Numerical Homogeneisation Technique with Domain Decomposition Based a-posteriori Error Estimates

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Summary. The purpose of the present work is to review some basic numerical homogeneisation techniques for the simulation of multiscale materials and to introduce an error control strategy at the local level. This error control uses an a posteriori error estimate built on a local problem coupling different representative volume elements. It introduces a weakly coupled adjoint problem to be solved say by a direct Schur complement method. Mortar element techniques as introduced in domain decomposition techniques are used to couple in a weak and cheap form the different representative elements in the error analysis. The strategy is numerically assessed on a model two dimensional problem.

1 Introduction

In many practical situations, there is a significant separation of scales between the global macroscopic problem and the local heterogeneities governing the response of the constitutive materials. Metals, elastomers, construction materials present a microstructure at micronic or submicronic scales which influence their constitutive laws. Dynamic contact problems, cable matrix interactions inside composite materials are similar situations where the physical response of the system occurs at very small scales (millimiter or less) compared to the overall dimensions of the global structure. These scales are out of reach by a direct simulation of the global problem, even when using sophisticated domain decomposition algorithms. Homogeneisation techniques at large propose a general methodology to handle such situations.

The methodology is quite simple [7, 8, 12, 15]. It is based on the notion of representative volume elements (RVE). Each volume element is a microscopic sample of the system under study. Its size H is very small compared to the macroscopic characteristic length L of the global problem, and very large compared to the size ε of the heterogeneities $L >> H >> \varepsilon$. Each sample is solved locally at a microscopic scale taking as boundary conditions uniform displacement data deduced from the pointwise value of the strain tensor observed at macroscopic scale. Once computed at a local scale, the averaged answer defines the macroscopic constitutive response of the material. In such a construction, the ratio between H and ε serves two purposes: a

large ratio reduces the effect of the artificial boundary conditions to be used on the RVE [10], and leaves room to include a statistically representative sample of the local heterogeneities. On the other hand, a smaller ratio reduces the cost of the solution of the local problems. Hence the idea of developing an a posteriori error estimate strategy to assess the choices of the sample size H and of the artificial boundary conditions used at local scale.

The purpose of the present work is therefore to review some basic numerical homogeneisation techniques for the simulation of nonlinear viscoelastic multiscale materials and to introduce a domain decomposition based error control strategy for the local problems. A model mechanical problem is introduced in Section 2. Numerical homogeneisation is reviewed in Section 3. Section 4 is devoted to the introduction of an a posteriori error estimate built on a reference extended local problem coupling different representative volume elements. This introduces a weakly coupled adjoint problem to be transformed into a small interface problem to be solved say by a direct Schur complement method. Mortar element techniques are used at this level to weakly couple the different representative elements in the error analysis. The strategy is assessed on a two dimensional problem in Section 5.

2 Mechanical Problem

Let us consider the quasi static evolution of a given macroscopic solid or structure which occupies the domain Ω at rest, which is fixed on a part $\partial\Omega_\xi$ of its boundary, and which is subjected to a known distribution $\underline{F}$ of specific loads and $\underline{T}$ of surface loads. The problem to solve combines the balance of momentum in reference configuration, a time dependent viscoelastic constitutive law and a time differential equation describing the evolution of the internal variables $\underline{\underline{\varepsilon}}^e_\tau$, each material relaxation time τ corresponding to one specific internal variable $\underline{\underline{\varepsilon}}^e_\tau$. After time discretisation, say by a uniformly stable time implicit Euler scheme, this problem reduces to a sequence of equilibrium problems to be solved at different times t_{n+1}:

Find $\underline{x}-\underline{x}_d \in \mathbf{V}$ and $\underline{\underline{\varepsilon}}^e_\tau$ solution of

$$\int_\Omega \underline{\underline{\sigma}} : \frac{\partial \underline{\hat{U}}^t}{\partial \underline{X}}\, d\Omega = \int_\Omega \rho \underline{F}(\underline{X})\cdot\underline{\hat{U}}\, d\Omega + \int_{\partial\Omega_T} \underline{T}(\underline{X})\cdot\underline{\hat{U}}\, da \quad \forall \underline{\hat{U}} \in \mathbf{V}, \tag{1}$$

$$\underline{\underline{\varepsilon}} = \frac{1}{2}\left(\frac{\partial(\underline{x}-\underline{X})}{\partial \underline{X}} + \frac{\partial(\underline{x}-\underline{X})^t}{\partial \underline{X}}\right), \tag{2}$$

$$\underline{\underline{\sigma}} = \rho\,\frac{\partial \psi_\infty}{\partial \underline{\underline{\varepsilon}}}(\underline{\underline{\varepsilon}}) + \sum_\tau \underline{\underline{\bar{\sigma}}}_\tau, \qquad \underline{\underline{\bar{\sigma}}}_\tau = \rho\,\frac{\partial \psi_\tau}{\partial \underline{\underline{\varepsilon}}^e_\tau}(\underline{\underline{\varepsilon}}^e_\tau), \tag{3}$$

$$\underline{\underline{\varepsilon}}^e_\tau = \underline{\underline{\varepsilon}}^{e\,n}_\tau + \underline{\underline{\varepsilon}} - \underline{\underline{\varepsilon}}^n - \Delta t\, \underline{\underline{\phi}}^{-1}_\tau(\underline{\underline{\bar{\sigma}}}_\tau) \quad \forall \tau. \tag{4}$$

In the above expression, $\mathbf{V}$ denotes the space of kinematically admissible test functions, ψ_∞ and ψ_τ are given free energy potentials characterizing the reversible parts of the stresses, $\underline{\underline{\phi}}^{-1}_\tau$ is a given dissipation function, $\underline{\underline{\varepsilon}}^n$ and $\underline{\underline{\varepsilon}}^{e\,n}_\tau$ are the strain and

internal variables values at previous time step. After elimination of the viscoelastic stress $\underline{\underline{\bar{\sigma}}}_\tau$ and linearisation, this problem reduces to a standard elasticity problem

$$\int_\Omega \frac{1}{2}\left(\frac{\partial \delta \underline{x}}{\partial \underline{X}} + \frac{\partial \delta \underline{x}}{\partial \underline{X}}^t\right) : \underline{\underline{\underline{\underline{C}}}} : \frac{\partial \hat{\underline{U}}}{\partial \underline{X}}^t \, d\Omega = R(\hat{\underline{U}}) \quad \forall \hat{\underline{U}} \in \mathbf{V}$$

with branch averaged elasticity tensor

$$\underline{\underline{\underline{\underline{C}}}} = \rho \frac{\partial^2 \psi_\infty}{\partial \underline{\underline{\varepsilon}}^2} + \sum_\tau \left(\frac{1}{\rho}\left(\frac{\partial^2 \psi_\tau}{\partial \underline{\underline{\varepsilon}}_\tau^{e\,2}}\right)^{-1} + \Delta t \frac{\partial \underline{\underline{\phi}}_\tau^{-1}}{\partial \underline{\underline{\bar{\sigma}}}_\tau}\right)^{-1}.$$

3 Numerical Homogeneisation

In the original problem, the Cauchy stress $\underline{\underline{\sigma}}$ oscillate rapidly in space at scale ε because the coefficients inside the free energy do so. In theory, one would need to solve this problem at the space scale ε over the whole domain Ω of size L, which is completely out of reach. To overcome this problem, homogeneisation techniques introduce an averaging scale H with $L >> H >> \varepsilon$ and construct around each macroscopic point $\underline{X}$ one sample or a collection of samples $\Omega_H(\underline{X})$ of the material, of size H. Space averages on the local RVE (Representative Volume Elements) $\Omega_H(\underline{X})$ with respect to the local space variable $Y \in \Omega_H(\underline{X})$ will be denoted by $\langle f \rangle_{\Omega_H(\underline{X})} := \frac{1}{|\Omega_H(\underline{X})|}\int_{\Omega_H(\underline{X})} f(\underline{Y}) d\Omega_H$. Using smooth test functions $\hat{\underline{U}}$ such that $\frac{\partial \hat{\underline{U}}}{\partial \underline{\underline{X}}} \approx \langle \frac{\partial \hat{\underline{U}}}{\partial \underline{\underline{Y}}} \rangle_{\Omega_H(\underline{X})}$, the power devoloped by the internal forces in the virtual motion $\hat{\underline{U}}$ can be reduced to

$$\int_\Omega \underline{\underline{\sigma}} : \frac{\partial \hat{\underline{U}}}{\partial \underline{X}}^t \, d\Omega \approx \int_\Omega \langle \underline{\underline{\sigma}} \rangle_{\Omega_H(\underline{X})} : \frac{\partial \hat{\underline{U}}}{\partial \underline{X}}^t \, d\Omega.$$

Compared to the original expression, we may assume that the variations in space of the average tensor $\langle \underline{\underline{\sigma}} \rangle_{\Omega_H(\underline{X})}$ will be very slow, meaning that the second integral can be approximated at macroscopic level by a Gaussian integration rule with few integration points X_G. As explained in [5], the challenge is to identify the averaged stress $\langle \underline{\underline{\sigma}} \rangle_{\Omega_H(\underline{X})}$ at each macroscopic point X. The stress tensor must summarize the local heterogeneous constitutive response of the material as function of the strain field inherited from the macroscopic displacement field. The idea [7, 8, 11] is then to solve the original problem on each local domains Ω_H with imposed strain average

$$\lim_{\underline{Y} \to \partial \Omega_H(\underline{X})} \underline{x}(\underline{Y}) - \underline{Y} - \langle \underline{\underline{\varepsilon}} \rangle_{\Omega_H(\underline{X}_G)} \cdot \underline{Y} = \underline{0}, \tag{5}$$

using Dirichlet or periodic boundary conditions to impose this macroscopic strain field. The choice of boundary conditions does not affect the asymptotic limit of the solution as $H/\varepsilon \to \infty$, but may affect the size of the error for bounded ratios H/ε [10]. In that respect, periodic boundary conditions are usually found to be less intrusive.

The local problem defines a H homogeneized constitutive law

$$\langle \underline{\underline{\sigma}} \rangle (\langle \underline{\underline{\varepsilon}} \rangle_{\Omega_H(\underline{X})}) = \left\langle \rho \frac{\partial \psi_\infty}{\partial \underline{\underline{\varepsilon}}} (\underline{\underline{\varepsilon}}_Y) + \sum_\tau \rho \frac{\partial \psi_\tau}{\partial \underline{\underline{\varepsilon}}^e_\tau} (\underline{\underline{\varepsilon}}^e_\tau) \right\rangle_{\Omega_H(\underline{X})} \tag{6}$$

which may directly be used in a continuous writing of the problem on the whole domain Ω. This leads to a regularized macroscopic problem with unknown $\underline{x}$, which hopefully is the right limit of our original problem when the size of the heterogeneities go to zero and which writes

$$\int_\Omega \langle \underline{\underline{\sigma}} \rangle (\langle \underline{\underline{\varepsilon}}(\underline{x}) \rangle_{\Omega_H(\underline{X})}) : \frac{\partial \underline{\hat{U}}^t}{\partial \underline{X}} \, d\Omega = \int_\Omega \rho \underline{F}(\underline{X}) \cdot \underline{\hat{U}} \, d\Omega + \int_{\partial \Omega_T} \underline{T}(\underline{X}) \cdot \underline{\hat{U}} \, da \quad \forall \underline{\hat{U}} \in \mathbf{V}. \tag{7}$$

The two scales homogeneized formulation of our original problem is obtained by simultaneously writing the global equilibrium problem (7) and the local evolution problems. The downscale coupling comes from the boundary condition (5) used in the local problem which is function of the global solution. The upscale coupling occurs through the averaged constitutive law (6).

We could see in the above numerical homogeneisation a nonlinear domain decomposition technique, with representative volume elements playing the roles of subdomains, and where the restriction and extension operators would be simple averages of strains and stresses respectively. One could also view the global problem as the reduction of the problem to a coarse space built with functions whose restriction on each representative element is linear. The difference is that the decomposition of the original problem as done in the numerical homogeneisation technique does not really build an additive decomposition of our original multiscale problems because of the simplified nonconforming boundary conditions applied to the small scale solutions and because the local domains do not necessarily build a complete partition of the full global domain. Therefore, homogeneisation techniques are inexact in nature, and can only be approximation of the real solutions at the limit of large ratios H/ε and L/H.

4 Error Control

4.1 Motivation and Reference Local Solution

The above methodology is very general. It is arbitrary with respect to the choice of the ratio between the size H of the representative volume element Ω_H and the size ε of the heterogeneities, the choice of the boundary conditions to be imposed on the local problem to be solved on each RVE and the construction of the local geometry and material coefficients inside the RVE.

The theoretical answer is to use as large RVE as possible, the theory proving the asymptotic convergence of the method at the limit $H/\varepsilon \to \infty$ [1]. But such a methodology has a cost, which is the solution of the local problems on the different

domains Ω_{mH}. Since calculating over large RVE is costly, compromises must be found using smaller samples and improved boundary conditions. The validity of the resulting approach must then be checked by a posteriori error estimates [16].

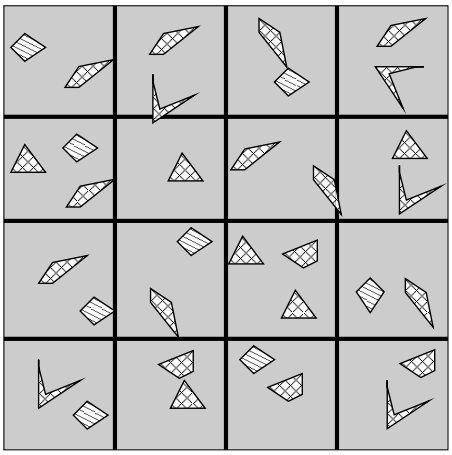

Fig. 1. The reference geometry at local scale, and its decomposition into subcells.

Error estimates must first define a local reference problem. For this purpose, we assume that we can specify a local reference problem at a sufficiently large scale $\bar{H} = NH$, with geometry $\overline{\Omega}_{\bar{H}}$, imposed macroscopic strain, and an adequate choice of boundary conditions (typically periodic boundary conditions in space). This reference geometry is partitioned into subcells (Fig. 1)

$$\overline{\Omega}_{\bar{H}} = \cup_{K=1}^{N^3} \overline{\Omega}_{kH},$$

on which we can introduce a hierarchy of local numerical solutions. The coarsest is the solution of the local problem on a single subcell $\overline{\Omega}_{0H}$ with imposed averaged strain. The second level solves the local problem on each subcell $\overline{\Omega}_{kH}, \forall k = 1, N^3$, with say periodic boundary conditions. This constructs a two scale local solution $(\underline{x}_H, \underline{\underline{\sigma}}_H)$ by juxtaposition of the local fields $\underline{x}_H|_{\Omega_{kH}} = \underline{x}_{kH}, \quad \underline{\underline{\sigma}}_H|_{\Omega_{kH}} = \underline{\underline{\sigma}}_{kH}$ and an empirical stress average (and associated variance)

$$\langle \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}) \rangle = \frac{1}{N^3} \sum_k \langle \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}) \rangle_{\Omega_{kH}}.$$

The third level would be to compute the full solution $(\underline{x}, \underline{\underline{\sigma}})$ of the nonlinear problem on the large local domain $\overline{\Omega}_{\bar{H}}$.

The problem is then to estimate the distance $(\delta\underline{x}, \delta\underline{\underline{\sigma}})$ between the two scales local solution $(x_H, \underline{\underline{\sigma}}_H)$ and the full local solution $(\underline{x}, \underline{\underline{\sigma}})_{\Omega_{\bar{H}}}$ without computing the full solution. Since the proposed two scales solution may be discontinuous across inter-domain boundaries, we must first propose a framework which handles discontinuous

fields. This can be achieved by using mortar techniques as in [3, 14] which introduce a finite element notion of weak continuity by constructing local interface finite elements $\mathbf{M}_{kl} = \mathbf{M}_{lk}$ on each interface $\partial\Omega_{kH} \cap \partial\Omega_{lH}$ between neighboring subdomains Ω_{kH} and $\partial\Omega_{lH}$ and by weakly imposing the interface continuity requirement in $\mathbf{M}_{kl}$. In this framework, the full local problem reduces to the following sequence of coupled problems:

Find the displacement $(\underline{x}_k)_k \in \Pi_k \mathbf{V}_{kH}$ and the interface tractions $(\underline{\lambda}_{kl})_{kl} \in \Pi_{kl} \mathbf{M}_{kl}$ such that

$$\begin{aligned} \int_{\Omega_{kH}} \left(\rho \frac{\partial \psi_\infty}{\partial \underline{\underline{\varepsilon}}}(\underline{\underline{\varepsilon}}_Y) + \sum_\tau \rho \frac{\partial \psi_\tau}{\partial \underline{\underline{\varepsilon}}^e_\tau}(\underline{\underline{\varepsilon}}^e_\tau(\underline{Y})) \right) : \frac{\partial \underline{\hat{U}}^t}{\partial \underline{Y}} \, d\Omega_H \\ + \sum_l \int_{\partial\Omega_{kH} \cap \partial\Omega_{lH}} \underline{\lambda}_{kl} \cdot \underline{\hat{U}} \, da = 0 \quad \forall \underline{\hat{U}} \in \mathbf{V}_{kH}, \ \forall k, \end{aligned} \tag{8}$$

$$\underline{\underline{\varepsilon}}_Y(\underline{Y}) = \frac{1}{2} \left(\frac{\partial (\underline{x}_k - \underline{Y})}{\partial \underline{Y}} + \frac{\partial (\underline{x}_k - \underline{Y})^t}{\partial \underline{Y}} \right)(\underline{Y}), \tag{9}$$

$$\underline{\underline{\varepsilon}}^e_\tau = \underline{\underline{\varepsilon}}^{e\,n}_\tau + \underline{\underline{\varepsilon}}_Y - \underline{\underline{\varepsilon}}^n_Y - \Delta t \, \underline{\underline{\phi}}^{-1}_\tau \left(\rho \frac{\partial \psi_\tau}{\partial \underline{\underline{\varepsilon}}^e_\tau}(\underline{\underline{\varepsilon}}^e_\tau) \right), \tag{10}$$

$$\int_{\partial\Omega_{kH} \cap \partial\Omega_{lH}} \underline{\mu}_{kl} \cdot (\underline{x}_l - \underline{x}_k) da = 0 \quad \forall \underline{\mu}_{kl} \in \mathbf{M}_{kl}, \ \forall k < l, \tag{11}$$

$$\underline{\lambda}_{kl} + \underline{\lambda}_{lk} = 0 \quad \forall k < l. \tag{12}$$

In such formulations, the choice of the interface spaces $\mathbf{M}_{kl}$ cannot be completely arbitrary. The initial formulation of [2, 3] uses finite element displacements of degree q without stabilization, and continuous Lagrange multipliers of degree q. Limited modifications of the Lagrange multipliers are necessary on the boundaries of the interfaces. Alternatively, as shown in [13] for second order approximations of the displacements ($q \geq 2$), the formulation of [2, 3] can be used with continuous Lagrange multipliers of degree $q-1$. In order to make the mortar weak continuity constraint diagonal, one can also adopt the dual Lagrange multipliers of Wohlmuth [14]. A last choice advocated in [9] uses finite element displacements of degree q with proper stabilization (bubble additions) together with discontinuous Lagrange multipliers of degree $q-1$ as first developed for three-field matching formulations in [4]. All these choice guarantee an optimal order of convergence between the solution of the above discrete coupled problem and the continuous one [9, 14]. But here we are only interested in error estimates. Thus, for estimating the error, we can use very simple Lagrange multipliers as initially proposed in [6], namely simple polynomials globally defined on each interface and of low order p (typically $4 \leq p \leq 10$).

4.2 Adjoint Equation

The question is now to estimate the distance between the two scales local solution $(x_H, \underline{\underline{\sigma}}_H)$ and the reference solution of the mixed variational system (8-12) without solving the latter system. A first information on the error is given by the residual

observed in the formulation (8-12) when plugging our two scales solution. This is useful, but is hard to relate to a meaningful norm. A better strategy would be to solve the variational problem defining the error but its solution is out of reach because it couples all local subdomains together. A compromise must be found. Here, we are only interested in the local averages of the components of the Cauchy stress tensor

$$Q = \int_{\Omega_H} \underline{\underline{\sigma}} : \underline{e}_i \otimes \underline{e}_j \, d\Omega_H,$$

$$\frac{\partial Q_k}{\partial \underline{x}}(\underline{x}_H) \cdot \underline{\hat{U}} = \int_{\Omega_{kH}} \underline{e}_i \otimes \underline{e}_j : \left(\underline{\underline{\underline{\underline{C}}}}_Y : \frac{1}{2}\left(\frac{\partial \underline{\hat{U}}}{\partial \underline{Y}} + \frac{\partial \underline{\hat{U}}^t}{\partial \underline{Y}} \right) \right) d\Omega_H.$$

To estimate the accuracy of $Q(\underline{x})$ as predicted by the two scales local solution, one only needs to obtain an approximate solution of the adjoint equation defined on the collection of subdomains by:

Find the adjoint state $\underline{x}^a$ and the adjoint interface tractions $\underline{\lambda}^a$ such that

$$\begin{aligned} &\int_{\Omega_{kH}} \left(\underline{\underline{\underline{\underline{C}}}}_Y : \frac{1}{2}\left(\frac{\partial \underline{x}^a}{\partial \underline{X}} + \frac{\partial \underline{x}^{a\,t}}{\partial \underline{X}} \right) \right) : \frac{\partial \underline{\hat{U}}^t}{\partial \underline{X}} \, d\Omega_H + \sum_l \int_{\partial\Omega_{kH} \cap \partial\Omega_{lH}} \underline{\lambda}^a_{kl} \cdot \underline{\hat{U}} \, da \\ &\quad = \frac{\partial Q}{\partial \underline{x}}(\underline{x}_H) \cdot \underline{\hat{U}} \quad \forall \underline{\hat{U}} \in \mathbf{V}_{kH}, \ \forall k, \end{aligned} \tag{13}$$

$$\int_{\partial\Omega_{kH} \cap \partial\Omega_{lH}} \underline{\mu}_{kl} \cdot (\underline{x}^a_l - \underline{x}^a_k) da = 0 \quad \forall \underline{\mu}_{kl} \in \mathbf{M}_{kl}, \ \forall k < l, \tag{14}$$

$$\underline{\lambda}^a_{kl} + \underline{\lambda}^a_{lk} = 0 \quad \forall k < l. \tag{15}$$

4.3 Explicit a Posteriori Error Estimate

The adjoint state then allows a direct access to the error on $Q(\underline{x})$. Indeed, writing the adjoint problem (13)–(14) using as test functions $(\underline{\hat{U}}, \underline{\mu})$ the solution $(\delta\underline{x}, \underline{\lambda})$ of the linearized error problem yields

$$\begin{aligned} \frac{\partial Q}{\partial \underline{x}}(\underline{x}_H) \cdot \delta\underline{x} = &\sum_k \int_{\Omega_{kH}} \left(\underline{\underline{\underline{\underline{C}}}}_Y : \frac{1}{2}\left(\frac{\partial \underline{x}^a}{\partial \underline{X}} + \frac{\partial \underline{x}^{a\,t}}{\partial \underline{X}} \right) \right) : \frac{\partial \delta\underline{x}^t}{\partial \underline{X}} \, d\Omega_H \\ &+ \sum_{k<l} \int_{\partial\Omega_{kH} \cap \partial\Omega_{lH}} \underline{\lambda}^a_{kl} \cdot (\delta\underline{x}_l - \delta\underline{x}_k) da. \end{aligned}$$

Using the symmetry of the elasticity tensor, the continuity of the exact solution, the linearized error equations, and using the weak interface continuity of the adjoint state reduce the above expression to the *explicit error estimate*

$$\begin{aligned} \frac{\partial Q}{\partial \underline{x}}(\underline{x}_H) \cdot \delta\underline{x} &= \sum_k \int_{\Omega_{kH}} \left(\underline{\underline{\underline{\underline{C}}}}_Y : \delta\underline{\underline{\varepsilon}} \right) : \frac{\partial \underline{x}^{a\,t}}{\partial \underline{X}} \, d\Omega_H \\ &\quad - \sum_{k<l} \int_{\partial\Omega_{kH} \cap \partial\Omega_{lH}} \underline{\lambda}^a_{kl} \cdot (\underline{x}_{lH} - \underline{x}_{kH}) da \\ &= -\sum_k \int_{\Omega_{kH}} \underline{\underline{\sigma}}_H : \frac{\partial \underline{x}^{a\,t}}{\partial \underline{X}} \, d\Omega_H - \sum_{k<l} \int_{\partial\Omega_{kH} \cap \partial\Omega_{lH}} \underline{\lambda}^a_{kl} \cdot (\underline{x}_{lH} - \underline{x}_{kH}) da. \end{aligned}$$

4.4 Numerical Solution of the Adjoint Problem

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For solution purposes, the adjoint problem can be rewritten as a Schur complement problem set on the interface with unknown $\bar{X}^a = (Tr_{kl}\underline{x}^a)_{kl} \in \Pi_{k<l} M'_{kl}$. By introducing the local trace

$$Tr_k = \begin{pmatrix} \vdots \\ Tr_{kl} \\ \vdots \end{pmatrix} \quad \text{and restriction} \quad R_k\bar{X} = \begin{pmatrix} \vdots \\ \bar{X}_{kl} \\ \vdots \end{pmatrix},$$

we can immediately rewrite the adjoint problem as the algebraic system

$$\left(\sum_k R_k^t \begin{pmatrix} 0 & I \end{pmatrix} \begin{pmatrix} K_k & Tr_k^T \\ Tr_k & 0 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ I \end{pmatrix} R_k \right) \bar{X}^a = - \sum_k R_k^t \begin{pmatrix} 0 & I \end{pmatrix} \begin{pmatrix} K_k & Tr_k^T \\ Tr_k & 0 \end{pmatrix}^{-1} \begin{pmatrix} \frac{\partial Q_k}{\partial \underline{x}}(\underline{x}_H) \\ 0 \end{pmatrix}. \quad (16)$$

This symmetric reduced system is of smalll dimension when one uses low order interface mortars. It can be solved by a direct solver in $\bar{X}^a$. It can also be solved by a few iterations of a domain decomposition algorithm.

5 Numerical Results

The proposed strategy has been tested on a simple two dimensional situation in anisotropic elasticity. The reference local problem uses a periodic geometry at scale $\bar{H}$ made of $n_x \times n_y = 30$ unit subcells of size $l_x \times l_y$ with a non periodic variation of the stiffness coefficients as represented in Fig. 2. In crystal coordinates, the stiffness coefficients C_{1111}, C_{1122} and C_{1212} have a space periodic distribution at the subcell level

$$C_{ijkl} = C^0_{ijkl} * \left(1.1 + \sin\left(\frac{2\pi x}{l_x}\right)\right) * \left(1.1 + \sin\left(\frac{2\pi y}{l_y}\right)\right)$$

with $C^0_{1111} = 3000\,Gpa, C^0_{1122} = 100\,Gpa, C^0_{1212} = 200\,Gpa$ and the crystal direction has a non periodic space variation with a local angle given by

$$\theta = \frac{1}{4}\left(\frac{2\pi x}{n_x l_x} + \frac{2\pi y}{n_y l_y}\right).$$

The global sample (the local geometry built with the 30 subcells) is subjected at infinity to a uniform shear deformation of one percent. A solution computed for the whole local sample cell yields a non periodic shear stress distribution as represented on Fig. 2, with a shear localisation in the weak parts of the sample.

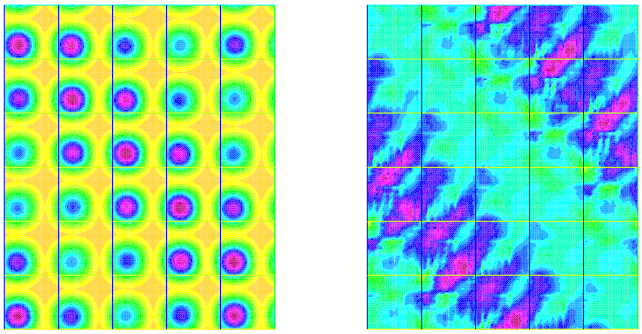

Fig. 2. (Left) Representation of the space variation of the stiffness coefficient C_{xxxx}. The ratio between the minimal and the maximal values is 400. (Right) Representation of the shear stress when computed globally on the full sample.

The two scales solution $\underline{x}_H$ computed independently on each subcell using periodic boundary conditions is represented on Fig. 3. Observe the displacement jumps at the interface in this local construction. The averaged shear stress obtained by this two scales local approach differs from the exact one by $50.6 MPa$. The solution of the dual problem is then obtained using polynomial Lagrange multipliers of order 4. In this simple case, the error on the average shear as predicted from the dual solution is equal to $50.3 MPa$ to be compared to the real error of $50.6 MPa$. This clearly indicates the good accuracy of our error estimate.

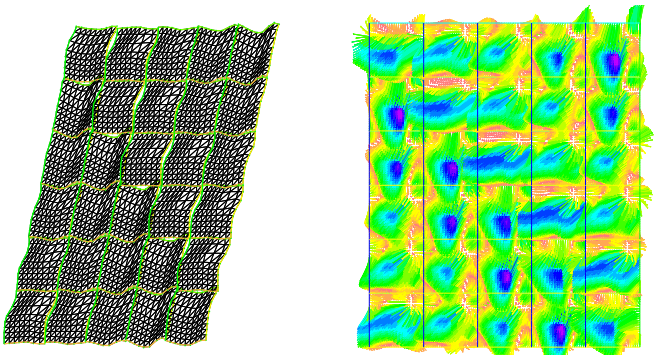

Fig. 3. Representation of the two scale solution computed subcell by subcell using periodic boundary conditions. Deformed mesh and displacement field.

6 Conclusions

In the framework of first order numerical homogeneisation techniques, the present paper has introduced an a-posteriori error estimate to qualify the choice of the local representative volume elements to be used in a two scale finite element method.

The error estimate was developed in the framework of nonlinear viscoelastic materials in small strains but can readily be extended to large strains situations. Its performance was assessed on two dimensional problems. A lot of numerical assessment is still to be done. Recovering microscopic data, implementing mortars in an industrial framework is challenging. Moreover, the local problems are stochastic in nature. What is then the best treatment of the random nature of the material heterogeneities and processes?

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