

MULTISCALE METHODS FOR ADVECTION-DIFFUSION PROBLEMS

ASSYR ABDULLE

Mathematics Department
University of Basel
Rheinsprung 21
CH-4051 Switzerland

Abstract. The development of numerical methods for multiscale advection-diffusion problems presents a number of challenges. The fine-scale structures may significantly influence the coarser properties of the system, but are often impossible to solve in full details. The time integration of the evolution system is stiff due to the diffusion term and its stability properties have to be taken into account for its resolution. We discuss in this paper an algorithm, which combines Heterogeneous Multiscale Methods (HMM) with Orthogonal Runge-Kutta Chebyshev (ROCK) methods, for the efficient numerical resolution of multiscale advection-diffusion problems.

1. Introduction. A broad range of scientific problems involve multi-scale phenomena. We face multi-scale problems when studying for example the flow and contaminant transport through aquifers in hydromecanic and ground water modeling, heat and mass transport in chemical engineering, filtration processes and transport of fluids and chemicals in lungs and other organs in biomedical engineering, to mention but a few.

Let $\Omega \in \mathbb{R}^d$, $d = 2, 3$ be an open and bounded domain and $I = [t_0, T]$ a time interval. We consider the following advection-diffusion problem, describing the transport of a scalar quantity $c(t, x)$ immersed in a flow $v(x)$:

$$\frac{\partial c}{\partial t}(t, x) = -\nabla \cdot (v(x)c(t, x)) + \nabla \cdot (D\nabla c(t, x)) + g(t, x), \quad (t, x) \in I \times \Omega \quad (1)$$

$$c(t_0, x) = \bar{c}(x), \quad x \in \Omega, \quad (2)$$

together with suitable boundary conditions, where $g(t, x)$ is a source term and D is a diffusivity tensor which we suppose, for simplicity, to be a positive constant. The flow field $v(x)$ is determined by Darcy's Law

$$v(x) = -a(x)\nabla u(x), \quad (3)$$

(or a generalized form of it), where $u(x)$ is given by an elliptic equation

$$-\nabla \cdot (a(x)\nabla u(x)) = f, \quad (4)$$

together with suitable boundary conditions, where $a(x)$ represents the conductivity of the medium.

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The multiscale nature of the problems (1)–(4) comes from the fact that in many situations, the conductivity $a(x)$ exhibits (at least) two scales of variation: a macro length scale, characteristic scale at which the transport behavior is observed and a micro length scale due to the microstructures of the medium. We denote by ε the typical length of the micro scale (representing for example a characteristic self-similar structure). The multiscale nature of the conductivity will induce a multiscale behavior of the velocity field and the concentration. In the sequel, we will add a superscript to these quantities $c^\varepsilon, v^\varepsilon$, to emphasize their dependence on ε .

Solving numerically the details of equations such as (1) and (4) is often impossible due to the amount of work needed. On the other hand, eliminating the small scales involved in the problem can lead to very inaccurate descriptions for practical applications.

In this paper we propose two algorithms to compute the fine scale advection-diffusion equation and an upscaled (homogenized) version of it, respectively. These algorithms are based on numerically reconstructed and upscaled velocity fields, and on a combination of the Finite Element Heterogeneous Multiscale Method (FE-HMM) for elliptic problems and Orthogonal Runge-Kutta Chebyshev methods (ROCK) for stiff ordinary differential equations (ODEs). The paper is organized as follows. In section 2 we briefly recall the homogenization theory for advection-diffusion equations and we recall the ROCK and the FE-HMM methods. In section 3 we propose an algorithm to compute the fine scale solution of problems (1-4) as well well an algorithm to compute an upscaled version of it. A priori error estimates are given. We close with numerical examples illustrating the proposed method.

2. Homogenization of transport equation. A goal in upscaling and homogenization strategies is to obtain effective equations of motion, at large scales and long times, for the *mean* passive scalar density or the *mean* velocity field. Homogenization was first developed as an analytical tool to derive macroscopic models and effective coefficients for partial differential equations with rapidly varying coefficients and was pioneered by DeGiorgi, Spagnolo, Babuska, Bensoussan, Lions and Papanicolaou (see [8] and the references therein). For advection-diffusion equations, the most studied case is when the velocity field is divergence free, i.e., $\nabla \cdot v = 0$, that is, $f = 0$ in (3). In this case problem (1) reads

$$\frac{\partial c}{\partial t} = -v \nabla c + D \nabla^2 c, \quad (5)$$

where we set $g(t, x) = 0$ for simplicity. Among the large literature on the subject we cite the review [14] and the references therein. For non-divergence free velocity field, we refer to [13] and the reference therein for recent progress.

We briefly describe the homogenization procedure for advection-diffusion equations with divergence free velocity field. We suppose that there are two typical length scales in the problem (1): l the typical length of the microscopic variations and L the length scale at which the transport behavior is observed. We define $\varepsilon = l/L$, the ratio between both length scale and study the situation where $l \ll L$. If we write (5) in a non dimensional form (using a parabolic scaling $x/L, tD/L^2$ and writing again x, t for the new variables) the advection-diffusion equation (5) reads

$$\frac{\partial c^\varepsilon}{\partial t} = -Pe_g v^\varepsilon \nabla c^\varepsilon + \nabla^2 c^\varepsilon, \quad (6)$$

where ε emphasizes the dependence on the small scale. Here $Pe_g = VL/D$ is the global (large scale) Peclet number, where V and L are the characteristic macroscopic

velocity and length, respectively. The Peclet number Pe_g sets the diffusion coefficient into relation with the transport velocity and the length scale of the large scale problem. We suppose that $v^\varepsilon = v(x, x/\varepsilon) = v(x, y)$, is 1-periodic with respect to the micro scale (or fast length scale), where $y = x/\varepsilon \in Y = (0, 1)^d$. The velocity field $v^\varepsilon(x) = \bar{v}(x) + \tilde{v}(x)$ is further split into a large scale mean part $\bar{v}(x) := \int_Y v(x, y) dy$ and a fluctuating zero mean part $\tilde{v}(x) := v^\varepsilon(x) - \bar{v}(x)$.

The derivation of the homogenized equation is achieved by assuming a formal asymptotic expansion for the concentration $c^\varepsilon(t, x, y) = c_0(t, x) + \varepsilon c_1(t, x, y) + \varepsilon^2 c_2(t, x, y) + \dots$, in the limit $\varepsilon \rightarrow 0$, where c_0 is the homogenized solution we are looking for (and does thus not depend on the micro scale y) and where we assume that the c_j functions are periodic in the y variable. Inserting the asymptotic expansion for c^ε and the splitted velocity field in (6), taking into account that $\nabla = \nabla_x + (1/\varepsilon)\nabla_y$ and identifying the power of ε , we obtain a cascade of equations. The ε^0 term gives the ‘‘homogenized’’ equation [17],[14],[6]

$$\frac{\partial c_0}{\partial t} = -Pe_g \bar{v} \nabla c_0 + \nabla \cdot D_0 \nabla c_0, \quad (7)$$

where D_0 is the effective diffusion tensor, defined by $D_0 = I + \int_Y Pe_l \tilde{v} \otimes \eta dy$, where the functions $\eta_i, i = 1, \dots, d$ are given by so-called cell problems

$$\nabla_y^2 \eta_i - Pe_l v^\varepsilon \nabla_y \eta_i = Pe_l \tilde{v}_i, \quad (8)$$

where $Pe_l = \varepsilon Pe_g$ is the small scale Peclet number. These problems can either be solved numerically or approximated through a perturbation theory expansion in case of large Peclet number (see [6] and the references therein).

The convergence result $\|c^\varepsilon(t, x) - c_0(t, x)\|_{L^\infty((t_0, T); \mathbb{R}^d)} \leq \varepsilon(C_1 + C_2 T)$ can be obtained (see [14] and the references therein) in case of zero, constant or weak mean flow $\bar{v}(x)$ (by weak mean flow we mean $v^\varepsilon(x) = \varepsilon \bar{v}(x) + \tilde{v}(x)$). It has been partially generalized for strong mean flow in [17]. Observe finally that both, the fine scale model (6) and the homogeneous large scale model (7), need informations on the fine scale fluctuating velocity field.

2.1. ROCK and Heterogeneous Multiscale Methods. In this section we recall the ROCK and HMM methods, which we will use to solve (6) or (7).

2.2. ROCK methods. For solving time dependent partial differential equations of the type (1), a widely used approach is to discretize the space variable by finite differences, leading to a (possibly large) system of ODEs

$$\frac{d}{dt} y(t) = F(t, y(t)), \quad y(t_0) = y_0, \quad (9)$$

where $y \in \mathbb{R}^n$, $F : I \times \mathbb{R}^n \rightarrow \mathbb{R}^n$. The dimension n is related to the space discretization of the spatial domain $\Omega \subset \mathbb{R}^d$ by $n = \mathcal{O}((\Delta x)^{-d})$, where Δx is the meshsize of the finite difference space discretization. For the advection-diffusion equation (1), taking second-order central difference schemes for the discretization of ∇c , $\nabla^2 c$, respectively, gives a system of ODEs with $F(t, y(t)) = Ay(t) + G(t)$, where A is a $n \times n$ matrix and $G(t)$ is a vector in \mathbb{R}^n which contains the discretized source term $g(t, x)$ and may also contains some boundary values. It is known that standard explicit solvers (forward Euler scheme, explicit Runge-Kutta methods for example) will have a restriction on the step size, governed by the largest eigenvalue (in modulus) of A . These eigenvalues are located, for the central discretization of (1), on an ellipse in the left half-plane \mathbb{C}^- and the aforementioned restriction reads

$\tau \leq C(\Delta x)^2$, where τ is the step size of the time integration method. The constant $C > 0$ depends on the spatial dimension and on the diffusion and advection coefficients of the equation (1) and may also depend on the stability properties of the numerical methods. However, for a standard explicit Runge-Kutta scheme, C is almost independent of the method [12]. Such ODEs, originating from the space discretization of (1) are called *stiff* in the literature [12]. It is also known that implicit solver have better stability properties, but at the expense of solving linear systems of dimension $n \times n$, which is costly if n is large.

Chebyshev methods (to which belong the ROCK methods discussed below) are a class of explicit one step methods with extended stability domains along the negative real axis. The basic ideas for such methods go back to the sixties with Saul'ev, Franklin and Guillou & Lago (see the references in [12]), and are the following: chose a sequence of time steps h_1, \dots, h_s with $\tau = h_1 + \dots + h_s$ and define *one step* of the method as the composition of s one step methods $\Psi_\tau = (\Psi_{h_s} \circ \dots \circ \Psi_{h_1})(y_0)$, and denote by $R_s(z) = \prod_{i=1}^s (1 + h_i z)$ its corresponding stability polynomial. Next, given s (called the the stage number), optimize the sequence $\{h_i\}_{i=1}^s$, to achieve

$$|R_s(z)| \leq 1 \text{ for } z \in [-l_s, 0], \quad l_s > 0 \text{ as large as possible.}$$

The solution of this problem is given by $R_s(z) = T_s(1 + z/s^2)$, where $T_s(x)$ are the Chebyshev polynomials, i.e. the optimal sequence of $\{h_i\}_{i=1}^s$ is given by $h_i = -1/z_i$, where z_i are the zeros of $R_s(z)$, and $l_s = 2s^2$. We see that the stability domain increases *quadratically* with the number of stages s , which represent also the numerical work per step. Based solely on stability consideration, if the integration of (9) from $t_0 = 0$ to $t_m = T$ requires N functions evaluation for the forward Euler method it will only need \sqrt{N} functions evaluation for the Chebyshev method.

The above method has order one, which means that after one step of the method $y_1 - y(t_1) = \mathcal{O}(\tau^2)$. Construction of higher order methods, say of order p require higher order stability polynomials, i.e., polynomials $R_s^p(z) - e^z = \mathcal{O}(z^{p+1})$, which remains for a given degree s bounded in the largest interval $[-l_s^p, 0] \subset \mathbb{R}^-$. These “optimal polynomials” are known to exist for all p and s but have no explicit analytic formulas for $p > 1$. Different strategies have been proposed to overcome this difficulty (see [12] and the references therein). Recently, a new strategy to construct higher order Chebyshev methods with “quasi” optimal stability polynomials has been proposed [2],[3]. It is based on the following decomposition of the optimal polynomials proved in [1].

Theorem 1. *The optimal polynomials $R_s^p(z)$ possess exactly p complex zeros if p is even and exactly $p - 1$ complex zeros if p is odd. The remaining real zeros are distinct and are all in the stability interval $[-l_s^p, 0]$.*

As a consequence, the decomposition $R_s^p(z) = w_p(z)P_{s-p}(z)$, holds, where $w_p(z)$ is a polynomial of degree p with p complex zeros (p odd) and $P_{s-p}(z)$ is a polynomial of degree $s - p$ with only real zeros. These polynomials can be approximated by

$$\tilde{R}_s^p(z) = \tilde{w}_p(z)\tilde{P}_{s-p}(z),$$

with $\tilde{R}_s^p(z) - e^z = \mathcal{O}(z^{p+1})$ and where $\tilde{P}_{s-p}(z)$ is an orthogonal polynomial with respect to the weight function $\tilde{w}_p(z)^2/(\sqrt{1-z^2})$ (see [2],[3]). For a given s , we consider also the orthogonal polynomials $\tilde{P}_j(z)$ ($j = 1, \dots, s-p$) associated with the same weight function. These polynomials possess a three-term recurrence relation

$$\tilde{P}_j(z) = (\mu_j z - \nu_j)\tilde{P}_{j-1}(z) - \kappa_j\tilde{P}_{j-2}(z), \quad j = 1, \dots, s-p, \quad (10)$$

which can be used to define a $s - p$ stages numerical method ψ^{s-p} . The remaining p stages are constructed as to have $\tilde{w}_p(z)$ as stability function and such that $\Psi = \psi^p \circ \psi^{s-p}$ is of order p . The methods ROCK2 and ROCK4 for $p = 2$ and $p = 4$, respectively, are implemented in the following way [2],[3]:

1. Compute the spectral radius of the Jacobian.
2. Determine an s-stage formula to satisfy the stability requirement.
3. Compute an integration step.
4. Determine the error (with an embedded method) and a new step size.

The codes ROCK2-4 are available at <http://www.math.unibas.ch/~abdulle/> and we refer to [2],[3] for numerical experiments, and comparison with other methods.

2.3. Heterogeneous Multiscale Methods. In order to obtain the mean and the fine scale fluctuating velocity fields \bar{v} and \tilde{v} , respectively, we need to compute the elliptic equation (4). We will discuss the solution of (4) in the case of periodically oscillating coefficients, but we emphasize that the method presented below is also applicable in the *non-periodic case* [4],[15]. We consider

$$-\nabla \cdot (a^\varepsilon \nabla u^\varepsilon) = f \text{ in } \Omega, \quad u^\varepsilon = 0 \text{ on } \partial\Omega, \quad (11)$$

where we assume that the tensor $a^\varepsilon(x) = a(x, \frac{x}{\varepsilon}) = a(x, y)$ is symmetric, coercive and periodic with respect to each component of y in the unit cube $Y = (0, 1)^d$. For simplicity we take zero Dirichlet boundary conditions. We further assume that $f \in L^2(\Omega)$, $a_{ij}(x, \cdot) \in L^\infty(\mathbb{R}^d)$, that $x \rightarrow a_{ij}(x, \cdot)$ is smooth from $\bar{\Omega} \rightarrow L^\infty(\mathbb{R}^d)$ and that $\Omega \subset \mathbb{R}^d$ is a convex polygon. As for the advection-diffusion, (11) can be homogenized and it is known (see e.g. [8, Chap.1]) that u^ε converges (usually in a weak sense) to a ‘‘homogenized solution’’ u^0 , which solves the homogenized problem

$$-\nabla \cdot (a^0(x) \nabla u^0) = f(x) \in \Omega, \quad u^0 = 0 \quad \text{on } \partial\Omega, \quad (12)$$

where the homogenized diffusion tensor a^0 is smooth and coercive with coefficients given by $a_{ij}^0(x) = \int_Y \left(a_{ij}(x, y) + \sum_{l=1}^d a_{il}(x, y) \frac{\partial \chi^j}{\partial y_l}(x, y) \right) dy$, and where $\chi^j(x, y)$, $j = 1, \dots, d$ are the (unique) solutions of the cell problems

$$\int_Y \nabla \chi^j a(x, y) (\nabla z)^T dy = - \int_Y e_j^T a(x, y) (\nabla z)^T dy, \quad \forall z \in W_{per}^1(Y), \quad (13)$$

where $Y = (0, 1)^d$ and $\{e_j\}_{j=1}^d$ is the standard basis of \mathbb{R}^d and $W_{per}^1(Y) = \{v \in H_{per}^1(Y); \int_Y v dx = 0\}$, where $H_{per}^1(Y)$ is defined as the closure of $C_{per}^\infty(Y)$ (the subset of $C^\infty(\mathbb{R}^d)$ of periodic functions in $Y = (0, 1)^d$) for the H^1 norm.

For the numerical method, we consider the macro Finite Element (FE) space

$$S_0^1(\Omega, \mathcal{T}_H) = \{u^H \in H_0^1(\Omega); u^H|_K \in \mathcal{P}^1(K), \forall K \in \mathcal{T}_H\}, \quad (14)$$

where $\mathcal{P}^1(K)$ is the space of linear polynomials on the triangle K , and \mathcal{T}_H is a quasi-uniform triangulation of $\Omega \subset \mathbb{R}^d$ with ‘‘macro’’ meshsize H of shape regular triangles K . We consider also the micro FE space

$$S_{per}^1(K_\varepsilon, \mathcal{T}_h) = \{z^h \in W_{per}^1(K_\varepsilon); z^h|_T \in \mathcal{P}^1(T), T \in \mathcal{T}_h\}, \quad (15)$$

where $K_\varepsilon \subset K$ is a sampling subdomain of K , $\mathcal{P}^1(T)$ is the space of linear polynomials on the triangle T and \mathcal{T}_h is a quasi-uniform triangulation of K_ε . By macro and micro triangulation we mean that H can be much larger than ε and $h < \varepsilon$ resolves the fine scale.

The FE-HMM for elliptic homogenization problems has been introduced in [9] and analyzed in [10] and [5]. Define a *modified macro bilinear form*

$$B(u^H, v^H) := \sum_{K \in \mathcal{T}_H} \frac{|K|}{|K_\varepsilon|} \int_{K_\varepsilon} \nabla u^h a(x_k, x/\varepsilon) (\nabla v^h)^T dx, \quad (16)$$

where $K_\varepsilon = x_k + \varepsilon[-1/2, 1/2]^d$ is a sampling domain centered at the barycenter x_k of K , where $|K|, |K_\varepsilon|$ denote the measure of K and K_ε , respectively and u^h is given by the following *micro problem*: find u^h such that $(u^h - u^H) \in S_{per}^1(K_\varepsilon, \mathcal{T}_h)$ and

$$b_{K_\varepsilon}(u^h, z^h) := \int_{K_\varepsilon} \nabla u^h a(x_k, x/\varepsilon) (\nabla z^h)^T dx = 0 \quad \forall z^h \in S_{per}^1(K_\varepsilon, \mathcal{T}_h). \quad (17)$$

We obtain v^h by replacing u^H with v^H in (17). The macro FE-HMM solution is defined by the following variational *macro problem*: find $u^H \in S_0^1(\Omega, \mathcal{T}_H)$ such that

$$B(u^H, v^H) = \langle f, v^H \rangle, \quad \forall v^H \in S_0^1(\Omega, \mathcal{T}_H). \quad (18)$$

It can be shown that the problem (18) is well posed and has a unique solution [5],[10]. We define (similarly to [16]) an approximation of the fine scale solution u^ε

$$u^{\varepsilon,h}(x)|_K := u^H(x) + (u^h(x) - u^H(x))|_K^\# \quad \text{for } x \in K \in \mathcal{T}_H, \quad (19)$$

where $|_K^\#$ denotes the periodic extension of the fine scale solution $(u^h - u^H)$, available in K_ε , on the element K . We also define a broken H^1 norm $\|u\|_{\bar{H}^1(\Omega)} := (\sum_{K \in \mathcal{T}_H} \|\nabla u\|_{L^2(K)}^2)^{1/2}$, since $u^{\varepsilon,h}$ can be discontinuous across the macro elements K . In the sequel, we assume that the solutions χ^j of the cell problems (13) satisfy $\chi^j(x_k, \cdot) \in W^{2,\infty}(Y)$. If one sets $\chi^j(x_k, y) = \chi^j(x_k, x/\varepsilon)$, then by the chain rule (assuming χ^j is smooth)

$$\|D_x^\alpha (\chi^j(x_k, x/\varepsilon))\|_{L^\infty(K_\varepsilon)} \leq C \varepsilon^{-|\alpha|}, \quad |\alpha| \leq 2, \quad \alpha \in \mathbb{N}^d. \quad (20)$$

The following convergence results have been obtained in [5].

Theorem 2. *Let u^0 be the solution of the homogenized problem (12) and assume u^0 is H^2 -regular and that (20) holds. Let u^H be the solution of problem (18) and consider $u^{\varepsilon,h}$ defined in (19). Then*

$$\|u^0 - u^H\|_{H^1(\Omega)} \leq C(H + M^{-\frac{2}{d}}) \|f\|_{L^2(\Omega)}, \quad (21)$$

$$\|u^\varepsilon - u^{\varepsilon,h}\|_{\bar{H}^1(\Omega)} \leq C(\sqrt{\varepsilon} + H + M^{-\frac{1}{d}}) \|f\|_{L^2(\Omega)}, \quad (22)$$

where H is the size of the triangulation of the macro FE space (14) and M is the dimension of the micro FE space (15).

Notice that the meshsize h of the micro FE space on K_ε (of measure $|K_\varepsilon| = \varepsilon^d$) is given by $h \simeq \varepsilon M^{-\frac{1}{d}}$. Therefore the quantity h/ε does only depend on M and we write it as $M^{-\frac{1}{d}}$ in the above theorem and in the sequel.

We see that the FE-HMM gives a procedure to obtain an approximation u^H of the homogenized solution u^0 (without computing explicitly the homogenized equations) and an approximation $u^{\varepsilon,h}$ of the fine scale solution u^ε , at a much lower cost than solving the equation (11), since we solve the fine scales only in sampling domains of size ε^d in the periodic case, within a macro mesh of Ω . Furthermore, the micro problems are independent and can be solved in parallel, In the non-periodic case, K_ε should be chosen as to sample enough information of the local variations of a^ε .

3. Numerical velocity fields. In this section, we define and analyze a fine scale numerical approximation $v^{\varepsilon,h}$ of the velocity field (3) and an upscaled numerical approximation v^H of the mean velocity field of (7). Before giving more details, we state the algorithms for solving the multiscale advection-diffusion equations (6),(7).

Algorithm 1. *Fine scale problem (6)*

1. Compute $v^{\varepsilon,h}$ given below by (23).
2. Discretize the space variables of (6) with the approximated velocity field $v^{\varepsilon,h}$ and solve the time dependent problem with ROCK2-4 (subsection 2.2).

Algorithm 2. *Upscaled problem (7)*

1. Compute $v^{\varepsilon,h}$ and v^H given below by (23) and (33).
2. Compute the fluctuating field $\tilde{v}^h(x) := v^{\varepsilon,h}(x) - \frac{1}{|K_\varepsilon|} \int_{K_\varepsilon} v^{\varepsilon,h} dx$, $K_\varepsilon = x + \varepsilon[-1/2, 1/2]^d$.
3. Use \tilde{v}^h to solve (8) and derive an effective diffusion tensor D_0 . Discretize the space variables of (7) with the approximated mean velocity field v^H and solve the time dependent problem with ROCK2-4 (subsection 2.2).

Let $u^{\varepsilon,h}$ be given by (19). We define a numerical approximation of the velocity field $v^\varepsilon := -a^\varepsilon \nabla u^\varepsilon$ by

$$v^{\varepsilon,h}(x)|_K := -a(x_k, x/\varepsilon) \nabla u^{\varepsilon,h}(x) \text{ for } x \in K \in \mathcal{T}_H, \quad (23)$$

where x_k is at the barycenter of K . The following theorem estimates the error introduced by the approximation (23). In the sequel, $C > 0$ denotes a generic constant independent of the various discretization parameters.

Theorem 3. *Suppose that the assumptions of Theorem 2 hold, that a^ε is bounded and $a^\varepsilon(x, \cdot)$ is smooth. Then*

$$\|v^\varepsilon - v^{\varepsilon,h}\|_{\bar{L}^2(\Omega)} \leq C(\sqrt{\varepsilon} + H + M^{-\frac{1}{d}}), \quad (24)$$

where H is the size of the triangulation of the macro FE space (14), M is the dimension of the micro FE space (15) and \bar{L}^2 is a broken L^2 norm similar as defined for (19).

Proof. We have $\|v^\varepsilon - v^{\varepsilon,h}\|_{\bar{L}^2(K)}^2 \leq$

$$\int_K |(a(x, x/\varepsilon) - a(x_k, x/\varepsilon)) \nabla u^\varepsilon|^2 dx + \int_K |a(x_k, x/\varepsilon) (\nabla u^\varepsilon - \nabla u^{\varepsilon,h})|^2 dx.$$

Summing over $K \in \mathcal{T}_H$, the result follows from (22) the boundedness of a^ε and

$$\max_{x \in K} |(a(x, x/\varepsilon) - a(x_k, x/\varepsilon))| \leq CH, \quad (25)$$

since $a(x, \cdot)$ is smooth. \square

For the mean velocity involved in (7), we consider the approximation $\bar{v} \simeq v^0 = -a^0 \nabla u^0$. The motivation is as follows. Consider $v_1^\varepsilon = -a^\varepsilon \nabla u_1^\varepsilon = -a^\varepsilon \nabla (u^0(x) + \varepsilon \sum_{j=1}^d \chi^j(x, x/\varepsilon) \frac{\partial u^0}{\partial x_j})$, where χ^j are the solutions of the cell problems (13). As for v^ε , we split $v_1^\varepsilon = \bar{v}_1 + \tilde{v}_1$, where $\bar{v}_1(x) := \int_Y v_1(x, y) dy$ and $\tilde{v}_1 := v_1^\varepsilon - \bar{v}_1$. We have

$$\|v^\varepsilon - v_1^\varepsilon\|_{L^2(\Omega)} \leq C_1 \|\nabla(u^\varepsilon - u_1^\varepsilon)\|_{L^2(\Omega)} \leq C_2 \sqrt{\varepsilon},$$

using that a^ε is bounded and classical result (see [11, Chap.1.4]) for the last inequality. A simple computation, using $\nabla = \nabla_x + (1/\varepsilon) \nabla_y$ and $u^0 \in H^2(\Omega)$, yields

$$\bar{v}_1 = -a^0(x) \nabla u^0(x) + \mathcal{O}(\varepsilon).$$

To approximate v^0 , we first need the two following lemmas.

Lemma 1. *The solution u^h of the problem (17) for $x \in K_\varepsilon \subset K \in \mathcal{T}_H$ is given by*

$$u^h(x) = u^H(x) + \varepsilon \sum_{j=1}^d \chi^{j,h}(x_k, x/\varepsilon) \frac{\partial u^H(x_k)}{\partial x_j}, \quad (26)$$

where x_k is at the barycenter of $K \in \mathcal{T}_H$ and $\chi^{j,h}(x_k, x/\varepsilon)$, $j = 1, \dots, d$ are the solutions of (13) in $S_{per}^1(K_\varepsilon, \mathcal{T}_h)$.

Proof. Inserting (26) in (17), and using that ∇u^H is constant in K give the result. \square

Lemma 2. *Let $u^H, v^H \in S_0^1(\Omega, \mathcal{T}_H)$ and u^h, v^h be the solution of the cell problems (17) such that $(u^h - u^H), (v^h - v^H) \in S_{per}^1(K_\varepsilon, \mathcal{T}_h)$. Then*

$$\frac{1}{|K_\varepsilon|} \int_{K_\varepsilon} \nabla u^h a(x_k, x/\varepsilon) (\nabla v^h)^T dx = \frac{1}{|K|} \int_K \nabla u^H a^{0,h}(x_k) (\nabla v^H)^T dx, \quad (27)$$

where x_k is at the barycenter of $K \in \mathcal{T}_H$ and $a^{0,h}$ defined below is the numerical homogenized tensor with $\chi^{j,h}$ solution of (13) in $S_{per}^1(Y, \mathcal{T}_h)$. Furthermore, the error between the homogenized tensor a^0 and $a^{0,h}$ is given by

$$|a_{ij}^0(x_k) - a_{ij}^{0,h}(x_k)| \leq CM^{-\frac{1}{d}}, \quad (28)$$

where M is the dimension of the micro FE space defined in (15).

Proof. Inserting (26) in (17) gives

$$\begin{aligned} \frac{1}{|K_\varepsilon|} \int_{K_\varepsilon} \nabla u^h a(x_k, x/\varepsilon) (\nabla v^h)^T dx &= \frac{1}{|K_\varepsilon|} \int_{K_\varepsilon} \nabla u^H a(x_k, x/\varepsilon) (\nabla v^h)^T dx = \\ &= \sum_{i,j=1}^d \frac{\partial u^H(x_k)}{\partial x_i} \frac{1}{|K_\varepsilon|} \int_{K_\varepsilon} e_i^T a(x_k, x/\varepsilon) (e_j + \sum_{l=1}^d e_l \frac{\partial \chi^{j,h}(x_k, x/\varepsilon)}{\partial x_l}) dx \frac{\partial v^H(x_k)}{\partial x_j}, \end{aligned}$$

where $\{e_j\}_{j=1}^d$ is the standard basis of \mathbb{R}^d and we used that $b_{K_\varepsilon}(u^h, \chi^{j,h}) = 0$ (see (17)) and that $\nabla u^H, \nabla v^H$ are constant. One term, for i, j chosen, of the integral of the last equality gives, after the change of variables $y = x/\varepsilon$,

$$\frac{1}{|Y|} \int_Y a_{ij}(x_k, y) + \sum_{l=1}^d a_{il}(x_k, y) \frac{\partial \chi^{j,h}(x_k, y)}{\partial x_l} dy =: a_{ij}^0(x_k), \quad (29)$$

and (27) follows. Formula (29) is similar to the formula for the component of the homogenized tensor a_{ij}^0 (see (12)), but with $\chi^{j,h}$ solution of (13) in $S_{per}^1(Y, \mathcal{T}_h)$. The formula (28) follows from $\|\frac{\partial \chi^j}{\partial x_l} - \frac{\partial \chi^{j,h}}{\partial x_l}\|_{L^2(Y)} \leq CM^{-\frac{1}{d}}$, which is a consequence of standard H^1 error estimates in FEM with H^2 regularity of χ^j . \square

We show next how the homogenized tensor $a^{0,h}$ can be computed during the stiffness assembly process. Consider a triangle $K \in \mathcal{T}_H$, and $S_K \subset S_0^1(\Omega, \mathcal{T}_H)$ the collection of the nodal basis functions associated with the vertices of K . Consider

$$B(\varphi_i^H, \varphi_j^H) = \frac{1}{|K_\varepsilon|} \int_{K_\varepsilon} \nabla \varphi_i^h a(x_k, x/\varepsilon) (\nabla \varphi_j^h)^T dx, \quad (30)$$

where $\varphi_i^H, \varphi_j^H \in S_K$ and φ_i^h is a solution of (17) such that $(\varphi_i^h - \varphi_i^H) \in S_{per}^1(K_\varepsilon, \mathcal{T}_h)$ (similarly for φ_j^h). Define the affine mapping $\phi_K : \hat{K} \rightarrow K$, $\phi_K(\xi) = x$, which maps the reference simplex $\hat{K} = \{\xi \in \mathbb{R}^2; \xi_i > 0, \sum_{i=1}^d \xi_i < 1\}$ onto K . The nodal basis of the reference simplex is defined by $\hat{\varphi}_i^H = \xi_i$, $i = 1, \dots, d$, $\hat{\varphi}_0^H = 1 - \sum_{i=1}^d \xi_i$. We

order the nodal basis of S_K so that $\varphi_i^H(\phi_K(\xi)) = \hat{\varphi}_i^H(\xi)$, $i = 0, \dots, d$ and define the matrix $M_K^h \in \mathbb{R}^{d \times d}$ by $(M_K^h)_{ij} = B(\varphi_i^H, \varphi_j^H)$, $i, j = 1, \dots, d$. We can now show

Lemma 3. *The numerical homogenized tensor $a^{0,h}(x_k)$, where x_k is at the barycenter of $K \in \mathcal{T}_H$ is given by*

$$a^{0,h}(x_k) = JM_K^h J^T, \quad (31)$$

where M_K is defined above and J is the Jacobian of the mapping ϕ_K defined above.

Proof. Using Lemma 2 for (30) and a change of variables give

$$(M_K^h)_{ij} = B(\varphi_i^H, \varphi_j^H) = \frac{1}{|\hat{K}|} \int_{\hat{K}} \nabla \hat{\varphi}_i^H J^{-1} a^{0,h}(x_k) J^{-T} (\nabla \hat{\varphi}_j^H)^T d\xi \quad (32)$$

for $i, j = 1, \dots, d$.

The last integral is equal to $\nabla \hat{\varphi}_i^H J^{-1} a^{0,h}(x_k) J^{-T} (\nabla \hat{\varphi}_j^H)^T$ since the integrand is constant and $\nabla \hat{\varphi}_i^H = \nabla \xi_i = e_i^T$, $i = 1, \dots, d$, where $\{e_j\}_{j=1}^d$ is the standard basis of \mathbb{R}^d . These two observations give (31). \square

An approximation of the mean velocity $v^0(x) = -a^0(x) \nabla u^0(x)$ is defined as

$$v^H(x)|_K := -a^{0,h}(x_k) \nabla u^H(x) \text{ for } x \in K \in \mathcal{T}_H, \quad (33)$$

where x_k is at the barycenter of K and where u^H is the solution of (18). We have the following error estimate for the approximation (33) of the mean velocity.

Theorem 4. *Let u^0 be the solution of the homogenized problem (12) and suppose u^0 is H^2 -regular, $a^0(x)$ is smooth and bounded and (20) holds. Let u^H be the solution of problem (18). Then,*

$$\|v^H - v^0\|_{L^2(\Omega)} \leq C(H + M^{-\frac{1}{d}}) \quad (34)$$

where H is the size of the triangulation of the macro FE space (14) and M is the dimension of the micro FE space defined in (15).

Proof. We have

$$\begin{aligned} \|v^H - v^0\|_{L^2(\Omega)}^2 &= \sum_{K \in \mathcal{T}_H} \|v^H - v^0\|_{L^2(K)}^2 \leq \sum_{K \in \mathcal{T}_H} \|a^{0,h}(x_k) (\nabla u^H - \nabla u^0)\|_{L^2(K)}^2 \\ &+ \sum_{K \in \mathcal{T}_H} \|(a^{0,h}(x_k) - a^0(x_k)) \nabla u^0\|_{L^2(K)}^2 + \sum_{K \in \mathcal{T}_H} \|(a^0(x_k) - a^0(x)) \nabla u^0\|_{L^2(K)}^2. \end{aligned}$$

The first term of the right hand side of the inequality is bounded by $C(H + M^{-\frac{2}{d}})^2$ using (21), the boundedness of a^0 and (28), the second term is bounded by $C(M^{-\frac{1}{d}})^2$ using (28) and the last term is bounded by $C(H)^2$ using the smoothness of a^0 . Summing up these terms we obtain the stated result. \square

4. Numerical example. We present in this section numerical experiments which illustrate our algorithms. We concentrate here on the reconstructed velocity fields and refer to [7] for an application of the full algorithms proposed in this paper, involving the time dependent problem (1). Consider

$$-\nabla \cdot (a^\varepsilon \nabla u^\varepsilon) = 0 \quad \text{in } \Omega = (0, 1)^2, \quad (35)$$

$$u^\varepsilon|_{\Gamma_{D_0}} = u_{D_0}, \quad u^\varepsilon|_{\Gamma_{D_1}} = u_{D_1}, \quad (36)$$

$$n \cdot (a^\varepsilon \nabla u^\varepsilon)|_{\Gamma_N} = 0 \quad \Gamma_N := \partial\Omega \setminus (\Gamma_{D_0} \cup \Gamma_{D_1}), \quad (37)$$

where $\Gamma_{D_0} := \{(x_1, x_2); x_1 = 1, x_2 \in [\gamma_1, \gamma_2]\} \cup \{(x_1, x_2); x_1 \in [\gamma_1, \gamma_2], x_2 = 1\}$ and $\Gamma_{D_1} := \{(x_1, x_2); x_1 \in [\gamma_1, \gamma_2], x_2 = 0\} \cup \{(x_1, x_2); x_1 = 0, x_2 \in [\gamma_1, \gamma_2]\}$. We chose

$u_{D_0} = 0$, $u_{D_1} = 1$, an anisotropic diffusivity tensor $a^\varepsilon = \text{diag}(2 + \sin 2\pi x_1/\varepsilon, 2 + \sin 2\pi x_2/\varepsilon)$ and $\gamma_1 = \gamma_2 = 0.25$. We compute a reference solution via scale resolution and chose therefore a parameter $\varepsilon = 1/16$ not too small. We also compute the homogenized tensor a^0 and a reference solution for the homogenized problem corresponding to (35). We chose the micro mesh of the sampling domain K_ε small enough to minimize the influence of the term $M^{-\frac{1}{d}}$ in (24) and (34) (we refer to [5], where this influence has been discussed for the FE-HMM). For the macro mesh of the FE space $S_0^1(\Omega, \mathcal{T}_H)$, we take successively $H = 1/2, 1/4, 1/8, 1/16$. The amount of work needed to obtain a velocity approximation (23) or (33) is to solve $2 \cdot (1/H)^2$ micro problems of size $|K_\varepsilon| = \varepsilon^2$ and one macro problem with work $\sim (1/H)^2$.

In Figure 1 we study the convergence in the L^2 norm of $v^{\varepsilon,h}, v^H$ given by (23) and (33), respectively, towards a reference solution for v^ε and v^0 . We see that both approximations converge nicely. The reconstructed homogenized velocity field (right picture of Figure 1) converges slightly better than the reconstructed small scale field. For the latter field, the term $\sqrt{\varepsilon}$ may have an impact on the solution. Both fields converge with a slower rate than the macro linear rate expected from (24) and (34). The boundary conditions induce a sharp transition of the solution at the border of the domain Ω and a uniform (macro) grid, as chosen in these computations, may not capture sufficiently well this behavior.

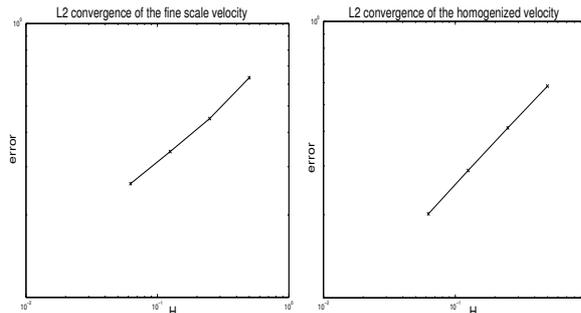


FIGURE 1. Convergence rate of $v^{\varepsilon,h}$ to v^ε (left pict.) and v^H to v^0 (right pict.). Macro mesh: $H = 1/2, 1/4, 1/8, 1/16$.

In Figure 2, we plot the small scale solution u^ε versus $u^{\varepsilon,h}$, defined in (19), upon which our numerical velocity fields are based, for a coarse macro mesh $H = 1/8$. We see that the fine scale solution is nicely captured in the interior of the domain, while at the corner of the boundary, a refinement should be applied. We emphasize that this is not a drawback of our method since this refinement would be required for a standard FEM applied to a smooth problem with the above boundary conditions.

For $\varepsilon \rightarrow 0$ the resolution of the fully detailed problem (35) becomes impossible, while our numerical approximations can still be computed with a complexity independent of ε (in the periodic case).

In conclusion, we see that the methods presented in this paper are able to capture the right behavior of the fine scale and the homogenized velocity fields for coarse macro meshes with a complexity independent of ε (for the periodic case) and a much lower cost than the work needed for resolving the full details of the problem. The combination of these reconstructed velocity fields with Chebyshev methods for the time integration as proposed here, gives efficient numerical methods (at the same time easy to implement) for the solution of multiscale advection-diffusion problems.

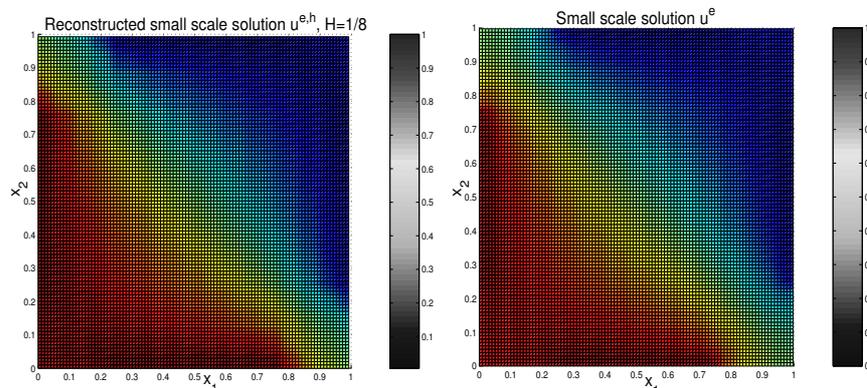


FIGURE 2. u^{ϵ} (right pict.) and $u^{\epsilon,h}$ (left pict.). Macro mesh $H = 1/8$.

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E-mail address: assyr.abdulle@unibas.ch