A MULTISCALE FINITE ELEMENT METHOD FOR TRANSPORT MODELING

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Abstract. This work proposes a new multiscale finite element method to solve convectiondiffusion problems where both velocity and diffusion coefficient exhibit strong variations at a much smaller scale than the domain of resolution. In that case, classical discretization methods, used at the scale of the heterogeneities, turn out to be too costly or useless. The method, introduced in this paper, aims at solving this kind of problems on coarser grids with respect to the size of the heterogeneities by means of particular basis functions. These basis functions are solutions to cell problems and are designed to reproduce the variations of the solution on an underlying fine grid. Since all cell problems are independent from each other, these problems can be solved in parallel, which makes the method very efficient when used on parallel architectures. The convergence proof of our method is still in progress. But, on the basis of results of periodic homogenization, an a priori error estimate, that represents a first step in the proof, is established in this paper. Numerical results are also presented to illustrate some homogenization results.

1 Introduction

A first multiscale finite element method was introduced by T.Y. Hou and X.H. Wu in [1] to efficiently solve elliptic problems with diffusion coefficients containing small-scale features. The novelty of this method consisted in computing basis functions associated to a grid with a coarser resolution than the fine scale and which contain the small-scale variations. This method was based on results of the periodic homogenization theory shown, for example, in [2], [3] and [4]. Other multiscale methods which also stem from homogenization results, were proposed in [5], [6], [7] and [8].

In [9], a multiscale method was first applied for the resolution of a convection-diffusion problem with high Péclet numbers. The problem we address in this paper is however different. Convection is still dominating but the scaling is not the same. For this second problem, a method called the Heterogeneous Multiscale Method (HMM) was proposed in [10]. This method can be used to compute more accurately a solution at the coarse scale but it is not designed to reproduce the variations of the solution at a finer scale. Moreover, this method assumes that the diffusion and velocity field only have a small scale behavior and that they are constant on the macro scale.

The problem considered in this paper is introduced in Section 2. Known homogenization results for the periodic case are then summarized and an a priori error estimate between the exact solution and the first two terms of its two-scale expansion is established in Section 3. Having proved that the two-scale expansion can be a good approximation of the solution, we introduce in Section 4 our new multiscale method to compute numerically this approximation. Section 5 presents our first numerical results.

2 Statement of the problem

We consider, in this work, the following advection-diffusion equation, defined on an open set $(0, \mathcal{T}) \times \Omega$, $\Omega \subset \mathbb{R}^d$ and $\mathcal{T} > 0$:

$$\begin{cases} \rho^{*}(x^{*})\frac{\partial c^{*}}{\partial t^{*}}(t^{*},x^{*}) + b^{*}(x^{*}) \cdot \nabla c^{*}(t^{*},x^{*}) - \operatorname{div}\left(A^{*}(x^{*})\nabla c^{*}(t^{*},x^{*})\right) &= 0 \text{ in } (0,\mathcal{T}) \times \Omega \\ c^{*}(0,x^{*}) &= c^{0}(x^{*}) \text{ in } \Omega. \end{cases}$$
(1)

In (1), ρ^* represents the porosity, b^* the velocity, A^* the diffusion tensor, c^* a concentration and we assume that

$$\operatorname{div}\left(b^{*}\right) = 0.$$

Problem (1) can be rescaled following the same ideas as in [11], [12] and [13]. Let l be a characteristic length of the variations of the properties, L_R a characteristic length of the size of the domain Ω and let T_R represent our time scale. We set $\varepsilon = \frac{l}{L_R}$, we denote by ρ_R , b_R , c_R , A_R characteristic values for the porosity, velocity, concentration and diffusion and define adimensionalized variables which are

$$\begin{aligned} x &= \frac{x^*}{L_R}, \quad t = \frac{t^*}{T_R}, \quad \rho^{\varepsilon}(x) = \frac{\rho^*(x^*)}{\rho_R}, \\ b^{\varepsilon}(x) &= \frac{b^*(x^*)}{b_R}, \quad A^{\varepsilon}(x) = \frac{A^*(x^*)}{A_R}, u_{\varepsilon}(t,x) = \frac{c^*(t^*,x^*)}{c_R}. \end{aligned}$$

The dimensionless equation thus reads

$$\rho^{\varepsilon} \frac{\partial u_{\varepsilon}}{\partial t} + \frac{b_R T_R}{L_R} b^{\varepsilon} \cdot \nabla_x u_{\varepsilon} - \frac{A_R T_R}{L_R^2} \operatorname{div}_x \left(A^{\varepsilon} \nabla_x u_{\varepsilon} \right) = 0 \quad \text{in} \ (0, T) \times \Omega_{\varepsilon}, \tag{2}$$

with $\Omega_{\varepsilon} = \left\{ \frac{x^*}{L_R} \mid x^* \in \Omega \right\}$. For this problem, depending on the scale, two Péclet numbers can be defined:

• a local one defined by

$$\mathbf{Pe}_{loc} = \frac{lb_R}{A_R}$$

• and a macroscopic one defined by

$$\mathbf{Pe} = \frac{L_R b_R}{A_R}.$$

Using these definitions, we have $\mathbf{Pe} = \frac{1}{\varepsilon} \mathbf{Pe}_{loc}$. Furthermore, we set $T_R = \frac{L_R^2}{A_R}$ and rewrite (2) in

$$\rho^{\varepsilon} \frac{\partial u_{\varepsilon}}{\partial t} + \mathbf{Pe} \, b^{\varepsilon} \cdot \nabla_x u_{\varepsilon} - \operatorname{div}_x \left(A^{\varepsilon} \nabla_x u_{\varepsilon} \right) = 0 \quad \text{in} \, (0, T) \times \Omega_{\varepsilon}.$$

Assuming that our local Péclet number is equal to 1, $Pe = \frac{1}{\varepsilon}$, and our initial problem (1) becomes:

$$\begin{cases} \rho^{\varepsilon}(x)\frac{\partial u_{\varepsilon}}{\partial t} + \frac{1}{\varepsilon}b^{\varepsilon}(x)\cdot\nabla u_{\varepsilon} - \operatorname{div}\left(A^{\varepsilon}(x)\nabla u_{\varepsilon}\right) &= 0 & \operatorname{in}\left(0,T\right)\times\Omega_{\varepsilon}\\ u_{\varepsilon}\left(0,x\right) &= u^{0}\left(x\right) & \operatorname{in}\Omega_{\varepsilon}. \end{cases}$$
(3)

In the following, our study will only deal with this dimensionless problem. We assume in the next section that the parameters ρ^{ε} , b^{ε} , A^{ε} are periodic functions, which will allow us to state some homogenization results.

Remark 1: In [9], T.Y. Hou and D. Liang are concerned with the following equation:

$$\begin{cases} \frac{\partial u_{\varepsilon}}{\partial t} + b^{\varepsilon}(x) \cdot \nabla u_{\varepsilon} - \varepsilon^{m} \operatorname{div} \left(A^{\varepsilon}(x) \nabla u_{\varepsilon} \right) &= 0 & \operatorname{in} \mathbb{R}_{+} \times \Omega_{\varepsilon}, \\ u_{\varepsilon}(0, x) &= u^{0}(x) & \operatorname{in} \Omega_{\varepsilon}, \end{cases}$$
(4)

where $m \in [2, +\infty[$. Our case corresponds to m = 1. Moreover, a time of order 1 in (4) is equivalent to a time of order ε in (3).

3 The periodic case

From now on, Ω is the entire space \mathbb{R}^d . Let us consider the following problem defined on $\mathbb{R}^d \times (0,T)$: Find u_{ε} such that

$$\begin{cases} \rho\left(\frac{x}{\varepsilon}\right)\partial_{t}u_{\varepsilon} + \frac{1}{\varepsilon}b\left(\frac{x}{\varepsilon}\right)\cdot\nabla u_{\varepsilon} - \operatorname{div}\left(A\left(\frac{x}{\varepsilon}\right)\nabla u_{\varepsilon}\right) = 0 \quad \text{in } (0,T)\times\mathbb{R}^{d}, \\ u_{\varepsilon}(0,x) = u^{0}(x) \quad \text{in } \mathbb{R}^{d}. \end{cases}$$
(5)

 $\rho(y)$, b(y) and A(y) are assumed to be Y-periodic functions where $Y = (0, 1)^d$ is the unit cube. We also assume that:

- $\forall y \in Y, \rho(y) \ge \rho_{min} > 0$ and ρ is bounded,
- $\operatorname{div}(b) = 0, b \in L^{\infty}(Y),$
- A is bounded and coercive:

$$\forall \xi \in \mathbb{R}^d, \quad C_{sta} \left\| \xi \right\|^2 \leqslant A \xi \cdot \xi \leqslant C_{bnd} \left\| \xi \right\|^2,$$

 $\|\cdot\|$ being the Euclidean norm, C_{sta} and C_{bnd} positive constants.

In the following, $\bar{\rho}$ stands for the mean value of ρ :

$$\bar{\rho} = \int_{Y} \rho(y) dy.$$

3.1 Asymptotic expansion with drift

As in [14], [12] or [15], we assume that the solution u_{ε} can be expressed by means of an asymptotic expansion with drift:

$$u_{\varepsilon}(t,x) = \sum_{i=0}^{+\infty} \varepsilon^{i} u_{i} \left(t, x - \frac{b^{*}t}{\varepsilon}, \frac{x}{\varepsilon} \right),$$
(6)

where,

- for i = 0, ..., d, $u_i(t, x, y)$ are Y-periodic functions with respect to y,
- *b*^{*} is a constant vector which represents the homogenized velocity. Its expression will be given later.

We insert this expansion into equation (5). The identification of the terms corresponding to each power of ε leads to the following set of equations:

$$b(y) \cdot \nabla_y u_0 - \operatorname{div}_y \left(A(y) \nabla_y u_0 \right) = 0, \tag{7}$$

$$-\rho(y)b^* \cdot \nabla_x u_0 + b(y) \cdot (\nabla_x u_0 + \nabla_y u_1) - \operatorname{div}_y (A(y) (\nabla_x u_0 + \nabla_y u_1)) = 0,$$
(8)

$$b(y) \cdot \nabla_y u_2 - \operatorname{div}_y \left(A(y) \nabla_y u_2 \right) = -\rho(y) \partial_t u_0 + \rho(y) b^* \cdot \nabla_x u_1 - b(y) \cdot \nabla_x u_1 + \operatorname{div}_y \left(A(y) \nabla_x u_1 \right) + \operatorname{div}_x \left(A(y) \left(\nabla_y u_1 + \nabla_x u_0 \right) \right).$$
(9)

From equation (7), we deduce that $u_0(t, x, y)$ does not depend on the third variable $y \in Y$ so that we can set

$$\forall y \in Y, \quad u_0(t, x, y) = u(t, x).$$

From the compatibility condition of equation (8), we deduce that the homogenized velocity b^* is given by

$$b^* = \frac{\int_Y b(y)dy}{\bar{\rho}}.$$
(10)

Morevoer, for each i = 1, ..., d, we introduce the function w_i , solution to the cell problem

$$b(y) \cdot (\nabla_y w_i + e_i) - \operatorname{div}_y \left(A(y) \left(\nabla_y w_i + e_i \right) \right) = \rho(y) b^* \cdot e_i, \text{ on } Y.$$
(11)

Using equation (8), u_1 can be computed, up to a function of x, using the formula

$$u_1\left(t, x - \frac{b^*t}{\varepsilon}, y\right) = \sum_{i=1}^d \frac{\partial u}{\partial x_i} \left(t, x - \frac{b^*t}{\varepsilon}\right) w_i(y).$$
(12)

From the compatibility condition of (9) we deduce that the homogenized problem for u is

$$\bar{\rho}\partial_t u - \operatorname{div}\left(A^*\nabla u\right) = 0,\tag{13}$$

where

$$A_{i,j}^* = \int_Y A(y) \left(\nabla_y w_i + e_i \right) \cdot \left(\nabla_y w_j + e_j \right) dy.$$
(14)

The results presented here are deduced from a formal analysis. In [16], the following convergence theorem is proved:

Theorem 1. Let u_{ε} be the sequence of solutions to (5). Then

$$\int_0^T \int_{\mathbb{R}^d} \left| u_{\varepsilon}(t,x) - u\left(t,x - \frac{b^*t}{\varepsilon}\right) \right|^2 dx dt \xrightarrow[\varepsilon \to 0]{} 0,$$

where b^* and u are given by equations (10)-(14).

The proof of this theorem results from the theory of the two-scale convergence with drift. This result, which states that u is a good approximation of u_{ε} with respect to the L^2 norm, is not sufficient for higher order approximations and will be improved in the next section.

3.2 A priori error estimate

The aim of this section is to prove the following a priori error estimate.

Theorem 2. Let u_{ε} be the sequence of solutions to (5) and u and u_1 be given by equations (10)-(12). Then

$$\left\| u_{\varepsilon}(t,x) - u\left(t,x - \frac{b^{*}t}{\varepsilon}\right) - \varepsilon u_{1}\left(t,x - \frac{b^{*}t}{\varepsilon},\frac{x}{\varepsilon}\right) \right\|_{L^{2}\left((0,T),H^{1}\left(\mathbb{R}^{d}\right)\right)} \leqslant C\varepsilon,$$
(15)

where C depends on the final time T and not on ε .

Inequality (15) allows us to justify the approximation

$$u_{\varepsilon}(t,x) \approx u\left(t,x-\frac{b^{*}t}{\varepsilon}\right) + \varepsilon \sum_{i=1}^{d} \frac{\partial u}{\partial x_{i}}\left(t,x-\frac{b^{*}t}{\varepsilon}\right) w_{i}\left(\frac{x}{\varepsilon}\right)$$
(16)

which will be the starting point of our new multiscale method.

To prove Theorem 2, we use the same method as the one used in [17] for the elliptic case. A first intermediate result is given by the following Lemma.

Lemma 3. Let u_{ε} be the sequence of solutions to (5) and u and u_1 be given by equations (10)-(12). Then

$$\|r_{\varepsilon}\|_{L^{\infty}\left((0,T),L^{2}\left(\mathbb{R}^{d}\right)\right)}+\|\nabla r_{\varepsilon}\|_{L^{2}\left((0,T)\times\mathbb{R}^{d}\right)^{d}}\leqslant C,$$

where

$$r_{\varepsilon}(t,x) = \varepsilon^{-1} \left(u_{\varepsilon}(t,x) - u_0 \left(t, x - \frac{b^* t}{\varepsilon} \right) - \varepsilon u_1 \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \right).$$

Theorem 2 is then a consequence of Lemma 3. Indeed, using the Cauchy-Schwarz inequality, we can notice that

$$\|u\|_{L^{2}((0,t_{1}),H^{1}(\mathbb{R}^{d}))}^{2} \leq t_{1} \|u\|_{L^{\infty}((0,t_{1}),L^{2}(\mathbb{R}^{d}))}^{2} + \|\nabla u\|_{L^{2}((0,t_{1})\times\mathbb{R}^{d})}^{2}.$$

Proof. First, let us notice that, since b^* , u and u_1 are defined by equations (10)-(12), equations (7)-(9) are also verified with a function u_2 that can be defined as the solution of equation (9). In fact, replacing $\partial_t u$ with $\frac{1}{2} \operatorname{div} (A^* \nabla u)$ in equation (9), u_2 can be defined up to a function

of x by $u_2(t, x, y) = \sum_{i,j=1}^d \chi_{i,j}(y) \frac{\partial^2 u}{\partial x_i \partial x_j}(t, x)$, where each function $\chi_{i,j}$ is the periodic solution of the second-order cell problem:

$$b(y) \cdot \nabla_y \chi_{i,j}(y) - \operatorname{div}_y \left(A(y) \nabla_y \chi_{i,j}(y) \right) = -\frac{\rho(y)}{\bar{\rho}} A_{i,j}^* + \left(\rho(y) b_i^* - b_i(y) \right) w_j(y)$$
$$+ \sum_{k=1}^d \left(\frac{\partial}{\partial y_k} \left(w_i A_{k,j} \right) (y) + A_{i,k}(y) \frac{\partial w_j}{\partial y_k}(y) \right) + A_{i,j}(y), \quad \text{in } Y. \quad (17)$$

It is important to notice that, using the De Giorgi-Nash-Moser theorem, the functions w_i and $\chi_{i,j}$ are bounded in $L^{\infty}(Y)$. Consequently, the space norms of u_1 and u_2 can be bounded, up to a multiplicative constant, respectively by the derivatives and by the second-order derivatives of u:

$$\left\| u_1\left(t,\cdot,\frac{\cdot}{\varepsilon}\right) \right\|_{L^2(\Omega)} \leqslant C \left\| \nabla u(t,\cdot) \right\|_{L^2(\Omega)^d}, \quad \left\| u_2\left(t,\cdot,\frac{\cdot}{\varepsilon}\right) \right\|_{L^2(\Omega)} \leqslant C \left\| \nabla^2 u(t,\cdot) \right\|_{L^2(\Omega)^{d\times d}}.$$

Let $B(r_{\varepsilon})$ be defined by

$$B\left(r_{\varepsilon}(t,x)\right) = \rho\left(\frac{x}{\varepsilon}\right)\partial_{t}r_{\varepsilon} + \frac{1}{\varepsilon}b\left(\frac{x}{\varepsilon}\right)\cdot\nabla r_{\varepsilon} - \operatorname{div}\left(A\left(\frac{x}{\varepsilon}\right)\nabla r_{\varepsilon}\right).$$

The expression of r_{ε} is inserted in $B(r_{\varepsilon}(t, x))$ and we use the fact that

$$abla =
abla_x + rac{1}{arepsilon}
abla_y.$$

Developing all terms and using equation (5) as well as equations (7)-(9), we have:

$$B(r_{\varepsilon}(t,x)) = \varepsilon^{-1} \left(b\left(\frac{x}{\varepsilon}\right) \cdot \nabla_{y} u_{2} - \operatorname{div}_{y} \left(A\left(\frac{x}{\varepsilon}\right) \nabla_{y} u_{2} \right) \right) - \rho\left(\frac{x}{\varepsilon}\right) \partial_{t} u_{1} + \operatorname{div}_{x} \left(A\left(\frac{x}{\varepsilon}\right) \nabla_{x} u_{1} \right).$$

Using the fact that div(b) = 0, this can be rewritten as:

$$B(r_{\varepsilon}(t,x)) = \operatorname{div}\left(b\left(\frac{x}{\varepsilon}\right)u_{2}\right) -\operatorname{div}\left(A\left(\frac{x}{\varepsilon}\right)\nabla_{y}u_{2}\right) - b\left(\frac{x}{\varepsilon}\right)\cdot\nabla_{x}u_{2} + \operatorname{div}_{x}\left(A\left(\frac{x}{\varepsilon}\right)\nabla_{y}u_{2}\right) -\rho\left(\frac{x}{\varepsilon}\right)\partial_{t}u_{1} + \operatorname{div}_{x}\left(A\left(\frac{x}{\varepsilon}\right)\nabla_{x}u_{1}\right).$$

Multiplying this equation by r_{ε} and integrating with respect to t and x, for any $t_1 \in [0, T]$, we get:

$$\begin{split} \iint_{(0,t_1)\times\mathbb{R}^d} B\left(r_{\varepsilon}(t,x)\right) r_{\varepsilon}(t,x) dt dx &= -\iint_{(0,t_1)\times\mathbb{R}^d} \left(b\left(\frac{x}{\varepsilon}\right) u_2\left(t,x-\frac{b^*t}{\varepsilon},\frac{x}{\varepsilon}\right) \cdot \nabla r_{\varepsilon}(t,x) \right. \\ &+ A\left(\frac{x}{\varepsilon}\right) \nabla_y u_2\left(t,x-\frac{b^*t}{\varepsilon},\frac{x}{\varepsilon}\right) \cdot \nabla r_{\varepsilon}(t,x) \\ &+ \left(-b\left(\frac{x}{\varepsilon}\right) \cdot \nabla_x u_2\left(t,x-\frac{b^*t}{\varepsilon},\frac{x}{\varepsilon}\right) \right. \\ &+ \operatorname{div}_x \left(A\left(\frac{x}{\varepsilon}\right) \left(\nabla_y u_2\left(t,x-\frac{b^*t}{\varepsilon},\frac{x}{\varepsilon}\right) + \nabla_x u_1\left(t,x-\frac{b^*t}{\varepsilon},\frac{x}{\varepsilon}\right)\right)\right) \\ &- \rho\left(\frac{x}{\varepsilon}\right) \partial_t u_1\left(t,x-\frac{b^*t}{\varepsilon},\frac{x}{\varepsilon}\right)\right) r_{\varepsilon}(t,x) \right) dt dx. \end{split}$$

If u is sufficiently regular, we have:

$$\left| \iint_{(0,t_1)\times\mathbb{R}^d} B\left(r_{\varepsilon}(t,x)\right) r_{\varepsilon}(t,x) dt dx \right| \leq C\left(\left\| r_{\varepsilon} \right\|_{L^{\infty}\left((0,t_1),L^2\left(\mathbb{R}^d\right)\right)} + \left\| \nabla r_{\varepsilon} \right\|_{L^2\left((0,t_1)\times\mathbb{R}^d\right)^d} \right),$$

where the constant C depends on T, $||b||_{\infty}$, C_{bnd} , $||u||_{L^2((0,T),H^3(\mathbb{R}^d))}$ and $||\partial_t u||_{L^2((0,T),H^2(\mathbb{R}^d))}$. Furthermore, using equation (13), $\partial_t u$ is equivalent to $\nabla^2 u$. Therefore, C depends on T, $||b||_{\infty}$, C_{bnd} and $||u||_{L^2((0,T),H^4(\mathbb{R}^d))}$. Besides, the definition of B gives:

$$B\left(r_{\varepsilon}(t,x)\right)r_{\varepsilon}(t,x) = \frac{1}{2}\rho\left(\frac{x}{\varepsilon}\right)\partial_{t}\left(r_{\varepsilon}^{2}\right) + \frac{1}{2\varepsilon}b\left(\frac{x}{\varepsilon}\right)\cdot\nabla\left(r_{\varepsilon}^{2}\right) - \operatorname{div}\left(A\left(\frac{x}{\varepsilon}\right)\nabla r_{\varepsilon}\right)r_{\varepsilon}.$$

Integrating with respect to x and t and integrating by parts with respect to x, we have, since $\operatorname{div} b^{\varepsilon} = 0$:

$$\begin{split} \iint_{(0,t_1)\times\mathbb{R}^d} B\left(r_{\varepsilon}(t,x)\right) r_{\varepsilon}(t,x) dt dx &= \frac{1}{2} \int_{\mathbb{R}^d} \rho\left(\frac{x}{\varepsilon}\right) r_{\varepsilon}\left(t_1,x\right)^2 dx - \frac{1}{2} \int_{\mathbb{R}^d} \rho\left(\frac{x}{\varepsilon}\right) r_{\varepsilon}(0,x)^2 dx \\ &+ \iint A\left(\frac{x}{\varepsilon}\right) \nabla r_{\varepsilon} \cdot \nabla r_{\varepsilon}(t,x) dt dx. \end{split}$$

Since A is coercive, we have

$$\left| \iint A\left(\frac{x}{\varepsilon}\right) \nabla r_{\varepsilon}(t,x) \cdot \nabla r_{\varepsilon}(t,x) dt dx \right| \ge C_{sta} \left\| \nabla r_{\varepsilon} \right\|_{L^{2}\left((0,t_{1}) \times \mathbb{R}^{d}\right)}^{2}$$

Moreover, as ρ is bounded and positive, there exist ρ_{min} , ρ_{max} positive constants such that:

$$\frac{1}{2} \int_{\mathbb{R}^d} \rho\left(\frac{x}{\varepsilon}\right) r_{\varepsilon} \left(t_1, x\right)^2 dx \ge \rho_{\min} \left\| r_{\varepsilon} \left(t_1, \cdot\right) \right\|_{L^2(\mathbb{R}^d)}^2,$$

and

$$\frac{1}{2} \int_{\mathbb{R}^d} \rho\left(\frac{x}{\varepsilon}\right) r_{\varepsilon}(0,x)^2 dx \leqslant \rho_{max} \left\| r_{\varepsilon}(0,\cdot) \right\|_{L^2(\mathbb{R}^d)}^2.$$

Thus,

$$C_{sta} \left\| \nabla r_{\varepsilon} \right\|_{L^{2}\left((0,t_{1})\times\mathbb{R}^{d}\right)^{d}}^{2} + \rho_{min} \left\| r_{\varepsilon}\left(t_{1},\cdot\right) \right\|_{L^{2}\left(\mathbb{R}^{d}\right)}^{2} - \rho_{max} \left\| r_{\varepsilon}\left(0,\cdot\right) \right\|_{L^{2}\left(\mathbb{R}^{d}\right)}^{2}$$

$$\leqslant \iint_{(0,t_{1})\times\mathbb{R}^{d}} B\left(r_{\varepsilon}\left(t,x\right) \right) r_{\varepsilon}\left(t,x\right) dtdx$$

$$\leqslant C\left(\left\| r_{\varepsilon} \right\|_{L^{\infty}\left((0,t_{1}),L^{2}\left(\mathbb{R}^{d}\right)\right)}^{2} + \left\| \nabla r_{\varepsilon} \right\|_{L^{2}\left((0,t_{1})\times\mathbb{R}^{d}\right)^{d}}^{2} \right).$$

Let us prove that $||r_{\varepsilon}(0, \cdot)||^{2}_{L^{2}(\mathbb{R}^{d})}$ is bounded. First of all, using the definition of r_{ε} , we have

$$r_{\varepsilon}(0,x) = \varepsilon^{-1} \left(u_{\varepsilon}(0,x) - u_{0}(0,x) - \varepsilon u_{1}\left(0,x,\frac{x}{\varepsilon}\right) \right)$$
$$= -u_{1}\left(0,x,\frac{x}{\varepsilon}\right)$$
$$= -\sum_{i=1}^{d} \frac{\partial u^{0}}{\partial x_{i}}(x)w_{i}\left(\frac{x}{\varepsilon}\right).$$

Since the gradient of the initial value u^0 is assumed to be bounded in $L^2(\mathbb{R}^d)^d$ and the functions w_i are bounded in $L^{\infty}(Y)$, we get

$$\left\|r_{\varepsilon}\left(0,\cdot\right)\right\|_{L^{2}\left(\mathbb{R}^{d}\right)} \leqslant C.$$

Hence:

$$C_{sta} \left\|\nabla r_{\varepsilon}\right\|_{L^{2}\left((0,t_{1})\times\mathbb{R}^{d}\right)^{d}}^{2} + \rho_{min} \left\|r_{\varepsilon}\left(t_{1},\cdot\right)\right\|_{L^{2}\left(\mathbb{R}^{d}\right)}^{2} - C'$$

$$\leq C\left(\left\|r_{\varepsilon}\right\|_{L^{\infty}\left((0,t_{1}),L^{2}\left(\mathbb{R}^{d}\right)\right)} + \left\|\nabla r_{\varepsilon}\right\|_{L^{2}\left((0,t_{1})\times\mathbb{R}^{d}\right)^{d}}\right), \quad (18)$$

with C', C > 0. The function r_{ε} is in $\mathcal{C}^0((0,T), L^2(\mathbb{R}^d))$ so there exists $T_0 \leq T$ such that

$$\left\| r_{\varepsilon} \left(T_{0}, \cdot \right) \right\|_{L^{2} \left(\mathbb{R}^{d} \right)} = \left\| r_{\varepsilon} \right\|_{L^{\infty} \left((0,T), L^{2} \left(\mathbb{R}^{d} \right) \right)}$$

and in this case:

$$\|r_{\varepsilon}\|_{L^{\infty}\left((0,T_{0}),L^{2}\left(\mathbb{R}^{d}\right)\right)} = \|r_{\varepsilon}\|_{L^{\infty}\left((0,T),L^{2}\left(\mathbb{R}^{d}\right)\right)}.$$

Applying inequality (18) with $t_1 = T_0$ gives:

$$C_{sta} \left\| \nabla r_{\varepsilon} \right\|_{L^{2}\left((0,T_{0})\times\mathbb{R}^{d}\right)^{d}}^{2} + \rho_{min} \left\| r_{\varepsilon} \right\|_{L^{\infty}\left((0,T),L^{2}\left(\mathbb{R}^{d}\right)\right)}^{2} - C'$$
$$\leq C \left(\left\| \nabla r_{\varepsilon} \right\|_{L^{2}\left((0,T_{0})\times\mathbb{R}^{d}\right)^{d}}^{2} + \left\| r_{\varepsilon} \right\|_{L^{\infty}\left((0,T),L^{2}\left(\mathbb{R}^{d}\right)\right)}^{2} \right).$$

Let us now use the following result.

Lemma 4. If X_{ε} is a sequence of positive real numbers, verifying:

$$X_{\varepsilon}^2 - C_1 \leqslant C_2 X_{\varepsilon}, \text{ with } C_1, C_2 \geqslant 0$$
(19)

then, there exists a constant C such that

 $X_{\varepsilon} \leqslant C.$

Thus, using Lemma 4 with $X_{\varepsilon} = \|\nabla r_{\varepsilon}\|_{L^{2}((0,T_{0})\times\mathbb{R}^{d})^{d}} + \|r_{\varepsilon}\|_{L^{\infty}((0,T),L^{2}(\mathbb{R}^{d}))}$, we have:

$$\|\nabla r_{\varepsilon}\|_{L^{2}\left((0,T_{0})\times\mathbb{R}^{d}\right)^{d}}+\|r_{\varepsilon}\|_{L^{\infty}\left((0,T),L^{2}\left(\mathbb{R}^{d}\right)\right)}\leqslant C,$$

which implies

$$\|r_{\varepsilon}\|_{L^{\infty}\left((0,T),L^{2}\left(\mathbb{R}^{d}\right)\right)} \leqslant C.$$
(20)

Using inequality (18) with $t_1 = T$ and the fact that $||r_{\varepsilon}||_{L^{\infty}((0,T),L^2(\mathbb{R}^d))}$ is bounded, we deduce from (18) that:

$$C_{sta} \left\| \nabla r_{\varepsilon} \right\|_{L^{2}\left((0,T) \times \mathbb{R}^{d}\right)^{d}}^{2} + 0 - C' \leqslant C \left(\left\| \nabla r_{\varepsilon} \right\|_{L^{2}\left((0,T) \times \mathbb{R}^{d}\right)^{d}}^{2} + C \right)$$

A new application of Lemma 4 with $X_{\varepsilon} = \|\nabla r_{\varepsilon}\|_{L^{2}((0,T)\times\mathbb{R}^{d})^{d}}$ gives:

$$\left\|\nabla r_{\varepsilon}\right\|_{L^{2}\left((0,T)\times\mathbb{R}^{d}\right)^{d}} \leqslant C.$$
(21)

Gathering equations (20) and (21), we finally obtain

$$\|\nabla r_{\varepsilon}\|_{L^{2}\left((0,T)\times\mathbb{R}^{d}\right)^{d}}+\|r_{\varepsilon}\|_{L^{\infty}\left((0,T),L^{2}\left(\mathbb{R}^{d}\right)\right)}\leqslant C.$$

4 A new multiscale finite element method

In this section, we again consider problem (3) defined on Ω . The domain is assumed to be a rectangular cuboid: $\Omega = \prod_{i=1}^{d} (0, l_i)$, so that periodic boundary conditions can be set on the boundary of the domain $\partial \Omega$. Our problem consists in finding a solution u_{ε} to

$$\begin{cases} \rho^{\varepsilon}(x) \partial_{t} u_{\varepsilon} + \frac{1}{\varepsilon} b^{\varepsilon}(x) \cdot \nabla u_{\varepsilon} - \operatorname{div} \left(A^{\varepsilon}(x) \nabla u_{\varepsilon} \right) = 0 \quad \text{in } \Omega \times (0, T) \\ u_{\varepsilon}(0, x) = u^{0}(x) \quad \text{in } \Omega, \end{cases}$$
(22)

where $\varepsilon > 0$ and ρ^{ε} , b^{ε} , A^{ε} and u^{0} are Ω -periodic functions. Here A^{ε} and b^{ε} are not assumed to be ε -periodic functions. However, A^{ε} is assumed to be bounded and coercive, b^{ε} is assumed to be bounded and div $(b^{\varepsilon}) = 0$. We denote by $H^{1}_{\#}(\Omega)$ the set of the Ω -periodic functions of $H^{1}(\Omega)$.

4.1 Idea of the method

As suggested in [18], we introduce oscillating test functions \hat{w}_i^{ε} which stand for $x_i + \varepsilon w_i\left(\frac{x}{\varepsilon}\right)$, each $w_i\left(\frac{x}{\varepsilon}\right)$ being the solution of equation (11). With this definition, we have

$$\nabla \widehat{w}_i^{\varepsilon}(x) = e_i + \left(\nabla_y w_i\right) \left(\frac{x}{\varepsilon}\right).$$

Since $\operatorname{div}_y = \varepsilon \operatorname{div}$, equation (11) becomes:

$$b\left(\frac{x}{\varepsilon}\right) \cdot \nabla \widehat{w}_{i}^{\varepsilon}(x) - \varepsilon \operatorname{div}\left(A\left(\frac{x}{\varepsilon}\right) \nabla \widehat{w}_{i}^{\varepsilon}(x)\right) = \rho\left(\frac{x}{\varepsilon}\right) b^{*} \cdot e_{i}.$$

Thus, each $\widehat{w}_i^{\varepsilon}$ is the ε -periodic solution to:

$$\frac{1}{\varepsilon}b\left(\frac{x}{\varepsilon}\right)\cdot\nabla\widehat{w}_{i}^{\varepsilon} - \operatorname{div}\left(A\left(\frac{x}{\varepsilon}\right)\nabla\widehat{w}_{i}^{\varepsilon}\right) = \frac{1}{\varepsilon}\rho\left(\frac{x}{\varepsilon}\right)b^{*}\cdot e_{i} \quad \text{in } \varepsilon Y.$$
(23)

Using approximation (16), u_{ε} verifies

$$u_{\varepsilon}(t,x) \approx u\left(t, x - \frac{b^*t}{\varepsilon}\right) + \sum_{i=1}^{d} \left(\widehat{w}_i^{\varepsilon}(x) - x_i\right) \frac{\partial u}{\partial x_i} \left(t, x - \frac{b^*t}{\varepsilon}\right)$$

Here, one important point is to notice that the right hand side of this approximation is a first order Taylor expansion with respect to the space variable. Thus, equivalently, we have:

$$u_{\varepsilon}(t,x) \approx u\left(t, \widehat{w}^{\varepsilon}(x) - \frac{b^{*}t}{\varepsilon}\right).$$

If we set

$$\tilde{u}(t,x) = u\left(t, x + \frac{b^*t}{\varepsilon}\right),$$

we have

$$u\left(t,\widehat{w}^{\varepsilon}\left(x\right)-\frac{b^{*}t}{\varepsilon}\right)=\widetilde{u}(t,\widehat{w}^{\varepsilon}(x))$$

and the previous approximation can be rewritten as:

$$u_{\varepsilon}(t,x) \approx \tilde{u}(t,\cdot) \circ \hat{w}^{\varepsilon}(x).$$
(24)

The multiscale method presented in this paper is based on this approximation and a set of multiscale basis functions is built following this idea of composition. We detail this new numerical scheme in the next section.

4.2 Discretization

Let \mathcal{K}_H be a mesh of resolution H with $\overline{\Omega} = \bigcup_{K \in \mathcal{K}_H} \overline{K}$. In the following, \mathcal{K}_H will be referred to as the *coarse mesh*. On each coarse cell $K \in \mathcal{K}_H$, we define the functions $\tilde{w}_i^{\varepsilon, K}$ by:

$$\begin{cases} \frac{1}{\varepsilon}b^{\varepsilon}(x)\cdot\nabla\tilde{w}_{i}^{\varepsilon,K} - \operatorname{div}\left(A^{\varepsilon}\left(x\right)\nabla\tilde{w}_{i}^{\varepsilon,K}\right) = \frac{1}{\varepsilon}\rho^{\varepsilon}(x)b_{K}^{*}\cdot e_{i} \quad \text{in } K,\\ \tilde{w}_{i}^{\varepsilon,K} = x_{i} \quad \text{on } \partial K, \end{cases}$$
(25)

where

$$b_K^* = \frac{\int_K b^\varepsilon(x) dx}{\int_K \rho^\varepsilon(x) dx}.$$

In practice, equation (25) is solved, on each cell K, using a finite element method on a local fine mesh of resolution $h \ll H$. A function $w_i^{\varepsilon,H}$ is then defined on Ω by gathering all functions $\tilde{w}_i^{\varepsilon,K}$ of each cell K. Defining the operator $D_{t,x}^{\varepsilon} = \partial_t + \frac{1}{\varepsilon} b^*(x) \cdot \nabla$, Problem (22) can be rewritten in the form: $\forall v \in H^1_{\#}(\Omega)$,

$$\begin{split} \int_{\Omega} \rho^{\varepsilon}(x) D_{t,x}^{\varepsilon} \left(\tilde{u}\left(t,\cdot\right) \circ w^{\varepsilon,H}(x) \right) \left(v \circ w^{\varepsilon,H} \right)(x) dx \\ &+ \int_{\Omega} \left(A^{\varepsilon}(x) \nabla \left(\tilde{u}\left(t,\cdot\right) \circ w^{\varepsilon,H}(x) \right) \cdot \nabla \left(v \circ w^{\varepsilon,H} \right)(x) \right. \\ &+ \frac{1}{\varepsilon} \left(b^{\varepsilon}(x) - \rho^{\varepsilon}(x) b^{*}(x) \right) \cdot \nabla \left(\tilde{u}\left(t,\cdot\right) \circ w^{\varepsilon,H}(x) \right) \left(v \circ w^{\varepsilon,H} \right)(x) \right) dx = 0. \end{split}$$

4.2.1 Time discretization

We now use the characteristic-Galerkin method, presented in [19], to compute the time derivative. This method introduces, for each time t^{n+1} , a function χ which satisfies the ordinary differential equation:

$$\frac{d}{dt}\chi(t) = \frac{1}{\varepsilon}b^*\left(\chi(t)\right), \ \chi\left(t^{n+1}\right) = x.$$

This definition implies

$$\frac{\partial}{\partial t} \left(\tilde{u} \left(t, w^{\varepsilon, H} \circ \chi(t) \right) \right) \left(t^{n+1} \right) = D_{t, x}^{\varepsilon} \left(\tilde{u} \left(t, w^{\varepsilon, H}(x) \right) \right) \left(t^{n+1}, x \right).$$

Then, we compute a function X^n defined by

$$X^{n}(x) = \chi \left(t^{n+1} - \delta t \right).$$

Having introduced this time discretization, the problem now consists in finding a solution $u^{n+1} \in H^1_{\#}(\Omega)$ such that for all $v \in H^1_{\#}(\Omega)$:

$$\int_{\Omega} \rho^{\varepsilon}(x) \frac{u^{n+1} \circ w^{\varepsilon,H}(x) - u^{n} \circ w^{\varepsilon,H} \circ X^{n}(x)}{\delta t} v \circ w^{\varepsilon,H}(x) dx + \int_{\Omega} \left(A^{\varepsilon}(x) \nabla \left(u^{n+1} \circ w^{\varepsilon,H} \right) (x) \cdot \nabla \left(v \circ w^{\varepsilon,H} \right) (x) \right) dx = 0. \quad (26)$$
$$+ \frac{1}{\varepsilon} \left(b^{\varepsilon}(x) - \rho^{\varepsilon}(x) b^{*}(x) \right) \cdot \nabla \left(u^{n+1} \circ w^{\varepsilon,H} \right) (x) \left(v \circ w^{\varepsilon,H} \right) (x) \right) dx = 0. \quad (26)$$

This method is unconditionally stable, which means that there is no restriction on the value of the time step δt . However, when $\chi (t^{n+1} - \delta t)$ does not belong to the domain Ω , its value cannot be properly defined. In the general case, one often assigns the boundary value to $\chi (t^{n+1} - \delta t)$. Here, since periodic boundary conditions are imposed, we use, for one side of the domain, the value available on the opposite one. There is therefore no constraint on the value of δt .

4.2.2 Definition of the multiscale finite element space

Let V_H be a linear subspace of $H^1_{\#}(\Omega)$ associated to the coarse mesh \mathcal{K}_H , D_H the dimension of this space i.e. the number of degrees of freedom, $(\Phi_l^H)_l$ the set of basis functions of the space V_H . We define a new space $V_{\varepsilon,H}$ generated by the multiscale basis functions:

$$\Phi_l^{\varepsilon,H} = \Phi_l^H \circ w^{\varepsilon,H}, \quad l = 1, \dots, D_H$$

where we will compute our approximation of u_{ε} . The variational formulation (26) then amounts to finding $u_{\varepsilon,H}^{n+1} \in V_{\varepsilon,H}$ such that $\forall v_{\varepsilon,H} \in V_{\varepsilon,H}$:

$$\int_{\Omega} \rho^{\varepsilon}(x) \frac{u_{\varepsilon,H}^{n+1}(x) - u_{\varepsilon,H}^{n} \circ X^{n}(x)}{\delta t} v_{\varepsilon,H}(x) dx + \int_{\Omega} \left(A^{\varepsilon}(x) \nabla u_{\varepsilon,H}^{n+1}(x) \cdot \nabla v_{\varepsilon,H}(x) + \frac{1}{\varepsilon} \left(b^{\varepsilon}(x) - \rho^{\varepsilon}(x) b^{*}(x) \right) \cdot \nabla u_{\varepsilon,H}^{n+1}(x) v_{\varepsilon,H}(x) \right) dx = 0.$$
 (27)

4.3 Building the global system

Since

$$u_{\varepsilon,H}^n(x) = \sum_{i=1}^{D_H} u_i^n \Phi_i^{\varepsilon,H}(x),$$
(28)

testing equation (27) with each basis function $\Phi_i^{\varepsilon,H}$ leads to a system of D_H equations, with, for each $i = 1, \ldots, D_H$:

$$\begin{split} &\sum_{j=1}^{D_H} \int_{\Omega} \bigg(\frac{u_j^{n+1}}{\delta t} \rho^{\varepsilon}(x) \Phi_j^{\varepsilon,H}(x) \Phi_i^{\varepsilon,H}(x) - \frac{u_j^n}{\delta t} \rho^{\varepsilon}(x) \Phi_j^{\varepsilon,H} \circ X^n(x) \Phi_i^{\varepsilon,H}(x) \\ &+ u_j^{n+1} A^{\varepsilon}(x) \nabla \Phi_j^{\varepsilon,H}(x) \cdot \nabla \Phi_i^{\varepsilon,H}(x) + u_j^{n+1} \frac{1}{\varepsilon} \left(b^{\varepsilon}(x) - \rho^{\varepsilon}(x) b^*(x) \right) \cdot \nabla \Phi_j^{\varepsilon,H}(x) \Phi_i^{\varepsilon,H}(x) \bigg) dx = 0. \end{split}$$

As shown previously, u is a good zero-order approximation of u_{ε} in the L^2 -norm but not in the H^1 -norm. Similarly, Φ_i is a good zero-order approximation of $\Phi_i^{\varepsilon,H}(x)$ in the L^2 -norm. Therefore, when its gradient is not involved, the function $\Phi_i^{\varepsilon,H}(x)$ is replaced by Φ_i . As a result, for all $i = 1, \ldots, D_H$, the system to solve is:

$$\begin{split} \sum_{j=1}^{D_H} u_j^{n+1} \bigg(\int_{\Omega} \bigg(\rho^{\varepsilon}(x) \Phi_i(x) \Phi_j(x) + \delta t A^{\varepsilon}(x) \nabla \Phi_i^{\varepsilon,H}(x) \cdot \nabla \Phi_j^{\varepsilon,H}(x) \\ &+ \frac{\delta t}{\varepsilon} \left(b^{\varepsilon}(x) - \rho^{\varepsilon}(x) b^*(x) \right) \cdot \nabla \Phi_j^{\varepsilon,H}(x) \Phi_i^{\varepsilon,H}(x) \bigg) dx \bigg) \\ &= \sum_{j=1}^{D_H} u_j^n \int_{\Omega} \rho^{\varepsilon}(x) \Phi_j \circ X^n(x) \Phi_i(x) dx. \end{split}$$

This system can be rewritten in matrix form as

$$RU^{n+1} = F^n, (29)$$

with

$$\begin{split} U^{n+1} \in \mathbb{R}^{D_H}, \quad U^{n+1}_i &= u^{n+1}_i, \\ R \in \mathbb{R}^{D_H \times D_H}, \quad R_{i,j} &= \int_{\Omega} \left(\rho^{\varepsilon}(x) \Phi_i(x) \Phi_j(x) + \delta t A^{\varepsilon}(x) \nabla \Phi_i^{\varepsilon,H}(x) \cdot \nabla \Phi_j^{\varepsilon,H}(x) \right) \\ &\quad + \frac{\delta t}{\varepsilon} \left(b^{\varepsilon}(x) - \rho^{\varepsilon}(x) b^*(x) \right) \cdot \nabla \Phi_j^{\varepsilon,H}(x) \Phi_i^{\varepsilon,H}(x) \right) dx, \\ F^n \in \mathbb{R}^{D_H}, \qquad F^n_i &= \sum_{j=1}^{D_H} u^n_j \int_{\Omega} \rho^{\varepsilon}(x) \Phi_j \circ X^n(x) \Phi_i(x) dx. \end{split}$$

The computation of the basis functions and the resolution of system (29) was implemented using the finite-element platform FreeFem++ [20]. This implementation is presented in the next section.

Remark 2: In [10], P. Henning and M. Ohlberger apply a Heterogeneous Multiscale Method to the case presented in this paper. This method computes u_H^n an approximation of $u(t^n, x)$ solution to equation (13) at time t^n , whereas our method computes an approximation of the reconstructed solution:

$$u\left(t^n, x - \frac{b^*t^n}{\varepsilon}\right) + \varepsilon u_1\left(t^n, x - \frac{b^*t^n}{\varepsilon}, \frac{x}{\varepsilon}\right).$$

According to theorems 1 and 2, this second approximation is more precise than the first one. Note also that u_H^n is computed using moving coordinates.

In [10], u_H^n is defined as the solution of

$$\left(u_{H}^{n},\Phi_{H}\right)_{L^{2}\left(\mathbb{R}^{d}\right)}=\left(u_{H}^{n+1},\Phi_{H}\right)_{L^{2}\left(\mathbb{R}^{d}\right)}+\Delta tA_{H}\left(u_{H}^{n+1},\Phi_{H}\right),$$

where $(\cdot, \cdot)_{L^2(\mathbb{R}^d)}$ is the usual scalar product in $L^2(\mathbb{R}^d)$ and A_H represents the homogenized operator. In the non-periodic case, A_H is not uniform and needs to be computed on each coarse cell by solving local problems. Nevertheless, a change of variable is required to be in the same coordinates system as u_H^n . To avoid this change of variable, the properties A^{ε} , b^{ε} and ρ^{ε} are assumed to only depend on the micro-scale.

In our approach, the multiscale solution is in the same coordinates system as the solution u_{ε} . As a result, no change of variable is necessary and the coarse scale variations of the properties can be taken into account.

5 Application case

Let us consider the domain $\Omega = (0, 1)^2$. The initial condition u^0 is depicted in figure 1(a). It is a piecewise linear function which is equal to 1 on the central node of the coarse mesh and to 0 on the other nodes. As mentioned before, periodic boundary conditions are imposed on $\partial\Omega$. The parameters of the problem were chosen in the following way:

•
$$\varepsilon = \frac{1}{200}$$
,



Figure 1: On the left, the initial condition over the whole domain. On the right, two periods of the x-component of the velocity field b^{ε} .



Figure 2: Cell problem solution obtained using a \mathbb{P}_1 -Lagrange method.

•
$$b^{\varepsilon}(x) = \begin{pmatrix} -\delta \sin\left(\frac{2\pi x}{\varepsilon}\right) \cos\left(\frac{2\pi y}{\varepsilon}\right) + b_x^0 \\ \delta \cos\left(\frac{2\pi x}{\varepsilon}\right) \sin\left(\frac{2\pi y}{\varepsilon}\right) + b_y^0 \end{pmatrix}$$
, with $\delta = 100$ and $b_x^0 = b_y^0 = 1$,

```
• A = 1.
```

Intentionally, we chose a high value for δ in order to highlight the effective diffusion created by the velocity field. Two periods of the horizontal component of the velocity are represented in figure 1(b).

The coarse mesh is composed of 800 triangles of size $H = \frac{1}{20} = 10\varepsilon$. Each coarse cell is composed of 5000 fine triangles of size $h = \frac{1}{1000} = \frac{\varepsilon}{5}$. Note that our method can avoid generating the whole fine mesh. In this case, this mesh would contain 4000000 triangles.

Figures 5 and 6 show the solutions obtained at time $t = 1.8 \times 10^{-3}$.

5.1 Cell problem resolution

The cell problem (25) features a large convection term which requires a special numerical treatment. Indeed, if simple \mathbb{P}_1 -Lagrange finite elements are used, then numerical instabilities appear (figure 2). In order to avoid these instabilities, we introduce the following non-stationary



Figure 3: Solution of the cell problem (25) obtained using a transient approach.

problem:

$$\begin{cases} \partial_t w_i^{t,\varepsilon,K} + \frac{1}{\varepsilon} b^{\varepsilon}(x) \cdot \nabla w_i^{t,\varepsilon,K} - \operatorname{div} \left(A^{\varepsilon}(x) \nabla w_i^{t,\varepsilon,K} \right) = \frac{1}{\varepsilon} \rho^{\varepsilon}(x) b_K^* \cdot e_i \text{ in } K, \\ w_i^{t,\varepsilon,K} = x_i \text{ on } \partial K. \end{cases}$$
(30)

Using a fixed time step δt_0 satisfying the CFL condition:

$$\delta t_0 \leqslant \frac{\varepsilon h}{b_{max}^{\varepsilon}},$$

where $b_{max}^{\varepsilon} = \|b^{\varepsilon}\|_{\infty}$. Equation (30) is solved until a stationary solution is obtained. More precisely, we iterate until a time t_0 is reached for which

$$\frac{\left\|w_{i}^{t_{0},\varepsilon,K}-w_{i}^{t_{0}+\delta t_{0},\varepsilon,K}\right\|_{L^{2}(\Omega)}}{\delta t_{0}\left\|w_{i}^{t_{0},\varepsilon,K}\right\|_{L^{2}(\Omega)}} < \eta$$

where η is a threshold equal to 0.01 in our case. The solution $w_i^{t_0,\varepsilon,K}$ is then taken as solution to cell problem (25). Figure 3 shows the solution computed with this algorithm with $\eta = 0.01$. We can observe that we obtain a more stable solution.

This algorithm still requires a high number of iterations. For the case introduced in the previous paragraph, the solution is reached after 2000 iterations with $\eta = 0.01$ on each coarse cell. However, the basis functions being time-invariant, these resolutions only need to be done once.

5.2 Visualization of the solution

The matrix R and the right hand side F^n in equation (29) are completed after each resolution of cell problem (25). Once this system is solved on the coarse mesh, the multiscale solution is computed using (28).

Since the basis functions $\Phi_i^{\varepsilon,H}$ are defined on local fine meshes, plotting $u_{\varepsilon,H}^n$ would require to build the whole fine mesh. To avoid that, a reconstruction of the solution at the fine scale is only done on a particular area of the domain, involving a limited number of basis functions. Outside this area, and only for visualization purposes, we replace $\Phi_i^{\varepsilon,H}$ by Φ_i^H . For example, figure 4 shows the difference between a classical basis function and a multiscale basis function. These functions are plotted on a local fine mesh corresponding to the support of the basis functions.

Figure 5(b) shows the *coarse multiscale solution* for which all basis functions $\Phi_i^{\varepsilon,H}$ are replaced by Φ_i^H . In figure 6(b), a few basis functions $\Phi_i^{\varepsilon,H}$ are used. This solution will be referred to as the *partially refined multiscale solution*.



Figure 4: A coarse basis function (Φ_i^H) and the corresponding multiscale basis function $(\Phi_i^{\varepsilon,H})$ represented on their support.

5.3 Analysis of the results in the periodic case

In the following, the *coarse solution* will stand for the solution to the convection-diffusion problem with constant velocity $\frac{1}{c}b^*$ and diffusivity A.

Since this practical case features ε -periodic coefficients, the multiscale solution can be directly compared to the *homogenized solution* \tilde{u}^n , defined by

$$\tilde{u}^n = u^n \left(x - \frac{b^* t^n}{\varepsilon} \right),$$

where u^n is the solution of the homogenized equation (13) at time $t^n = n\delta t$. This function is represented in figure 5(c). The matrix A^* obtained in this case is:

$$A^* = \left(\begin{array}{rrr} 4.30702 & 0.0132418\\ 0.0132418 & 4.30702 \end{array}\right)$$

In fact, the homogenized coefficient A^* includes an additional diffusion induced by the velocity through the functions w (see equations (14) and (11)). This phenomenon, known as Taylor dispersion, can be observed in figure 5(c): the solution of the homogenized problem is more diffusive than in figure 5(a) where the transport problem was simulated with the velocity $\frac{1}{\varepsilon}b^*$ and the diffusivity A. We notice that the coarse multiscale solution, depicted in figure 5(b), is also able to reproduce this coarse scale diffusion. The multiscale method does not compute explicitly the homogenized coefficient A^* but the use of the basis functions $\Phi_i^{\varepsilon,H}$ allows us to reproduce the Taylor dispersion at the macro scale.

Moreover, using equation (24), we saw that a better approximation of the exact solution is given by

$$\tilde{u}_T^n = u^n \left(x - \frac{b^* t^n}{\varepsilon} + \varepsilon w \left(\frac{x}{\varepsilon} \right) \right).$$

This function is used to improve locally the approximation \tilde{u}^n and will be called the *partially* refined homogenized solution (figure 6(a)). In order to see the refinements more clearly, figures 6(a) and 6(b) only feature a part of the mesh (12 coarse cells in the direction x and 9 coarse cells in the direction y). Figure 6(c) shows the fine scale oscillations of the multiscale solution.



Figure 5: Comparison over the whole domain between the coarse solution, the coarse multiscale solution and the homogenized solution \tilde{u}^n .



(a) Partially refined homogenized so- (b) Partially refined multiscale solu- (c) Zoom on the multiscale solution lution

Figure 6: Comparison over a part of the domain between the partially refined multiscale solution and the partially refined homogenized solution. On the right, a zoom is made on the pink area represented in 6(b).

REFERENCES

- [1] T.Y. Hou and X.H. Wu. A multiscale finite element method for elliptic problems in composite materials and porous media. *J. Comput. Phys.*, 134(1):169-189, 1997.
- [2] A. Bensoussan, J.L. Lions, and G. Papanicolaou. *Asymptotic analysis for periodic structures*. North Holland, 1978.
- [3] E. Sanchez-Palencia. *Non-homogeneous media and vibration theory*. Springer-Verlag, 1980.
- [4] V.V. Zhikov, S.M. Kozlov, and O.A. Oleinik. *Homogenization of differential operators and integral functionals*. Springer-Verlag, 1994.
- [5] T. Arbogast. Numerical subgrid upscaling of two-phase flow in porous media. In Numerical Treatment of Multiphase Flows in Porous Media, volume 552 of Lecture Notes in Physics, pages 35-49. Springer, 2000.
- [6] A.M. Matache, I. Babuška, and C. Schwab. Generalized p-fem in homogenization. *Numer. Math.*, 86(2) :319-375, 2000.
- [7] W. E and B. Engquist. The heterogeneous multiscale methods. *Comm. Math. Sci.*, 1(1) :87-132, 2003.
- [8] Y. Efendiev and T.Y. Hou. *Multiscale finite element methods : theory and applications*. Springer-Verlag, 2009.
- [9] T.Y. Hou and D. Liang. Multiscale analysis for convection dominated transport equations. *DCDS*, 23(1-2) :281-298, 2009.
- [10] P. Henning and M. Ohlberger. The heterogeneous multiscale finite element method for advection-diffusion problems with rapidly oscillating coefficients and large expected drift. *Netw. Heterog. Media*, 5(4):711-744, 2010.
- [11] G. Allaire and A.L. Raphael. Homogenization of a convection-diffusion model with reaction in a porous medium. *C. R., Math., Acad. Sci. Paris*, 344(8):523-528, 2007.
- [12] P. Donato and A. Piatnitski. Averaging of nonstationary parabolic operators with large lower order terms. *Math. Sci. Appl.*, 24 :153-165, 2005.
- [13] G. Allaire, R. Brizzi, A. Mikelić, and A.L. Piatnitski. Two-scale expansion with drift approach to the Taylor dispersion for reactive transport through porous media. *Chem. Eng. Sci.*, 65(7) :2292-2300, 2010.
- [14] G. C. Papanicolaou, Diffusion in random media. Surv. Appl. Math., 1:205-253, 1995.
- [15] E. Marušić-Paloka and A.L. Piatnitski. Homogenization of a nonlinear convectiondiffusion equation with rapidly oscillating coefficients and strong convection, J. London Math. Soc., 72(2) :391-409, 2005.
- [16] G. Allaire, A. Mikelić and A. Piatnitski, Homogenization approach to the dispersion theory for reactive transport through porous media. *SIAM J. Math. Anal.*, 42(1) :125-144, 2010.

- [17] G. Allaire and M. Amar. Boundary Layer tails in periodic homogenization, *COCV*, 4(1) :209-243, 1999.
- [18] G. Allaire and R. Brizzi. A multiscale finite element method for numerical homogenization. *Multiscale Modeling and Simulation*, 4(3):125-144, 2006.
- [19] O. Pironneau, J. Liou, and T. Tezduyar. Characteristic-galerkin and galerkin/least-squares space-time formulations for the advection-diffusion equation with time-dependent domains, *Comput. Methods Appl. Mech. Eng.*, 100(1):117-141, 1992.
- [20] F. Hecht, O. Pironneau, A. Le Hyaric, and K. Ohtsuka. *Freefem++*. Laboratoire J.-L. Lions, University of Paris VI, France, 1998.