameters k, P_{xy} for stagnation flows. It yields the common solution $y_0 = y_0^{st}$.

can try to find the gas parameters $M_c, b^0, g(\rho_0)$, and k to satisfy simultaneously the equations (64b) for ξ and P_{xy} , the equations (67) for ξ and (65), (66) for P_{xy} .

For example, in the case $P_{xy} = 0$, the inverse function $k(\xi)$ (see Fig. 8) for small ξ has the form

$$k(\xi) = -0.373 + 0.916 \xi + \dots$$

The solution $y_0^{st} = 0.5$ if $k = -0.25$ can be reached for

$$\xi = \xi^{st}(k = -0.25, P_{xy} = 0) = 1/6.$$

Thus, unfortunately, the common solution y_0^{st} cannot be equal to 0.5 only by choosing $k = -0.25$ as for Poiseuille flow (cf. (49), (61)). For instance, if the stagnation solution is obtained by the Boltzmann model with $k = -0.25$, the distance y_{0b} between the last lattice node and the point $v = 0$, defined by the equation (58b) may differ widely from $y_{0u} = 0.5$. This is illustrated in figure 9.

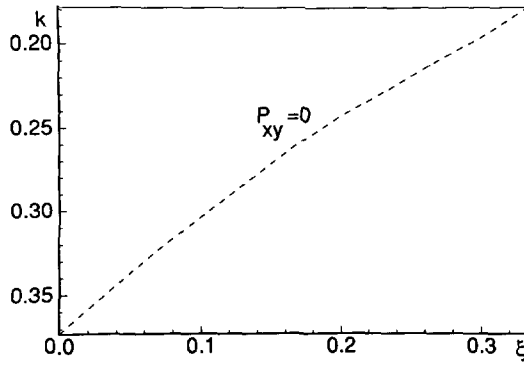


Fig. 8. — Inverse function $k = k^{st}(\xi)$ for $P_{vv} = 0$. Stagnation flow.

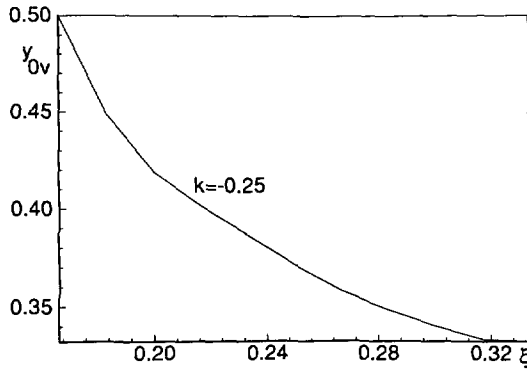


Fig. 9. — Solution y_{0v} to no slip condition $v = 0$ as a function of the parameter ξ for $k = -0.25$, $P_{vy} = 0$. Stagnation flow.

Generally speaking, the previous analysis allows us to choose the parameters M_c , b^0 , $g(\rho_0)$, ν , k of the model as functions of the physical parameter a^2 to obtain the equality (64a). In this respect, it is interesting to note that in contrast with u , the condition on the component v cannot be satisfied by choosing only the eigenvalues of the collision matrix A . The parameter $P_{vy}^0(y_0)$ can be derived in terms of $f(y_0)$ from the relations (C.9), (C.10a)

$$P_{vy}^0 = 27 \nu g(\rho_0) (a^2 + f(y_0))^2 + O(a^2 + f(y_0))^3, \quad E = 0. \tag{65}$$

Then $f(y_0)$ may be evaluated by substituting (C.10) with (65) into the stagnation solution (56a). The resulting expression for $f(y_0)$ is rather long. Let us give a simplified form obtained when the terms $f(y_0)^2$ as well as the ones of order $O(a^4)$ are neglected

$$f(y_0) = ka^2(k + 6 \nu^2) / [\nu \{ 18 ga^2 k^2 + (27 \nu a^2 - 1) (6k + 1) \}], \quad E = 0. \tag{66}$$

The relation (66) for $f(y_0)$ or a more exact one can be introduced into (59) to express the parameter ξ in terms of the parameters of the model and of the physical parameter a^2 .

$$\xi = \nu^2 \{ 18 ga^2 k^2 + (27 \nu^2 a^2 - 1) (6k + 1) \} / k(k + 6 \nu^2), \quad E = 0. \tag{67}$$

Hence, the parameters M_c , b^0 if $M_c \neq 0$ and $g(\rho_0)$, ν , k can be chosen *a priori* to satisfy the relation (64b) where the function $\xi^{st}(k, P_{\nu})$ can be found numerically (see Fig. 7, for example), and P_{xy} can be evaluated by (59b), with (65), (66).

For example, one can try to find a numerical solution to the parameter $k(\lambda_2)$ to satisfy (64b), (65-67) for chosen values $g(\rho_0)$, ν , a^2 if $M_c = 0$. Analogical equations can be obtained for $M_c \neq 0$ ($E \neq 0$).

7. Concluding remarks.

From the previous analysis, it seems obvious that for an arbitrary flow, we have no grounds to state that all the velocity components vanish at the same point when the bounce back condition is used at the wall. Hence, the boundary conditions are imposed with an error of order ε^2 as it can be seen from (48) for instance. This is a serious problem because it means that the precision of the overall scheme is of order ε , and thus much less precise than usual finite routines based on finite difference schemes with errors of order ε^2 or ε^4 (see [12]). In three dimensions, the three solutions y_{0u} , y_{0v} , y_{0w} are different even for the choice $k = -0.25$.

An even more precise analysis of the population solutions (10) has been developed up to the next order $O(\varepsilon^3)$. For this purpose, the 4-order invariant tensor was determined. However, the calculation of the coefficients of these terms is tedious. Let us only say that such an analysis confirms the previous conclusions about the choice of the parameter $k = -0.25$. The real position of the solid walls imposed by the bounce-back reflection depends on the velocity field close to the solid. Even for Poiseuille-like flows, the choice $k = -0.25$ (or equivalently $\lambda_2 = \lambda_{2c}$) is only valid for horizontal channels.

Hence a very fruitful path of research could be the determination of new boundary conditions which would replace the classical bounce back conditions. It is important to note that a precise analysis of solid boundary location is crucial for real porous media simulations.

One possible way to change momentum at the nodes close to the solid walls in order to introduce the no slip conditions at the same distance y_0 is to use a combination of bounce-back and specular reflections [5, 13]. The combination itself would be found numerically since it is thought to depend upon the nearby velocity field. Such an investigation has recently been started.

Acknowledgments.

A grant from the Institut Français du Pétrole (F. Kalaydjian) which partially supports this work, is gratefully acknowledged.

Appendix A.

The linear collision operator.

The major well-known properties associated with a linear collision operator [10, 6] are summarized in this Appendix. The mass and momentum conservation equations (2) imply that the coefficients of **A** verify

$$\begin{aligned} \sum A'_{ij} &= -b^0 M_c, \quad i = 1, \dots, b_m \\ b^0 b_m &= -c^0 M_c \\ \sum A'_{ij} c_{j\alpha} &= 0, \quad i = 1, \dots, b_m; \quad \alpha = 1, \dots, D \end{aligned} \quad (\text{A.1})$$

or equivalently, one obtains the three conditions

$$\begin{aligned} a_0 + 8 a_{60} + 6 a_{90} + 8 a_{120} + a_{180} &= -b^0 M_c \\ a_0 + 4 a_{60} - 4 a_{120} - a_{180} &= 0 \\ b^0 b_m &= -c^0 M_c. \end{aligned} \quad (\text{A.2})$$

One can show that the 24 + 1 eigenvalues of \mathbf{A} can be expressed as

$$\begin{aligned} \lambda_0 &= 0, & \text{multiplicity } 5 \\ \lambda_1 &= 1.5 a_0 + 6 a_{90} + a_{180} + 12 b^0 M_c / b_m, & \text{multiplicity } 2 \\ \lambda_2 &= 1.5 a_0 - a_{180}, & \text{multiplicity } 8 \\ \lambda_\psi &= a_0 - 2 a_{90} + a_{180}, & \text{multiplicity } 9 \\ \lambda_c &= -b^0 (M_c + b_m / M_c), & \text{multiplicity } 1 \end{aligned} \quad (\text{A.3})$$

The eigenvectors corresponding to the eigenvalues λ_2 and λ_ψ can be shown to be

$$\begin{aligned} \sum A_{ij} Q_{j\alpha\beta} &= \lambda_\psi Q_{i\alpha\beta}, \quad \forall \alpha, \beta, Q_{0\alpha\beta} = 0 \\ \sum A_{ij} R_{j\alpha\beta} &= \lambda_2 R_{i\alpha\beta}, \quad \forall \alpha \neq \beta \end{aligned}$$

with the eigenvector

$$R_{i\alpha\beta} = c_{i\alpha} - (D + 2) c_{i\alpha} c_{i\beta}^2 / c^2 \quad R_{0\alpha\beta} = 0. \quad (\text{A.4a})$$

Note that there is no summation on the Greek indices α, β .

The eigenvalue λ_ψ is related to the shear viscosity (13b) by

$$\lambda_\psi = d' / \Psi \quad (\text{A.4b})$$

or equivalently,

$$\nu = -\frac{c^2}{D + 2} \left(\frac{1}{\lambda_\psi} + \frac{1}{2} \right). \quad (\text{A.4c})$$

In order to summarize this presentation, it can be said that among the seven unknown a 's, b^0, c^0 , three are fixed by (A.2). Four extra conditions can be imposed by the eigenvalues (A.3) which are only requested to be in the interval $(-2, 0)$. Following [10], one can choose $\lambda_1 = \lambda_2 = \lambda_c = -1$ and λ_ψ as close as possible to -2 in order to accelerate the relaxation to equilibrium.

It is usually demanded that the Galilean factor $g(\rho)$ be equal to 1 (cf. (13a))

$$[Db(1 - 2d)] / [(D + 2)b_m(1 - d)] = 1. \quad (\text{A.5a})$$

In the FCHC lattice, since $D = 4$, $b_m = 24$, the density d is equal to

$$d_0 = (M_c - 12)[2(M_c + 6)]^{-1} \quad (\text{A.5b})$$

and because of (6)

$$\rho_0 = (M_c + 24) d_0. \quad (\text{A.5c})$$

Appendix B.**Second-order terms for the FCHC lattice.**

The general form of second-order tensors invariant under the isometry group L of the lattice was given in [9] and it can be conveniently written in the form (cf. (29))

$$\mathbf{S}_i = E' \mathbf{Q}_i + F' \mathbf{I}. \quad (\text{B.1a})$$

The extension of this property to third-order tensors is straightforward and can be written as

$$\mathbf{T}_i = A c_i c_i c_i + B c_i \mathbf{I} + C \mathbf{I} c_i + D (\mathbf{I} c_i)^t \quad (\text{B.1b})$$

where the transposed operator t acts on the last two indices.

However the general form of this tensor has to be restricted because of the conservation conditions (40). The mass conservation is automatically verified since all the terms in (B.1b) are odd powers of c_i . The momentum condition yields some interesting consequences. Let us consider the particular case where the two first indices of \mathbf{T}_i are equal to α ; hence, without any summation on α , (40) implies that

$$\sum_{i=1}^{b_m} T_{i\alpha\alpha\beta} c_{i\delta} = A \sum_{i=1}^{b_m} c_{i\alpha}^2 c_{i\beta} c_{i\delta} + C \sum c_{i\beta} c_{i\delta}.$$

Note that the first summation is restricted to the case where $c_{i\alpha}^2$ is not zero. Hence, because of (20),

$$\sum_{i=1}^{b_m} T_{i\alpha\alpha\beta} c_{i\delta} = d'^{-1} \{A c^2 / (D + 2) + C\} = 0.$$

The same reasoning can be made for any couple of indices with the same result. The general form of (B.1b) is restricted to

$$\mathbf{T}_i = C \{ -c_i c_i c_i (D + 2) / c^2 + c_i \mathbf{I} + \mathbf{I} c_i + (\mathbf{I} c_i)^t \}. \quad (\text{B.2})$$

This tensor is automatically symmetric for its last two indices; a possible antisymmetric component on these last two indices would have been automatically cancelled by the contraction with $\nabla' \nabla'(\rho \mathbf{u})$.

This expression can be somewhat modified in order to use the eigenvectors of the matrix \mathbf{A} (cf. (A.4)). It is obvious from (B.2) that

$$\begin{aligned} T_{i\alpha\beta\gamma} &= 0, \quad \text{if } \alpha \neq \beta \neq \gamma, \\ T_{i\alpha\alpha\alpha} &= 0, \quad \text{without summation.} \end{aligned} \quad (\text{B.3})$$

Hence the only components which are non zero are the ones where only two indices are equal and different from the third. Hence, within a multiplicative constant, the components of \mathbf{T}_i may be written as linear combinations of the eigenvectors $R_{i\alpha\beta}$ corresponding to λ_2 (cf. (A.4))

$$T_{i\alpha\beta\gamma} = R_{i\alpha\beta} (1 - \delta_{\alpha\beta}) + R_{i\beta\gamma} (1 - \delta_{\beta\gamma}) + R_{i\alpha\gamma} (1 - \delta_{\alpha\gamma}). \quad (\text{B.4})$$

Introduction of (B.1a) and (B.4) into (41) yields the general expression $N_i^2(\mathbf{r}, t)$. Because of the future application of the collision equation (39), it is more convenient to use the eigenvectors \mathbf{Q}_i and \mathbf{R}_i (cf. (B.1a))

$$N_i^2(\mathbf{r}, t) = \sigma_1 E' \mathbf{Q}_i : \nabla' \nabla' \rho + \sigma_1 F' \nabla' \cdot \nabla' \rho + \sigma_2 E' \mathbf{Q}_i : \nabla'(\rho \mathbf{f}) + \sigma_2 F' \nabla' \cdot (\rho \mathbf{f}) + \\ + \sum_{\alpha \neq \beta} R_{i\alpha\beta} [\tau \partial_{\beta'} \partial_{\beta'}(\rho u_\alpha) + 2 \tau \partial_{\beta'} \partial_{\alpha'}(\rho u_\beta)], \quad i = 1, \dots, b_m \quad (\text{B.5a})$$

$$N_0^2(\mathbf{r}, t) = -b_m \{ \sigma_1 F' \nabla' \cdot \nabla' \rho + \sigma_2 F' \nabla' \cdot (\rho \mathbf{f}) \} / M_c. \quad (\text{B.5b})$$

This last formula for N_0^2 necessarily follows from the mass conservation (40).

The remaining calculations are now tedious but not difficult. The expressions (B.5) are inserted into the left-hand side of the second-order equation (39). One takes into account the eigenvalues and the eigenvectors of (A.4). Then the factors of the various gradients are identified and the coefficients of (B.5) are determined. To illustrate the process, let us consider the equation for $i = 0$ in (39). It can be proved to be

$$(\chi b_m / M_c + (2b)^{-1}) \{ \nabla' \cdot (\rho \mathbf{f}) - c_s^2 \nabla' \cdot \nabla' \rho \} = \\ = (b_m / M_c + 1) b^0 b_m \{ \sigma_2 F' \nabla' \cdot (\rho \mathbf{f}) + \sigma_1 F' \nabla' \cdot \nabla' \rho \}$$

from which the values of $\sigma_2 F'$ and $\sigma_1 F'$ readily follow.

The same development can be applied to the terms $i = 1, \dots, b_m$ and one obtains

$$\sigma_1 E' = -c_s^2 \sigma_2 E'; \quad \sigma_2 E' = -3 d' \nu / \lambda_\psi, \\ \sigma_1 F' = -c_s^2 \sigma_2 F'; \quad \sigma_2 F' = (\chi / b^0 b + M_c / (2 b^2 b^0 b_m)); \quad (\text{B.6}) \\ \tau = d' \nu / \lambda_2; \quad \sigma_1^0 = -b_m / M_c \sigma_1; \quad \sigma_2^0 = -b_m / M_c \sigma_2.$$

Appendix C.

Bounce back conditions for stagnation flow.

First the mean population is evaluated up to the second-order in ε thanks to (5), (29), (31), (32), (B.5) with two components (u, v) of the velocity field

$$N_i(\mathbf{r}) = d + d' \rho \{ u c_{ix} + v c_{iy} + \\ + G(\rho) (d' b)^{-1} [u^2 \cdot \{ Q_{ixx} + (c^2/D - c_s^2) \} + v^2 \{ Q_{ivy} + (c^2/D - c_s^2) \} + 2 uv Q_{ixy}] \\ + \lambda_\psi^{-1} [\partial_y u Q_{ixy} + \partial_x u Q_{ixx} + \partial_y v Q_{iyy}] \\ + \nu \lambda_\psi^{-1} [\partial_y \partial_y u (c_{ix} - 3 c_{ix} c_{iy}^2) + 2 \partial_x \partial_y u (c_{iy} - 3 c_{iy} c_{ix}^2)] \} \\ + \lambda_\psi^{-1} 3 \nu d' c_s^2 [\partial_x \partial_x \rho Q_{ixx} + \partial_y \partial_y \rho Q_{iyy}] + E \nabla^2 \rho, \\ N_0(\mathbf{r}) = d [1 - G(\rho) \{ u^2 + v^2 \}] - b_m / M_c E \nabla^2 \rho \quad (\text{C.1})$$

with $E = \sigma_1 F'$ (cf. (B.5), (B.6)).

Note that no external force \mathbf{f} has been included in these mean populations.

Before we start considering the precise bounce back conditions, it might be useful to consider a node close to a wall in the FCHC lattice as displayed in figure 5. The node y_0 is located, half a lattice unit above the wall; there are 6 possible virtual nodes located half a lattice unit below the wall; two of them possess a velocity component c_{ix} along the x -axis; four of them do not have such a component. Let us number them from +1 to +6 as indicated in figure 5. The real nodes which are connected to the node y_0 by the reverse velocities are numbered from -1 to -6.

When the node \mathbf{r} is at $y = y_0$ and when the node $\mathbf{r}_0 + \mathbf{c}_i$ belongs to the solid, the bounce back condition (17) applies. Instead of considering N_{+1} and N_{+2} individually, it is more physical and mathematically equivalent to consider $N_{+1} - N_{+2}$ and $N_{+1} + N_{+2}$, which are directly related to the components u and v of the velocity (cf. (3b)). In a steady state, this condition reads as

$$N_{-1}(\mathbf{r}_0, t) \pm N_{-2}(\mathbf{r}_0, t) = N_{+1}(\mathbf{r}_0, t) \pm N_{+2}(\mathbf{r}_0, t) + \sum_{j=0}^{b_m} (A_{+1j} \pm A_{+2j}) [N_j(\mathbf{r}_0, t) - N_j^0(\mathbf{r}_0, t)] W_j. \quad (\text{C.2})$$

This condition can be evaluated with the help of the expression (C.1) for $N_i(\mathbf{r}, t)$. For instance, the equation for the mean population difference yields for $y = y_0$

$$\begin{aligned} uc_{-1x} + 2G(\rho)(d'b)^{-1} [2uvQ_{-1xy}] + \lambda_\psi^{-1} Q_{-1xy} \partial_y u + \nu \lambda_2^{-1} (c_{-1x} - 3c_{-1x}c_{-1y}^2) \partial_y \partial_y u = \\ = uc_{+1x} + 2G(\rho)(d'b)^{-1} [2uvQ_{+1xy}] + (\lambda_\psi^{-1} + 1) Q_{-1xy} \partial_y u \\ + \nu (\lambda_2^{-1} + 1) (c_{-1x} - 3c_{-1x}c_{-1y}^2) \partial_y \partial_y u. \end{aligned} \quad (\text{C.3})$$

This equation can be further simplified by using various properties of the flow field and one obtains

$$\{2u - \partial_y u - 2\nu(1 + 2\lambda_2^{-1}) \partial_y \partial_y u\} (y_0) = 0. \quad (\text{C.4a})$$

The same development can be made for the mean population sum $N_{+1} + N_{+2}$; it yields a second condition

$$\begin{aligned} 0 = \{2v - 4\nu(1 + 2\lambda_2^{-1}) \partial_x \partial_y u + \rho^{-1} [-3\nu(1 - c^2/D) + Eb^0 b] \nabla^2 (c_s^2 \rho')\} (y_0), \\ \rho' = \rho - \rho_0 \end{aligned} \quad (\text{C.4b})$$

where the density fluctuations have been incorporated.

This completes the analysis for the populations N_{+1} and N_{+2} , i.e. with a non zero c_{ix} component.

The analysis for the populations N_{+3} and N_{+4} can be made along the same lines. Because of the translational symmetry along the z -axis, these two populations are equal and the difference vanishes identically; the same holds for N_{+5} and N_{+6} because of the translational symmetry along the fourth dimension. The sums of the mean populations $N_{+3} + N_{+4}$ and $N_{+5} + N_{+6}$ yield the same equation which can be expressed as

$$\begin{aligned} 0 = \{2v - \partial_y v + 2\nu(1 + 2\lambda_2^{-1}) \partial_x \partial_y u + \rho^{-1} [-3\nu(1 - c^2/D) + Eb^0 b] \nabla^2 (c_s^2 \rho') + \\ + 3\nu\rho^{-1} \partial_x \partial_x (c_s^2 \rho')\} (y_0). \end{aligned} \quad (\text{C.4c})$$

Hence the bounce back conditions (17) written for the 6 virtual nodes +1 to +6 are equivalent to the three conditions (C.4). By the use of the function f (cf. (55)), the conditions (C.4) can be simplified into the following expressions if square velocity squared terms are neglected (cf. (C.6b), (12))

$$2f'(y_0) - f''(y_0) - kf'''(y_0) = 0 \quad (\text{C.5a})$$

$$2f(y_0) + 2kf''(y_0) - P_{xy}^0 = 0 \quad (\text{C.5b})$$

$$2f(y_0) - f'(y_0) - kf''(y_0) - P_{xy}^0 + 3\nu a^2 = 0 \quad (\text{C.5c})$$

where with the use of (55)

$$\partial_x \partial_x (c_s^2 \rho') = -a^2 \rho \quad (\text{C.6a})$$

$$\nabla^2 (c_s^2 \rho') = - [a^2 + 0.5 a^2 F''(y)] \rho \quad (\text{C.6b})$$

and we have denoted

$$P_{vy}^0 = [-3 \nu (1 - c^2/D) + Eb^0 b] \nabla^2 (c_s^2 \rho') / \rho, \quad (\text{C.7})$$

the constant k is defined as

$$k = 2 \nu (1 + 2 \lambda_2^{-1}). \quad (\text{C.8})$$

With equations (56) and (C.6b), the parameter P_{vy}^0 (C.7) can be represented in terms of $f'(y)$

$$P_{xy}^0 = -2 g(\rho_0) [f'(y)]^2 \{-3 \nu (1 - c^2/D) + Eb^0 b\}. \quad (\text{C.9})$$

Then one can solve the linear system (C.5) for the first derivatives of $f(y)$; first $P_{vy}^0/f(y_0)$ is considered as a parameter in the numerical solution of the equation (64a)

$$f'(y_0) = 3 \{f(y_0) + \nu a^2 - 0.5 P_{vy}^0\} \quad (\text{C.10a})$$

$$f''(y_0) = -k^{-1} \{f(y_0) - 0.5 P_{vy}^0\} \quad (\text{C.10b})$$

$$f'''(y_0) = k^{-2} \{6 k [f(y_0) + \nu a^2 - 0.5 P_{vy}^0] + [f(y_0) - 0.5 P_{vy}^0]\}. \quad (\text{C.10c})$$

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