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# NUMERICAL HOMOGENIZATION OF A NONLINEARLY COUPLED ELLIPTIC-PARABOLIC SYSTEM, REDUCED BASIS METHOD, AND APPLICATION TO NUCLEAR WASTE STORAGE

ANTOINE GLORIA, THIERRY GOUDON, AND STELLA KRELL

**Abstract.** We consider the homogenization of a coupled system of PDEs describing flows in highly heterogeneous porous media. Due to the coupling, the effective coefficients always depend on the slow variable, even in the simple case when the porosity is taken purely periodic. Therefore the most important part of the computational time for the numerical simulation of such flows is dedicated to the determination of these coefficients. We propose a new numerical algorithm based on Reduced Basis techniques, which significantly improves the computational performances.

**Keywords:** porous media, homogenization, reduced basis method.

**2010 Mathematics Subject Classification:** 35B27, 65M60, 65Z05, 76M50, 76M10

## 1. INTRODUCTION

This work is concerned with the numerical treatment of a nonlinearly coupled elliptic-parabolic system of equations involving coefficients varying on a fast scale. Resolving the finest scales induces a prohibitive numerical cost, both in terms of computational time and memory storage. Our goal consists in finding relevant “averaged” models, combined with efficient numerical methods. It turns out that the main part of the computational effort is precisely devoted to the evaluation of the coefficients of the effective equations which are obtained by the homogenization analysis. We shall propose methods which lead to a considerable speed-up of this crucial step.

A strong motivation relies on the modeling of radionuclide transport in devices for the storage of nuclear waste. This leads to consider nonlinear systems of parabolic equations, coupling the time-evolution of the radionuclide concentration  $C(t, x)$  (for the sake of simplicity we consider only one single species of radionuclides) to the velocity field  $U(t, x)$  of the water flow. The flow takes place in a complex porous medium made of clay, limestone and marl — so that the physical properties vary a lot from place to place. The modeling of radionuclide transport in disposal facilities of radioactive waste therefore requires to deal with PDEs whose coefficients are highly heterogeneous on short scales. The realization of routine simulations should however rely on fast computations, which excludes to resolve the finest scales. Homogenization is the natural tool to derive effective models, which hopefully smoothes out in a consistent way the small scale features of the problem. In the case of the nonlinearly coupled system treated here, (periodic) homogenization alone is not enough to drastically reduce the computational cost, since a so-called cell-problem (which is itself an elliptic PDE) has to be solved at each Gauss point of the computational

domain — this could surprise the expert: although diffusion coefficients are assumed to be purely periodic, and the equations are linear, the nonlinear coupling condition makes the homogenized diffusion matrix depend on the space variable. This is where the reduced basis (RB) method comes into the picture: these cell-problems can be viewed as a  $d$ -parameter ( $d$  being the space dimension) family of elliptic equations, which is an ideal setting for the RB method. A further practical issue is related to the dependence of the elliptic operator upon the parameters, which is not affine (according to the terminology of the RB approach) and therefore requires a specific treatment. This article is devoted to the homogenization and numerical approximation of solute transfer equations driven by diffusion and convection, with a coupling with hydrodynamics in porous media.

A typical set of equations describing radionuclides transport is as follows:

$$\phi(R\partial_t C + a\partial_t p) - \operatorname{div}_x(D(U)C - UC) + \phi R\lambda C = S, \quad (1.1)$$

$$\mu U = -k(\nabla_x p + \rho g \mathbf{e}_d), \quad (1.2)$$

$$\phi b \partial_t p + \operatorname{div}_x(U) = q, \quad (1.3)$$

for  $t \geq 0$  and  $x$  lying in some given bounded domain  $\Omega \subset \mathbb{R}^d$ , with  $d = 2$  or  $d = 3$ . The system is completed by initial and boundary conditions, which can be of Dirichlet, Neumann, or mixed type. In this system, the fluid velocity  $U(t, x)$  is related to the pressure  $p(t, x)$  through the Darcy law (1.2) where  $\rho > 0$  stands for the fluid density,  $g > 0$  is the gravity acceleration, and  $\mathbf{e}_d$  stands for the vertical unit vector. The physical properties of the porous medium are embodied into the porosity  $\phi > 0$  and the permeability tensor  $k$ , which are both functions of the space variable  $x \in \Omega$ . In simple cases the permeability is scalar, but in general it takes into account the anisotropy of the porous medium. Thus  $x \mapsto k(x)$  is matrix-valued, and throughout this work it will be assumed to satisfy an ellipticity condition, uniformly over  $\Omega$ . The latency retardation factor  $R > 0$ , and the degradation coefficient  $\lambda = \frac{\ln(2)}{T}$ , only depend on the species of radionuclide under consideration, with  $T$  the half-time of the element. Couplings are due to several physical effects:

- The constituents of the mixture have different compressibility, which are described by the coefficients  $a, b$ . A typical formula reads  $a = (\zeta_1 - \zeta_2)C(1 - C)$ , and  $b = \zeta_2 + (\zeta_1 - \zeta_2)C$ , for some  $\zeta_1 \geq \zeta_2 > 0$ . In practice the coefficients  $\zeta_1, \zeta_2$  are small, and we usually assume that the flow is indeed incompressible. In particular, we shall consider  $\zeta_1 = \zeta_2 = 0$ , and therefore also  $a = b = 0$ . The incompressibility assumption greatly simplifies the model, and we shall make this assumption in the rest of this work.
- The viscosity  $\mu > 0$  depends on a complex way on the concentration. For instance Koval's law reads  $\mu : C \in [0, 1] \mapsto \frac{\mu_0}{(1 + ((\mu_0/\mu_1)^{1/4} - 1)C)^4}$ , for some  $0 < \mu_0 < \mu_1$ .
- The diffusion tensor  $D$  depends on the velocity  $U$ . To be more specific it splits as follows

$$D = D_0 + \mathbb{D}(U).$$

The leading part reads  $D_0 = \phi D_{\text{ref}}$  with  $D_{\text{ref}}$  the molecular diffusion coefficient of the species and  $\phi > 0$  the porosity. The correction depends on the velocity field as follows

$$\mathbb{D}(U) = \alpha |U| \mathbb{I} + \beta \frac{U \otimes U}{|U|}, \quad \alpha, \beta \geq 0. \quad (1.4)$$

This correction has dispersive effects. Note that, unless  $U$  lies in  $L^\infty$ , the diffusion tensor has unbounded coefficients.

Of course, these nonlinear couplings are sources of difficulties from the mathematical viewpoint. In the incompressible case, a definitive breakthrough is due to [23]. The theory has been completed in [24] with existence–uniqueness results in dimension 2 and in [15] with results on the existence of weak solutions, including nonlinear models with possible degeneracy due to concentration dependent viscosity, and unbounded diffusion and convection coefficients in the concentration equation. Compressible effects are dealt with in [2], assuming a constant viscosity, and in [3], restricting to the one-dimension framework. A more general case is discussed in [17]. We also mention [16] where, additionally, temperature variations are accounted for in the model, [29] where further nonlinear reaction terms are treated, and [4] where the case of vanishing  $D_0$  is analyzed, which potentially yields degenerate diffusion. Note that the models above describe the miscible displacement of two fluids in a porous medium. The immiscible case rises new difficulties and requires different techniques, see [25] and the references therein.

As said above, the transfer of radionuclides takes place in a highly heterogeneous medium. Simulations resolving the finest scales, that means with a mesh size far smaller than the smallest characteristic scales of the space heterogeneities, would lead to a prohibitive numerical cost, both in terms of memory capacities and computational time. This observation motivates the quest of an effective model, that corresponds to the limit where the scale of heterogeneities is small compared to the length scale of observation. Assuming periodic variations, we can guess formulae for the effective coefficients by means of two-scale ansatz, as described in e. g. [6]. The justification of the asymptotic model then relies on the use of “two-scale convergence” techniques, following [30] and [1] (the extension of these techniques to random media is described in [9]). The asymptotic analysis faces the difficulties mentioned above: nonlinear couplings, unbounded coefficients... Results in this direction can be found in [18] and the references therein. However, even if homogenized models can be derived, it is likely that the obtained formulae are not very useful on a practical viewpoint. Indeed, the effective coefficients are usually defined, at each space point  $x \in \Omega$ , by an average over the elementary cell  $\mathbb{Y}$  of the periodic medium

$$F_{\text{effective}}(x) = \int_{\mathbb{Y}} f(x, y) dy$$

of a function  $y \mapsto f(x, y)$  which is itself defined by solving a PDE, say of elliptic type, on the cell  $\mathbb{Y}$ , endowed with periodic boundary conditions. Therefore, the determination of the effective coefficients has still an important numerical cost since at each Gauss point  $x$  of  $\Omega$  one needs to solve an elliptic PDE and compute such integrals!

This work precisely addresses the questions

- (1) of finding effective equations for the transport of radionuclides in porous media, at least in some simplified framework,
- (2) of designing numerical methods to compute efficiently the coefficients of the effective models, without using the brutal and prohibitive method consisting of solving independently the cell-problems and computing the suitable averages at each Gauss point of the computational domain.

The model under investigation here has been derived for the benchmark COUPLEX, see [8]. This benchmark is based on a set of simplified but realistic models for the transport of radionuclides around a nuclear waste repository. It allows to evaluate the pros and cons of several numerical strategies that can be used in this context. We wish to complete the benchmark by considering the corresponding homogenization problem. In this work, we restrict to the simplest situation where the hydraulic regime is established and governed by a mere diffusion equation. For the sake of completeness, let us remind the basis of the modeling. It is convenient to define the hydrodynamic load (or piezoelectric height)  $\Theta = \frac{p}{\rho g} + z$ ,  $z = x_d \in \mathbb{R}$  being the height coordinate. We neglect the dependence of the viscosity upon the concentration (in which case  $\mu$  is a constant), so that we are led to

$$U(x) = -K(x)\nabla_x\Theta(x). \quad (1.5)$$

together with

$$\nabla_x \cdot U(x) = q(x). \quad (1.6)$$

In (1.5)–(1.6), we have set  $K = \frac{\rho g}{\mu}k$ . Equations (1.5)–(1.6) define the convection and diffusion terms to be used in the PDE that describes the migration of radionuclides dissolved in the saturated porous medium. The concentration  $C(t, x)$  obeys the equation

$$R\phi\partial_t C - \nabla \cdot (D(U)\nabla C - UC) + R\phi\lambda C = S \quad (1.7)$$

with  $D(U) = D_0 + \mathbb{D}(U)$ , and  $\mathbb{D}$  as in (1.4). We shall write the system (1.5)–(1.7) in dimensionless form, and we shall make a small parameter  $0 < \varepsilon \ll 1$  appear, which is the ratio of the typical period of the heterogeneities over the length scale of reference. The rescaled system has the same form as (1.5)–(1.7), but now the permeability matrix takes the form  $K(x/\varepsilon)$ , with  $K$  a periodic function. We can consider oscillating source terms  $q, S$  and diffusion coefficient  $D_0$  as well. As it will be shown in the next section, the effective model in the regime  $\varepsilon \rightarrow 0$  has the form

$$\begin{cases} \nabla \cdot U^* = q^*, \\ \partial_t C^* - \nabla \cdot (D^*\nabla C^* - U^*C^*) + \lambda C^* = S^*. \end{cases} \quad (1.8)$$

where the coefficients  $S^*, q^*$  are determined by suitable “average” operations on the oscillating coefficients  $S, q$ , while the velocity field  $U^*$  and the diffusion coefficient  $D^*$  are given by relation of the form

$$U^* = \mathcal{U}(K, q), \quad D^* = \mathcal{D}(D_0, U^*), \quad (1.9)$$

involving suitable functionals  $\mathcal{U}$  and  $\mathcal{D}$ . This paper is organized as follows. In Section 2 we present the existence–uniqueness theory for the system (1.5)–(1.7), together with the homogenization result, which provides formulae for the effective coefficients in the regime of fast oscillations of the properties of the medium. We pay a specific attention to the discussion of the uniqueness of weak solutions, which is not standard due to the fact that the diffusion term  $D$  is unbounded. Section 3 is devoted to the numerical approximation of the homogenized system. Since the direct approach for the computation of the effective coefficients remains prohibitive in terms of computational cost, we develop a numerical strategy based on the RB method (see [28] and the references therein for elliptic equations, and [10] for an application to homogenization). The guideline of the RB approach is the construction of a suitable Galerkin basis “adapted” to the parametrized set of equations. We present in detail the application of the RB method to the system (1.5)–(1.7). Again, the fact that the diffusion coefficients are unbounded raises some interesting problems, this time not only for the analysis but also for the practical implementation of the RB

method and the choice of the estimator. Numerical results demonstrate the ability of the method to provide accurate results with a substantial speed-up.

We shall make use of the following notation:

- $\mathbb{R}^+ = [0, +\infty)$ ;
- $0 < T < \infty$  is a final time;
- $d \geq 1$  denotes the space dimension;
- $\mathcal{M}_d(\mathbb{R})$  is the set of  $d \times d$  real matrices,  $\mathbb{I}$  is the identity matrix;
- $\Omega$  is an open bounded Lipschitz domain of  $\mathbb{R}^d$ ;
- For all  $p \in [1, \infty]$  and  $s \in \mathbb{N}$ ,  $L^p(\Omega)$  denotes the space of  $p$ -integrable functions on  $\Omega$ ,  $W^{s,p}(\Omega)$  denotes the Sobolev space of  $p$ -integrable functions whose  $s$ -first distributional derivatives are  $p$ -integrable,  $W_0^{1,p}(\Omega)$  the closure in  $W^{1,p}(\Omega)$  of the space  $C_0^\infty(\Omega)$  of smooth functions compactly supported in  $\Omega$ ;
- For  $p = 2$ , we denote the Hilbert spaces  $W^{1,2}(\Omega)$  and  $W_0^{1,2}(\Omega)$  by  $H^1(\Omega)$  and  $H_0^1(\Omega)$ , respectively.
- $\mathbb{Y} = (0, 1)^d$  is the periodic cell, and  $H_{\#}^1(\mathbb{Y})$  denotes the closure of the subspace of  $C^\infty(\mathbb{R}^d)$  made of  $\mathbb{Y}$ -periodic functions with vanishing mean.

## 2. WELL-POSEDNESS AND HOMOGENIZATION

**2.1. Main results.** We consider the following weakly coupled system of PDEs:

$$\begin{cases} U = -K\nabla\Theta & \text{in } \Omega, \\ \nabla \cdot U = q & \text{in } \Omega, \\ \partial_t C - \nabla \cdot (D(U)\nabla C - UC) + \lambda C = S & \text{in } ]0, T[ \times \Omega. \end{cases} \quad (2.1)$$

We let  $\lambda > 0$ , and for the source terms we let  $q \in L^\infty(\Omega)$  and  $S \in L^2(0, T; H^{-1}(\Omega))$ . The weak coupling condition reads

$$D(U)(x) := D_0(x) + \alpha|U(x)|\mathbb{I} + \beta \frac{U(x) \otimes U(x)}{|U(x)|}, \quad (2.2)$$

for a. e.  $x \in \Omega$ , where  $\alpha > 0, \beta \geq 0$ . The functions  $x \mapsto K(x)$  and  $x \mapsto D_0(x)$  are matrix-valued; they both satisfy uniform bounds and strong ellipticity condition, uniformly over  $\Omega$ : namely, there exists  $\Lambda > 0$  such that for a. e.  $x \in \Omega$  and all  $\xi \in \mathbb{R}^d$

$$\begin{aligned} |K(x)\xi| &\leq \Lambda|\xi|, & \xi \cdot K(x)\xi &\geq \Lambda^{-1}|\xi|^2, \\ |D_0(x)\xi| &\leq \Lambda|\xi|, & \xi \cdot D_0(x)\xi &\geq \Lambda^{-1}|\xi|^2. \end{aligned}$$

The system (2.1) is completed by boundary conditions and an initial condition, which for simplicity we take as follows (mixed Neumann-Dirichlet boundary conditions could be considered as well)

$$\begin{cases} \Theta = 0 & \text{on } \partial\Omega, \\ C(0, \cdot) = C_{\text{init}} & \text{in } \Omega, \\ C = 0 & \text{on } ]0, T[ \times \partial\Omega, \end{cases} \quad (2.3)$$

for some  $C_{\text{init}} \in L^2(\Omega)$ .

We are interested in the case when  $K$  is an  $\varepsilon$ -periodic matrix, and  $\varepsilon \rightarrow 0$ . Before we turn to this problem, we first define a notion of weak solution for the coupled system (2.1)–(2.3), and give an existence and uniqueness result.

**Definition 2.1.** A weak solution of (2.1)–(2.3) is a pair  $(\Theta, C) \in H_0^1(\Omega) \times L^2(0, T; H_0^1(\Omega)) \cap C^0(0, T; L^2(\Omega))$  such that  $\partial_t C \in L^2(0, T; H^{-1}(\Omega))$ ,  $\int_0^T \int_\Omega \nabla C \cdot D(U) \nabla C < \infty$  with  $U = -K \nabla \Theta$ , and which satisfies (2.1)–(2.3) in the following sense:

- $\Theta$  is a weak solution in  $H_0^1(\Omega)$  to (2.1)<sub>1,2</sub> & (2.3)<sub>1</sub>;
- For all  $v \in L^2(0, T; H_0^1(\Omega)) \cap L^2(0, T; L^\infty(\Omega))$  such that  $\int_0^T \int_\Omega \nabla v \cdot D(U) \nabla v < \infty$ , we have

$$\begin{aligned} \int_0^T \langle \partial_t C, v \rangle_{H^{-1}, H_0^1} + \int_0^T \int_\Omega \nabla v \cdot D(U) \nabla C + \int_0^T \int_\Omega v U \cdot \nabla C \\ + \int_0^T \int_\Omega C v (q + \lambda) = \int_0^T \langle S, v \rangle_{H^{-1}, H_0^1}. \end{aligned}$$

The following theorem states the existence and uniqueness of such weak solutions.

**Theorem 1.** *For all  $q \in L^\infty(\Omega)$ ,  $S \in L^2(0, T; H^{-1}(\Omega))$ , and  $C_{\text{init}} \in L^2(\Omega)$ , there exists a unique weak solution to (2.1)–(2.3) in the sense of Definition 2.1.*

We now turn to the periodic homogenization of (2.1)–(2.3). Let  $K$  be a  $\mathbb{Y} = (0, 1)^d$ -periodic matrix. For all  $\varepsilon > 0$ , we consider the coupled system

$$\begin{cases} U_\varepsilon = -K_\varepsilon \nabla \Theta_\varepsilon & \text{in } \Omega, \\ \nabla \cdot U_\varepsilon = q & \text{in } \Omega, \\ \partial_t C_\varepsilon - \nabla \cdot (D(U_\varepsilon) \nabla C_\varepsilon - U_\varepsilon C_\varepsilon) + \lambda C_\varepsilon = S & \text{in } ]0, T[ \times \Omega, \\ \Theta_\varepsilon = 0 & \text{on } \partial\Omega, \\ C_\varepsilon(0, \cdot) = C_{\text{init}} & \text{in } \Omega, \\ C_\varepsilon = 0 & \text{on } ]0, T[ \times \partial\Omega, \end{cases} \quad (2.4)$$

where  $q, S, C_{\text{init}}$  and the function  $D$  are as above, and  $K_\varepsilon$  is defined by  $K_\varepsilon(x) := K(x/\varepsilon)$  on  $\Omega$ . Theorem 1 ensures the existence and uniqueness of a weak solution  $(\Theta_\varepsilon, C_\varepsilon)$  of (2.4) for any  $\varepsilon > 0$ . The following result characterizes the asymptotic behavior of  $(\Theta_\varepsilon, C_\varepsilon)$  as  $\varepsilon \rightarrow 0$ .

**Theorem 2.** *Let  $q \in L^\infty(\Omega)$ ,  $S \in L^2(0, T; H^{-1}(\Omega))$ ,  $C_{\text{init}} \in L^2(\Omega)$ ,  $D$  be as in (2.2), and  $K$  be a  $\mathbb{Y}$ -periodic bounded and strongly elliptic matrix. For all  $\varepsilon > 0$ , we set  $K_\varepsilon := K(\cdot/\varepsilon)$ . Then the unique weak solution  $(\Theta_\varepsilon, C_\varepsilon)$  to (2.4) converges to some  $(\Theta_0, C_0)$  in the following senses: strongly in  $L^2(\Omega)$  and  $L^2((0, T) \times \Omega)$ , and weakly in  $H^1(\Omega)$  and  $L^2(0, T; H^1(\Omega))$ . In addition  $C_\varepsilon$  converges in  $C^0([0, T], L^2(\Omega))$  – weak to  $C_0$ , and  $(\Theta_0, C_0)$  is the unique weak solution to*

$$\begin{cases} U_0 = -K^* \nabla \Theta_0 & \text{in } \Omega, \\ \nabla \cdot U_0 = q & \text{in } \Omega, \\ \partial_t C_0 - \nabla \cdot (D^* \nabla C_0 - U_0 C_0) + \lambda C_0 = S & \text{in } ]0, T[ \times \Omega, \\ \Theta_0 = 0 & \text{on } \partial\Omega, \\ C_0(0, \cdot) = C_{\text{init}} & \text{in } \Omega, \\ C_0 = 0 & \text{on } ]0, T[ \times \partial\Omega, \end{cases} \quad (2.5)$$

where  $K^*$  is a constant matrix, and  $D^*(x)$  is a function of  $\nabla \Theta_0(x)$  which we define below. To this aim we need to introduce auxiliary quantities. For all  $i \in \{1, \dots, d\}$ , we let  $\varphi_i$  denote the unique periodic weak solution in  $H_{\#}^1(\mathbb{Y})$  to

$$-\nabla \cdot K(\mathbf{e}_i + \nabla \varphi_i) = 0. \quad (2.6)$$

The matrix  $K^*$  is strongly elliptic and characterized by: for all  $i, j \in \{1, \dots, d\}$

$$\mathbf{e}_j \cdot K^* \mathbf{e}_i = \int_{\mathbb{Y}} (\mathbf{e}_j + \nabla \varphi_j) \cdot K (\mathbf{e}_i + \nabla \varphi_i). \quad (2.7)$$

This allows to uniquely define the function  $\Theta_0$  through the homogenized Darcy equation (2.5)<sub>1,2</sub>. The homogenized drift is then given by

$$U_0 = -K^* \nabla \Theta_0.$$

It remains to define  $D^*$ . Let  $\tilde{U}, \tilde{D}$  be defined on  $\Omega \times \mathbb{Y}$  as follows:

$$\tilde{U}(x, y) = -K(y)(\mathbb{I} + \nabla \varphi(y)) \nabla \Theta_0(x), \quad (2.8)$$

$$\tilde{D}(x, y) = D_0(x) + \alpha |\tilde{U}(x, y)| \mathbb{I} + \beta \frac{\tilde{U}(x, y) \otimes \tilde{U}(x, y)}{|\tilde{U}(x, y)|} = D_0(x) + \mathbb{D}(\tilde{U}(x, y)), \quad (2.9)$$

where  $\varphi = (\varphi_1, \dots, \varphi_d)$ . For all  $i \in \{1, \dots, d\}$  and a. e.  $x \in \Omega$ , we let  $\Phi_i(x, \cdot)$  denote the unique periodic weak solution in  $H_{\#}^1(\mathbb{Y})$  to the elliptic equation parametrized by  $x$ :

$$-\nabla_y \cdot \tilde{D}(x, y)(\mathbf{e}_i + \nabla_y \Phi_i(x, y)) = 0.$$

The homogenized coefficients  $D^*$  are then characterized by: for all  $x \in \Omega$  and all  $i, j \in \{1, \dots, d\}$ ,

$$\mathbf{e}_j \cdot D^*(x) \mathbf{e}_i = \int_{\mathbb{Y}} (\mathbf{e}_j + \nabla_y \Phi_j(x, y)) \cdot \tilde{D}(x, y)(\mathbf{e}_i + \nabla_y \Phi_i(x, y)) dy. \quad (2.10)$$

Although the diffusion  $D^*$  is not of the form (2.2), for all  $x \in \Omega$ ,  $D^*(x)$  only depends on  $\nabla \Theta_0(x)$ , and  $D^* \in L^2(\Omega)$ . Hence existence and uniqueness of weak solutions for the homogenized system can be proved the same way as for Theorem 1, and we leave the details to the reader. From the homogenization point of view, Theorem 2 is a rather direct application of two-scale convergence and Theorem 1. Although  $D(U)$  is unbounded, it is square-integrable and the homogenized system remains elliptic-parabolic (for the homogenization of elliptic equations with unbounded coefficients which are not equi-integrable, nonlocal effects may appear, and we refer the reader to [5] and [11]). In the case of strong coupling, homogenization has been proved in [18]. Yet [18] is an overkill for the problem under consideration (uniqueness is not discussed in [18] though), and we display the main arguments of a simpler proof in Appendix A.

**Remark 2.1.** In this statement we have considered only the case of a purely periodic oscillating matrix  $K$ . Note that, even in this simple case, the matrix  $\tilde{D}$  depends on both the slow variable  $x \in \Omega$  and the fast variable  $y \in \mathbb{Y}$ . The result generalizes readily to the case of a modulated matrix  $K(x, x/\varepsilon)$ . Similarly, oscillating source terms and diffusion coefficients  $D_0$ , depending on  $x$  and  $x/\varepsilon$ , can be considered.

Since the specific feature of the coupled model under investigation is the uniqueness of weak solutions, we prove Theorem 1 in detail in the following subsection.

**2.2. Proof of Theorem 1.** The difference with respect to previous contributions on the strongly coupled system is the fact that weak solutions can be proved to be unique for the weakly coupled system. The only subtle feature of the system is the integrability condition on  $D$  and  $U$ , which are square-integrable but not necessarily essentially bounded. The proof is based on regularization and compactness arguments. We shall only prove the uniqueness of weak solutions in detail.



For the reader convenience we quickly sketch the proof of existence of weak solutions as well. We divide the proof into six steps, and proceed by regularization. In the first step we recall a standard result essentially due to J.-L. Lions. In the second step we introduce the regularizations for  $U$  and  $D(U)$ . In the third step we apply Step 1 and derive a priori estimates. In Step 4 from these a priori estimates we deduce by compactness and Aubin-Simon's arguments that the weakly coupled system admits a distributional solution. We then show in Step 5 that this solution satisfies a weak formulation of the equation. We prove uniqueness of weak solutions in Step 6.

*Step 1.* Case of bounded coefficients and drifts.

Let  $D : \Omega \rightarrow \mathcal{M}_d(\mathbb{R})$  be uniformly bounded and strongly elliptic, and  $U \in L^\infty(\Omega, \mathbb{R}^d)$ . We consider the equation

$$\begin{cases} \partial_t C - \nabla \cdot (D \nabla C - UC) + \lambda C = S & \text{in } ]0, T[ \times \Omega, \\ C(0, \cdot) = C_{\text{init}} & \text{in } \Omega, \\ C = 0 & \text{on } ]0, T[ \times \partial\Omega, \end{cases} \quad (2.11)$$

Then for all  $S \in L^2(0, T; H^{-1}(\Omega))$  and  $C_{\text{init}} \in L^2(\Omega)$  there exists a unique function  $C \in L^2(0, T; H_0^1(\Omega)) \cap C^0(0, T; L^2(\Omega))$  such that  $\partial_t C \in L^2(0, T; H^{-1}(\Omega))$ , which satisfies the weak form of (2.11): for all  $v \in L^2(0, T; H_0^1(\Omega))$  and all  $T > 0$ ,

$$\begin{aligned} \int_0^T \langle \partial_t C, v \rangle_{H^{-1}, H_0^1} + \int_0^T \int_\Omega \nabla v \cdot D \nabla C - \int_0^T \int_\Omega CU \cdot \nabla v \\ + \lambda \int_0^T \int_\Omega Cv = \int_0^T \langle S, v \rangle_{H^{-1}, H_0^1}. \end{aligned}$$

Note that by an exponential change of time, one may assume  $\lambda$  to be as large as desired (which then ensures the coercivity of the bilinear form). We refer the reader to [31, Chapter 12] for details. In the sequel we shall use the following equivalent weak formulation: for all  $v \in L^2(0, T; H_0^1(\Omega))$  and all  $T > 0$ ,

$$\begin{aligned} \int_0^t \langle \partial_t C, v \rangle_{H^{-1}, H_0^1} + \int_0^t \int_\Omega \nabla v \cdot D \nabla C + \int_0^t \int_\Omega \nabla C \cdot Uv \\ + \int_0^t \int_\Omega (q + \lambda)Cv = \int_0^t \langle S, v \rangle_{H^{-1}, H_0^1}, \end{aligned} \quad (2.12)$$

which we obtain by using the divergence theorem and the identity  $\nabla \cdot U = q$ .

*Step 2.* Regularizations.

First note that the elliptic part of the system

$$\begin{cases} U = -K \nabla \Theta & \text{in } \Omega, \\ \nabla \cdot U = q & \text{in } \Omega, \\ \Theta = 0 & \text{on } \partial\Omega, \end{cases} \quad (2.13)$$

admits a unique weak solution  $\Theta \in H_0^1(\Omega)$ . The associated drift  $U = -K \nabla \Theta$  is not essentially bounded, but square-integrable. Likewise the associated diffusion coefficients  $D(U)$  are not essentially bounded, but square-integrable. In particular, the advection-diffusion equation

$$\begin{cases} \partial_t C - \nabla \cdot (D(U) \nabla C - UC) + \lambda C = S & \text{in } ]0, T[ \times \Omega, \\ C(0, \cdot) = C_{\text{init}} & \text{in } \Omega, \\ C = 0 & \text{on } ]0, T[ \times \partial\Omega, \end{cases} \quad (2.14)$$

does not satisfy the assumptions of Step 1. We regularize  $D(U)$  and  $U$ , and begin with the diffusion coefficients. Since  $D(U)$  is a symmetric matrix, for a. e.  $x \in \Omega$  there exist  $\alpha_1(x), \dots, \alpha_d(x) \geq 0$ , and a unitary matrix  $P(x)$  such that  $D(U)(x) = P^T(x)\text{diag}(\alpha_1(x), \dots, \alpha_d(x))P(x)$ . For all  $M > 0$  and a. e.  $x \in \Omega$ , we define  $D^M(x)$  as follows:

$$D^M(x) := P^T(x)\text{diag}(\min\{\alpha_1(x), M\}, \dots, \min\{\alpha_d(x), M\})P(x).$$

In particular,  $D^M$  converges monotonically to  $D(U)$  in  $L^2(\Omega)$  as  $M \rightarrow \infty$ . For the regularization of  $U$ , we prefer to regularize the defining equation  $\nabla \cdot U = q$  rather than using truncation. We consider  $K^M$  and  $q^M$  two sequences of smooth functions such that  $K^M$  and  $q^M$  converge to  $K$  and  $q$  in  $L^r(\Omega)$  for all  $r < \infty$ , respectively. We define  $\Theta^M$  as the unique weak solution in  $H_0^1(\Omega)$  to

$$-\nabla \cdot (K^M \nabla \Theta^M) = q^M,$$

and set  $U^M := -K^M \nabla \Theta^M$ . By elliptic regularity,  $U^M$  belongs to  $L^\infty(\Omega)$ . Furthermore,  $U^M$  converges to  $U$  in  $L^2(\Omega)$  (the argument relies on Meyers' estimate, which implies that  $\nabla \Theta^M$ , and thus  $U^M$ , converge in  $L^p(\Omega)$  for some  $p > 2$  depending only on the constant  $\Lambda$ ).

Hence, for all  $M > 0$ , Step 1 implies there exists a unique weak solution  $C^M \in L^2(0, T; H_0^1(\Omega)) \cap C^0(0, T; L^2(\Omega))$  such that  $\partial_t C^M \in L^2(0, T; H^{-1}(\Omega))$  to the regularized equation

$$\begin{cases} \partial_t C^M - \nabla \cdot (D^M \nabla C^M - U^M C^M) + \lambda C^M = S & \text{in } ]0, T[ \times \Omega, \\ C^M(0, \cdot) = C_{\text{init}} & \text{in } \Omega, \\ C^M = 0 & \text{on } ]0, T[ \times \partial\Omega. \end{cases} \quad (2.15)$$

It remains to pass to the limit as  $M \rightarrow \infty$ .

*Step 3.* A priori estimates.

The weak form of (2.15) with test-function  $C^M$  itself yields for all  $0 < t \leq T$ ,

$$\begin{aligned} \int_0^t \langle \partial_t C^M, C^M \rangle_{H^{-1}, H_0^1} + \int_0^t \int_\Omega \nabla C^M \cdot D^M \nabla C^M - \int_0^t \int_\Omega C^M U^M \cdot \nabla C^M \\ + \lambda \int_0^t \int_\Omega (C^M)^2 = \int_0^t \langle S, C^M \rangle_{H^{-1}, H_0^1}. \end{aligned}$$

Since  $\nabla \cdot U^M = q^M$ , we have by the divergence theorem

$$-\int_0^t \int_\Omega C^M U^M \cdot \nabla C^M = -\frac{1}{2} \int_0^t \int_\Omega U^M \cdot \nabla (C^M)^2 = \frac{1}{2} \int_0^t \int_\Omega q(C^M)^2$$

so that the weak form turns into

$$\begin{aligned} \frac{1}{2} \int_\Omega (C^M(\cdot, t))^2 + \int_0^t \int_\Omega \nabla C^M \cdot D^M \nabla C^M \\ + \int_0^t \int_\Omega (C^M)^2 \left( \frac{1}{2} q^M + \lambda \right) = \frac{1}{2} \int_\Omega C_{\text{init}}^2 + \int_0^t \langle S, C^M \rangle_{H^{-1}, H_0^1}. \end{aligned}$$

Recalling that one may take  $\lambda$  such that  $\frac{1}{2} \inf q^M + \lambda \geq \frac{1}{2} \inf q + \lambda = \lambda^* > 0$ , we finally deduce by coercivity of  $D^M$  (and arbitrariness of  $t$ ):

$$\begin{aligned} \frac{1}{2} \sup_{0 < t \leq T} \int_{\Omega} (C^M(\cdot, t))^2 + \Lambda^{-1} \|\nabla C^M\|_{L^2(0, T; L^2(\Omega))}^2 + \lambda^* \|C^M\|_{L^2(0, T; L^2(\Omega))}^2 \\ \leq \|S\|_{L^2(0, T; H^{-1}(\Omega))} \|C^M\|_{L^2(0, T; H_0^1(\Omega))} + \frac{1}{2} \|C_{\text{init}}\|_{L^2(\Omega)}^2. \end{aligned}$$

Using this estimate and the equation again, we finally obtain that  $C^M$  is bounded in  $L^2(0, T; H_0^1(\Omega)) \cap L^\infty(0, T; L^2(\Omega))$  and that  $\partial_t C^M$  is bounded in  $L^2(0, T; H^{-1}(\Omega))$ , uniformly in  $M$ .

*Step 4. Compactness and existence of distributional solutions.*

By weak compactness and Aubin-Simon's theorem (see [33]), there exists a function  $C \in L^2(0, T; H_0^1(\Omega)) \cap C^0(0, T; L^2(\Omega))$  with  $\partial_t C \in L^2(0, T; H^{-1}(\Omega))$  such that  $C^M$  converges weakly to  $C$  in  $L^2(0, T; H_0^1(\Omega))$ , strongly in  $L^2(0, T; L^2(\Omega))$ , and such that  $\partial_t C^M$  converges weakly to  $\partial_t C$  in  $L^2(0, T; H^{-1}(\Omega))$ .

It is easy matter to check that  $C$  solves (2.14) in the sense of distributions, and satisfies the initial condition as a continuous function in time taking values in  $L^2(\Omega)$ .

*Step 5. Weak formulation of the system.*

In this step, we shall prove that  $(\Theta, C)$  is a weak solution of (2.1)–(2.3) in the sense of Definition 2.1. We start by showing that  $\int_0^T \int_{\Omega} \nabla C \cdot D(U) \nabla C < \infty$ , which is not obvious a priori since  $\nabla C \in L^2(\Omega)$  and  $D(U) \in L^2(\Omega)$ . Let  $M' > 0$  be fixed. By weak lower-semicontinuity, since  $\nabla C^M$  converges weakly to  $\nabla C$  in  $L^2(0, T; L^2(\Omega))$ ,

$$\int_0^T \int_{\Omega} \nabla C \cdot D^{M'} \nabla C \leq \liminf_{M \rightarrow \infty} \int_0^T \int_{\Omega} \nabla C^M \cdot D^{M'} \nabla C^M.$$

Since  $M \mapsto D^M$  is an increasing function in the sense of symmetric matrices, the a priori estimate of Step 3 implies for all  $M \geq M'$ ,

$$\int_0^T \int_{\Omega} \nabla C^M \cdot D^{M'} \nabla C^M \leq \int_0^T \int_{\Omega} \nabla C^M \cdot D^M \nabla C^M \leq \|C_{\text{init}}\|_{L^2(\Omega)}^2 + \|S\|_{L^2(0, T; H^{-1}(\Omega))}^2.$$

Hence,

$$\int_0^T \int_{\Omega} \nabla C \cdot D^{M'} \nabla C \leq \|C_{\text{init}}\|_{L^2(\Omega)}^2 + \|S\|_{L^2(0, T; H^{-1}(\Omega))}^2,$$

and the desired estimate

$$\int_0^T \int_{\Omega} \nabla C \cdot D(U) \nabla C \leq \|C_{\text{init}}\|_{L^2(\Omega)}^2 + \|S\|_{L^2(0, T; H^{-1}(\Omega))}^2$$

follows from the monotone convergence theorem as  $M' \rightarrow \infty$ , using again the monotonicity of  $M \mapsto D^M$ .

Let  $v \in L^2(0, T; H_0^1(\Omega)) \cap L^2(0, T; L^\infty(\Omega))$  be such that  $\int_0^T \int_{\Omega} \nabla v \cdot D(U) \nabla v < \infty$ . In order to prove that  $C$  is a weak solution, we need to pass to the limit as  $M \rightarrow \infty$  in

the weak formulation (2.12) for  $C^M$ , that is,

$$\begin{aligned} \int_0^t \langle \partial_t C^M, v \rangle_{H^{-1}, H_0^1} + \int_0^t \int_{\Omega} \nabla v \cdot D^M \nabla C^M + \int_0^t \int_{\Omega} \nabla C^M \cdot U^M v \\ + \int_0^t \int_{\Omega} (q + \lambda) C^M v = \int_0^t \langle S, v \rangle_{H^{-1}, H_0^1}. \end{aligned}$$

In view of the regularity of  $v$ , the convergence of  $U^M$  to  $U$  in  $L^2(\Omega)$ , and the weak compactness of  $C^M$  obtained in Step 4, the only nontrivial term to treat is the second-order term, and we shall prove that

$$\lim_{M \rightarrow \infty} \int_0^T \int_{\Omega} \nabla v \cdot D^M \nabla C^M = \int_0^T \int_{\Omega} \nabla v \cdot D(U) \nabla C.$$

Let  $M' > 0$  be fixed. We rewrite the above term as

$$\int_0^T \int_{\Omega} \nabla v \cdot D^M \nabla C^M = \int_0^T \int_{\Omega} \nabla v \cdot (D^M - D^{M'}) \nabla C^M + \int_0^T \int_{\Omega} \nabla v \cdot D^{M'} \nabla C^M. \quad (2.16)$$

We focus on the second term of the r. h. s. and first take the limit as  $M \rightarrow \infty$ . Since  $D^{M'}$  is bounded, this yields

$$\lim_{M \rightarrow \infty} \int_0^T \int_{\Omega} \nabla v \cdot D^{M'} \nabla C^M = \int_0^T \int_{\Omega} \nabla v \cdot D^{M'} \nabla C.$$

We conclude by the dominated convergence theorem that

$$\lim_{M' \rightarrow \infty} \lim_{M \rightarrow \infty} \int_0^T \int_{\Omega} \nabla v \cdot D^{M'} \nabla C^M = \int_0^T \int_{\Omega} \nabla v \cdot D(U) \nabla C$$

since by Young's inequality and monotonicity of  $M \mapsto D^M$ ,

$$|\nabla v \cdot D^{M'} \nabla C| \leq \frac{1}{2} (\nabla v \cdot D(U) \nabla v + \nabla C \cdot D(U) \nabla C),$$

which is integrable.

It remains to prove that the first term of the r. h. s. of (2.16) vanishes as  $M'$  and  $M$  go to infinity. By Cauchy-Schwarz inequality and monotonicity of  $M \mapsto D^M$ , we have

$$\begin{aligned} \left| \int_0^T \int_{\Omega} \nabla v \cdot (D^M - D^{M'}) \nabla C^M \right| \\ \leq \left( \int_0^T \int_{\Omega} \nabla v \cdot (D - D^{M'}) \nabla v \right)^{1/2} \left( \int_0^T \int_{\Omega} \nabla C^M \cdot D^M \nabla C^M \right)^{1/2}. \end{aligned}$$

The second factor of the r. h. s. is bounded by Step 3 uniformly in  $M$ . We therefore focus on the first factor. Since  $D - D^{M'} \leq D$  in the sense of symmetric matrices and  $\nabla v \cdot D \nabla v \in L^1(\Omega)$ , the dominated convergence theorem yields

$$\lim_{M' \rightarrow \infty} \int_0^T \int_{\Omega} \nabla v \cdot (D - D^{M'}) \nabla v = 0,$$

and therefore

$$\lim_{M' \rightarrow \infty} \limsup_{M \rightarrow \infty} \left| \int_0^T \int_{\Omega} \nabla v \cdot (D^M - D^{M'}) \nabla C^M \right| = 0,$$

which concludes the proof of this step.

*Step 6.* Uniqueness of weak solutions.

Since equation (2.14) is linear with respect to  $C$ , uniqueness follows formally from the weak formulation tested with the solution  $C$  itself. However, we cannot directly proceed this way since  $C \notin L^2(0, T; L^\infty(\Omega))$  a priori and it is not clear whether it can be used as an admissible test function. Instead we use a standard truncation argument: for all  $N > 0$  we define a function  $\varphi_N : \mathbb{R} \rightarrow \mathbb{R}$  as

$$\varphi_N(x) := \begin{cases} -N & \text{for } x < -N, \\ x & \text{for } |x| \leq N, \\ N & \text{for } x > N, \end{cases}$$

and we test the weak formulation of (2.14) with  $C_N := \varphi_N(C) \in L^2(0, T; H_0^1(\Omega)) \cap L^\infty((0, T) \times \Omega)$ . This yields

$$\begin{aligned} \int_0^T \langle \partial_t C, C_N \rangle_{H^{-1}, H_0^1} + \int_0^T \int_\Omega \nabla C_N \cdot D(U) \nabla C + \int_0^T \int_\Omega C_N U \cdot \nabla C \\ + \int_0^T \int_\Omega C C_N (q + \lambda) = \int_0^T \langle S, C_N \rangle_{H^{-1}, H_0^1}. \end{aligned} \quad (2.17)$$

It is easy to prove that  $C_N \rightarrow C$  in  $L^2(0, T; H^1(\Omega))$  as  $N \rightarrow \infty$  so that we can pass to the limit in the first and last terms of the l. h. s. and in the r. h. s. of (2.17). It remains to treat the last two terms. We begin with the Dirichlet form. By definition of  $\varphi_N$  and  $C_N$ ,

$$\nabla C_N \cdot D(U) \nabla C = \nabla C \cdot D(U) \nabla C 1_{|C| \leq N} \leq \nabla C \cdot D(U) \nabla C.$$

Hence, the dominated convergence theorem yields

$$\lim_{N \rightarrow \infty} \int_0^T \int_\Omega \nabla C_N \cdot D(U) \nabla C = \int_0^T \int_\Omega \nabla C \cdot D(U) \nabla C.$$

We now turn to the third term of the l. h. s. of (2.17), which we treat together with the term involving  $q$ . In particular since  $\nabla \cdot U = q$ , the divergence theorem yields

$$\int_0^T \int_\Omega C_N U \cdot \nabla C + \int_0^T \int_\Omega C C_N q = - \int_0^T \int_\Omega C U \cdot \nabla C_N.$$

Note that by definition of  $\varphi_N$  and  $C_N$  we can rewrite this identity as

$$\int_0^T \int_\Omega C_N U \cdot \nabla C + \int_0^T \int_\Omega C C_N q = - \int_0^T \int_\Omega C_N U \cdot \nabla C_N.$$

Using that  $\nabla \cdot U = q$  and the divergence theorem again, this turns into

$$\begin{aligned} \int_0^T \int_\Omega C_N U \cdot \nabla C + \int_0^T \int_\Omega C C_N q &= - \int_0^T \int_\Omega C_N U \cdot \nabla C_N \\ &= - \frac{1}{2} \int_0^T \int_\Omega U \cdot \nabla C_N^2 \\ &= \frac{1}{2} \int_0^T \int_\Omega q C_N^2. \end{aligned}$$

Passing to the limit in the last identity yields

$$\lim_{N \rightarrow \infty} \left( \int_0^T \int_\Omega C_N U \cdot \nabla C + \int_0^T \int_\Omega C C_N q \right) = \frac{1}{2} \int_0^T \int_\Omega q C^2.$$

Gathering the results of this step, we obtain the following identity:

$$\begin{aligned} \frac{1}{2} \int_{\Omega} C^2(T, \cdot) + \int_0^T \int_{\Omega} \nabla C \cdot D(U) \nabla C \\ + \int_0^T \int_{\Omega} C^2 \left( \frac{1}{2} q + \lambda \right) = \int_0^T \langle S, C \rangle_{H^{-1}, H_0^1} + \frac{1}{2} \int_{\Omega} C_{\text{init}}^2, \end{aligned}$$

since  $\int_0^T \langle \partial_t C, C \rangle_{H^{-1}, H_0^1} = \frac{1}{2} \int_{\Omega} C^2(T, \cdot) - \frac{1}{2} \int_{\Omega} C^2(0, \cdot)$ . This implies uniqueness of weak solutions, and concludes the proof of Theorem 1.

### 3. NUMERICAL APPROXIMATION OF THE HOMOGENIZED SYSTEM

In this section we propose a numerical strategy to approximate the weak solution to the homogenized system (2.5). There are essentially three steps to solve (2.5):

- (1) the computation of  $K^*$  and the approximation of  $\Theta_0$ . The latter is solution of a standard elliptic equation once  $K^*$  is known, see (2.5)<sub>1,2</sub>.
- (2) the approximation of  $D^*(x)$  at every Gauss point  $x$  of  $\Omega$ . This requires to solve a family of elliptic equations on the periodic cell  $\mathbb{Y}$ , parametrized by the Gauss points  $x$  via  $\nabla \Theta_0(x)$ .
- (3) To find the solution of the advection-diffusion equation (2.5)<sub>3</sub>.

As we shall see, the bottleneck of the numerical approximation of (2.5) in terms of computational cost is the approximation of  $D^*$  in the second step. A large part of this section is dedicated to this problem, and we shall use a reduced basis approach to drastically reduce this computational cost. We have chosen not to focus on the numerical strategy to solve the advection-diffusion equation (2.5)<sub>3</sub> since the equation is rather “standard” once  $D^*$  is known. In particular, for the numerical tests of the coupled system we use a naive  $\mathbb{P}_1$ -finite element method in space combined with the implicit Euler method in time. For more efficient and modern methods, we refer the reader to [32, 21, 22, 34, 35, 13, 14]. The main contribution of this section (a numerical method for the computation of  $D^*$ ) can indeed be combined with any strategy to solve the advection-diffusion equation (2.5)<sub>3</sub>.

In the first subsection we present a direct approach to solve (2.5), and complement the homogenization result of Theorem 2 by numerical tests showing the rate of convergence of  $(\Theta_\varepsilon, C_\varepsilon)$  towards  $(\Theta_0, C_0)$ . As expected, the computational time to approximate  $D^*$  becomes rapidly prohibitive as the number of discretization points increases. In the second subsection we turn to the RB method. We first quickly recall the rationale of the approach, and discuss what can be expected in terms of convergence. We then turn to the practical implementation of the method, propose an a posteriori estimator adapted to homogenization problems (but not limited to the specific one treated here), and present an original and effective way of fast-assembling of the RB matrix, which is the major difficulty encountered in the RB method when the dependence of the diffusion matrix upon the parameter is not affine — as it is the case here.

Before we turn to the core of this section let us point out that, as the attentive reader may have already noticed, it is not clear a priori that the finite element method converges since the diffusion matrix in (2.5)<sub>3</sub> is unbounded. The method does indeed converge to the expected solution. This property can be proved along the lines of the existence-uniqueness theory developed in Section 2.

### 3.1. Direct approach.

3.1.1. *Space and time discretizations.* We discretize the homogenized problem (2.5) with a finite element method in space and the implicit Euler scheme in time. Let  $T_{\Omega, h_0}$  and  $T_{\mathbb{Y}, h_1}$  be regular tessellations of  $\Omega$  and of  $\mathbb{Y}$ , respectively, into  $d$ -simplices of meshsizes  $h_0, h_1 > 0$ . We denote by  $\mathcal{V}_{\Omega, h_0}^k$  the space of  $\mathbb{P}_k$  finite elements associated with  $T_{\Omega, h_0}$  for  $k = 0$  and 1 (for  $k = 1$ , we only consider functions which vanish on the boundary), and by  $\mathcal{V}_{\mathbb{Y}, h_1}^1$  (resp.  $\mathcal{V}_{\mathbb{Y}, h_1}^0$ ) the subspace of  $H_{\#}^1(\mathbb{Y})$  (resp.  $L^2(\mathbb{Y})$ ) made of  $\mathbb{P}_1$ -periodic (resp.  $\mathbb{P}_0$ ) finite elements associated with  $T_{\mathbb{Y}, h_1}$ . As quickly mentioned above, a natural strategy to solve (2.5) is as follows:

**Algorithm 1.** (1) Numerical approximation  $K_{h_1}^*$  of  $K^*$ : compute for all  $k \in \{1, \dots, d\}$  Galerkin approximations  $\varphi_k^{h_1}$  of  $\varphi_k$  in  $\mathcal{V}_{\mathbb{Y}, h_1}^1$  defined by: For all  $\psi \in \mathcal{V}_{\mathbb{Y}, h_1}^1$

$$\int_{\mathbb{Y}} \nabla \psi \cdot K(\mathbf{e}_k + \nabla \varphi_k^{h_1}) = 0. \quad (3.1)$$

Define then for all  $k, l \in \{1, \dots, d\}$ ,

$$\mathbf{e}_l \cdot K_{h_1}^* \mathbf{e}_k = \int_{\mathbb{Y}} (\mathbf{e}_l + \varphi_l^{h_1}) \cdot K(\mathbf{e}_k + \nabla \varphi_k^{h_1}).$$

For future reference, we set  $\varphi^{h_1} = (\varphi_1^{h_1}, \dots, \varphi_d^{h_1}) \in H_{\#}^1(\mathbb{Y}, \mathbb{R}^d)$ .

(2) Compute the Galerkin approximation  $\Theta_0^{h_0} \in \mathcal{V}_{\Omega, h_0}^1$  of the solution to (2.5)<sub>1,2,4</sub> with  $K_{h_1}^*$  in place of  $K^*$ , unique solution in  $\mathcal{V}_{\Omega, h_0}^1$  to: for all  $w \in \mathcal{V}_{\Omega, h_0}^1$ ,

$$\int_{\Omega} \nabla w \cdot K_{h_1}^* \nabla \Theta_0^{h_0} = \int_{\Omega} qw.$$

It defines  $U_0^{h_0} = -K_{h_1}^* \nabla \Theta_0^{h_0}$ , too.

(3) Approximation  $D_{h_0}^* \in \mathcal{V}_{\Omega, h_0}^0$  (each entry of the matrix is piecewise constant on  $T_{\Omega, h_0}$ ) of the homogenized diffusion  $D^*$ . Let  $\Pi_{\mathcal{V}_{\Omega, h_0}^0}$  denote the  $L^2$ -projection onto  $\mathcal{V}_{\Omega, h_0}^0$ . For every element  $T$  of the tessellation  $T_{\Omega, h_0}$ ,  $\nabla \Theta_0^{h_0}|_T$  is constant, and we define  $D_{h_0}^*|_T$  as follows: for all  $k, l \in \{1, \dots, d\}$ ,

$$\mathbf{e}_l \cdot D_{h_0}^*|_T \mathbf{e}_k = \int_{\mathbb{Y}} (\mathbf{e}_l + \nabla \Phi_l^{h_1}|_T) \cdot \tilde{D}^{h_1}|_T (\mathbf{e}_k + \nabla \Phi_k^{h_1}|_T),$$

where

$$\begin{aligned} \tilde{D}^{h_1}|_T(y) &:= \Pi_{\mathcal{V}_{\Omega, h_0}^0} D_0|_T + \mathbb{D}(\tilde{U}^{h_1}|_T(y)), \\ \tilde{U}^{h_1}|_T(y) &:= -K(y)(\mathbb{I} + \nabla \varphi^{h_1}(y)) \nabla \Theta_0^{h_0}|_T, \end{aligned}$$

and  $\Phi_k^{h_1}|_T \in \mathcal{V}_{\mathbb{Y}, h_1}^1$  is the unique periodic weak solution to: for all  $\Psi \in \mathcal{V}_{\mathbb{Y}, h_1}^1$ ,

$$\int_{\mathbb{Y}} \nabla \Psi \cdot \tilde{D}^{h_1}|_T (\mathbf{e}_k + \nabla \Phi_k^{h_1}|_T) = 0. \quad (3.2)$$

(4) Approximation of  $C_0$ . Let  $N \in \mathbb{N}^*$ . The time interval  $[0, T]$  is uniformly discretized with a fixed time step  $\Delta t = \frac{T}{N}$ . For all  $n \in \{0, \dots, N\}$ , we set  $t_n = n\Delta t$ , and

define the approximation  $C_0^{\text{h}_0, n} \in \mathcal{V}_{\Omega, \text{h}_0}^1$  of  $C_0(t_n, \cdot)$  by induction as the unique solution to: for all  $v \in \mathcal{V}_{\Omega, \text{h}_0}^1$ ,

$$\int_{\Omega} \frac{C_0^{\text{h}_0, n+1} - C_0^{\text{h}_0, n}}{\Delta t} + \int_{\Omega} \nabla v \cdot (D_{\text{h}_0}^* \nabla C_0^{\text{h}_0, n+1} - U_0^{\text{h}_0} C_0^{\text{h}_0, n+1}) + \int_{\Omega} \lambda C_0^{\text{h}_0, n+1} v = \int_{\Omega} S^{n+1} v.$$

Since we use an implicit time discretization, there is no CFL condition — note that we could have used a semi-implicit scheme as well (see for instance [31]).

**3.1.2. Numerical tests.** To illustrate Theorem 2 when the homogenized system is solved using the direct approach of Algorithm 1, we consider a numerical test suggested by ANDRA<sup>1</sup>. We take  $d = 2$  and let  $\Omega = ]0, 2[^2$  be a square domain, and  $[0, T]$  be the time interval with  $T = 1$ . The permeability is defined on the domain  $\mathbb{Y} = ]0, 1[^2$  by:

$$\forall y = (y_1, y_2) \in \mathbb{Y}, \forall y_1 \in ]0, 1[, K(y_1, y_2) = \begin{cases} 4.94064, & \text{if } y_2 \geq 0.5, \\ 0.57816, & \text{if } y_2 < 0.5. \end{cases}$$

We consider boundary conditions which are slightly different than in Theorem 2 and Algorithm 1 — note that the adaptations are straightforward in both cases — :

$$\left\{ \begin{array}{l} \text{Dirichlet boundary conditions: Let } x = (x_1, x_2) \in \partial\Omega \\ \text{For } x_1 \in (0, 2), h_0(x_1, x_2) = \begin{cases} \frac{5}{3}, & \text{if } x_2 = 2, \\ \frac{5}{3} + 0.5, & \text{if } x_2 = 0, \end{cases} \\ \text{For } x_2 \in (0, 2), C_0(x_1, x_2) = \begin{cases} 1, & \text{if } x_1 = 0, \\ 0, & \text{if } x_1 = 2. \end{cases} \\ \text{Homogeneous Neumann boundary conditions elsewhere.} \end{array} \right. \quad (3.3)$$

The parameters used in the numerical tests are gathered in Table 1.

$T = 1$	$D_0 = 4.38 \text{ II}$	$\alpha = \frac{2}{10}$	$\beta = \frac{2}{100}$	$\lambda = \frac{\ln(2)}{1.57}$	$\Delta t = 10^{-3}$
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TABLE 1. Parameters

In Table 2 we compare the approximations  $(\Theta_{\varepsilon}^{\text{h}_1}, C_{\varepsilon}^{\text{h}_1})$  of the solutions to the heterogeneous system (2.4) to the approximation  $(\Theta_0^{\text{h}_0}, C_0^{\text{h}_0})$  of the solution to the homogenized system (2.5), for several values of  $\varepsilon$  (the discretization parameters  $\text{h}_1$  and  $\text{h}_0$  being fixed). The periodic cell  $\mathbb{Y}$  is discretized with 8 elements per dimension (note that the correctors  $\varphi_1$  and  $\varphi_2$  happen to belong to the finite element space  $\mathcal{V}_{\mathbb{Y}, \text{h}_1}^1$  in the case treated here because of the laminate structure of  $K$ ), and the macroscopic domain  $\Omega$  is discretized using  $2 \times 8/\varepsilon$  elements per dimension to compute  $(\Theta_{\varepsilon}^{\text{h}_1}, C_{\varepsilon}^{\text{h}_1})$ . For the approximation of  $(\Theta_0^{\text{h}_0}, C_0^{\text{h}_0})$ , we take  $\text{h}_0 = 1/100$ . This yields

- $\mathcal{V}_{\mathbb{Y}, \text{h}_1}^1$  has dimension 81;
- $\mathcal{V}_{\Omega, \text{h}_0}^1$  has dimension  $\sim 40000$ ;
- $\mathcal{V}_{\Omega, \text{h}_0, \varepsilon}^1$  has dimension  $\sim 256\varepsilon^{-2}$ .

<sup>1</sup>Agence nationale pour la gestion des déchets radioactifs — <http://www.andra.fr>



We display in Table 2 the  $L^2(\Omega)$  norm of the error  $\Theta_0^{h_0} - \Theta_\varepsilon^{h_1}$  and the  $L^2(\Omega \times ]0, T])$ -norm of the error  $C_0^{h_0} - C_\varepsilon^{h_1}$  for  $\varepsilon \in \{0.2, 0.1, 0.05, 0.025\}$ . These results have been obtained using `FreeFem++` (see [27]). The linear systems are solved with a direct solver. We obtain a first order of convergence for both errors.

$\varepsilon$	$\frac{\ h_0^{h_0} - h_\varepsilon^{h_1}\ _{L^2}}{\ h_0^{h_0}\ _{L^2}}$	Rate	$\frac{\ C_0^{h_0} - C_\varepsilon^{h_1}\ _{L^2(L^2)}}{\ C_0^{h_0}\ _{L^2(L^2)}}$	Rate
0.2	1.667e-3	-	5.528e-4	-
0.1	8.095e-4	1.04	2.525e-4	1.13
0.05	3.992e-4	1.02	1.270e-4	0.99
0.025	1.983e-4	1.01	6.704e-5	0.92

TABLE 2. Error in function of  $\varepsilon$

As can be seen on Table 2 the apparent convergence rates are of order 1, which is consistent with a formal two-scale expansion, and shows the interest of replacing  $(\Theta_\varepsilon, C_\varepsilon)$  by its homogenized counterpart  $(h_0, C_0)$ . Although the computational time for the approximation of  $(\Theta_0, C_0)$  is much smaller than the computational time for the approximation of  $(\Theta_\varepsilon, C_\varepsilon)$  when  $\varepsilon$  is small, this method rapidly becomes prohibitive when the tessellation of  $\mathbb{Y}$  gets finer since the approximation of  $D^*$  then becomes quite expensive.

The last part of this article is devoted to the speed up of the approximation of  $D^*$ , with a numerical cost which should ideally be independent of the meshsize  $h_1$  of  $T_{\mathbb{Y}, h_1}$ . From now on we assume  $\tilde{D}$  in (2.9) to be a symmetric matrix (that is, we assume  $D^0$  to be symmetric).

**3.2. Reduced basis method for homogenization problems.** In this section we describe how to apply the reduced basis method to the homogenized problem under consideration, assuming in addition that  $D_0$  in (2.2) is a constant matrix.

**3.2.1. General presentation.** The reduced basis method was introduced for the accurate online evaluation of (outputs of) solutions to a parameter-dependent family of elliptic PDEs. The basis of the method and further references can be found in [28]. The application to the homogenization of elliptic equations is discussed in [10]. Abstractly, it can be viewed as a method to determine a “good”  $N$ -dimensional space  $\mathcal{S}_N$  to be used in approximating the elements of a set  $\mathcal{F} = \{(\overline{\Phi}_1(\xi), \dots, \overline{\Phi}_d(\xi)), \xi \in \mathcal{P}\}$  of parametrized elements lying in a Hilbert space  $\mathcal{S}$ , the parameter  $\xi$  ranging a certain subset  $\mathcal{P} \subset \mathbb{R}^n$ .

Let us describe how the computation of the effective coefficients we are concerned with belongs to such a framework. First of all, the auxiliary function  $\Theta_0$  is simply determined by solving the problem (2.5)<sub>1,2</sub>, with effective coefficients obtained by solving the cell equations (2.6). There is no difficulty in this step and  $\nabla_x \Theta_0$  can be considered as given in this discussion. Then, we write the effective coefficient (2.9) for the concentration equation (2.5)<sub>3</sub> as follows

$$\tilde{D}(x, y) = \widehat{\mathcal{D}}(\nabla_x \Theta_0(x))(y)$$

where  $\xi \in \mathbb{R}^d \mapsto \widehat{\mathcal{D}}(\xi) \in L^\infty(\mathbb{Y}, \mathcal{M}_d(\mathbb{R}))$  is defined by

$$\begin{aligned} \widehat{\mathcal{D}}(\xi)(y) &= D_0 + \alpha |M(y)\xi| \mathbb{I} + \beta \frac{M(y)\xi \otimes M(y)\xi}{|M(y)\xi|} = D_0 + \mathbb{D}(M(y)\xi), \\ M(y) &= K(y)(\mathbb{I} + \nabla\varphi(y)), \\ \varphi &= (\varphi_1, \dots, \varphi_d) \quad \text{solutions of (2.6)}. \end{aligned} \tag{3.4}$$

We recall that  $\alpha, \beta > 0$ , and  $D_0$  is a positive-definite symmetric matrix while  $M : \mathbb{Y} \rightarrow \mathcal{M}_d(\mathbb{R})$  is a square-integrable function. We are interested in the solution  $\overline{\Phi}_k(\xi)$  to the problem: for all  $\overline{\Psi} \in H_{\#}^1(\mathbb{Y})$ ,

$$\int_{\mathbb{Y}} \nabla \overline{\Psi}(y) \cdot \widehat{\mathcal{D}}(\xi)(y)(\mathbf{e}_k + \nabla \overline{\Phi}_k(\xi)(y)) \, dy = 0.$$

In the present context,  $\mathcal{S} = H_{\#}^1(\mathbb{Y})$  and we wish to find a convenient finite dimensional approximation space  $\mathcal{S}_N$  which allows to describe those solutions. The working plan faces the following technical difficulties:

- Here the parameter  $\xi$  ranges over the whole  $\mathbb{R}^d$  while the method is designed to deal with parameters lying in a compact set.
- The method simplifies significantly when the dependence of  $\mathcal{D}$  upon  $\xi$  is affine. In such a case it is described and analyzed in full details, but here the dependence with respect to the parameter is more intricate and the implementation of the method will require additional devices.
- The matrix  $M$  is square-integrable only and not essentially bounded, so that the available statements that could be useful to analyze the method simply do not apply.

We will go back to these issues later on; let us now introduce the basis of the RB method.

Let  $n \geq 1$  and let  $\mathcal{D} : \mathbb{R}^n \rightarrow L^\infty(\mathbb{Y}, \mathcal{M}_d(\mathbb{R}))$  be a function taking values in a set of ( $y \in \mathbb{Y}$ )-dependent  $d \times d$  symmetric real matrices, satisfying uniform bounds and elliptic estimates. We suppose that  $\mathcal{D}(\xi)$  depends continuously on the parameter  $\xi \in \mathbb{R}^n$ . Given a compact subset  $\overline{\mathcal{K}}$  of  $\mathbb{R}^n$ , we set  $\mathcal{F}_{\overline{\mathcal{K}}} = \{(\overline{\Phi}_1(\xi), \dots, \overline{\Phi}_d(\xi)), \xi \in \overline{\mathcal{K}}\}$ , where  $\overline{\Phi}_k(\xi) \in H_{\#}^1(\mathbb{Y})$  denotes the unique periodic weak solution to the problem: for all  $\overline{\Psi} \in H_{\#}^1(\mathbb{Y})$ ,

$$\int_{\mathbb{Y}} \nabla \overline{\Psi}(\xi)(y) \cdot \mathcal{D}(\xi)(y)(\mathbf{e}_k + \nabla \overline{\Phi}_k(\xi)(y)) \, dy = 0.$$

The set  $\mathcal{F}_{\overline{\mathcal{K}}}$  is therefore compact in  $H_{\#}^1(\mathbb{Y})$ .

To construct the  $N$ -finite dimensional space  $\mathcal{S}_N$  intended to approximate  $\mathcal{S} = H_{\#}^1(\mathbb{Y})$ , we proceed by induction using a greedy algorithm. To this aim we need a reliable estimator which measures the error between  $\overline{\Phi}_k(\xi)$  for some  $\xi \in \overline{\mathcal{K}}$  and its approximation  $\overline{\Phi}_k^j(\xi)$  in  $\mathcal{S}_j$  for  $0 \leq j \leq N$ , which is defined as the unique weak solution  $\overline{\Phi}_k^j(\xi) \in \mathcal{S}_j$  to: for all  $\overline{\Psi}^j \in \mathcal{S}_j$ ,

$$\int_{\mathbb{Y}} \nabla \overline{\Psi}^j(\xi)(y) \cdot \mathcal{D}(\xi)(y)(\mathbf{e}_k + \nabla \overline{\Phi}_k^j(\xi)(y)) \, dy = 0. \tag{3.5}$$

Recalling that we are dealing with a homogenization problem, the quantity of interest is the symmetric homogenized matrix  $\overline{D}^*(\xi)$  defined for all  $k, l \in \{1, \dots, d\}$  by (see (2.10))

$$\mathbf{e}_l \cdot \overline{D}^*(\xi) \mathbf{e}_k = \int_{\mathbb{Y}} (\mathbf{e}_l + \nabla \overline{\Phi}_l(\xi)) \cdot \mathcal{D}(\xi) (\mathbf{e}_k + \nabla \overline{\Phi}_k(\xi)) dy.$$

We denote by  $\overline{D}^{*,j}(\xi)$  the approximation of  $\overline{D}^*(\xi)$  using  $\mathcal{S}_j$ , that is for all  $k, l \in \{1, \dots, d\}$

$$\mathbf{e}_l \cdot \overline{D}^{*,j}(\xi) \mathbf{e}_k = \int_{\mathbb{Y}} (\mathbf{e}_l + \nabla \overline{\Phi}_l^j(\xi)) \cdot \mathcal{D}(\xi) (\mathbf{e}_k + \nabla \overline{\Phi}_k^j(\xi)) dy.$$

A standard calculation using (3.5) and the symmetry of  $\mathcal{D}$  yields

$$\mathbf{e}_l \cdot (\overline{D}^*(\xi) - \overline{D}^{*,j}(\xi)) \mathbf{e}_k = \int_{\mathbb{Y}} (\nabla \overline{\Phi}_l(\xi) - \nabla \overline{\Phi}_l^j(\xi)) \cdot \mathcal{D}(\xi) (\nabla \overline{\Phi}_k(\xi) - \nabla \overline{\Phi}_k^j(\xi)) dy.$$

This shows that the error on the homogenized matrix is a suitable estimator. We thus define the estimator  $\overline{\mathcal{E}}^j : \overline{\mathcal{K}} \times \{1, \dots, d\} \rightarrow \mathbb{R}^+$  as

$$\overline{\mathcal{E}}^j(\xi, k) = \sqrt{\frac{|\mathbf{e}_k \cdot (\overline{D}^*(\xi) - \overline{D}^{*,j}(\xi)) \mathbf{e}_k|}{\mathbf{e}_k \cdot \overline{D}^*(\xi) \mathbf{e}_k}}.$$

So defined, and recalling that  $\mathcal{D}$  is assumed to take values in the set of uniformly elliptic symmetric matrices (say with ellipticity constants  $0 < \underline{\nu} \leq \overline{\nu} < \infty$ ), the estimator is such that there exist  $C_1, C_2 > 0$  verifying for all suitable  $j, k, \xi$  the inequality

$$C_1 \overline{\mathcal{E}}^j(\xi, k) \leq \|\nabla \overline{\Phi}_k(\xi) - \nabla \overline{\Phi}_k^j(\xi)\|_{L^2(\mathbb{Y})} \leq C_2 \overline{\mathcal{E}}^j(\xi, k). \quad (3.6)$$

The induction procedure is then as follows. For all  $j \in \{0, \dots, N-1\}$ , choose  $\xi_{j+1} \in \overline{\mathcal{K}}$  and  $k_{j+1} \in \{1, \dots, d\}$  such that

$$(\xi_{j+1}, k_{j+1}) = \operatorname{argmax}_{\overline{\mathcal{K}}, \{1, \dots, d\}} \overline{\mathcal{E}}^j,$$

define

$$\overline{\Psi}_{j+1} = \frac{\overline{\Phi}_{k_{j+1}}(\xi_{j+1}) - \overline{\Phi}_{k_{j+1}}^j(\xi_{j+1})}{\|\nabla \overline{\Phi}_{k_{j+1}}(\xi_{j+1}) - \nabla \overline{\Phi}_{k_{j+1}}^j(\xi_{j+1})\|_{L^2(\mathbb{Y})}}$$

and set

$$\mathcal{S}_{j+1} := \operatorname{span} \{\overline{\Psi}_1, \dots, \overline{\Psi}_{j+1}\}.$$

By induction, for all  $j \in \{0, \dots, N\}$ ,  $\dim \mathcal{S}_{j+1} = j+1$ , since by construction  $\overline{\Psi}_{j+1}$  is orthogonal to  $\mathcal{S}_j$  for the following scalar product of  $H_{\#}^1(\mathbb{Y})$

$$(\overline{\Psi}_1, \overline{\Psi}_2) \mapsto \int_{\mathbb{Y}} \nabla \overline{\Psi}_1 \cdot \mathcal{D}(\xi_{j+1}) \nabla \overline{\Psi}_2 dy.$$

Note that usually, in the RB literature, the vectors  $\overline{\Psi}_j$  are orthogonalized using the same scalar product for all  $j$  (whereas here, the scalar product depends on  $j$ ). The choice made here makes the computation of the reduced basis simpler (and the generated space  $\mathcal{S}_{j+1}$  is the same).

What convergence rate can be expected in terms of  $N$ ? In the case when  $n = 1$  and  $\mathcal{D}$  has a dependence of the form  $\mathcal{D}(\xi) = D_0 + \xi D_1$  (that is  $\mathcal{D}$  is an affine function on the real line, and  $\overline{\mathcal{K}}$  is just a segment), the combination of results from [28] (see also the more

general case treated in [19]) and [7] (see also [12]) shows that there exist  $c, C > 0$  such that for all  $N \geq 1$ ,

$$\sup_{\bar{\mathcal{K}}, \{1, \dots, d\}} \bar{\mathfrak{E}}^N \leq C \exp(-cN).$$

The convergence being exponential in  $N$ , the reduced basis method is expected to yield accurate results for moderate  $N$  (say for  $N$  which is much smaller than the dimension of the finite element space  $\mathcal{V}_{\mathbb{Y}, h_1}^1$  for instance). Note that this yields a complete control of the error on the homogenized coefficients since for all  $k, l \in \{1, \dots, d\}$  by Cauchy-Schwarz' inequality and definition of the estimator,

$$\begin{aligned} |\mathbf{e}_l \cdot (\bar{D}^*(\xi) - \bar{D}^{*,N}(\xi)) \mathbf{e}_k| &= \left| \int_{\mathbb{Y}} (\nabla \bar{\Phi}_l(\xi) - \nabla \bar{\Phi}_l^N(\xi)) \cdot \mathcal{D}(\xi) (\nabla \bar{\Phi}_k(\xi) - \nabla \bar{\Phi}_k^N(\xi)) \right| \\ &\leq \sqrt{(\mathbf{e}_l \cdot \bar{D}^*(\xi) \mathbf{e}_l) (\mathbf{e}_k \cdot \bar{D}^*(\xi) \mathbf{e}_k)} \bar{\mathfrak{E}}^N(\xi, k) \bar{\mathfrak{E}}^N(\xi, l) \\ &\leq \tilde{C} \exp(-2cN) \end{aligned}$$

for some constant  $\tilde{C}$  depending only on  $C$  and  $d, \underline{\nu}, \bar{\nu}$ .

In the case under consideration here things are more complex than in [28] and [7] for the following three reasons:

- the parameter  $\xi$  is in  $\mathbb{R}^d$  (that is  $n = d > 1$  in the cases of interest);
- a priori  $\bar{\mathcal{K}} = \mathbb{R}^d$ , which is not a compact set;
- the function  $\xi \mapsto \mathcal{D}(\xi)$  is nonlinear.

The algorithm described in this paragraph is not of any practical use yet since in order to choose  $\xi_{j+1}$  and  $k_{j+1}$ , one needs to know  $\bar{\mathfrak{E}}^j(\xi, k)$  for all  $\xi$  and  $k$ . In the following paragraph we describe the standard way to proceed in practice.

**3.2.2. Practical reduced basis method.** In practice we do not have access to  $\{\bar{\mathfrak{E}}^j(\xi, k), \xi \in \bar{\mathcal{K}}, k \in \{1, \dots, d\}\}$  since:

- the corrector  $\bar{\Phi}_k(\xi)$  has to be approximated in a finite-dimensional subspace  $\mathcal{V}$  of  $H_{\#}^1(\mathbb{Y})$ , so that  $\bar{\mathfrak{E}}^j$  is approximated by some  $\mathfrak{E}^j$ .
- the space  $\bar{\mathcal{K}}$  has to be replaced by some finite set  $\mathcal{K}$ .

The construction of the reduced basis is then as follows.

**Algorithm 2.** Let  $N \in \mathbb{N}$ ,  $p \geq N$ ,  $\mathcal{K} = \{\xi_m, m \in \{1, \dots, p\}\}$  be a subset of  $\bar{\mathcal{K}}$ , and  $\mathcal{V}$  be a finite-dimensional subspace of  $H_{\#}^1(\mathbb{Y})$ .

- (1) For all  $m \in \{1, \dots, p\}$  and  $k \in \{1, \dots, d\}$ , let  $\Phi_k(\xi_m) \in \mathcal{V}$  be an approximation of the corrector  $\bar{\Phi}_k(\xi_m)$  in  $\mathcal{V}$ , that is the unique element of  $\mathcal{V}$  such that for all  $\Psi \in \mathcal{V}$

$$\int_{\mathbb{Y}} \nabla \Psi(y) \cdot \mathcal{D}(\xi_m)(y) (\mathbf{e}_k + \nabla \Phi_k(\xi_m)(y)) dy = 0,$$

and let  $D_{kk}^*(\xi_m)$  be the approximation of  $\mathbf{e}_k \cdot \bar{D}^*(\xi_m) \mathbf{e}_k$  given by

$$D_{kk}^*(\xi_m) = \int_{\mathbb{Y}} (\mathbf{e}_k + \nabla \Phi_k(\xi_m)) \cdot \mathcal{D}(\xi_m) (\mathbf{e}_k + \nabla \Phi_k(\xi_m)) dy.$$

- (2) Set  $\mathcal{V}_0 = \{0\}$ .
- (3) While  $0 \leq j < N$

- (a) For all  $m \in \{1, \dots, p\}$  and  $k \in \{1, \dots, d\}$ , let  $\Phi_k^j(\xi_m) \in \mathcal{V}$  be an approximation of the corrector  $\Phi_k(\xi_m)$  in  $\mathcal{V}_j$ , that is the unique element of  $\mathcal{V}_j$  such that for all  $\Psi^j \in \mathcal{V}_j$

$$\int_{\mathbb{Y}} \nabla \Psi^j(y) \cdot \mathcal{D}(\xi_m)(y)(\mathbf{e}_k + \nabla \Phi_k^j(\xi_m)(y)) dy = 0,$$

and let  $D_{kk}^{*,j}(\xi_m)$  be the approximation of  $D_{kk}^*(\xi_m)$  given by

$$D_{kk}^{*,j}(\xi_m) = \int_{\mathbb{Y}} (\mathbf{e}_k + \nabla \Phi_k^j(\xi_m)) \cdot \mathcal{D}(\xi_m)(\mathbf{e}_k + \nabla \Phi_k^j(\xi_m)) dy.$$

- (b) For all  $m \in \{1, \dots, p\}$  and  $k \in \{1, \dots, d\}$ , define the estimator  $\mathfrak{E}^j(m, k)$  as

$$\mathfrak{E}^j(m, k) = \sqrt{\frac{|\mathbf{e}_k \cdot D^*(\xi_m)\mathbf{e}_k - D_{kk}^{*,j}(\xi_m)|}{\mathbf{e}_k \cdot D^*(\xi_m)\mathbf{e}_k}},$$

and set

$$(m_j, k_j) = \operatorname{argmax}_{\mathcal{K}, \{1, \dots, d\}} \mathfrak{E}^j(m, k).$$

- (c) Define

$$\Psi_{j+1} := \frac{\Phi_{k_j}(\xi^m) - \Phi_{k_j}^j(\xi^m)}{\|\nabla \Phi_{k_j}(\xi^m) - \nabla \Phi_{k_j}^j(\xi^m)\|_{L^2(\mathbb{Y})}},$$

and set

$$\mathcal{V}_{j+1} = \operatorname{span} \{\Psi_i, 1 \leq i \leq j+1\}.$$

- (d)  $j = j + 1$ .

Provided  $p$  is chosen large enough and  $\mathcal{V}$  has dimension larger than  $N$ , one has as in the previous paragraph  $\dim \mathcal{V}_N = N$ .

What convergence rate can be expected in terms of  $N$ ? Going back to the example mentioned in the previous paragraph, that is for  $\mathcal{D}(\xi) = D_0 + \xi D_1$  and  $\bar{\mathcal{K}}$  a segment, the answer is given in [7]. In particular it is proved that the exponential estimate is stable in the sense that if the reduced basis  $\mathcal{V}_N$  is constructed starting from approximations of the correctors  $\{\bar{\Phi}_k(\xi), \xi \in \bar{\mathcal{K}}, k \in \{1, \dots, d\}\}$  within an error  $e$ , then the error estimate is of the form

$$\sup_{\bar{\mathcal{K}}, \{1, \dots, d\}} \bar{\mathfrak{E}}^N \leq C \exp(-cN) + Ce.$$

In Algorithm 2 there are two origins for the error  $e$ :

- The fact that  $H_{\#}^1(\mathbb{Y})$  is replaced by a finite-dimensional space  $\mathcal{V}$ , so that for all  $\xi \in \mathcal{K}$  and  $k \in \{1, \dots, d\}$ ,  $\Phi_k(\xi)$  is a finite-dimensional approximation of  $\bar{\Phi}_k$ ;
- The fact that for the greedy algorithm, the argmax of the estimator is taken in  $\mathcal{K}$  and not in  $\bar{\mathcal{K}}$ .

The first source of error is standard and can be controlled by a priori or a posteriori estimates. In the affine case above, the second source of error can also be estimated. Indeed, as proved in [20], the maps  $\bar{\Phi}_k : \bar{\mathcal{K}} \rightarrow H_{\#}^1(\mathbb{Y}), \xi \mapsto \bar{\Phi}_k(\xi)$  are analytic for all  $k \in \{1, \dots, d\}$ . In particular, if  $\mathcal{K}$  is a sampling of  $\bar{\mathcal{K}}$  with “meshsize”  $h$ , for all  $\xi \in \bar{\mathcal{K}}$ ,  $\bar{\Phi}_k(\xi)$  can be approximated by interpolation in  $\{\bar{\Phi}_k(\xi_m), m \in \{1, \dots, p\}\}$  within an error of order  $h^q$  for any  $q \in \mathbb{N}$ . Hence the practical reduced basis method remains efficient in

this specific case. However, this analysis is restricted to the affine case and it does not apply in our context.

3.2.3. *About fast-assembly of the matrix.* Let  $\overline{\mathcal{K}}$ ,  $\mathcal{K}$ , and  $N \in \mathbb{N}$  and  $\mathcal{V}_N$  be as in Algorithm 2. For all  $\xi \in \overline{\mathcal{K}}$  and  $k \in \{1, \dots, d\}$ , the approximation of  $\overline{\Phi}_k(\xi)$  in the reduced basis  $\mathcal{V}_N$  is given by the unique function  $\Phi_k^N(\xi) \in \mathcal{V}_N$  such that for all  $\Psi^N \in \mathcal{V}_N$ ,

$$\int_{\mathbb{Y}} \nabla \Psi^N \cdot \mathcal{D}(\xi)(\mathbf{e}_k + \nabla \Phi_k^N(\xi)) \, dy = 0. \quad (3.7)$$

Expanding  $\Phi_k^N(\xi)$  in the basis  $\mathcal{V}_N$  as  $\Phi_k^N(\xi) = \sum_{j=1}^N u_j(\xi) \Psi_j$ , the above equation is equivalent to the linear system

$$\mathbb{M}(\xi)U = B(\xi, k),$$

where for all  $j \in \{1, \dots, N\}$ ,  $U_j = u_j(\xi)$  and  $B(\xi, k)_j = -\int_{\mathbb{Y}} \nabla \Psi_j \cdot \mathcal{D}(\xi) \mathbf{e}_k \, dy$ , and the  $N \times N$  matrix  $\mathbb{M}(\xi)$  is given by its entries  $\mathbb{M}(\xi)_{j_1 j_2} = \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot \mathcal{D}(\xi) \nabla \Psi_{j_2}$  for all  $1 \leq j_1, j_2 \leq N$ . In particular, in order to compute  $\Phi_k^N(\xi)$ , one needs to solve (3.7), and therefore construct the matrix  $\mathbb{M}(\xi)$  and the r. h. s.  $B(\xi, k)$ .

Without further assumption on the function  $\xi \mapsto \mathcal{D}(\xi)$ , the exact calculation of  $\mathbb{M}(\xi)$  and  $B(\xi, k)$  requires:

- the storage of the coordinates of each vector  $\Psi_j$  of the reduced basis  $\mathcal{V}_N$  in the finite dimensional space  $\mathcal{V}$ ,
- the computation of integrals over  $\mathbb{Y}$ .

In particular, both the information to be stored and the computational cost to construct  $\mathbb{M}(\xi)$  and  $B(\xi, k)$  scale like the dimension  $\dim(\mathcal{V})$  of the finite-dimensional space  $\mathcal{V}$  (which can be prohibitively large). Yet, if  $\xi \mapsto \mathcal{D}(\xi)$  has specific structural properties, the information to be stored and the computational cost can be drastically reduced. This is the case when  $\xi \mapsto \mathcal{D}(\xi)$  is affine. Let us go back to the example of  $\mathcal{D}(\xi) = D_0 + \xi D_1$ . Then, the entries of the matrix  $\mathbb{M}(\xi)$  and of the r. h. s.  $B(\xi, j)$  take the form: for all  $1 \leq j, j_1, j_2 \leq N$ ,

$$\begin{aligned} \mathbb{M}(\xi)_{j_1 j_2} &= \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot D_0 \nabla \Psi_{j_2} + \xi \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot D_1 \nabla \Psi_{j_2} \, dy, \\ B(\xi, k)_j &= \int_{\mathbb{Y}} \nabla \Psi_j \cdot D_0 \mathbf{e}_k + \xi \int_{\mathbb{Y}} \nabla \Psi_j \cdot D_1 \mathbf{e}_k \, dy. \end{aligned}$$

In particular, provided we store the two  $N \times N$  matrices  $M_1$  and  $M_2$ , and the two  $d \times N$  matrices  $B_1$  and  $B_2$  defined by: for all  $1 \leq j, j_1, j_2 \leq N$  and  $k \in \{1, \dots, d\}$ ,

$$\begin{aligned} (M_1)_{j_1 j_2} &= \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot D_0 \nabla \Psi_{j_2} \, dy, & (M_2)_{j_1 j_2} &= \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot D_1 \nabla \Psi_{j_2} \, dy, \\ (B_1)_{kj} &= \int_{\mathbb{Y}} \nabla \Psi_j \cdot D_0 \mathbf{e}_k \, dy, & (B_2)_{kj} &= \int_{\mathbb{Y}} \nabla \Psi_j \cdot D_1 \mathbf{e}_k \, dy, \end{aligned}$$

one may reconstruct  $\mathbb{M}(\xi)$  and  $B(\xi, k)$  by the simple formulae

$$\mathbb{M}(\xi) = M_1 + \xi M_2, \quad B(\xi, k) = (B_1)_k + \xi (B_2)_k,$$

where  $(B_1)_k$  and  $(B_2)_k$  are the  $k$ -th column of  $B_1$  and  $B_2$ , respectively.

The gain is twofold:

- the dimension of the information to store is  $2N^2 + 2dN$ , which is independent of  $\dim(\mathcal{V})$ ,

- the computation of  $\mathbb{M}(\xi)$  and  $B(\xi, k)$  only requires  $N^2 + N$  multiplications and  $N^2 + N$  additions, and not the computation of  $N^2 + N$  integrals on  $\mathbb{Y}$  (using an integration rule which should be exact for functions of  $\mathcal{V}$ ).

The same strategy allows one to easily compute the approximation  $D^{*,N}(\xi)$  of the homogenized matrix  $\overline{D}^*(\xi)$ , via the formula: for all  $k, l \in \{1, \dots, d\}$ ,

$$\begin{aligned} \mathbf{e}_k \cdot D^{*,N}(\xi) \mathbf{e}_l &= \int_{\mathbb{Y}} (\mathbf{e}_k + \nabla \Phi_k^N(\xi)) \cdot \mathcal{D}(\xi) (\mathbf{e}_l + \nabla \Phi_l^N(\xi)) \, dy \\ &= \mathbf{e}_k \left( \int_{\mathbb{Y}} D_0 \, dy + \xi \int_{\mathbb{Y}} D_1 \, dy \right) \mathbf{e}_l \\ &\quad + \sum_{j=1}^N u_j(\xi) \mathbf{e}_k \cdot \left( \int_{\mathbb{Y}} D_0 \nabla \Psi_j \, dy + \xi \int_{\mathbb{Y}} D_1 \nabla \Psi_j \, dy \right), \end{aligned}$$

so that one only has to store  $2d^2 + 2dN$  real numbers to compute the approximation of the homogenized matrix.

This fast-assembly method is very convenient and efficient, but requires the diffusion matrix  $\mathcal{D}(\xi)$  to be affine with respect to  $\xi$ .

**3.3. Application of the reduced basis method to the homogenized system.** As said above, the evaluation of the effective coefficients for the homogenized problem involves the parametrized matrices  $\widehat{\mathcal{D}}$  defined in (3.4) where the parameter  $\xi$  ranges the unbounded set  $\mathbb{R}^d$ . In the following paragraph we shall rewrite the problem in an equivalent form so that we end up with a set of parameters which is compact. We address the issue of fast assembly in the second paragraph, bearing in mind that the dependence with respect to the parameter is not affine, and we provide with a numerical study of the method in the last paragraph.

**3.3.1. Rewriting of the problem.** The starting point to rewrite the problem is the following fact: for all  $\xi \in \mathbb{R}^d$  and all  $k \in \{1, \dots, d\}$ , the corrector  $\overline{\Phi}_k(\xi) \in H_{\#}^1(\mathbb{Y})$  is solution to

$$-\nabla \cdot \frac{\widehat{\mathcal{D}}(\xi)}{1 + |\xi|} (\mathbf{e}_k + \nabla \overline{\Phi}_k(\xi)) = 0. \quad (3.8)$$

Let  $S^{d-1}$  denote the unit hypersphere in dimension  $d$  and let  $\mathcal{P} = [0, 1] \times S^{d-1}$  (which is nothing but the closed unit ball). Define

$$\begin{aligned} \mathcal{D} : [0, 1] \times S^{d-1} &\longrightarrow L^2(\mathbb{Y}, \mathcal{M}_d(\mathbb{R})) \\ (\rho, X) &\longmapsto \mathcal{D}(\rho, X) \end{aligned}$$

by

$$\mathcal{D}(\rho, X) : y \mapsto (1 - \rho)D_0 + \rho \left( \alpha |M(y)X| \mathbb{I} + \beta \frac{M(y)X \otimes M(y)X}{|M(y)X|} \right), \quad (3.9)$$

For all  $(\rho, X) \in [0, 1] \times S^{d-1}$  and  $k \in \{1, \dots, d\}$ , we define  $\overline{\Phi}_k(\rho, X)$  as the unique weak solution in  $H_{\#}^1(\mathbb{Y})$  to

$$-\nabla \cdot \mathcal{D}(\rho, X) (\mathbf{e}_k + \nabla \overline{\Phi}_k(\rho, X)) = 0. \quad (3.10)$$

Let  $\xi \in \mathbb{R}^d$ , and set

$$\rho = \frac{|\xi|}{1 + |\xi|}, \quad X = \frac{\xi}{|\xi|}$$

so that

$$\frac{\widehat{\mathcal{D}}(\xi)}{1+|\xi|} = \mathcal{D}(\rho, X);$$

the identity (3.8) and (3.10) imply that

$$\overline{\Phi}_k(\xi) \equiv \overline{\Phi}_k(\rho, X)$$

by uniqueness of correctors. In particular, this shows that

$$\left\{ \overline{\Phi}_k(\xi), \xi \in \mathbb{R}^d, k \in \{1, \dots, d\} \right\} = \left\{ \overline{\Phi}_k(\rho, X), (\rho, X) \in [0, 1] \times S^{d-1}, k \in \{1, \dots, d\} \right\}.$$

What we gain by applying the reduced basis method on this new formulation is that the parameters now belong to the compact set  $\mathcal{P} := [0, 1] \times S^{d-1}$ .

To complete the description of the RB method, we need to choose an estimator. We shall make use of the estimator defined in the previous subsection. Let  $j \in \mathbb{N}$  and let  $\mathcal{V}_j$  be a subspace of  $H_{\#}^1(\mathbb{Y})$  of dimension  $j$ . Set for all  $(\rho, X) \in [0, 1] \times S^{d-1}$  and  $k \in \{1, \dots, d\}$ ,

$$\overline{\mathfrak{E}}^j(\rho, X, k) = \sqrt{\frac{|\mathbf{e}_k \cdot (\overline{D}^*(\rho, X) - \overline{D}^{*,j}(\rho, X))\mathbf{e}_k|}{\mathbf{e}_k \cdot \overline{D}^*(\rho, X)\mathbf{e}_k}}, \quad (3.11)$$

where, denoting by  $\overline{\Phi}_k^j(\rho, X)$  the approximation of  $\overline{\Phi}_k(\rho, X)$  in  $\mathcal{V}_j$ , we have

$$\begin{aligned} \mathbf{e}_k \cdot \overline{D}^*(\rho, X)\mathbf{e}_k &= \int_{\mathbb{Y}} (\mathbf{e}_k + \nabla \overline{\Phi}_k(\rho, X)) \cdot \mathcal{D}(\rho, X)(\mathbf{e}_k + \nabla \overline{\Phi}_k(\rho, X)) \, dy, \\ \mathbf{e}_k \cdot \overline{D}^{*,j}(\rho, X)\mathbf{e}_k &= \int_{\mathbb{Y}} (\mathbf{e}_k + \nabla \overline{\Phi}_k^j(\rho, X)) \cdot \mathcal{D}(\rho, X)(\mathbf{e}_k + \nabla \overline{\Phi}_k^j(\rho, X)) \, dy. \end{aligned} \quad (3.12)$$

Note that this estimator is consistent with the estimator associated with  $\widehat{\mathcal{D}}$  since we have for all  $\xi \in \mathbb{R}^d$ ,

$$\widetilde{\mathfrak{E}}^j(\xi, k) = \overline{\mathfrak{E}}^j(\rho, X, k)$$

for  $\rho = \frac{|\xi|}{1+|\xi|}$  and  $X = \frac{\xi}{|\xi|}$ , the estimator  $\widetilde{\mathfrak{E}}^j(\xi, k)$  (and the matrices  $\overline{D}^*(\xi)$ ,  $\overline{D}^{*,j}(\xi)$ ) being defined with the matrix  $\widehat{\mathcal{D}}(\xi)$ . Since we also have for all  $\xi \in \mathbb{R}^d$

$$\begin{aligned} \overline{D}^*(\rho, X) &= \frac{1}{1+|\xi|} \overline{D}^*(\xi), \\ \overline{D}^{*,j}(\rho, X) &= \frac{1}{1+|\xi|} \overline{D}^{*,j}(\xi), \end{aligned}$$

for  $\rho = \frac{|\xi|}{1+|\xi|}$  and  $X = \frac{\xi}{|\xi|}$ , it is equivalent to approximate  $\overline{D}^*$  and  $\overline{D}^{*,j}$ . We will focus on the former in what follows.

Before we turn to fast-assembly, let us make a comment of the RB method used here. The estimator (3.11) satisfies the second inequality of (3.6), namely there exists  $C_2 > 0$  such that for all  $j \in \mathbb{N}$ ,  $(\rho, X) \in [0, 1] \times S^{d-1}$ , and  $k \in \{1, \dots, d\}$ ,

$$\|\nabla \overline{\Phi}_k(\rho, X) - \nabla \overline{\Phi}_k^j(\rho, X)\|_{L^2(\mathbb{Y})} \leq C_2 \overline{\mathfrak{E}}^j(\rho, X, k).$$



Yet the converse inequality only holds in a weaker sense. In particular, using that  $\overline{D}^*(\rho, X)$  and  $\overline{D}^{*,j}(\rho, X)$  can be defined as

$$\begin{aligned} \mathbf{e}_k \cdot \overline{D}^*(\rho, X) \mathbf{e}_k &= \int_{\mathbb{Y}} \mathbf{e}_k \cdot \mathcal{D}(\rho, X) (\mathbf{e}_k + \nabla \overline{\Phi}_k(\rho, X)) \, dy, \\ \mathbf{e}_k \cdot \overline{D}^{*,j}(\rho, X) \mathbf{e}_k &= \int_{\mathbb{Y}} \mathbf{e}_k \cdot \mathcal{D}(\rho, X) (\mathbf{e}_k + \nabla \overline{\Phi}_k^j(\rho, X)) \, dy, \end{aligned}$$

if  $M \in L^2(\mathbb{Y}, \mathcal{M}_d(\mathbb{R}))$  is square-integrable but not *essentially unbounded*, we end up with

$$C_1 \overline{\mathcal{E}}^j(\rho, X, k) \leq \|\nabla \overline{\Phi}_k(\rho, X) - \nabla \overline{\Phi}_k^j(\rho, X)\|_{L^2(\mathbb{Y})}^{1/2},$$

for some  $C_1 > 0$ , a weaker estimate than the first inequality of (3.6). As a consequence, the analysis of the reduced basis method and of the greedy algorithm in this case does not follow from [12, 19, 20, 7]. Filling the gap for analyzing the convergence of the RB method when dealing with such unbounded coefficients remains beyond the scope of the present work. Nevertheless, the numerical experiments show the efficiency of the algorithm to treat this case.

**3.3.2. Fast-assembly procedure.** In this section, we restrict our discussion to  $d = 2$  for notational convenience. The case  $d > 2$  can be treated similarly. In dimension 2, the unit sphere  $S^1$  is parametrized by  $[0, 2\pi]$ , so that from now on, we write the element of  $S^1$  as

$$X = \mathbf{e}(\theta) = \cos(\theta) \mathbf{e}_1 + \sin(\theta) \mathbf{e}_2, \quad (3.13)$$

and consider  $\mathcal{D}$  as a function of  $\rho$  and  $\theta$  (instead of  $\rho$  and  $X$ ). The diffusion matrix  $\mathcal{D} : [0, 1] \times [0, 2\pi] \rightarrow L^2(\mathbb{Y}, \mathcal{M}_d(\mathbb{R}))$  given by (3.9), that is

$$\mathcal{D}(\rho, \theta) : y \mapsto (1 - \rho)D_0 + \rho \left( \alpha |M(y) \mathbf{e}(\theta)| \mathbb{I} + \beta \frac{M(y) \mathbf{e}(\theta) \otimes M(y) \mathbf{e}(\theta)}{|M(y) \mathbf{e}(\theta)|} \right),$$

is affine with respect to  $\rho$ , but not with respect to  $\theta \in [0, 2\pi]$ .

To circumvent this difficulty we use a partial Fourier series expansion in the  $\theta$ -variable, and write:

$$\mathcal{D}(\rho, \theta)(y) = (1 - \rho)D_0 + \rho \left( \frac{a_0(y)}{2} + \sum_{n=1}^{\infty} (a_n(y) \cos(n\theta) + b_n(y) \sin(n\theta)) \right),$$

where the functions  $y \mapsto a_n(y)$  and  $y \mapsto b_n(y)$  are matrices which depend only on  $y \mapsto M(y)$ .

Given a finite-dimensional space  $\mathcal{V}_N = \text{span}\{\Psi_1, \dots, \Psi_N\}$  of dimension  $N \geq 1$ , and some parameters  $(\rho, \theta) \in [0, 1] \times [0, 2\pi]$  and  $k \in \{1, \dots, d\}$ , in order to approximate the corrector  $\overline{\Phi}_k$  in  $\mathcal{V}_N$ , it is enough to solve the linear system

$$\mathbb{M}(\rho, \theta)U = B(\rho, \theta, k),$$

where  $U$  is the vector of coordinates of  $\overline{\Phi}_k$  in  $\mathcal{V}_N$ ,  $\mathbb{M}(\rho, \theta)$  is the  $N \times N$ -matrix given for all  $1 \leq j_1, j_2 \leq N$  by

$$\begin{aligned} \mathbb{M}(\rho, \theta)_{j_1 j_2} &= (1 - \rho) \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot D_0 \nabla \Psi_{j_2} \, dy + \rho \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot \frac{a_0(y)}{2} \nabla \Psi_{j_2} \, dy \\ &\quad + \sum_{n=1}^{\infty} \rho \cos(n\theta) \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot a_n(y) \nabla \Psi_{j_2} \, dy + \sum_{n=1}^{\infty} \rho \sin(n\theta) \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot b_n(y) \nabla \Psi_{j_2} \, dy, \end{aligned}$$

and the r. h. s. is the  $N$ -vector given for all  $1 \leq j \leq N$  by

$$B(\rho, \theta, k)_j = -(1 - \rho) \int_{\mathbb{Y}} \nabla \Psi_j \cdot D_0 \mathbf{e}_k \, dy - \rho \int_{\mathbb{Y}} \nabla \Psi_j \cdot \frac{a_0(y)}{2} \mathbf{e}_k \, dy \\ - \sum_{n=1}^{\infty} \rho \cos(n\theta) \int_{\mathbb{Y}} \nabla \Psi_j \cdot a_n(y) \mathbf{e}_k \, dy - \sum_{n=1}^{\infty} \rho \sin(n\theta) \int_{\mathbb{Y}} \nabla \Psi_j \cdot b_n(y) \mathbf{e}_k \, dy.$$

In particular, provided we truncate the Fourier series expansion up to some order  $L \in \mathbb{N}$ , a fast assembly procedure can be devised if the  $2(L+1)$  following matrices of order  $N$  and  $2Lk(L+1)$  following vectors of order  $N$  are stored:

$$\left( \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot D_0 \nabla \Psi_{j_2} \, dy \right)_{j_1, j_2}, \quad \left( \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot \frac{a_0(y)}{2} \nabla \Psi_{j_2} \, dy \right)_{j_1, j_2}, \\ \left( \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot a_n(y) \nabla \Psi_{j_2} \, dy \right)_{j_1, j_2}, \quad \left( \int_{\mathbb{Y}} \nabla \Psi_{j_1} \cdot b_n(y) \nabla \Psi_{j_2} \, dy \right)_{j_1, j_2} \quad \text{for } n \in \{1, \dots, L\}, \quad (3.14)$$

and for  $\in \{1, \dots, d\}$ ,

$$\left( \int_{\mathbb{Y}} \nabla \Psi_j \cdot D_0 \mathbf{e}_k \, dy \right)_j, \quad \left( \int_{\mathbb{Y}} \nabla \Psi_j \cdot \frac{a_0(y)}{2} \mathbf{e}_k \, dy \right)_j, \\ \left( \int_{\mathbb{Y}} \nabla \Psi_j \cdot a_n(y) \mathbf{e}_k \, dy \right)_j, \quad \left( \int_{\mathbb{Y}} \nabla \Psi_j \cdot b_n(y) \mathbf{e}_k \, dy \right)_j \quad \text{for } n \in \{1, \dots, L\}. \quad (3.15)$$

Note that the number of real numbers to be stored for the fast-assembly only depends on  $L$  and  $N$ . In particular, if the reduced basis vectors  $\Psi_j$  are approximated in a finite-dimensional subspace of  $H_{\#}^1(\mathbb{Y})$ , this number is independent of the size of that subspace, as desired.

In practice, once we are given the reduced basis  $\{\Psi_1, \dots, \Psi_N\}$ , the matrices (3.14) and vectors (3.15) can be obtained by performing a fast Fourier transform of

$$\theta \mapsto \alpha |M(y) \mathbf{e}(\theta)| \mathbb{I} + \beta \frac{M(y) \mathbf{e}(\theta) \otimes M(y) \mathbf{e}(\theta)}{|M(y) \mathbf{e}(\theta)|}$$

at each Gauss point  $y \in \mathbb{Y}$  to evaluate the values of  $a_n(y)$  and  $b_n(y)$ .

**3.3.3. Numerical results.** Let  $d = 2$ ,  $\mathbb{T}_{\mathbb{Y}, h_1}, \mathbb{T}_{\mathbb{Y}, \bar{h}_1}$  be regular tessellations of  $\mathbb{Y}$  of meshsize  $h_1, \bar{h}_1 > 0$ , and  $\mathcal{V}_{\mathbb{Y}, h_1}^1, \mathcal{V}_{\mathbb{Y}, \bar{h}_1}^1$  be the subspaces of  $H_{\#}^1(\mathbb{Y})$  made of  $\mathbb{P}_1$ -periodic finite elements associated with  $\mathbb{T}_{\mathbb{Y}, h_1}$  and  $\mathbb{T}_{\mathbb{Y}, \bar{h}_1}$ , respectively. The diffusion matrix  $M \in L^2(\mathbb{Y}, \mathcal{M}_d(\mathbb{R}))$  is defined by

$$M(y) = K(y)(\mathbb{I} + \nabla \varphi^{\bar{h}_1}(y)),$$

where  $K$  is a standard checkerboard: for all  $y = (y_1, y_2) \in \mathbb{Y}$ ,

$$K(y_1, y_2) = \begin{cases} 4.94064, & \text{if } \{y_1 \geq 0.5, y_2 \geq 0.5\} \text{ or } \{y_1 < 0.5, y_2 < 0.5\}, \\ 0.57816, & \text{elsewhere,} \end{cases}$$

and  $\varphi^{\bar{h}_1} = (\varphi_1^{\bar{h}_1}, \dots, \varphi_d^{\bar{h}_1})$  is defined as in (3.1). In the actual computations, we take  $\bar{h}_1 \in \{1/10, 1/20, 1/40\}$  so that  $\dim \mathcal{V}_{\mathbb{Y}, \bar{h}_1}^1 \sim 100, 400, 1600$ . The other parameters are the

$p$ and $\bar{h}_1$	1/10	1/20	1/40
10	41	61	61
20	41	61	61
40	49	95	175

TABLE 3. Dependence of  $L$  upon  $\bar{h}_1$  and  $p$ 

$p$ and $\bar{h}_1$	1/10	1/20	1/40
10	21	24	25
20	23	38	44
40	24	47	60

TABLE 4. Dependence of  $N$  upon  $\bar{h}_1$  and  $p$ 

same as in Table 1. In the rest of this paragraph, we assume that the corrector equations are solved in  $\mathcal{V}_{\bar{h}_1}^1$ , so that the reduced basis will be a subspace of  $\mathcal{V}_{\bar{h}_1}^1$  as well.

For the reduced basis method we replace the compact space  $\mathcal{D} = [0, 1] \times [0, 2\pi]$  by the finite set  $\{(\rho_i, \theta_j), i, j \in \{1, \dots, p\}\}$ , with  $p \geq 2$ ,  $\theta_j = j\frac{2\pi}{p}$ , and  $\rho_i = (i-1)\frac{1}{p-1}$ . Let us denote by  $\mathcal{D}_L$  the diffusion matrix obtained by a truncation of the Fourier series expansion of  $\mathcal{D}$  at order  $L$ , and let  $\bar{D}^*$  denote the homogenized coefficients defined in (3.12) (where the correctors  $\bar{\Phi}_k(\rho, X)$  is in fact approximated in  $\mathcal{V}_{\bar{h}_1}^1$ , and with  $X$  related to  $\theta$  through (3.13)), and let  $\bar{D}_L^*$  be defined by

$$\mathbf{e}_k \cdot \bar{D}_L^*(\rho, \theta) \mathbf{e}_k = \int_{\mathbb{Y}} (\mathbf{e}_k + \nabla \bar{\Phi}_k(\rho, \theta)) \cdot \mathcal{D}_L(\rho, \theta) (\mathbf{e}_k + \nabla \bar{\Phi}_k(\rho, \theta)) dy.$$

We choose  $L$  such that

$$\sup_{i,j \in \{1, \dots, p\}} \frac{|\bar{D}^*(\rho_i, \theta_j) - \bar{D}_L^*(\rho_i, \theta_j)|}{|\bar{D}^*(\rho_i, \theta_j)|} \leq 10^{-6}.$$

Numerical tests show that  $L$  depends both on  $\bar{h}_1$  and on  $p$ , but not on  $h_1$ . As can be expected, the smaller  $\bar{h}_1$ , the finer the approximation  $\varphi^{\bar{h}_1}$  of the correctors  $\varphi$  of the Darcy equation, and therefore the more complex  $\mathcal{D}$  (it should however stabilize as  $\bar{h}_1 \rightarrow 0$ ). We display the results of the numerical tests on  $L$  in Table 3.

For all  $N \leq p^2$ , we denote by  $\mathcal{V}_N$  the RB space of dimension  $N$ . We then choose  $N$  such that

$$\sup_{\mathcal{D}} (\mathfrak{E}_L^N(\rho, \theta))^2 \leq 10^{-6},$$

where  $\mathfrak{E}_L^N$  is the estimator associated with  $\mathcal{D}_L$  and the space  $\mathcal{V}_N$ , when the equations are solved in  $\mathcal{V}_{\bar{h}_1}^1$ . As expected,  $N$  depends both on  $\bar{h}_1$  and on  $p$ , but not on  $h_1 \in \{1/10, 1/20, 1/40, 1/80, 1/160, 1/320\}$  (which is the desired scaling property). The dimension  $N$  of the reduced basis in fonction of  $\bar{h}_1$  and on  $p$  is displayed in Table 4.

$p$ and $\bar{h}_1$	1/10	1/20	1/40
10	1.3e-03	1.1e-03	1.7e-03
20	3.4e-05	1.7e-04	2.6e-04
40	8.0e-06	2.8e-05	4.1e-05

 TABLE 5. Dependence of the RB error upon  $\bar{h}_1$  and  $p$  on a random sampling

In order to check a posteriori the efficiency of the method (both in terms of  $L$  and  $N$ ), we have picked at random a set  $\tilde{\mathcal{P}}$  of 100 pairs of parameters  $(\rho, \theta) \in [0, 1] \times [0, 2\pi]$ , computed the corresponding approximations  $\bar{D}^*(\rho, \theta)$  of the homogenized coefficients in  $\mathcal{V}_{\bar{y}, \bar{h}_1}^1$ , and compared them to the approximations  $\bar{D}_L^{*,N}(\rho, \theta)$  using the reduced basis method of order  $N$  and a Fourier series expansion of  $\mathcal{D}$  truncated at order  $L$ . The numerical tests show that this error

$$\sup_{\tilde{\mathcal{P}}} \frac{|\bar{D}^*(\rho, \theta) - \bar{D}_L^{*,N}(\rho, \theta)|}{|\bar{D}^*(\rho, \theta)|}$$

does not depend on  $h_1$  but depends again on  $\bar{h}_1$  and  $p$ . More precisely, the error increases as  $\bar{h}_1 \rightarrow 0$  and decreases as  $p$  increases. These results are displayed in Table 5.

A last comment is as follows. A close look at the points which are chosen by the greedy algorithm shows that most of the information lies in the region  $\rho$  close to 1 and  $\theta$  in  $[0, \pi]$  (this latter fact is indeed a consequence of the identity  $\mathcal{D}(\rho, \theta) = \mathcal{D}(\rho, \pi - \theta)$ ). This motivates us to put more points in this region rather than in the rest of  $\mathcal{P}$ , and allows us to focus on the right region of the parameters.

In conclusion, these tests widely confirm the efficiency of the method.

Note that in order to reduce the effect of the aliasing phenomena in the fast Fourier transform, we compute twice as many coefficients as needed (that is, up to  $2L$  for an effective truncation of order  $L$ ).

**Remark 3.1.** As in Remark 2.1, we can consider modulated coefficients depending on both the the slow and the fast variables, provided the dependence with respect to the slow variable is smooth enough. Of course price to be paid is to increase the size of the set of parameters  $\mathcal{P}$  accordingly.

#### 4. CONCLUSION

We consider a simple model of radionuclide transport in porous media: the radionuclide concentration satisfies a convection–diffusion equation where the coefficients are determined through the Darcy law by solving an non homogeneous elliptic equation. A remarkable feature of the model relies on the fact that the diffusion coefficient depends non linearly on the velocity and does not satisfy an uniform  $L^\infty$  estimate.

Nevertheless, existence-uniqueness statements can be established for this model. We can also perform the homogenization analysis but, due to the coupling, the effective coefficients remain non homogeneous, even in the simple case of purely periodic oscillations. It impacts strongly the computational cost when using direct evaluation of the coefficients. We propose an algorithm based on Reduced Basis methods in order to speed up

the computation. The method relies on a suitable parametrization of the problem, which in particular allows to make use of Fast Fourier Transform algorithms. Working with unbounded coefficients is clearly identified as a difficulty for analyzing the convergence properties of the method, but simulations demonstrate the efficiency of the scheme which is a valuable tool for the computation of such complex flows.

#### APPENDIX A. PROOF OF THEOREM 2

We decompose the proof into two steps and homogenize the Darcy equation and the advection-diffusion equation separately.

*Step 1.* Homogenization of the Darcy equation, and two-scale convergence of  $U_\varepsilon$  and  $D(U_\varepsilon)$ .

By standard two-scale convergence arguments (see [1, Theorem 2.3], and see also [30]), the function  $\Theta_\varepsilon$  two-scale converges to  $\Theta_0$  and  $\nabla\Theta_\varepsilon$  two-scale converges to the function  $(x, y) \in \Omega \times \mathbb{Y} \mapsto (\mathbb{I} + \nabla\varphi(y))\nabla\Theta_0(x)$ . Likewise the flux  $K_\varepsilon\nabla\Theta_\varepsilon$  two-scale converges to  $(x, y) \mapsto K(y)(\mathbb{I} + \nabla\varphi(y))\nabla\Theta_0(x) = -\tilde{U}(x, y)$ . In order to homogenize the advection-diffusion equation, we need the function  $K_\varepsilon\nabla\Theta_\varepsilon$  to be an admissible test-function for two-scale convergence, see [1, Definition 1.4]. It is enough to prove that  $K_\varepsilon\nabla\Theta_\varepsilon$  strongly two-scale converges to  $-\tilde{U}$ , that is, in addition of two-scale convergence, to prove that we have

$$\lim_{\varepsilon \rightarrow 0} \int_{\Omega} |K_\varepsilon(x)\nabla\Theta_\varepsilon(x)|^2 dx = \int_{\Omega} \int_{\mathbb{Y}} |\tilde{U}(x, y)|^2 dy dx. \quad (\text{A.1})$$

This is essentially a consequence of the following convergence of the energy:

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \int_{\Omega} \nabla\Theta_\varepsilon(x) \cdot K_\varepsilon(x)\nabla\Theta_\varepsilon dx \\ = \int_{\Omega} \int_{\mathbb{Y}} (\nabla\Theta_0(x) + \nabla_y\Theta_1(x, y)) \cdot K(y)(\nabla\Theta_0(x) + \nabla_y\Theta_1(x, y)) dy dx, \end{aligned}$$

where  $\Theta_1(x, y) = \sum_{i=1}^d \nabla_i\Theta_0(x)\varphi_i(y)$ . In particular, since  $K$  is positive-definite, we may rewrite this identity as

$$\lim_{\varepsilon \rightarrow 0} \int_{\Omega} |K_\varepsilon(x)^{1/2}\nabla\Theta_\varepsilon(x)|^2 dx = \int_{\Omega} \int_{\mathbb{Y}} |K(y)^{1/2}(\nabla\Theta_0(x) + \nabla_y\Theta_1(x, y))|^2 dy dx,$$

which upgrades the two-scale convergence of  $K_\varepsilon^{1/2}\nabla\Theta_\varepsilon$  to  $(x, y) \mapsto K(y)^{1/2}(\nabla\Theta_0(x) + \nabla_y\Theta_1(x, y))$  into strong two-scale convergence. We now consider a sequence  $v_\varepsilon : \Omega \rightarrow \mathbb{R}^d$  which two-scale converges to  $(x, y) \mapsto v_0(x, y)$ . The sequence  $V_\varepsilon := K_\varepsilon^{1/2}v_\varepsilon$  then two-scale converges to  $(x, y) \mapsto K(y)^{1/2}v_0(x, y)$ . Since we have proved that  $K_\varepsilon^{1/2}\nabla\Theta_\varepsilon$  is an admissible test-function for the two-scale convergence, we have

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \int_{\Omega} K_\varepsilon(x)^{1/2}\nabla\Theta_\varepsilon(x) \cdot V_\varepsilon(x) dx \\ = \int_{\Omega} \int_{\mathbb{Y}} K(y)^{1/2}(\nabla\Theta_0(x) + \nabla_y\Theta_1(x, y)) \cdot K(y)^{1/2}v_0(x, y) dy dx. \end{aligned}$$

Taking  $v_\varepsilon = K_\varepsilon\nabla\Theta_\varepsilon$  then proves (A.1).

We conclude this step by the proof of the strong two-scale convergence of  $D(U_\varepsilon)$  to  $(x, y) \mapsto \tilde{D}(x, y)$ . This is a direct consequence of [26, Proposition 4] since  $(x, U) \mapsto$

$D(U)(x)$  is a Lipschitz function with respect to  $U$  uniformly in  $x$ , and  $U_\varepsilon$  strongly two-scale converges to  $\tilde{U}$ .

*Step 2.* Homogenization of the advection-diffusion equation.

In view of the results of Step 1, this is now standard matter to prove the two-scale convergence of  $C_\varepsilon$  to  $C_0$ . The proof of Theorem 1 provides uniform bounds on  $C_\varepsilon$  which gives weak compactness. Hence, up to extraction,  $C_\varepsilon$  two-scale converges to some  $C_0$ , and  $\nabla C_\varepsilon$  to some  $(x, y) \mapsto \nabla C_0(x) + \nabla_y C_1(x, y)$  (time is treated as a parameter). Since  $D(U_\varepsilon)$  and  $U_\varepsilon$  strongly two-scale converge to  $\tilde{D}$  and  $\tilde{U}$ , respectively, there is no difficulty to pass at the two-scale limit in the equation for  $C_\varepsilon$  tested with functions  $(t, x) \mapsto \psi(t)\phi(x, x/\varepsilon)$  and  $\phi \in C^\infty(\Omega, C^\infty_{\text{per}}(\mathbb{Y}))$  and  $\psi \in C^\infty(0, T)$ .

It remains to note that following the arguments of Step 5 in the proof of Theorem 1, we obtain

$$\int_0^T \int_\Omega \nabla C_0 \cdot D^* \nabla C_0 = \int_\Omega \int_{\mathbb{Y}} (\nabla C_0(x) + \nabla_y C_1(x, y)) \cdot \tilde{D}(x, y) (\nabla C_0(x) + \nabla_y C_1(x, y)) dy dx \leq \|C_{\text{init}}\|_{L^2(\Omega)}^2 + \|S\|_{L^2(0, T; H^{-1}(\Omega))}^2,$$

so that  $(\Theta_0, C_0)$  is the unique weak solution of the homogenized system, and the whole sequence  $C_\varepsilon$  converges.

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