

An optimization-based multiscale coupling method

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Abstract

An optimization based algorithm is proposed for solving elliptic problems with highly oscillatory coefficients that do not exhibit scale separation in a subregion of the physical domain. The given method, written as a constrained minimization problem couples a numerical homogenization method in the subregion of the physical domain with scale separation with a fine scale solver in subregions without scale separation. The unknown boundary conditions of both problems in the overlap region are determined by minimizing the discrepancy of the corresponding solutions in this overlap.

Un algorithme basé sur le principe d'optimisation est proposé pour résoudre des problèmes elliptiques à coefficients oscillants sans séparation d'échelles dans une région du domaine. La méthode, qui s'écrit comme un problème de minimisation sous contraintes, couple une méthode d'homogénéisation numérique dans la région avec séparation d'échelles avec une méthode avec discrétisation fine dans les régions sans séparation d'échelles. Les conditions au bord des deux problèmes sur l'intersection des deux domaines sont déterminées par la minimisation de la différence entre les deux solutions dans le domaine commun.

Version française abrégée

Dans ce papier, nous présentons une méthode basée sur le principe d'optimisation inspirée de travaux récents [OBL13] sur un couplage atomistique-à-continu. Considérons le problème elliptique (1) avec $a \in (L^\infty(\Omega))^{d \times d}$ un tenseur oscillant, symétrique, borné et uniformément elliptique. L'homogénéisation classique [BLP78, JKO94] nous permet d'obtenir une solution effective u^0 d'un problème similaire à (1) avec un tenseur homogénéisé a^0 au lieu de a . Un grand nombre de méthodes d'homogénéisation numérique ont été développées ces dernières années (voir les références de [Abd09]) afin d'approximer u à un coût indépendant de l'échelle la plus fine. Cependant, les coefficients du tenseur doivent être localement périodiques ou avoir une séparation d'échelles. Nous nous intéressons à un problème où l'homogénéisation numérique ne peut pas être appliquée dans l'ensemble du domaine et doit être couplée avec une méthode capable de résoudre la plus fine échelle. Des problèmes de ce type ont déjà été traités dans la littérature

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avec l'approche dite globale-à-locale, dans laquelle les conditions aux bords des régions à échelles fines sont données par la solution homogénéisée [OdV00]. Nous mentionnons aussi la méthode récente [BaL11] basée sur des projections L^2 de la solution homogénéisée sur des espaces créés par des solutions de problèmes locaux. Finalement, nous rappelons que notre approche est basée sur les travaux effectués sur le couplage entre atomistique et continu [OBL13]. Soit $\omega \Subset \Omega$, une région où l'homogénéisation ne s'applique pas, nous proposons de résoudre deux problèmes sur ω et $\omega_2 = \Omega \setminus \omega$. Afin d'assurer continuité des solutions sur ω et ω_2 , dénotées respectivement u_1 et u_2 , nous construisons une région de chevauchement ω_0 entre ω et ω_2 et introduisons des contrôles virtuels sur le bord de ω_0 . Le couplage se fait via la minimisation de $u_1 - u_2$ sur ω_0 et nous obtenons un problème d'optimisation sous les contraintes (2) et (3) qui est résolu via multiplicateurs de Lagrange afin de déterminer les solutions "optimales" sur $\omega \cup \omega_0$ et ω_2 .

1. Introduction

Let $\Omega \subset \mathbb{R}^d, d > 1$ be a bounded domain and $f \in L^2(\Omega)$ and consider the following elliptic problem: find $u \in H_0^1(\Omega)$ satisfying

$$-\operatorname{div}(a\nabla u) = f, \text{ in } \Omega, \quad (1)$$

with $u = 0$ on $\partial\Omega$. We assume that the tensor $a \in (L^\infty(\Omega))^{d \times d}$ is uniformly elliptic, symmetric, bounded and highly oscillatory. Classical homogenization theory [BLP78, JKO94] is the standard tool to derive an effective solution u^0 of a problem similar to (1) with an effective tensor a^0 known as the homogenized tensor. Various numerical homogenization methods have been developed in the past few years to capture the effective solution at a cost independent of the smallest scale in the problem (see [Abd09] and the references therein). However, they usually rely on scale separation or locally periodic structure of the coefficients. In this paper we are interested in the situation where numerical homogenization can only be performed in subregions of the computational domain and must be coupled with fine scale computations in other subregions. Such problems are usually treated in the literature with so called global local approach in which the boundary conditions for the fine scale subregions are given by the homogenized solution [OdV00]. We also mention the recent approach in [BaL11] based on L^2 -projections onto a function space spanned by the solutions of local problems.

In this paper we present an optimization based coupling inspired by the recent work [OBL13] for atomistic-to-continuum coupling. The problem at hand is to solve two boundary value problems on ω and $\omega_2 = \Omega \setminus \omega$. To ensure continuity of the solutions, we introduce a blending or overlap region ω_0 between the two regions and use virtual controls on the boundary of ω_0 . This coupling between the solutions on the two subdomains, denoted u_1 and u_2 is achieved by minimizing the difference $u_1 - u_2$ in an appropriate norm on the overlap region. Such ideas have been used in the past in [GPT90] for coupling viscous and inviscid flows, in [LiP98] for optimal control on elliptic and parabolic differential equations and in [GLQ01] for the coupling of advection and advection-diffusion problems. To the best of our knowledge such optimization based coupling has not been used for numerical homogenisation problems.

2. Optimization

Let Ω be a domain decomposed as follows $\Omega = (\Omega \setminus \omega) \cup \omega = \omega_2 \cup \omega$. Consider (1) and assume that a can be decomposed into $a = \tilde{a}(x)\chi_\omega + a^\varepsilon(1 - \chi_\omega)$, where χ_ω is the indicator function on ω . We further assume that $\omega \Subset \omega_1 \Subset \Omega$ and denote the overlap by $\omega_1 \cap \omega_2 = \omega_0$. Suppose that numerical homogenization holds in ω_2 , thus in principle, the solution u can be approximated by $u^0 + \varepsilon u^1$, where u^0 is the solution of (3)

in ω_2 with a^0 instead of a [BLP78,JKO94]. In contrast, we want to compute a fine scale approximation of u in the domain ω , where we do not assume scale separation or stationarity. The above considerations lead to the following coupled problem: denote $\Gamma = \partial\Omega, \Gamma_1 = \partial\omega_1, \Gamma_2 = \partial\omega_2$ and consider $u_1 \in H^1(\omega_1), u_2 \in H^1(\omega_2)$ the solutions of

$$-\operatorname{div}(a\nabla u_1) = f, \text{ in } \omega_1, \quad u_1 = \varphi_1, \text{ on } \Gamma_1, \quad (2)$$

$$-\operatorname{div}(a^0\nabla u_2) = f, \text{ in } \omega_2, \quad u_2 = \varphi_2, \text{ on } \Gamma_2, u_2 = 0 \text{ on } \partial\Omega, \quad (3)$$

where the boundary conditions $\varphi_1 \in H^{1/2}(\Gamma_1)$ and $\varphi_2 \in H^{1/2}(\Gamma_2)$ are to be determined. We note that we could have considered the coupled problem with a^ε instead of a^0 in (3). For practical computation an approximation of a^0 could then be obtained by a numerical homogenization method such as the finite element heterogeneous multiscale method (FE-HMM) [Abd09,Abd11]. This is the situation considered in our numerical implementation in Section 4 but for simplicity we consider the above situation to state and analyze our algorithm.

Solving the above problem in an constrained optimization setting such as proposed in [GLQ01] leads to consider the artificial boundary conditions $\varphi_i, i = 1, 2$ as control variables and the functions $u_i \in H^1(\omega_i), i = 1, 2$ as state variables. The cost functional to minimize reads

$$J(u_1, u_2) = \frac{1}{2} \|u_1 - u_2\|_{L^2(\omega_0)}^2, \quad (4)$$

under the constraints that u_1 and u_2 should satisfy (2) and (3). To solve the above problem, it is convenient to split the solutions u_1 and u_2 into a part depending on the controls and a part solving a homogeneous Dirichlet elliptic problem, as

$$u_1 = u_{1,0} + v_1(\varphi_1) \text{ and } u_2 = u_{2,0} + v_2(\varphi_2), \quad (5)$$

where $u_{1,0}$ and $u_{2,0}$ solve zero Dirichlet boundary value problems in ω_1 and ω_2 , respectively. The unknowns become v_1 and v_2 , depending on the virtual control and satisfying

$$-\operatorname{div}(a\nabla v_1) = 0, \text{ in } \omega_1 \text{ and } v_1 = \varphi_1, \text{ on } \Gamma_1, \quad (6)$$

$$-\operatorname{div}(a^0\nabla v_2) = 0, \text{ in } \omega_2 \text{ and } v_2 = \varphi_2, \text{ on } \Gamma_2, v_2 = 0 \text{ on } \partial\Omega. \quad (7)$$

For a practical implementation we use the Lagrangian formulation of the above constrained optimization problems, obtained by introducing the Lagrange multipliers $\lambda_1 \in H_0^1(\omega_1)$ and $\lambda_2 \in H_0^1(\omega_2)$ associated to the constraints. The problem then reads: find $(v_1, \lambda_1, v_2, \lambda_2) \in H^1(\omega_1) \times H^1(\omega_1) \times H_\Gamma^1(\omega_2) \times H_\Gamma^1(\omega_2)$ such that

$$\mathcal{L}(v_1, \lambda_1, v_2, \lambda_2) = J(u_1, u_2) + \langle f + \operatorname{div}(a\nabla u_1), \lambda_1 \rangle_{H^{-1}, H^1} + \langle f + \operatorname{div}(a^0\nabla u_2), \lambda_2 \rangle_{H^{-1}, H^1}, \quad (8)$$

where $H_\Gamma^1(\omega_2) = \{u \in H^1(\omega_2) \mid u = 0 \text{ on } \Gamma \text{ in the sense of the trace}\}$. Considering next the critical point of the Lagrangian formulation (8), leads to a saddle point problem,

$$(L1) \int_{\omega_0} (v_1 - v_2)\varphi - \int_{\omega_1} a\nabla\varphi\nabla\lambda_1 = - \int_{\omega_0} (u_{1,0} - u_{2,0})\varphi, \quad \forall\varphi \in H^1(\omega_1),$$

$$(L2) \int_{\omega_1} a\nabla v_1\nabla\xi_1 = \int_{\omega_1} f\xi_1 - \int_{\omega_1} a\nabla u_{1,0}\nabla\xi_1, \quad \forall\xi_1 \in H^1(\omega_1),$$

$$(L3) - \int_{\omega_0} (v_1 - v_2)\phi - \int_{\omega_2} a^0\nabla\phi\nabla\lambda_2 = \int_{\omega_0} (u_{1,0} - u_{2,0})\phi, \quad \forall\phi \in H_\Gamma^1(\omega_2),$$

$$(L4) \int_{\omega_2} a^0\nabla v_2\nabla\xi_2 = \int_{\omega_2} f\xi_2 - \int_{\omega_2} a^0\nabla u_{2,0}\nabla\xi_2, \quad \forall\xi_2 \in H_\Gamma^1(\omega_2).$$

We briefly state the main points of our numerical algorithm.

Algorithm.

(A1) Create meshes on ω, ω_0 and $\Omega \setminus \omega_2$.

(A2) Compute $u_{1,0}$ and $u_{2,0}$ using a FEM and the FE-HMM, respectively. Store the value of a^0 at quadrature point of ω_0 .

(A3) Solve the saddle point problem (L1) to (L4) using a FEM and obtain the solution $(v_1, \lambda_1, v_2, \lambda_2)^\top$.

(A4) Compute u_1 and u_2 , solutions of (2) and (3) respectively, by using (5).

Observe that we have given the algorithm for the practical situation where a^0 is not available and only a^ε is at hand, hence a numerical homogenization method such as the FE-HMM is needed in the step (A2) of the above algorithm.

3. Analysis

In this section we discuss the accuracy of our optimization based coupling method. To establish the well-posedness of the constrained optimization problem (4), we consider $J(u_1, u_2) = \tilde{J}(\varphi_1, \varphi_2)$ defined as

$$\tilde{J}(\varphi_1, \varphi_2) = \frac{1}{2} \|v_1(\varphi_1) - v_2(\varphi_2)\|_{L^2(\omega_0)}^2 + \frac{1}{2} \|u_{1,0} - u_{2,0}\|_{L^2(\omega_0)}^2 + \int_{\omega_0} (u_{1,0} - u_{2,0})(v_1(\varphi_1) - v_2(\varphi_2)) dx.$$

Let $\mathcal{U} := H^{1/2}(\Gamma_1) \times H^{1/2}(\Gamma_2)$, the constrained optimization problem then reads: find $(\varphi_1, \varphi_2) \in \mathcal{U}$ such that $J(\varphi_1, \varphi_2) = \frac{1}{2} \|u_1(\varphi_1) - u_2(\varphi_2)\|_{L^2(\omega_0)}$ is minimized subject to equations (2) and (3). The necessary optimality condition is obtained by the Euler-Lagrange equation: find $(\varphi_1, \varphi_2) \in \mathcal{U}$ such that

$$\pi(\{\varphi_1, \varphi_2\}, \{\mu_1, \mu_2\}) = - \int_{\omega_0} (u_{1,0} - u_{2,0})(v_1(\varphi_1) - v_2(\varphi_2)) dx, \quad \forall (\mu_1, \mu_2) \in \mathcal{U}, \quad (9)$$

where the bilinear form π is given by $\pi(\{\varphi_1, \varphi_2\}, \{\mu_1, \mu_2\}) = \int_{\omega_0} (v_1(\varphi_1) - v_2(\varphi_2))(v_1(\mu_1) - v_2(\mu_2)) dx$. Following standard arguments, it can be shown that π defines an inner product on the space \mathcal{U} and the existence and uniqueness of a minimizer in the space $\hat{\mathcal{U}}$, obtained by completion for the norm $\|\cdot\|_{L^*(\mathcal{U})}$ induced by π , is obtained using Riesz-representation theorem (see [GLQ01] for details).

Let u^{OB} denote the solution of the optimization-based coupling, given by

$$u^{OB} = \begin{cases} u_{1,0} + v_1(\theta_1) & \text{in } \omega_1, \\ u_{2,0} + v_2(\theta_2) & \text{in } \omega_2 \setminus \omega_0. \end{cases} \quad (10)$$

We give an error analysis for the error in H^1 -norm $\|u - u^{OB}\|_{H^1(\omega)}$. As the difference $u - u^{OB}$ is a -harmonic in ω_1 , Caccioppoli inequality can be used and we can bound the H^1 -norm on ω by the L^2 -norm over ω_1 . Let τ denote the width of ω_0 and $0 < \alpha < \beta$ be the coercivity constant of \tilde{a} , i.e. $\alpha|\xi|^2 \leq \xi^\top \tilde{a}(x)\xi \leq \beta|\xi|^2$, for $\xi \in \mathbb{R}^d$, we then have

$$\|u - u^{OB}\|_{H^1(\omega)} \leq C(\tau, \beta) \|u - u^{OB}\|_{L^2(\omega_1)}.$$

For any couple of virtual controls $\{\mu_1, \mu_2\} \in \mathcal{U}$, we define an operator $P : \mathcal{U} \rightarrow H_0^1(\Omega)$ by

$$\{\mu_1, \mu_2\} \mapsto P(\{\mu_1, \mu_2\}) = \begin{cases} u_{1,0} + v_1(\mu_1) & \text{in } \omega_1, \\ u_{2,0} + v_2(\mu_2) & \text{in } \omega_2 \setminus \omega_0, \end{cases}$$

which can be split into $P = U_0 + Q$, where U_0 is the constant part of P and

$$Q(\{\mu_1, \mu_2\}) = \begin{cases} v_1(\mu_1) & \text{in } \omega_1, \\ v_2(\mu_2) & \text{in } \omega_2 \setminus \omega. \end{cases}$$

Moreover, we define the trace operator $\gamma : H_0^1(\Omega) \rightarrow \mathcal{U}$ by $\gamma(u) = (\gamma_1(u), \gamma_2(u))$, where $\gamma_i : H^1(\omega_i) \rightarrow H^{1/2}(\Gamma_i)$, $i = 1, 2$ is given by $\gamma_i(u) = u|_{\Gamma_i}$ (in the sense of the trace). Using the exact trace of u as bound-

any condition in problem (7), we define $u^c = u_{2,0} + v_2(\gamma_2(u))$ and observe that $u|_{\omega_1} = (u_{1,0} + v_1(\gamma_1(u)))|_{\omega_1}$. Then, we have

$$\begin{aligned} \|u - u^{OB}\|_{L^2(\omega_1)} &= \|u - P(\{\theta_1, \theta_2\})\|_{L^2(\omega_1)} \leq \underbrace{\|u - P(\gamma(u))\|_{L^2(\omega_1)}}_{=0} + \|P(\gamma(u)) - P(\{\theta_1, \theta_2\})\|_{L^2(\omega_1)} \\ &\leq \|Q\| \|\gamma(u) - \{\theta_1, \theta_2\}\|_{L^*(\mathcal{U})}, \end{aligned} \quad (11)$$

where the norm of the operator Q is

$$\|Q\| = \sup_{\{\mu_1, \mu_2\}} \frac{\|Q(\{\mu_1, \mu_2\})\|_{L^2(\Omega)}}{\|\{\mu_1, \mu_2\}\|_{L^*(\mathcal{U})}}.$$

A bound on the norm $\|\gamma(u) - \{\theta_1, \theta_2\}\|$ is given in the next lemma that can be proved assuming local periodic coefficients a in ω_2 (details will be given in [AJS]).

Lemma 3.1 *Let u be the solution of (1) and let $\{\theta_1, \theta_2\}$ be the minimizer of (9). Then*

$$\|\gamma(u) - \{\theta_1, \theta_2\}\|_{L^*(\mathcal{U})} \leq \|u - u^c\|_{L^2(\omega_0)}.$$

Moreover, it hold

$$\|u - u^c\|_{L^2(\omega_0)} \leq C\varepsilon.$$

Finally, we obtain the following error bound.

Theorem 3.2 *Let u be the solution of (1) and let u^{OB} be defined by (10), it holds*

$$\|u - u^{OB}\|_{H^1(\omega)} \leq C\varepsilon,$$

where the constant depends on τ, β and Q .

The last step for the error analysis is to bound the norm of the operator Q in (11). This will be discussed in [AJS], as well as an error estimate for the FE discretization.

4. Numerical experiment

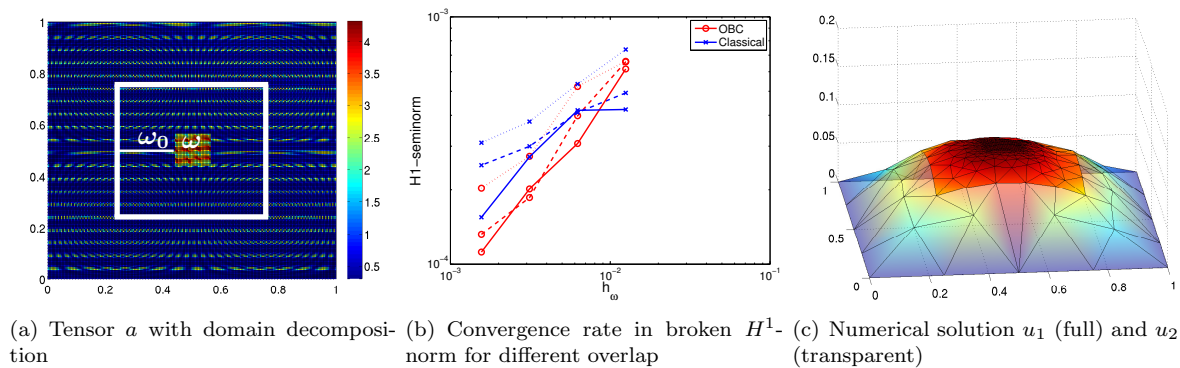
We present a two-dimensional experiment. We use P_1 -FE and compute a numerical approximation of u using FEM on Ω . Let $a(x_1, x_2) = \tilde{a}(x_1, x_2)\chi_\omega(x_1, x_2) + a^\varepsilon(x_1, x_2)(1 - \chi_\omega)(x_1, x_2)$, where

$$\begin{aligned} \tilde{a}(x_1, x_2) &= 3 + \frac{1}{7} \sum_{j=0}^4 \sum_{i=0}^j \frac{2}{j+1} \cos\left(\left\lfloor 8(ix_2 - \frac{x_1}{i+1}) \right\rfloor + \left\lfloor \frac{8ix_1}{\varepsilon} \right\rfloor + \left\lfloor \frac{8x_2}{\varepsilon} \right\rfloor\right) \\ a^\varepsilon(x_1, x_2) &= \frac{1}{6} \left(\frac{1.1 + \sin(2\pi(x_1/\varepsilon)(x_2/\varepsilon))}{1.1 + \sin(2\pi x_2/\varepsilon)} + \sin(4x_1^2 x_2^2) + 2 \right), \end{aligned}$$

where $\varepsilon = 1/160$, the tensor \tilde{a} is taken from [HMP13] and is represented in Figure 1(a). We compare the optimization-based method with a classical coupling [OdV00], where we solve

$$-\operatorname{div}(a\nabla u^C) = f, \text{ in } \omega_1, \quad u^C = u^0, \text{ on } \Gamma_1,$$

where u^0 is the homogenized solution computed with the FE-HMM on Ω . Figure 1(c) represent the numerical solutions u_1 (full) and u_2 (transparent). Convergence rates to the exact solution, $\|u - u^{OB}\|_{\bar{H}^1(\omega)}$ in red and $\|u - u^C\|_{\bar{H}^1(\omega)}$ in blue, are given in Figure 1(b). We chose to show the convergences for three different widths τ of the overlap $\tau = \frac{3}{16}$ (full), $\tau = \frac{1}{16}$ (dashed) and $\tau = \frac{3}{80}$ (dotted lines). We observe that the convergence deteriorate when the width gets smaller. Optimization based coupling produce better convergence rate than the classical method for tensor without scale-separation.



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