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COMPUTATION OF EFFECTIVE TRANSPORT COEFFICIENTS OF A MICROSCALE GAS FLOW

BY

PIERRE CHARRIER, BRUNO DUBROCA AND CHRISTOPHE PREUX

Abstract

The aim of the present paper is to propose efficient numerical methods for solving linear kinetic problems arising in the modeling of heat and mass transport in porous media. We propose a Galerkin approximation for the velocity variables (which can be also interpreted as a moment method in some cases), and a classical finite-volume approximation for the space variables. The Galerkin approximation for the velocity variables reduces the linear kinetic equation to a linear hyberbolic system of dimension N, where N is the number of basis functions used in the Galerkin method. To be efficient the approach must give correct prediction with small N. This can be obtained by a convenient choice of the basis functions which is governed by a mathematical analysis taking into account the physical regime. A modification of the space approximation is proposed to enforce the correct behavior in the fluid limit. Comparison of numerical results obtained by our method and direct solution of kinetic systems or experimental data are provided.

1. Introduction

In several applications such as flows in microdevices, fuel cells or material science we need precise mathematical models of heat and mass transfer in porous media for numerical simulations. In a recent paper ([5]) the authors

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propose a new approach for deriving such models from kinetic theory at a microscopic scale. In simple configurations this Asymptotic Transport Model (ATM) reduces to a set of two nonlinear diffusion equations. The main improvements of this approach are first to be able to treat various physical regimes in the same mathematical framework and also to allow to compute the effective transport coefficients from the microscopic properties of the medium. These coefficients are defined through the solution of auxiliary problems posed on the unit cell of the periodic medium.

Since these coefficients must be computed for a large number of values of density and temperature, we need efficient numerical methods to solve them. Some of this cell problems involve linear elliptic equations and efficient techniques of solution are well-known. Some other cell problems involve linear stationary kinetic equations depending on six independent variables (three space variables and three velocity variables) and the need of efficient numerical methods able to treat the various regime is a crucial issue in this context.

The aim of the present paper is to propose efficient numerical methods for solving the linear kinetic cell-problems. We propose a Galerkin approximation for the velocity variables (which can be also interpreted as a moment method in some cases), and a classical finite-volume approximation for the space variables. The Galerkin approximation for the velocity variables reduces the linear kinetic equation to a linear stationary hyberbolic system of dimension N, where N is the number of basis functions. To be efficient the approach must give correct prediction with small N. This can be obtained by a convenient choice of the basis functions which is governed by a mathematical analysis taking into account the physical regime. The fluid regime (where $\nu_w \ll \nu_b$) needs more work. Indeed by a rescaling and an asymptotic analysis we can prove that in the limit of high density (or small Knudsen number) the cell-problem tends to a Stokes system and that we recover the Darcy law at the macroscopic level. Therefore to adress this regime we must modify the space approximation of the hyperbolic system given by the Galerkin method in order to get an asymptotic preserving scheme. The paper is organized as follows. Section 2 contains some useful background on the ATM. The numerical strategy for solving the kinetic auxiliary problems is presented in Section 3. We derive the hyperbolic cell auxiliary problems and prove that some quite important properties of the kinetic cell auxiliary problems are preserved through the Galerkin approximation in velocity. Section 4 is devoted to space approximation and numerical modification of the

transport scheme to preserve the asymptotic limit. Section 5 contains numerical simulations including comparison with direct solution of the kinetic model and comparison with experiments.

2. The Asymptotic Transport Model

The ATM is based on the following microscopic model,

$$\begin{aligned}
\rho_s C_v \partial_t T &= \operatorname{div}(\lambda_s \nabla T), && \text{in } \Omega_s, && (1)\\
\partial_t f + v \cdot \nabla f &= Q(f,f), && \text{in } \Omega_f, && (2)\\
f(x,v,t)_{|x\in\Gamma,\ v.n>0} &= \sigma \int_{w\cdot n<0} |w\cdot n| f(x,w,t)dw\ M(T)(v) && && (3)\\
&+\ (1-\sigma) f(x, v-2v.n\ n, t) && && (4)\\
\lambda_s \nabla T \cdot n &= -\int \frac{1}{2}|v|^2 v\cdot n f(x,v,t)dv, && \text{on } \Gamma. && (5)
\end{aligned}$$

Here, Ω_s is the open set occupied by the solid phase, Ω_f is the open set occupied by the fluid phase, and Γ the interface between Ω_f and Ω_s. *In all the following* $n = n(x)$, $x \in \Gamma$, *denotes the normal to* Γ *at point* x, *outgoing from* Ω_s. The solid phase is characterized by its density ρ_s, its specific heat at constant volume C_v, and its thermal conductivity λ_s which are assumed to be known and constant. The only unknown in the solid phase is the temperature field $T(x,t)$ defined on Ω_s whose evolution is given by the classical heat equation (1). The fluid phase is a single species monoatomic gas, described by a kinetic model. We denote $f = f(x,t,v)$ the mass distribution function, and the evolution of the gas is given by the Boltzmann equation in Ω_f (2). The collision operator Q is defined by

$$Q(f,f)(v) = \int_{\mathrm{R}^3_w} \int_{S^2} f(v')f(w') - f(v)f(w)b(v-w,\omega)dwd\omega, \qquad (6)$$

where $v' = v - (v-w).\omega\ \omega$, $w' = w + (v-w).\omega\ \omega$ and where the scattering kernel $b(z,\omega) = |z|\Sigma(|z|, \cos(z,\omega))$ depends on the interaction potential between molecules which is considered and the cross-section Σ is given by (see [3])

$\Sigma(z, \cos\theta) = r^2 \cos\theta$, for the hard sphere potential,
$\Sigma(z, \cos\theta) = r^2 |z|^{\kappa-1} \cos\theta$, $\kappa \in [0,1[$, for the variable hard sphere potential.

In any case, the collision term satisfies the following fundamental properties insuring conservation laws and H-theorem

$$\forall f \geq 0, \quad \int_{\mathbf{R}^3_v} Q(f,f)\psi(v)dv \;=\; 0, \Leftrightarrow \psi(v) = a + b.v + c|v|^2, \tag{7}$$

$$\int_{\mathbf{R}^3_v} Q(f,f)\ln(f)dv \;\leq\; 0, \tag{8}$$

$$\int_{\mathbf{R}^3_v} Q(f,f)\ln(f)dv \;=\; 0 \Rightarrow Q(f,f) = 0. \tag{9}$$

Macroscopic quantities (density, momentum, total energy) are defined by

$$\rho = \langle f \rangle, \quad \rho u = \langle f v \rangle, \quad E = \langle \frac{1}{2}|v|^2 \rangle, \tag{10}$$

where $\langle \psi \rangle = \int_{\mathbf{R}^3} \psi(v)dv$. The coupling between the heat transfer in the solid and the gas flow is given by relation (4) which is a Maxwell reflection condition where $\sigma \in [0,1]$ is the accomodation coefficient and by relation (5) which ensures the continuity of the energy flux on Γ. $M(v,T)$ is a normalized Maxwellian distribution defined by :

$$M(v,T) = \frac{1}{2\pi(RT)^2} e^{\left(-\frac{|v|^2}{2RT}\right)}$$

We consider there the regime of weak thermal coupling ([4, 5]) where we assume that

- the frequency ν_b of binary collisions and the frequency ν_w of collisions of gas molecules with the boundary of the pores are of the same order,
- the thermal conductivity of the gas is much smaller than the thermal conductivity of the solid.

Then we can write the microscopic system in dimensionless form with respect to the small parameter which is the ratio between the length of an elementary representative volume of the porous medium and a representative length of the macroscopic structure and we obtain:

$$\rho_s C_v \partial_t T \;=\; \mathrm{div}(\lambda_s \nabla T), \qquad \text{in } \Omega_s, \tag{11}$$

$$\partial_t f + \frac{1}{\epsilon} v \cdot \nabla f \;=\; \frac{1}{\epsilon^2}\, Q(f,f), \qquad \text{in } \Omega_f, \tag{12}$$

$$f(x,v,t) \;=\; \sigma \int_{w\cdot n<0} |w \cdot n| f dw \; M(T) \tag{13}$$

$$+ (1-\sigma) f(x, v - 2v.nn) \quad \text{on } \Gamma \text{ for } v \cdot n > 0, \tag{14}$$

$$\lambda_s \nabla T \cdot n = -\int \frac{1}{2}|v|^2 v \cdot n f(x,v,t) dv, \quad \text{on } \Gamma. \tag{15}$$

To perform the asymptotic analysis ot this system we assume that the material is periodic. We denote Y the basic cell of periodicity, Y_s and Y_f the parts of this cell occupied by the solid and fluid phases and Γ_Y the interface. The unknown functions T and f have a dependence in space of the form $T = T(x,y)$ and $f = f(x,y)$, where $x \in \Omega$ is the slow variable and $y = \frac{x}{\epsilon} \in Y$ is the fast variable and we assume that T and f are Y-periodic functions. In the scaled model we look for T^ϵ and f^ϵ in the form $T^\epsilon = T^\epsilon(x, \frac{x}{\epsilon})$ and $f^\epsilon = f^\epsilon(x, \frac{x}{\epsilon})$. In order to find an asymptotic model at the macroscopic level we write the solutions T^ϵ and f^ϵ of the scaled microscopic system as power series in ϵ :

$$T^\epsilon(x) = T^\epsilon(x, y = \frac{x}{\epsilon}) = T_0^\epsilon(x, y = \frac{x}{\epsilon}) + \epsilon\, T_1^\epsilon(x, y = \frac{x}{\epsilon}) + \cdots \tag{16}$$

$$f^\epsilon(x,v) = f^\epsilon(x, y = \frac{x}{\epsilon}, v) = f_0^\epsilon(x, y = \frac{x}{\epsilon}) + \epsilon\, f_1^\epsilon(x, y = \frac{x}{\epsilon}) + \ldots \tag{17}$$

Inserting (16,17) in the microscopic system, and balancing order by order in ϵ, we can show that $f_0 = M(T_0, v)$ is a Maxwellian distribution, independent of y, with velocity $u_0 = 0$ and temperature T_0 constant on Y (see [5] for more details). Moreover, we look for T_1 and f_1 in the following form

$$T_1 = \gamma \cdot \nabla_x T_0, \tag{18}$$

$$f_1 = (\alpha \cdot \nabla_x T_0 + \beta \cdot \nabla_x \rho_0) f_0, \tag{19}$$

where $\alpha = (\alpha_i(y,v))_{i=1,2,3} \in \mathbb{R}^3$, $\beta(y,v) = (\beta_i(y,v))_{i=1,2,3} \in \mathbb{R}^3$ et $\gamma = (\gamma_i(y))_{i=1,2,3} \in \mathbb{R}^3$ are solutions of the following problems called *cell auxiliary problems* (see [5]):

$$(P_1) \quad \begin{cases} -\mathrm{div}_y(\lambda_s \nabla_y \gamma_i) = 0 & \text{in } Y_s, \\ \lambda_s \nabla_y \gamma_i \cdot n = -\lambda_s n_i & \text{on } \Gamma_Y, \end{cases}$$

$$(P_2) \quad \begin{cases} -L(f_0 \alpha_i) + f_0 v \cdot \nabla_y \alpha_i = -f_0 v_i \left(-\dfrac{3}{2T_0} + \dfrac{|v|^2}{2R{T_0}^2} \right) \text{ in } Y_f, \\ \alpha_i(y,v) = \sigma \left(\frac{|v|^2}{2R{T_0}^2} - \frac{2}{T_0} \right) \gamma_i + \sigma \int_{w.n<0} |w \cdot n| \alpha_i(w) M(T_0)\, dw \\ \qquad\qquad +(1-\sigma)\alpha_i(y, v - 2v.nn) \qquad \text{on } \Gamma_Y, \text{ for } v \cdot n > 0, \end{cases}$$

$$(P_3) \quad \begin{cases} -L(f_0\beta_i) + v \cdot \nabla_y(f_0\beta_i) = \dfrac{-f_0}{\rho_0} v_i \text{ in } Y_f, \\ \beta_i(y,v) = \sigma \displaystyle\int_{w\cdot n<0} |w\cdot n|\beta_i(w) M(T_0)\, dw + (1-\sigma)\beta_i(y, v - 2v.nn) \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{on } \Gamma_Y, \text{ for } v\cdot n > 0, \end{cases}$$

where L is the linearized collision operator defined by:

$$L(g) = L_{f_0}(g) = Q(f_0, g) + Q(g, f_0).$$

Finally, *the asymptotic transport model (ATM)* takes the following form:

$$\partial_t \rho_0 - \mathrm{div}_x(D\nabla_x \rho_0) - \mathrm{div}_x(\tilde{D}\nabla_x T_0) \;=\; 0, \tag{20}$$

$$\rho_s C_v \partial_t T_0 - \mathrm{div}_x(K\nabla_x T_0) \;=\; 0, \tag{21}$$

where

$$\tilde{D} = \langle -v f_0 \otimes [\alpha]_{Y_f} \rangle; \quad D = \langle -v f_0 \otimes [\beta]_{Y_f} \rangle; \quad K = [\lambda_s + \lambda_s \nabla_y \gamma(y)]_{Y_s} \tag{22}$$

where $\langle f \rangle = \int_{\mathrm{R}^3} f(v)dv$, $[g]_{Y_f} = \frac{1}{|Y_f|}\int_{Y_f} g(y)dy$ and $[g]_{Y_s} = \frac{1}{|Y_s|}\int_{Y_s} g(y)dy$.

The system (20)-(21) is a set of two coupled nonlinear diffusion equations. The first equation gives the mass transport and contains a mass diffusion term and a cross-diffusion term known as the *thermal transpiration* ([8]). In transport models the determination of the effective transport coeffficients is a crucial issue. They bring to the macroscopic scale a lot of informations coming from the microscopic scale including informations on the structure of the medium through the geometry of Y_s ans Y_f and on the regime of the flow through ρ and T. Let us notice that, though this model has been derived under the assumption that the flow is in a transition regime at the scale of the pores, the same mathematical framework can be used for the limit regimes of rarefied flow ($Kn \to +\infty$) or viscous flow ($Kn \to 0$). However, the regime of the flow greatly influences the solution of the cell auxiliary problems and must be taken into account in the solution strategy. Finally, it is important to quantify the relative weight of the mass diffusion and of the thermal transpiration. In one-dimensional configurations this is given by the dimensionless number (see [8])

$$\frac{\tilde{D}\ T}{D\ \rho}.$$

Let us remark that the effective transport coefficients $\tilde{D}$ and D are functions of ρ and T that are needed for numerical approximation of the macroscopic system. For that we compute in a pre-processing step a tabulation of $D(\rho, T)$ (and also of $\tilde{D}$) for some discrete values of ρ and T. Then this data base is used in the numerical approximation of the system in order to estimate by linear interpolation the quantities $D(\rho_i^n, T_i^n)$, where ρ_i^n and T_i^n are the time and space approximations of density and temperature. The discrete values of ρ and T are taken in intervals $[\rho_{Min}, \rho_{Max}]$ and $[T_{Min}, T_{Max}]$ large enough to contain all the values needed for a given computation. We have to solve three elliptic equations to get $\gamma_i,\ i = 1, 2, 3$ and for each value of ρ and T, six kinetic equations to get $\alpha_i, \beta_i,\ i = 1, 2, 3$. Since it can be necessary to take some hundred values of $\rho,\ T$ in order to have precision enough on the effective transport coefficients, it appears to be crucial to have fast numerical methods for solving these problems. To compute γ_i we use a seven point finite-volume approximation with a mesh of cubic cells with constant steps and the associated linear system is solved by a multigrid method using Conjugate Gradients as smoother. The solution strategy for the kinetic equations is more complex and is detailed in the following section.

3. Solving the Kinetic Cell Auxiliary Problems

3.1. Approximation in velocity variables: the Galerkin method

The method used to solve the auxilary problems (P_2) and (P_3) is based on the projection of the linear kinetic equations on a set of basis functions $\{m_j\}_{j=1,\ldots,N}$ through a Galerkin method on velocity variables. This can be seen as a generalization of a moment method, since the basis functions are not necessarily polynomial functions of v, as it will be seen later. Let us focus for example on the *kinetic cell auxiliary problem* (P_3). The equation writes

$$-L(f_0\beta_l) + v \cdot \nabla_y(f_0\beta_l) = \frac{-f_0}{\rho_0} v_l \text{ in } Y_f. \tag{23}$$

We introduce the following notations

$$\widehat{\beta}_l = \rho_0\beta_l, \quad g_0 = \frac{f_0}{\rho_0}. \tag{24}$$

Then $\widehat{\beta}_l$ is solution of the equation

$$-L(g_0\widehat{\beta}_l) + g_0 v \cdot \nabla_y(\widehat{\beta}_l) = -g_0 v_l \text{ in } Y_f. \tag{25}$$

Using Galerkin approximation we look for $\widehat{\beta}_l$ in the following form

$$\widehat{\beta}_l(y,v) = \sum_{j=1}^{N} b_j^l(y) m_j(v). \tag{26}$$

Inserting (26) in (25), multiplying by m_k and integrating in velocity space yields

$$\forall k \in \{1,\dots,N\} \ \sum_{j=1}^{N} \Big(-\langle L(g_0 m_j) m_k \rangle b_j^l + \langle g_0 v m_j m_k \rangle \cdot \nabla_y(b_j^l) \Big) = \langle g_0 v_l m_k \rangle. \tag{27}$$

Introducing the following notations

$$S_{kj} = \langle L(g_0 m_j) m_k \rangle, \ \ (A_p)_{kj} = \langle g_0 v_p m_j m_k \rangle, \ \ g_k^i = -\langle g_0 v_i m_k \rangle, \tag{28}$$

(27) writes as a stationary symmetric linear hyperbolic system :

$$-S\vec{b^l} + \sum_{p=1}^{3} A_p \partial_{y_p} \vec{b^l} = \vec{g^l}. \tag{29}$$

To write the boundary conditions for this system we start from the boundary conditions in (P_3), at the kinetic level (20), which can be written

$$\int_{w \in \mathbf{R}^3} \beta_l(y,w) w \cdot n dw \ = \ 0 \quad \text{ on } \Gamma_Y, \tag{30}$$

$$\beta_l(y,v)_{|\Gamma_Y,\ v.n>0} \ = \ \sigma K(y) M(T_0) \ + (1-\sigma)\beta_l(y, v - 2v.nn), \tag{31}$$

where $K(y)$ is a scalar determined by the first equation. This first equation is the condition of mass flux equal to zero, and thus writes for $\vec{b^l}$

$$A(n)\vec{b^l}.\vec{\theta}_{|_{\Gamma_Y}} = 0, \tag{32}$$

where $A(n) = \sum_{p=1}^{3} n_p A_p$ and $\vec{\theta}$ is defined by $\sum_{j=1}^{N} \theta_j m_j(v) = 1$. The second equation gives the distribution of particles coming into Y_f at the boundary. For the hyperbolic system, it consists in imposing the incoming Riemann

invariants, i.e.

$$A(n)^+ \vec{b^l}_{|\gamma} = A(n)^+ (\sigma K \vec{\theta} + (1-\sigma) R(n) \vec{b^l})_{|\Gamma_Y}, \tag{33}$$

where A^+ is the spectral positive part[1] of the matrix A and $R(n)$ is the matrix of the application $\beta(v) \longrightarrow \beta(v - 2(v.n)n)$ in the basis $\{m_j\}_{j=1,\dots,N}$. Moreover we have used the property $R(n)A(n)^+R(n) = -A(n)^-$ (see Lemma 1). Finally, the *hyperbolic cell auxiliary problem* for $\hat{\beta}_l$ writes

$$\begin{aligned}
-S\vec{b^l} + \sum_{p=1}^{3} A_p \partial_{y_p} \vec{b^l} &= g^l \text{ in } Y_f, && (34)\\
A(n)\vec{b^l}.\vec{\theta}_{|\gamma} &= 0, && (35)\\
A(n)^+ \vec{b^l}_{|\gamma} &= A(n)^+ (\sigma K \vec{\theta} + (1-\sigma) R(n) \vec{b^l})_{|\Gamma_Y} && (36)\\
\text{periodic conditions on} \quad & \partial Y_f - \Gamma_Y. && (37)
\end{aligned}$$

A similar system, associated with α_l can be written. The only slight differences come from the right-hand-side and the boundary condition.

3.2. Choice of the basis

To be efficient the approach described in the previous section must give correct predictions with small N. This can be obtained by a convenient choice of the basis functions in the Galerkin approach. This choice is governed by physical considerations which give some insight on the behavior of the solution according to the considered regime.

3.2.1. The collision and transition regimes

In collision regime the equation (25) is dominated by the linearized collision operator so that $L(g_0\widehat{\beta}_l) \approx 0$, and thus

$$\widehat{\beta}_l \approx a_0 + a_1 v + a_2 |v|^2.$$

That means that the collisionnal invariants $(1, v, |v|^2)$ must belong to the linear space spanned by the Galerkin basis. When the frequency of binary

[1] i.e., if $A = P\Lambda P^{-1}$ where Λ is a diagonal matrix then $A^+ = P\Lambda^+ P^{-1}$ where Λ^+ is the diagonal matrix whose diagonal elements are the positive part of the diagonal elements of matrix Λ.

collisions is smaller and close to the frequency of collisions with the boundary of the pores (i.e. in the transition regime), we enlarge the Galerkin approximation space by some polynomials in v of higher order : $v_i v_j,\ |v|^2 v_i$. This leads to an approximation space with dimension $N = 13$. Finally, taking into account the formula (28), it seems judicious to take a basis orthonormal with respect to the scalar product

$$(\alpha, \beta)_{T_0} = \langle \alpha(v)\beta(v) g_0(T_0, v) \rangle. \tag{38}$$

So the basis we consider for the collision and transition regimes is

$$\begin{aligned}
m_1 &= \frac{v_1}{\sqrt{RT_0}},\ m_4 = \frac{v_1^2 - RT_0}{\sqrt{2}RT_0},\ m_7 = \frac{v_2 v_3}{RT_0},\ m_{10} = \frac{|v|^2 - 5RT_0}{\sqrt{10R^3T_0^3}} v_1, \\
m_0 &= 1,\ m_2 = \frac{v_2}{\sqrt{RT_0}},\ m_5 = \frac{v_2^2 - RT_0}{\sqrt{2}RT_0},\ m_8 = \frac{v_1 v_3}{RT_0},\ m_{11} = \frac{|v|^2 - 5RT_0}{\sqrt{10R^3T_0^3}} v_2, \\
m_3 &= \frac{v_3}{\sqrt{RT_0}},\ m_6 = \frac{v_3^2 - RT_0}{\sqrt{2}RT_0},\ m_9 = \frac{v_1 v_2}{RT_0},\ m_{12} = \frac{|v|^2 - 5RT_0}{\sqrt{10R^3T_0^3}} v_3.
\end{aligned} \tag{39}$$

Any function of v belonging to the vector space generated by $(1, \vec{v}, |v|^2)$ is exactly represented on this basis, as stated above.

3.2.2. The Knudsen regime

We can expect that this basis is not quite suited for describing the solution of the auxiliary problems in the free-molecule limit where the frequency of binary collisions vanishes (Knudsen regime). To understand the behavior of the solution in this regime, we study the simplified configuration of a pipe with axis parallel to the y_1-axis and with a circular cross-section for fully diffusive reflection, i.e. for $\sigma = 1$. If y is a point of the section, v the velocity of a particle at point y, we denote $\hat{v} = (0, v_2, v_3) = |\hat{v}|\hat{\omega}(\hat{v})$, $z = z(y, \hat{\omega}(\hat{v}))$ the point $z = y + s\hat{\omega}(\hat{v}),\ s > 0$ such that z belongs to the boundary of the pore and $n = (0, n_2, n_3)$ the normal to the boundary of the pipe.

In Knudsen regime, i.e. without binary collisions, the auxiliary problem (P_3) writes

$$(P_3 - Knudsen) \quad \begin{cases} |v| \cdot \nabla_{\hat{\omega}} \beta &= -v_1 \text{ in } Y_f, \\ \beta(y, v)_{|\Gamma_Y,\ v.n>0} &= \int_{\xi . n<0} |\xi \cdot n| \beta(\xi) M(T_0)\, d\xi \end{cases}$$

The solutions of this problem write obviously $\beta(y, v) = -\frac{v_1}{|\hat{v}|}|y - z(y, \hat{\omega}(\hat{v}))| + \phi(z)$, where $\phi(z)$ is the incoming flux of particle at point $z \in \Gamma_Y$. To deter-

mine $\phi(z)$, we use the boundary condition, by replacing $\beta(y,v)$ by its value. After some algebra we find that ϕ satisfies on Γ_Y the following integral equation:

$$\phi(y) = \int_{\xi.n(y)<0} \phi(z)|\xi.n|M(T_0,\xi)d\xi.$$

The only solutions of this integral equation are constants. We take here $\phi(y) = 0$, and we obtain the solution for the system $(P_3 - Knudsen)$:

$$\beta(y,v) = -\frac{v_1}{|\hat{v}|}|y - z(y,\hat{\omega}(\hat{v}))| = b(y,\hat{\omega})\ \frac{v_1}{\hat{v}}. \tag{40}$$

This results shows the dependence of the solution in $\frac{v_i}{|\hat{v}|}$ in this example of a pipe. In a more general three-dimensional case the solution would depend on $\omega_i = \frac{v_i}{|v|}$. So, in order to improve the solution in the Knudsen regime, we suggest to include in the basis the following functions

$$\begin{array}{lll} m_{13} = \omega_1, & m_{16} = \omega_1^2, & m_{19} = \omega_2\ \omega_3, \\ m_{14} = \omega_2, & m_{17} = \omega_2^2 & m_{20} = \omega_1\ \omega_3, \\ m_{15} = \omega_3, & m_{18} = \omega_3^2, & m_{21} = \omega_1\ \omega_2. \end{array} \tag{41}$$

Finally, in order to have a code able to treat all regimes we want a basis containing the 13 functions suited for collision and transition regimes and the 9 functions introduced for the Knudsen regime. But since $\omega_1^2 + \omega_2^2 + \omega_3^2 = 1$, the final basis we use has only 21 functions.

Let us remark that there are some conditions for the validity of the asymptotic transport model in the Knudsen regime. A classical assumption is the property of *finite horizon* which ensures that every molecule of gas will touch the boundary Γ_Y before leaving the elementary cell Y (see for instance [2] for the diffusion limit of a collisionless gas).

3.3. The linearized BGK and ES-BGK collision operators

In the auxiliary problems, the operator L is the linearized Boltzmann collision operator defined by:

$$L(g) = Q(f_0,g) + Q(g,f_0).$$

To simplify the treatment we replace the Boltzmann collision operator by

the BGK- relaxation operator given by ([6])

$$C_{BGK}(f) = \frac{1}{\tau}[M(f) - f] = \frac{1}{\tau}[M(\vec{\rho}(f)) - f], \tag{42}$$

where $\tau = \mu/p$ is the relaxation time. In this relation the viscosity $\mu = CT^{\omega}$, where $\omega = (\kappa+1)/2$ depends on the interaction potential between molecules used in the Boltzmann equation. $\omega = 1/2$ corresponds to the "hard sphere" potential (HS), $\omega = 1$ to the Maxwellian potential and $\omega \in]0,1[$ to "variable hard sphere" (VHS) potential. Then the linearized BGK relaxation operator is given by

$$L_{BGK}(f) = C'_{BGK}(f_0)f = \frac{1}{\tau}\left(\frac{f_0}{\rho_0}\begin{pmatrix} \frac{5RT_0-|v|^2}{2RT_0} \\ \frac{v}{RT_0} \\ \frac{|v|^2-3RT_0}{3R^2T_0^2} \end{pmatrix}.\begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} - f\right) \tag{43}$$

Since it is well-known that in the fluid limit the BGK operator leads to an uncorrect Prandlt number ($Pr = 1$), it is sometimes prefered to use the ES-BGK operator ([1]) defined by

$$C_{ES-BGK}(f) = \frac{1-\nu}{\tau}[G(f) - f], \tag{44}$$

where

$$G(f) = \frac{\rho}{\sqrt{\det(2\pi\mathcal{T})}}\exp(\frac{1}{2}(v-u)^T\mathcal{T}^{-1}(v-u)), \tag{45}$$

and $\mathcal{T} = RT(1-\nu)Id + \nu\Theta$ and $\Theta = 2\mathcal{E} - \rho u \otimes u$.

The linearized ES-BGK operator writes

$$L_{ES-BGK}(f) = C'_{ES-BGK}(f_0)f = \frac{1-\nu}{\tau}\left(\partial_{\vec{\rho}_{13}}G(f_0).\vec{\rho}_{13} - f\right), \tag{46}$$

where

$$\begin{aligned}
\vec{\rho}_{13} &= (\rho, \rho u_1, \rho u_2, \rho u_3, E_{1,1}, E_{2,2}, E_{3,3}, E_{1,2}, E_{1,3}, E_{2,3}).\\
\partial_{\vec{\rho}_{13}}G(f_0) &= \Big(\frac{5RT_0-|v|^2}{2RT_0}, \frac{v1}{RT_0}, \frac{v2}{RT_0}, \frac{v3}{RT_0}, \frac{RT_0-(1-\nu)|v|_3^2\nu v_1^2}{3(RT_0)^2},\\
&\qquad \frac{RT_0-(1-\nu)|v|_3^2\nu v_2^2}{3(RT_0)^2}, \frac{RT_0-(1-\nu)|v|_3^2\nu v_3^2}{3(RT_0)^2},\\
&\qquad \frac{2\nu v_1v_2}{(RT_0)^2}, \frac{2\nu v_1v_3}{(RT_0)^2}, \frac{2\nu v_2v_3}{(RT_0)^2}\Big).
\end{aligned}$$

The Prandlt number associated with the ES-BGK collision operator is $Pr = 1/(1-\nu)$ and for $\nu = -1/2$ it gives the right Prandlt number $Pr = 2/3$ for monoatomic gas.

Both operators C_{BGK} and C_{ES-BGK} satisfy the main properties (7,8,9) of the Boltzmann collision operator (see [1] for the ES-BGK operator) and have also the following properties for the linearized operators ([3])

Proposition 1. *The linearized collision operators satisfy the following properties*

1. *L is symmetric,*
2. *$Ker\ (L) = Span(1, v, |v|^2)$;*
3. *$\exists \delta_0 > 0, \ - < L(\beta)\ \beta > \geq \delta_0 ||(I - P_K)\beta||^2$, where P_K is the projection on $Ker(L)$.*

3.4. Analysis of the hyperbolic cell auxiliary problems

In this paragraph we study the *hyperbolic cell auxiliary problem* and we prove that some important properties of the kinetic cell auxiliary problem are preserved by the Galerkin approximation. We make this analysis for the hyperbolic system derived by using the 13-element basis $\{m_j\}_{0\leq j\leq 12}$ (39). This greatly simplifies the notations and is enough but necessary for the asymptotic analysis in the fluid limit presented later.

3.4.1. Description and main properties

To clarify the expression of the hyperbolic cell auxiliary problem we introduce the following notations

$$b_V = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}, \quad b_E = \begin{pmatrix} b_{E_1} \\ b_{E_2} \\ b_{E_3} \end{pmatrix} = \begin{pmatrix} b_4 \\ b_5 \\ b_6 \end{pmatrix}, b_\tau = \begin{pmatrix} b_7 \\ b_8 \\ b_9 \end{pmatrix}, b_q = \begin{pmatrix} b_{10} \\ b_{11} \\ b_{12} \end{pmatrix}, \quad (47)$$

and

$$\bar{b}_E = \frac{1}{3}(b_{E1} + b_{E_2} + b_{E_3}) = \frac{1}{3}(b_4 + b_5 + b_6). \quad (48)$$

From (28), the matrix $S\vec{b}$, is given by:

$$(Sb)_i = 0 \quad \text{for } i \in \{0, 3\} \quad (49)$$

$$(Sb)_4 = \frac{1}{\tau}(\bar{b}_E - b_{E_1}) \quad (50)$$

$$(Sb)_5 = \frac{1}{\tau}(\bar{b}_E - b_{E_2}) \tag{51}$$

$$(Sb)_6 = \frac{1}{\tau}(\bar{b}_E - b_{E_3}) \tag{52}$$

$$(Sb)_j = -\frac{1}{\tau}b_j \quad \text{for } j \in \{7, 12\} \tag{53}$$

Then we have

Proposition 2. *The matrix S is symmetric and*

$$-S\vec{b}.\vec{b} \geq \frac{1}{\tau}||(I - P_{K_S})\vec{b}||^2, \tag{54}$$

$$KerS = \{(b_0, b_1, b_2, b_3, \bar{b}_E, \bar{b}_E, \bar{b}_E, 0, 0, 0, 0, 0, 0)\} \tag{55}$$

Proof. From the above relations, it is obvious that $\vec{b} \in KerS$ is equivalent to

$$b_{E_1} = b_{E_2} = b_{E_3} = \frac{1}{3}\bar{b}_E, \;\; b_7 = b_8 = b_9 = b_{10} = b_{11} = b_{12} = 0, \tag{56}$$

that is to say that

$$KerS = \{(b_0, b_1, b_2, b_3, \bar{b}_E, \bar{b}_E, \bar{b}_E, 0, 0, 0, 0, 0, 0)\}$$

Let us notice that this result means that $\vec{b} \in$ Ker S if and only if $\beta = \vec{b}.\vec{m}(v) = b_0 + b_V.v + \bar{b}_E|v|^2 \in$ Ker L. Moreover (28) gives:

$$S\vec{b}.\vec{b} = \sum_{i,j=1}^{13} S_{ij}b_ib_j = \sum_{i,j=1}^{13} \langle L(g_0m_j)b_i, m_jb_j\rangle \tag{57}$$

$$= -\langle L(g_0\beta)\beta\rangle, \tag{58}$$

and according to the properties of the collision operator L we conclude that (whatever basis is used in the Galerkin approximation), $-S\vec{b}.\vec{b} \geq 0$. More precisely, using the expression of S obtained by using the 13 moment basis, we have

$$-S\vec{b}.\vec{b} \geq 1/\tau||(I - P_{K_S})\vec{b}||^2. \qquad \square$$

We now write the hyperbolic system (34)

$$\sum_{p=1}^{3} A_p \partial_{y_p} \vec{b} \;=\; \mathcal{L}\vec{b} \;=\; \sqrt{RT_0} \begin{pmatrix} 0 & \mathcal{L}_{0,V} & 0 & 0 & 0 \\ \mathcal{L}_{V,0} & 0 & \mathcal{L}_{V,E} & \mathcal{L}_{V,\tau} & 0 \\ 0 & \mathcal{L}_{E,V} & 0 & 0 & \mathcal{L}_{E,q} \\ 0 & \mathcal{L}_{\tau,V} & 0 & 0 & \mathcal{L}_{\tau,q} \\ 0 & 0 & \mathcal{L}_{q,E} & \mathcal{L}_{q,\tau} & 0 \end{pmatrix} \begin{pmatrix} b_0 \\ b_V \\ b_E \\ b_\tau \\ b_q \end{pmatrix}$$

where

$$\mathcal{L}_{0,V} = (\partial_1,\ \partial_2,\ \partial_3) \tag{59}$$

$$\mathcal{L}_{V,0} = \begin{pmatrix} \partial_1 \\ \partial_2 \\ \partial_3 \end{pmatrix},\ \mathcal{L}_{V,E} = \sqrt{2} \begin{pmatrix} \partial_1 & 0 & 0 \\ 0 & \partial_2 & 0 \\ 0 & 0 & \partial_3 \end{pmatrix},\ \mathcal{L}_{V,\tau} = \begin{pmatrix} 0 & \partial_3 & \partial_2 \\ \partial_3 & 0 & \partial_1 \\ \partial_2 & \partial_1 & 0 \end{pmatrix}, \tag{60}$$

$$\mathcal{L}_{E,V} = \mathcal{L}_{V,E}; \quad \mathcal{L}_{E,q} = \frac{\sqrt{5}}{5} \begin{pmatrix} 3\partial_1 & \partial_2 & \partial_3 \\ \partial_1 & 3\partial_2 & \partial_3 \\ \partial_1 & \partial_2 & 3\partial_3 \end{pmatrix}, \tag{61}$$

$$\mathcal{L}_{\tau,V} = \mathcal{L}_{V,\tau}, \quad \mathcal{L}_{\tau,q} = \frac{\sqrt{10}}{5} \begin{pmatrix} 0 & \partial_3 & \partial_2 \\ \partial_3 & 0 & \partial_1 \\ \partial_2 & \partial_1 & 0 \end{pmatrix}, \tag{62}$$

$$\mathcal{L}_{q,E} = \mathcal{L}_{E,q}, \quad \mathcal{L}_{q,\tau} = \mathcal{L}_{\tau,q} \tag{63}$$

$$g^l = \sqrt{RT_0}(0,\ \delta_{l1},\ \delta_{l2},\ \delta_{l3},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0)$$

Since the quantity $\sqrt{RT_0}$ is a common factor in the the differential operator $\mathcal{L}$ and in the right-hand-side, it is simpler to divide the left and right-hand side of (34) by this quantity. This modifies the relaxation factor in the matrix S which is therefore $\rho_0\sqrt{RT_0}/\mu$ instead of $1/\tau$. This is done in all the following.

Finally to write the boundary condition (36), we need to precise the matrix $R(n)$. First we notice that the application $\beta \to \mathcal{R}(n)[\beta]$ defined by

$$\mathcal{R}(n)[\beta](v) = \beta(v - 2v.nn)$$

is a idempotent application and that

$$\mathcal{R}(n)\ \mathrm{Span}\{m_j(v), 0 \leq j \leq 12\} \subset \mathrm{Span}\{m_j(v), 0 \leq j \leq 12\}.$$

Then the matrix $R(n)$ is defined by

$$\sum_{j=1}^{N} b_j m_j(v - 2v.nn) = \sum_{p=1}^{N} \sum_{q+1}^{N} R(n)_{pq}\ b_q m_p(v), \tag{64}$$

and we have the following properties

Lemma 1. *The matrix $R(n)$ defined by* (64) *satisfies:*

- *If $\vec{b}$ is an eigenvector of the matrix $A(n)$ associated with the eigenvalue λ, then $R(n)\vec{b}$ is an eigenvector of the matrix $A(n)$ associated with the eigenvalue $-\lambda$.*
- $R(n)^2 = I, \quad R(n)A(n)^+R(n) = -A(n)^-.$

Sktech of the Proof. Let us remark that the properties (1) implies that

$$R(n)A(n)^-R(n) = -A(n)^+, \text{ and } R(n)A(n)R(n) = -A(n).$$

For the sake of simplicity we give the proof for $n = e^1$ so that $A(n) = A_1$. The first part of the lemma is obtained by using (28) and odd/even parity considerations, and as a consequence we have $R(n)Ker(A(n)) \subset Ker(A(n))$. The second part is obtained by writing any vector $\vec{b}$ on the basis of eigenvector of A_1, and using the properties proved in the first part. □

Lemma 2. *Let us assume that, $\forall y \in \Gamma_Y$,*

$$\vec{c}(y) = K(y)\ \vec{\theta}, \tag{65}$$

$$\vec{b}(y) = (b_0(y), b_V(y), \bar{b}_E(y), \bar{b}_E(y), \bar{b}_E(y), 0, 0, 0, 0, 0, 0) \tag{66}$$

$$0 = A_1(\vec{b}(y) - \vec{c}(y)).(\vec{b}(y) - \vec{c}(y)), \tag{67}$$

then

$$b(y) = K(y)\vec{\theta},\ \forall y \in \Gamma_Y.$$

Proof. The property is directly deduced from caracterization of

$$Ker(A_1) = Span\{\vec{k}^1, \vec{k}^2, \vec{k}^3, \vec{k}^4, \vec{k}^5\}$$

where

$$\begin{array}{rl|c|c|c|c|c|c|c|c|c|c|c|c|c|}
\vec{k}^1 = & (0 & 0 & \frac{-\sqrt{10}}{5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0) \\
\vec{k}^2 = & (0 & 0 & 0 & \frac{-\sqrt{10}}{5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1) \\
\vec{k}^3 = & (\sqrt{2} & 0 & 0 & 0 & -1 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0) \\
\vec{k}^4 = & (\sqrt{2} & 0 & 0 & 0 & -1 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0) \\
\vec{k}^5 = & (0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0)
\end{array}$$

□

Proposition 3. *Let $\vec{b}$ be satisfying the boundary conditions* (35-36 -37) *and let us denote*

$$E(\vec{b}) = \int_{Y_f} \Big(- S\vec{b}(y).b(y) + \sum_{p=1}^{3} A_p \partial_{y_p} \vec{b}(y).\vec{b}(y) \Big)\, dy.$$

Then

1. $\forall \vec{b},\ E(\vec{b}) \geq 0$,
2. $E(b) = 0 \Leftrightarrow \vec{b}(y) = (b_0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^T$, *where b_0 is a constant independent of y.*

Proof. We multiply (34) by $\vec{b}$ and we integrate over Y_f. It comes

$$E(\vec{b}) \ = \ -\int_{Y_f} S\vec{b}(y).\vec{b}(y)dy - \frac{1}{2}\int_{\Gamma_Y} A(n)\vec{b}(y).\vec{b}(y)dy, \tag{68}$$

From (54) we have

$$-\int_{Y_f} S\vec{b}(y).\vec{b}(y)dy \geq \frac{1}{\tau}\int_{Y_f} ||(I - P_{K_S})\vec{b}(y)||^2 dy > 0. \tag{69}$$

Writing $\vec{b}(y) = c(y) + (\vec{b}(y) - c(y))$, taking into account that $A(n)\vec{b}(y).\vec{c}(y) = 0$ and $A(n)\vec{c}(y).\vec{c}(y) = 0$ on Γ_Y, and using the Lemma 1, we finally obtain

$$\begin{aligned}
-\frac{1}{2}\int_{\Gamma_Y} A(n)(\vec{b}-\vec{c}).(\vec{b}-\vec{c})dy \ &= \ -\frac{(1-(1-\sigma)^2)}{2}\int_{\Gamma_Y} A(n)^-(\vec{b}-\vec{c}).(\vec{b}-\vec{c})dy, \\
&\geq \ 0,
\end{aligned}$$

which proves the first part of the proposition.

We assume now that $E(\vec{b}) = 0$. From the above computation this implies that

$$\int_{Y_f} S\vec{b}(y).\vec{b}(y)dy = 0, \quad \int_{\Gamma_Y} A(n)^-(\vec{b}(y) - \vec{c}(y)).(\vec{b}(y) - \vec{c}(y))dy \ = \ 0.$$

The first relation implies that $\vec{b}(y) = (b_0(y), b_V(y), \bar{b}_E(y), \bar{b}_E(y), \bar{b}_E(y), 0, 0, 0, 0, 0, 0)$, and the second relation implies that $A(n)^-(\vec{b}(y)-\vec{c}(y)).(\vec{b}(y)-\vec{c}(y)) = 0, \forall y \in \Gamma_Y$. But since we have $A(n)^+(\vec{b}(y)-\vec{c}(y)).(\vec{b}(y)-\vec{c}(y)) = 0, \forall y \in \Gamma_Y$, we get

$$A(n)(\vec{b}(y) - \vec{c}(y)).(\vec{b}(y) - \vec{c}(y)) = 0, \forall y \in \Gamma_Y, \tag{70}$$

Then, from Lemma 2 we get $\vec{b}(y) = \vec{c}(y)$, on Γ_Y, which implies that $b_V(y) = 0$, $\bar{b}_E(y) = 0$, on Γ_Y. Using now the expression of (34) we conclude that $\frac{\sqrt{5}}{5}\partial_{y_j}\bar{b}_E(y) = 0, (j \neq i)$ on Y_f and thus

$$b_0(y) = b_0, \ \ \bar{b}_E(y) = 0, \text{ on } Y_f,$$

which ends the proof of the second part of the proposition. □

Remark. The last proposition implies that the solution of the hyperbolic cell auxiliary problem is not unique and is defined up to an additive vector $\vec{\vec{b}} = (b_0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^T$. Nevertheless, as it is usual in homogeneization, the effective coefficients D and $\tilde{D}$ are uniquely defined because $\int_{Y_f} \vec{\vec{b}} < v_i f_0(v) > dy = 0$!

3.2.4. Asymptotic behavior for small Knudsen, the Darcy regime

As we have seen in a previous section, in the collision regime, the solution of the kinetic cell auxiliary problem $\hat{\beta}$ satisfies

$$\widehat{\beta}_l \approx a_0 + a_1 v + a_2 |v|^2,$$

and this property has been used to choose a convenient basis in our Galerkin approach in velocity variables. More precise results can be obtained when we consider the fluid limit corresponding to $\rho \to +\infty$. In ([4, 5]) an asymptotic analysis of the kinetic cell auxiliary problems shows that in this limit those problems lead to Stokes equations and that we recover at the macroscopic scale the well known Darcy law. This result can be seen as an extention to porous media of the analysis of the fluid limit of the linearized Boltzmann equation given in ([12]). It is quite important to check now that this asymptotic limit is preserved by the hyperbolic cell auxiliary problems.

Let us consider the cell auxiliary problem (34-35 -36-37) derived from the 13-element basis. We can write (34) in the following form

$$-\frac{\sqrt{RT_0}}{\mu\ \varepsilon}\hat{S}\vec{b}+\sum_{p=1,3}A_p\partial_{y_p}\vec{b}=\vec{g^l}, \tag{71}$$

where we have omitted for simplicity the index l for $\vec{b}$, where

$$\hat{S}=\ \mu/(\rho_0\sqrt{RT_0})\ S, \tag{72}$$

and

$$\varepsilon=\frac{1}{\rho_0}.$$

To make the asymptotic analysis of the hyperbolic cell auxiliary problem when $\varepsilon\to 0$ we look for a solution in the following form

$$\vec{b}=\frac{\vec{b}^{(-1)}}{\varepsilon}+\vec{b}^{(0)}+\varepsilon\ \vec{b}^{(1)}+\cdots \tag{73}$$

Inserting (73) in (71), and balancing ordre by order in ε we get

At the leading order

$$-\frac{\sqrt{RT_0}}{\mu}\hat{S}\vec{b}^{(-1)}=0, \tag{74}$$

so that

$$\vec{b}^{(-1)}=(b_0^{(-1)},b_V^{(-1)},\bar{b}_E^{(-1)},\bar{b}_E^{(-1)},\bar{b}_E^{(-1)},0,0,0,0,0,0,0). \tag{75}$$

Taking account of this result in the boundary condition (35-36) and using the properties of the matrix $R(n)$ leads to

$$b_{V|_\gamma}^{(-1)}=0\quad\text{ and }\quad b_{E|_\gamma}^{(-1)}=0. \tag{76}$$

At order $+1$

$$-\frac{\sqrt{RT_0}}{\mu}\hat{S}\vec{b}^{(0)}+\sum_{p=1,3}A_p\partial_{y_p}\vec{b}^{(-1)}=0. \tag{77}$$

Since

$$\hat{S}\vec{b}^{(0)}.\vec{d}=0,\forall\vec{d}\in\ \text{Ker}\ S,$$

the Fredholm alternative leads to

$$\sum_{p=1,3} A_p \partial_{y_p} \vec{b}^{(-1)}.\vec{d} = 0, \quad \forall \vec{d} \in \text{ Ker } S,$$

which writes

$$\begin{aligned}
\text{div}_y \ \vec{b}_V^{(-1)} &= 0, && (78)\\
\nabla_y b_0^{(-1)} + \sqrt{2}\nabla_y \ \bar{b}_E^{(-1)} &= 0, && (79)\\
b_E^{(0)} &= \bar{b}_E^{(0)}\vec{e} - \frac{\sqrt{2}\mu}{\sqrt{RT_0}} \sum_{i=1}^{3} \partial_{y_i} b_i e^i && (80)\\
\frac{\sqrt{RT_0}}{\mu} \ b_q^{(0)} &= -\sqrt{5} \ \nabla_y \bar{b}_E^{(-1)}, && (81)\\
\frac{\sqrt{RT_0}}{\mu} \ b_\tau^{(0)} &= \mathcal{L}_{\tau,V} \vec{b}_V^{(-1)} && (82)
\end{aligned}$$

At order $+2$

$$-\frac{\sqrt{RT_0}}{\mu} \hat{S}\vec{b}^{(1)} + \sum_{p=1,3} A_p \partial_{y_p} \vec{b}^{(0)} = g, \tag{83}$$

which gives, from Fredholm alternative

$$\begin{aligned}
\text{div}_y \ \vec{b}_V^{(0)} &= 0, && (84)\\
\nabla_y b_0^{(0)} + \sqrt{2}\sum_{i=1}^{3} \partial_{y_i} b_{E_i}^{(0)} e^i + \mathcal{L}_{V,\tau} b_\tau^{(0)} &= g_V^l, && (85)
\end{aligned}$$

Inserting (80) and (82) in (85) leads to

$$\nabla_y b_0^{(0)} + \sqrt{2}\nabla_y \bar{b}_E^{(0)} - \frac{2\mu}{\sqrt{RT_0}} \begin{pmatrix} \partial_{y_1}^2 \ b_{V_1}^{(-1)} \\ \partial_{y_2}^2 \ b_{V_2}^{(-1)} \\ \partial_{y_3}^2 \ b_{V_3}^{(-1)} \end{pmatrix} - \frac{\mu}{\sqrt{RT_0}} \mathcal{L}_{V,\tau}\mathcal{L}_{\tau,V} b_V^{(-1)} = g_V^l. \tag{86}$$

Denoting

$$\pi = (b_0 + \sqrt{2} \ \bar{b}_E), \tag{87}$$

and taking into account the definition of $\mathcal{L}_{V,\tau}$ and $\mathcal{L}_{\tau,V}$, and (78) we obtain

$$\begin{aligned}
-\frac{\mu}{\sqrt{RT_0}} \ \Delta_y b_V^{(-1)} + \nabla_y \pi^{(0)} &= e^l, && (88)\\
\text{div}_y \ b_v^{(-1)} &= 0, && (89)
\end{aligned}$$

$$b_V{}^{(-1)}_{|_\gamma} = 0, \tag{90}$$

$$\text{periodic conditions on} \qquad \partial Y - \Gamma_Y \tag{91}$$

which means that $b_V^{(-1)}$ is solution of a Stokes equation on Y_f.

The same analysis can be performed for the hyperbolic cell auxiliary problem associated to α_l. In that case we look for a solution

$$\vec{a} = \frac{\vec{a}^{(-1)}}{\varepsilon} + \vec{a}^{(0)} + \varepsilon\vec{a}^{(1)} + \cdots,$$

and $\vec{a}^{(-1)}$ is also solution of a Stokes equation but with a right hand side equal to e^l/T_0. Thus the vectors $b_V^{(-1)}$ and $a_V^{(-1)}$ are proportional. Taking into account that $\beta_l = \hat{\beta}_l/\rho_0$, we conclude that

$$\frac{\tilde{D}_{ij}T}{D_{ij}\rho} = 1.$$

This means that this ratio (which is independent of i, j) defines a dimensionless number which is the ratio of the mass diffusion over the thermal transpiration and

$$\tilde{D} = \frac{\rho}{T}D. \tag{92}$$

But in ATM, the macroscopic velocity of the fluid is given by

$$\rho\ u = -(D\ \nabla_x\ \rho + \ \tilde{D}\ \nabla_x\ T), \tag{93}$$

and thus using (92)

$$\rho\ u\ =\ -\rho D\left(\frac{\nabla_x\ \rho}{\rho} + \frac{\nabla_x\ T}{T}\right) = -\rho D\frac{\nabla_x p}{p} = -\frac{1}{RT}D\nabla_x p.$$

Moreover, since, $D_{ij} = -(\rho/|Y_f|)\int_{Y_f}\vec{b_j^i}(y)dy\int_v g_0(v)v_j^2 dv$, we obtain

$$u = -\frac{\epsilon}{\mu}B\nabla_x p, \tag{94}$$

where ϵ is the porosity and B defined by

$$B_{ij} = \int_{Y_s} b_j^i(y)dy, \tag{95}$$

is the *permeability tensor*. The relation (94) is the well known Darcy law. Thus we have proved that our approach, designed for the transition regime,

recovers the Darcy regime in the fluid limit. Of course there is no reason that the relation (92) is still true in other regime. This will be illustrated in the section of numerical results.

3.5. Approximation in space variables and solution

Since the hyperbolic-relaxation system (34) is obtained by closing a kinetic equation, a simple and efficient approximation consists in using a classical finite volume kinetic scheme. In a kinetic scheme, the half postive and negative fluxes must be computed to take into account the balance of particles between the boundary of the cells. As the flux in the p-direction is linear, with the associated matrix given A_p by (28), the half fluxes are also linear and the associated matrix $A_p^{(\pm)}$ can be computed simply by

$$A_p^{(\pm)} = (A_p^{(\pm)})_{i=1,N,j=1,N} = \left(\left\langle g_0(v) m_i(v) v_p^{\pm} m_j(v) \right\rangle\right)_{i,j}$$

where $v_p^{\pm} = (v_p \pm |v_p|)/2$. We work with a regular cartesian mesh where $\mathbf{i}$ denotes the multi-index (i, j, k) and we introduce the following notations

$$D_{y_1} f_{\mathbf{i}} = D_1 f_{\mathbf{i}} = \frac{f_{i+1,j,k} - f_{i-1,j,k}}{\Delta y_1}, \tag{96}$$

$$D^+_{y_1} f_{\mathbf{i}} = D^+_1 f_{\mathbf{i}} = \frac{f_{i+1,j,k} - f_{i,j,k}}{\Delta y_1}, \tag{97}$$

$$D^-_{y_1} f_{\mathbf{i}} = D^-_1 f_{\mathbf{i}} = \frac{f_{i,j,k} - f_{i-1,j,k}}{\Delta y_1}, \tag{98}$$

Then the kinetic scheme writes

$$-\frac{\rho_0 \sqrt{RT_0}}{\mu} \hat{S} \vec{b}_{\mathbf{i}} + \sum_{p=1}^{3} (A_p^{(+)} D_p^- \vec{b}_{\mathbf{i}} + A_p^{(-)} D_p^+ \vec{b}_{\mathbf{i}}) = g_{\mathbf{i}}, \tag{99}$$

where $\hat{S}$ is defined by (72) and the right-hand-side is $g^l_{\mathbf{i}} = \langle g_0(v) m_i(v) v_l \rangle = A_l (1, 0, \dots)^T$.

Unfortunately, a first order scheme is not accurate enough. Higher order extensions can be constructed by a MUSCL approach and since the problem is linear it is not necessary to use slope limiters. This leads to the canonical centered scheme :

$$-\frac{\rho_0 \sqrt{RT_0}}{\mu} \hat{S} \vec{b}_{\mathbf{i}} + \sum_{p=1}^{3} A_p D_p \vec{b}_{\mathbf{i}} = g_{\mathbf{i}}. \tag{100}$$

But this scheme can lead to some numerical instabilities known as odd-even uncoupling. To overcome this drawback, boundary conditions must be modify to couple the two nearest grid points of the boundaries. The boundary conditions are fulfilled with the help of ghost cells. In a regular mesh of hexaedra (cubic voxel), the boundary procedure is essentially one dimensional and can be explained for the direction 1. The extension from order one to order two can be viewed as

$$\begin{aligned}(A_1\vec{b})_{i+\frac{1}{2},j,k} &= A_1^{(+)}\vec{b}_{i,j,k} + A_1^{(-)}\vec{b}_{i+1,j,k} \\ &\approx A_1^{(+)}\frac{\vec{b}_{i,j,k}+\vec{b}_{i+1,j,k}}{2} + A_1^{(-)}\frac{\vec{b}_{i,j,k}+\vec{b}_{i+1,j,k}}{2} \\ &= A_1\frac{\vec{b}_{i,j,k}+\vec{b}_{i+1,j,k}}{2}.\end{aligned}$$

Near the boundary, we keep the ghost cell for the incoming half flux and we extrapolate the outgoing half flux respecting the upwinding direction of the first order scheme. If we denote $i = 0$ the ghost cell, the incoming half flux is $A_1^{(+)}\vec{b}_0$ and this value is not modified. On the other hand, the outgoing half flux $A_1^{(-)}\vec{b}_1$ is replaced by $A_1^{(-)}(\vec{b}_1+\vec{b}_2)/2$ instead of $A_1^{(-)}(\vec{b}_1+\vec{b}_0)/2$ as inside the domain of computation. The fulfill of $\vec{b}_0$ is the same for the two schemes and derived from the kinetic level of the problem. We simply express that the distribution in the ghost cell is proportional to a Maxwellian ($\beta = kg_0$ at the kinetic level or $\vec{b}_0 = k(1,0,\dots)^T$ at the hyperbolic level)and the constant k is founded by writing the balance of mass flux at the boundary which must be equal to 0. This gives

$$k = -\frac{A(n)^{(-)}\vec{b_1}.\vec{\theta}}{A(n)^{(+)}\vec{\theta}.\vec{\theta}}. \tag{101}$$

The space approximation leads to an algebraic linear system which is solved by using a non-symmetric matrix iterative solver GMRES (Generalized Minimum RESidual).

3.6. Asymptotic preserving scheme for the hyperbolic auxiliary cell problems

In the previous section we proposed a numerical approach to solve the kinetic cell auxiliary problems based on a Galerkin approximation for the velocity variables. Moreover we proposed a Galerkin basis able to take into

account both collisional and rarefied regimes inside the pores. Nevertheless we can expect some further difficulties in the fluid limit i.e. for high density (or small Knudsen number) gas flows as it is usual in kinetic models. Indeed we have proved in section 3.4.2 that the hyperbolic cell auxiliary problems leads in this limit to Stokes equations which are elliptic systems. It is well known in numerical approximation of kinetic models that usual upwind schemes designed for the transport regime have not the correct asymptotic behavior in the fluid limit and that we have to modify them so that they lead to a consistent and precise approximation of the asymptotic system in this limit. In our context it means that if we study the asymptotic limit of the scheme (99) for fixed space steps ($\Delta y_i,\ i = 1, 2, 3$) and for $Kn \to 0$ we would like to find a consistent approximation of the Stokes problem (88-89-90-91). But, as we can expect, this is not true and thus we have to modify the numerical scheme in the fluid limit to recover this property.

We denote in the following

$$\mathrm{Div}_h^{\pm} = \sum_{k=1}^{3} D_{y_k}^{\pm}, \tag{102}$$

$$\nabla_h^{+} = (D_1^{+}, D_2^{+}, D_3^{+})^T. \tag{103}$$

.

Introducing $\vec{b^*} = \rho^* \vec{b}$, where ρ^* is a reference density and $\varepsilon = \rho^*/\rho_0$, the numerical scheme introduced for the transport regime writes

$$-\frac{\sqrt{RT_0}}{\varepsilon\mu}\hat{S}\vec{b^*}_{\mathbf{i}} + \frac{1}{\rho^*}\sum_{p=1}^{3} A_p D_{y_p}\vec{b^*}_{\mathbf{i}} = g_{\mathbf{i}}. \tag{104}$$

In order to have the correct asymptotic limit as $\varepsilon \to 0$, we modify the numerical scheme as follows

$$-\frac{\sqrt{RT_0}}{\varepsilon\mu}\hat{S}\vec{b^*}_{\mathbf{i}} + \varepsilon^2\sum_{p=1}^{3} A_p D_{y_p}\vec{b^*}_{\mathbf{i}} + (1-\epsilon^2)\sum_{p=1}^{3} A_p \tilde{D}_{y_p}\vec{b^*}_{\mathbf{i}} = g_{\mathbf{i}}. \tag{105}$$

where $\tilde{D}_{y_p}$ is defined by

$$\tilde{D}_{y_1} = (D_1^{+}, D_1^{-}, D_1^{+}, D_1^{+}, D_1^{+}, D_1^{+}, D_1^{+}, D_1, D_1^{-}, D_1^{-}, D_1, D_1, D_1) \tag{106}$$

$$\tilde{D}_{y_2} = (D_2^{+}, D_2^{+}, D_2^{-}, D_2^{+}, D_2^{+}, D_2^{+}, D_2^{+}, D_2^{-}, D_2, D_2^{-}, D_2, D_2, D_2) \tag{107}$$

$$\tilde{D}_{y_3} = (D_3^{+}, D_3^{+}, D_3^{+}, D_3^{-}, D_3^{+}, D_3^{+}, D_3^{+}, D_3^{-}, D_3^{-}, D_3, D_3, D_3, D_3). \tag{108}$$

In this scheme we use a backward difference scheme for the components of $\vec{b}$ corresponding to odd basis functions and a forward difference scheme for the components corresponding to even basis functions. Introducing such a different treatment corresponds to have a different treatment of the odd and even parts of the distribution function, which is a usual way to obtain correct asmptotic behavior for kinetic equations.

For the asymptotic analysis when $\varepsilon \to 0$ we look for $b^*_{\mathbf{i}}$ as $b^*_{\mathbf{i}} = \frac{1}{\varepsilon} b_{\mathbf{i}}^{*(-1)} + b_{\mathbf{i}}^{*(0)} + \varepsilon b_{\mathbf{i}}^{*(1)} + \cdots$ .. Inserting in (105) and balancing order by order in ε, it comes

At the leading order

$$\frac{\sqrt{RT_0}}{\mu} \hat{S} b_i^{*(-1)} = 0,$$

and thus for the same reason as previously

$$b_{\mathbf{i}}^{*(-1)} = (b_{0\mathbf{i}}^{*(-1)}, b_{1\mathbf{i}}^{*(-1)}, b_{2\mathbf{i}}^{*(-1)}, b_{3\mathbf{i}}^{*(-1)}, b_{E\mathbf{i}}^{-\,*(-1)}, b_{E\mathbf{i}}^{-\,*(-1)}, b_{E\mathbf{i}}^{-\,*(-1)}, 0, 0, 0, 0, 0, 0) \tag{109}$$

At order $+1$

$$-\frac{\sqrt{RT_0}}{\mu} \hat{S} \vec{b}_{\mathbf{i}}^{*(0)} + \frac{1}{\rho^*} \sum_{p=1}^{3} A_p \tilde{D}_{y_p} \vec{b}_{\mathbf{i}}^{*(-1)} = 0. \tag{110}$$

Existence of $b_{\mathbf{i}}^{(0)}$ follows from Fredholm alternative under the condition

$$(\sum_{p=1}^{3} A_p \tilde{D}_{y_p} \vec{b}_{\mathbf{i}}^{*(-1)}, d) = 0, \ \forall \vec{d} \in \text{Ker } S,$$

which writes

$$\begin{aligned}
\text{Div}_h^-\ b_V^{*(-1)} &= 0, && (111)\\
\nabla_h^+ b_0^{*(-1)} + \sqrt{2}\ \nabla_h^+ b_E^{-\,*(-1)} \hat{e} &= 0, && (112)\\
b_{E\mathbf{i}}^{*(0)} &= b_{E\mathbf{i}}^{-\,*(0)} \hat{e} - \sqrt{2} \nabla_h^- b_{V\mathbf{i}}^{*(-1)}, && (113)\\
\frac{\sqrt{RT_0}}{\mu} b_\tau^{*(0)} &= -\frac{1}{\rho^*} \mathcal{L}_{\tau,V}^- b_{V\mathbf{i}}^{*(-1)}, && (114)\\
\frac{\sqrt{RT_0}}{\mu} b_{q\mathbf{i}}^{*(0)} &= -\frac{\sqrt{5}}{\rho^*} \nabla_h^+ b_{E\mathbf{i}}^{-\,*(-1)} \hat{e}, && (115)
\end{aligned}$$

where $\mathcal{L}_{\tau,V}^-$ is the approximation of the operator $\mathcal{L}_{\tau,V}$ (see 62) using backward

difference.

At order +2

$$-\frac{\sqrt{RT_0}}{\mu}\hat{S}\vec{b}_i^{*(1)} + \frac{1}{\rho^*}\sum_{p=1}^{3} A_p \tilde{D}_{y_p}\vec{b}_i^{*(0)} = g^i. \tag{116}$$

As previously Fredholm alternative leads to the condition

$$(\sum_{p=1}^{3} A_p \tilde{D}_{y_p}\vec{b}_{\mathbf{i}}^{*(0)} - g_{\mathbf{i}}, \vec{d}) = 0, \ \forall \vec{d} \in \text{Ker } S,$$

which writes

$$\nabla_h^+ {b_0}_{\mathbf{i}}^{*(0)} + \sqrt{2}\nabla_h^+ {b_E}_{\mathbf{i}}^{*(0)} + \mathcal{L}_{V,\tau}^+ {b_\tau}_{\mathbf{i}}^{*(0)} = g_V^i \tag{117}$$

Then inserting (114) and (117) in the previous relation and (111), and denoting $\pi = (b_0^* + \sqrt{2}\bar{b}_E^*$, we get

$$\begin{aligned}
-\frac{\sqrt{RT_0}}{\mu\rho^*}\text{Div}_h^+\nabla_h^- {b_V}_{\mathbf{i}}^{*(-1)} + \nabla_h^+ \pi_{\mathbf{i}}^{(0)} &= g_{\mathbf{i}}, && (118)\\
\text{Div}_h^- \ {b_V}_{\mathbf{i}}^{*(-1)} &= 0, && (119)\\
{b_V^{*(-1)}}_{|\gamma} &= 0, && (120)\\
\text{periodic conditions on} \quad \partial Y - \gamma. && (121)
\end{aligned}$$

The last step is to check that this scheme, writen back in $\vec{b} = \vec{b^*}/\rho^*$is consistent with the Stokes equation (88)-(89). We first notice from the definition of D^+ and D^-, $\text{Div}_h^+\nabla_h^-$ is the classical 7-point approximation scheme of the Laplace operator in $\mathbb{R}^3$. Moreover if ${b_V}_{\mathbf{i}}^{(-1)}$ is interpreted as defined on a staggered mesh, i.e.

$${b_V}_{\mathbf{i}}^{(-1)} = ({b_1}_{i+1/2,j,k}^{(-1)}, {b_2}_{i,j+1/2,k}^{(-1)}, {b_3}_{i,j,k+1/2}^{(-1)}),$$

then

$$\begin{aligned}
\text{Div}_h^- \ {b_V}_{\mathbf{i}}^{(-1)} &= ({b_1}_{i+1/2,j,k}^{(-1)} - {b_1}_{i-1/2,j,k}^{(-1)})/\Delta y_1 + ({b_2}_{i,j+1/2,k}^{(-1)} - {b_2}_{i,j-1/2,k}^{(-1)})/\Delta y_2\\
&\quad + ({b_3}_{i,j,k+1/2}^{(-1)} - {b_3}_{i,j,k-1/2}^{(-1)})/\Delta y_3,
\end{aligned}$$

and the above scheme gives the classical MAC scheme for the Stokes equation.

Let us precise now how the boundary conditions are implemented for this asymptotic preserving scheme. Let us recall that, in the continuous problem, we have in the asymptotic limit the relation

$$\frac{\sqrt{RT_0}}{\mu}\, b_\tau^{(0)} = \mathcal{L}_{\tau,V}\vec{b}_V^{(-1)} = \sum_{p=1}^{3} L_p \partial_{y_p} b_V^{(-1)}.$$

Thus, integrating on Y_f we obtain by using the boundary conditions

$$\frac{\sqrt{RT_0}}{\mu} \int_{Y_f} b_\tau^{(0)}(y)dy = -\int_{\Gamma_Y} (\sum_{p=1}^{3} n_p L_p) b_V^{(-1)} = 0,$$

In the numerical scheme this property is not automatically satisfied. To get it we must impose a convenient boundary condition on the boundary cells $\mathbf{i} = (i, j, k)$ of Γ_Y such that either $(i-1, j, k)$, $(i, j-1, k)$ or $(i, j, k-1)$ is an interior cell of Y_f (since $\mathcal{L}_{\tau,V}$ is approximated by using backward finite differences). These boundary values are used for the discretization of (117) which is based on forward finite differences.

4. Numerical Results

In this section we give numerical results testing the correctness and the efficiency of the method described in this paper. In all example the gas is Argon and for the space approximation we use regular cartesian meshes.The values of ρ and T used for computing the effective diffusion coefficients are chosen so that the physical domain of interest is covered (Example 3). Moreover we take a number of values large enough so that the interpolation error is small. As the depency of D and $\tilde{D}$ is smooth, as we see in the examples, this can be achieved with a reasonable number of sampling values.

In the first example we consider the flow of a gas between two parallel plates and we compute the diffusion coefficient D in a direction parallel to the plates. In this case the unit cell reduces to the normal segment to the two plates which is 1 m long. The temperature is $T = 400\ K$ and the diffusion coefficient D is given as a function of the density ρ. We compute the coefficient for 28 values of $\rho = 10^i,\ \rho = 5 \times 10^i,\ i \in \{-7, 2\}$. We compare the solution computed by our Galerkin approach (with the 21-element basis) with the results given in ([10]) (with the linearized Boltzmann collision operator) and in ([7]) (with the linearized BGK relaxation operator)

which are obtained by a direct solution of the kinetic cell auxiliary problems using a discretization of the velocity space. The results are given in Figure 1 (left) with a zoom (right).

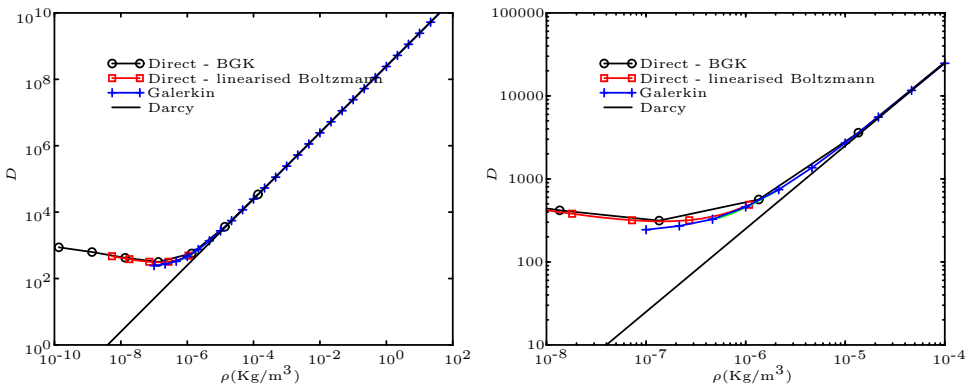

Figure 1. Coefficient D, comparison between the Galerkin approach and direct solution of kinetic problems.

The curves show a very good agreement between the direct computations on the kinetic problems and the Galerkin solution in the transition regime. For small values of ρ (or, which is equivalent, for small Knudsen numbers) the Galerkin solution gives a correct prediction up to the Knudsen minimum but, nevertheless, is less precise for smaller Knudsen number. Though the 21-element basis gives better results than the 13-element basis some more work is needed to capture the very rarefied flows. On the other hand, the Galerkin method is able to compute the solution for large values of ρ, where the direct computations are too much expensive. Moreover in this regime the results show a very good agreement with the asymptotic Darcy model.

In the second example we study the diffusion in a pipe with a square cross-section. We have to solve a two-dimensional cell auxiliary problem on the square $0.4mm \times 0.4mm$ with 40×40 grid cells. Figure 2 (left) shows the diffusion coefficient as function of ρ computed by the transport scheme (+), the asymptotic preserving scheme introduced in section 4.1 (x), and by solving the Stokes equation, which simplifies here in a Laplace equation (solid line). We observe a very good agreement between the solution given by the asymptotic preserving scheme and by Stokes equation in the Darcy regime. Figure 2 (right) shows the number of iterations needed for solving the cell auxiliary problem respectively with transport scheme (+) and asymptotic preserving scheme (x), as a function of ρ. It appears clearly that, contrary

to the transport scheme, the convergence rate of the asymptotic preserving scheme is almost independent of the value of ρ, which allows to treat efficiently problems with large density.

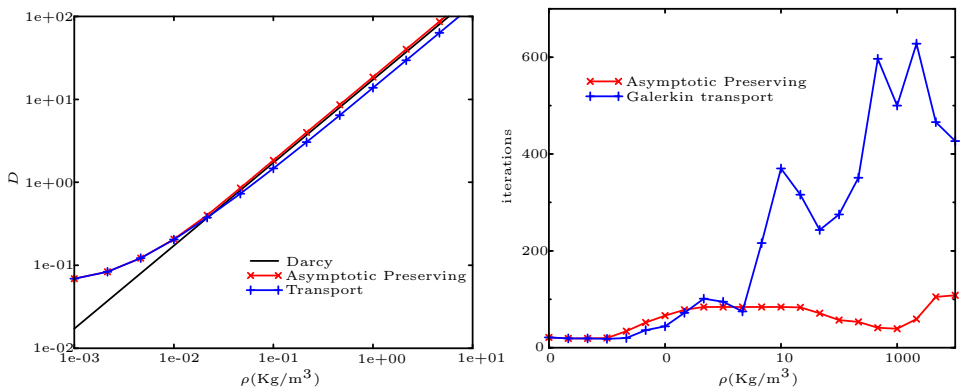

Figure 2. Coefficient D. Comparison between the transport scheme and the asymptotic preserving scheme.

In the third example we consider a pipe with a circular cross- section of 0.2 mm diameter. Figure 3 (left) shows the ratio $(\tilde{D}T)/(D\rho)$ as a function of ρ, for $T = 400K$ computed by the Galerkin method with the 21-element basis, using respectively a BGK relaxation operator (x) and a ES-BGK relaxation operator (+). In both case the ratio has a limit equal to 1 in the fluid regime and equal to 0.5 in the Knudsen regime which are the correct limits given by the theory.

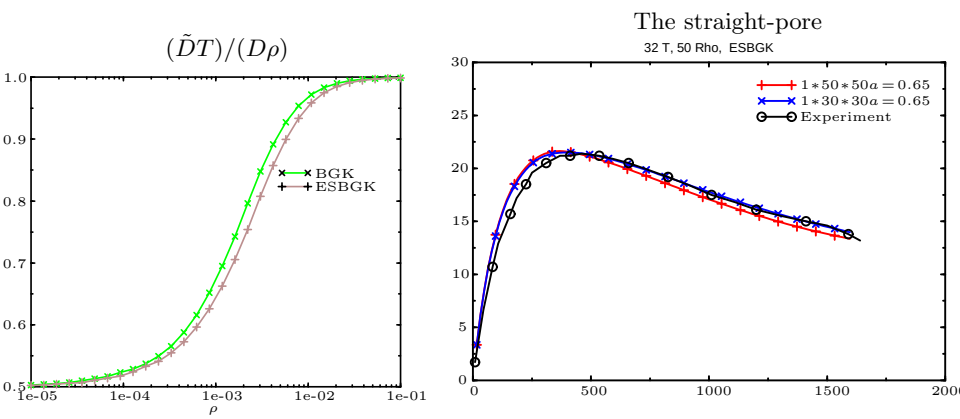

Figure 3. Flow in a pipe. Influence of the collison operator on the value of the ratio $(\tilde{D}T)/(D\rho)$ (left) and comparison with experimental data (right).

Nevertheless, in the transition regime there is a noticeable difference and the BGK operator overestimates the ratio compared to the ES-BGK. Those effective transport tensors D and $\tilde{D}$ are now used within the asymptotic transport model to make some comparisons between our approach and the experimental results reported in ([9]). Here we compute D and $\tilde{D}$ for 60 values of ρ (from 5×10^{-5} to 10^{-1}), and 30 values of T (from $T = 300K$ to $T = 600K$). In the experiment the two ends of the pipe (diameter= 0.2mm, length=76mm) were held at carefully monitored temperatures ($T_1 = 335.6K$ at the bottom end, and $T_2 = 569.8K$ at the top end), and the pressure difference between the two extremities ($\Delta P = P_1 - P_2$), chosen so that the mass flux in the tube vanishes, was recorded as a function of the absolute pressure at the top, hottest side (P_2). The hyperbolic cell auxiliary problems are solved with an accomodation coefficient $\sigma = 0.65$ and the ATM is solved with 100 cells along the pipe. The agreement between experimental data and numerical results is quite good. Finally it is worth noting that for this simulation we used the ES-BGK relaxation operator in the solution of the cell auxiliary problems. Results obtained using the BGK relaxation operator are notably less precise. This test case requires high precision of the numerical model in a large range of regimes and the results obtained with our approach are quite encouraging.

The last example is three dimensional. The porous media is between two horizontal plates distant from 0.3 mm and the unit cell is described by its horizontal rectangular section (1.6 mm $\times$ 3.2 mm) given on Figure 4 (left) where the solid phase is grey and the fluid phase dark grey.

The cell auxiliary problems are solved using the 21-element basis and a spatial mesh of cubic cells with $\Delta y = 0.2mm$. The eigenvectors of the tensor D for $T = 400K$ and $\rho = 10^{-2}kg/m^3$ are drawn on the figure. We see that the principal eigendirection is roughly parallel to the main channel of the porous media making an angle $\theta = 30^0$ with the y_1 axis, proving that the model brings to the macroscopic scale this geometric information from the microscopic scale. Moreover the anisotropy factor (i.e.the ratio between the largest and smallest eigenvalues) is equal to 3.13. On Figure 4 (right) is plotted the angle θ for the tensors D and $\tilde{D}$ as a function of ρ. The variation of θ is noticeable (about 5), giving the influence of the regime on the eigenvectors of D and $\tilde{D}$. Moreover we see that, as expected from the theory, these two tensors have the same eigendirections for small and large values of ρ, but that for intermediate values, here about $\rho = 10^{-4}$, their principal eigendirections are slightly different.

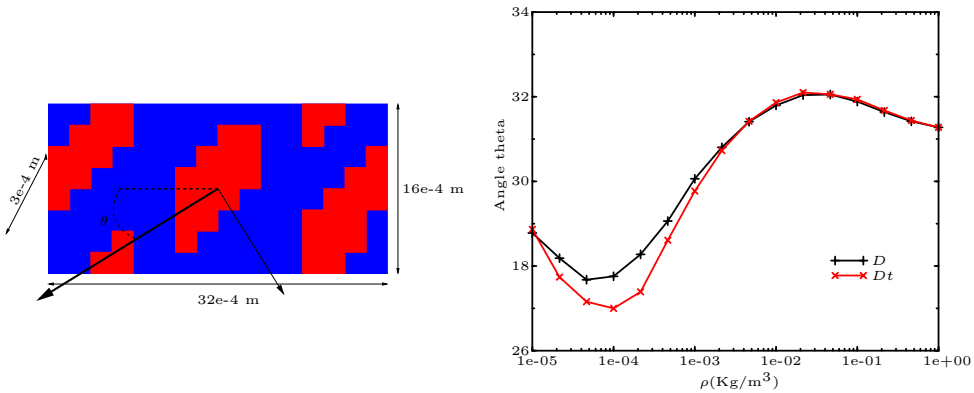

Figure 4. Geometry of a porous medium and principal directions of the tensor D (left), and variation of of the eigendirection with ρ (right).

5. Conclusion

We have presented a method for computing the solution of stationary linear kinetic equations allowing to determine the effective transport coefficients of macroscopic model for heat and mass transfer in porous media. Our approach is based on a Galerkin approximation in velocity variables and a classical kinetic scheme for space variables. The Galerkin approximation in velocity variables leads to an hyperbolic system which keeps the main properties of the original kinetic system. Numerical experiments show the efficiency of our method in the transition regime and the numerical scheme is modified in order to be extended in an asymptotic preserving scheme in the fluid limit. In forthcoming works we shall improve the precision of the method in the very rarefied regime.

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Applied Mathematics, University Bordeaux 1F-33405 Talence Cedex, France.
E-mail: Pierre.Charrier@math.u-bordeaux1.fr

Applied Mathematics, University Bordeaux 1F-33405 Talence Cedex, France.
E-mail: Bruno.Dubroca@math.u-bordeaux1.fr

Applied Mathematics, University Bordeaux 1F-33405 Talence Cedex, France.
E-mail: Christophe.Preux@math.u-bordeaux1.fr