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*A direct approach to numerical homogenization in
finite elasticity*

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Thème NUM



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A direct approach to numerical homogenization in finite elasticity

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Abstract: We describe, analyze, and test a direct numerical approach to a homogenized problem in nonlinear elasticity at finite strain. The main advantage of this approach is that it does not modify the overall structure of standard softwares in use for computational elasticity. Our analysis includes a convergence result for a general class of energy densities and an error estimate in the convex case. We relate this approach to the multiscale finite element method and show our analysis also applies to this method. Microscopic buckling and macroscopic instabilities are numerically investigated. The application of our approach to some numerical tests on an idealized rubber foam is also presented. For consistency a short review of the homogenization theory in nonlinear elasticity is provided.

Key-words: homogenization, nonlinear elasticity, large elastic deformations, finite elements

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Une approche directe de l'homogénéisation numérique en élasticité non linéaire

Résumé : Nous décrivons, analysons et testons une approche numérique directe pour un problème d'homogénéisation en hyperélasticité en grandes déformations. L'intérêt de cette approche est qu'elle ne modifie pas la structure des logiciels couramment utilisés en calcul des structures (comme Modulf dans notre cas). L'analyse inclut un résultat général de convergence pour une large classe de densités d'énergies élastiques ainsi qu'une estimation d'erreur dans le cas convexe. Cette approche est en fait liée à la méthode des éléments finis multiéchelles, à laquelle l'analyse sus-citée s'applique. Les problèmes de bifurcation microscopique et d'instabilité macroscopique sont abordés d'un point de vue numérique. Des tests sur une mousse de caoutchouc concluent le rapport. Par souci de clarté, quelques résultats de la théorie de l'homogénéisation en élasticité non linéaire sont rappelés au début de ce rapport.

Mots-clés : homogénéisation, élasticité non linéaire, grandes déformations, éléments finis

1 Physical motivation

Whereas the development of computational tools has helped engineers to design pieces with specific mechanical properties, chemists and physicists have developed new types of materials enjoying new types of properties and characterized by a high heterogeneity. Because of this heterogeneity the numerical methods commonly used by engineers cannot directly deal with these new materials. The reason is that classical analytical constitutive laws do not model correctly all the regimes encountered by these materials at the macroscopic scale.

A computational approach to circumvent the difficulty related to macroscopic constitutive laws could be to use a finite element method (FEM) at a scale for which classical constitutive laws are relevant. Unfortunately this is often out of reach of computers to date since the meshsize would have to be of the order of the micrometer e.g., which is prohibitive.

The landscape is then the following: direct computations at the microscopic scale are too expensive whereas computations at the macroscopic scale are delicate because of the lack of relevant analytical constitutive laws. An alternative track is provided by the homogenization approach.

The article is organized as follows. To start with, some results of the mathematical theory of periodic homogenization for nonlinear energy densities are recalled. The reader familiar with the state of the art of the homogenization theory for minimization problems and elliptic operators in divergence form can easily skip Section 2. Our specific contribution is detailed throughout Sections 3 to 6. Section 3 is devoted to an approximation result for a nonlinear elasticity problem with a homogenized constitutive law and to the derivation of an error estimate in the convex case. The numerical method introduced in Section 4 consists in replacing an unknown analytical constitutive law at the macroscopic scale by a numerical constitutive law computed at each macroscopic point by the resolution of a so-called *cell-problem* at the microscopic level. This approach is well developed and has been applied to linear materials (FE² method [11]) and nonlinear materials at small strain ([21]). It is adapted here to the finite strain case, for which convergence properties of Newton algorithms are very sensitive to the approximation of the second derivative of the constitutive law ([27],[17]). The computation of such a stiffness matrix has not been addressed in the literature to the knowledge of the author. This is one purpose of this article. In Section 5 this direct approach is related to the multiscale finite element method introduced by Hou and co-authors and the error estimate of Section 3 is proved to apply to the MsFEM, at least in the periodic case. Finally the question first introduced by Geymonat, Müller and Triantafyllidis in [12] concerning buckling in the cell-problem and instabilities of the homogenized energy density is numerically addressed. The convergence properties of the method for a class of energy densities which is not covered by the mathematical theory is also investigated.

2 A quick review of periodic homogenization theory

For consistency, some well-known results of the periodic homogenization theory applied to nonlinear energy densities with specific growth properties are recalled here. Such theoretical results guide the numerical strategy and tell in what sense mechanical quantities are approximated. To fully illustrate the situation, and for the sake of comparison, a synthesis of what is theoretically known for energy densities of several types and for general elliptic operators in divergence form is given (see [15] and [5]). The proofs of the results stated below can be found in the work of Müller [22] and the book of Braides and Defranceschi [5]. The theoretical point of view preferably uses the energy minimization problem whereas the PDE approach is more relevant for the numerical practice.

This theory makes use of the growth condition (1) introduced in Definition 3 below. In practice, several problems do not satisfy this condition. This is the case for porous materials and Ogden materials. To model porous media, we consider a perforated domain where the energy density satisfies (1) and we let the size of the holes, where the energy vanishes, go to zero. In a way this homogenization is also geometric since the domain is not fixed. Unlike porous materials, Ogden materials can violate (1) almost everywhere. Therefore the approach introduced in Section 4 is still to be justified mathematically. These limitations are summarized in the last paragraph of this section.

2.1 Convexity and minimization problems

Throughout the article Ω denotes an open bounded connected subset of \mathbb{R}^3 . The following definitions and results (see e.g. [25]) will be extensively used in the sequel.

Definition 1 *A function $W : \mathcal{M}_3(\mathbb{R}) \rightarrow [0, +\infty]$ is $W^{1,p}$ -quasiconvex if for all $A \in \mathcal{M}_3(\mathbb{R})$ (set of real square matrices of size 3), there exists an open bounded subset E of \mathbb{R}^3 with $|\partial E| = 0$ such that the linear function $A \cdot x$ is a local minimum in $W^{1,p}(E, \mathbb{R}^3)$:*

$$W(A) = \min \left\{ \frac{1}{|E|} \int_E W(A + \nabla \phi(x)) dx \mid \phi \in W_0^{1,p}(E; \mathbb{R}^3) \right\}$$

The function W is polyconvex when it can be expressed as a convex function of the minors of orders 1,2,3 of A .

Property 1 *If W is polyconvex then W is quasiconvex.*

Definition 2 *Let $(x, A) \mapsto W(x, A)$ be a quasiconvex energy density defined on $\Omega \times \mathcal{M}_3(\mathbb{R})$, for which there exist an integer $p \geq 1$, positive constants c and C , such that for almost all $x \in \Omega$ and for all $A \in \mathcal{M}_3(\mathbb{R})$,*

$$c|A|^p \leq W(x, A) \leq C(1 + |A|^p) \tag{1}$$

The function W is then said to satisfy a standard growth condition (of order p).

Definition 3 The function $W : \Omega \times \mathcal{M}_3(\mathbb{R}) \rightarrow \mathbb{R}$, $(x, A) \mapsto W(x, A)$ is a standard energy density if W is a quasiconvex Carathéodory function, that is:

- $W(\cdot, \cdot)$ is measurable in its first variable and continuous in its second variable
- $W(x, \cdot)$ is quasiconvex for almost every $x \in \Omega$

and if W satisfies (1).

Definition 4 A standard minimization problem refers in the literature to a minimization problem associated to a standard energy density that reads: given $\bar{u} \in W^{1,p}(\Omega, \mathbb{R}^3)$, solve

$$\inf \left\{ \int_{\Omega} W(x, \nabla(u + \bar{u})) dx \mid u \in W_0^{1,p}(\Omega, \mathbb{R}^3) \right\} \quad (2)$$

The direct method of the calculus of variations shows

Theorem 1 The minimization problem (2) admits at least a minimizer in $W_0^{1,p}(\Omega, \mathbb{R}^3)$.

Theorem 1 is a consequence of the following lemma.

Lemma 1 If $1 \leq p < \infty$, and $W : \mathcal{M}_3(\mathbb{R}) \rightarrow \mathbb{R}$ is a quasiconvex function satisfying

$$0 \leq W(A) \leq C(1 + |A|^p) \quad \text{for all } A \in \mathcal{M}_3(\mathbb{R}),$$

then the functional $J(u) = \int_{\Omega} W(\nabla u)$ is weakly lower semi-continuous on $W^{1,p}(\Omega)$.

2.2 Basic homogenization result

Periodic functions are defined as follows.

Definition 5 A function $\psi : \mathbb{R}^3 \rightarrow \mathbb{R}$ is said N -periodic, $N \in \mathbb{N}$, if for almost every (ae) $x \in \mathbb{R}^3$, and for all $(i, j, k) \in \mathbb{N}^3$,

$$\psi(x + ie_1 + je_2 + ke_3) = \psi(x)$$

with $e_1 = (N, 0, 0)$, $e_2 = (0, N, 0)$ and $e_3 = (0, 0, N)$.

For convenience, in the sequel of the article, only 1-periodic energy densities are considered, instead of general periodic functions. Theoretical results still hold *mutatis mutandis* for periodic functions with periodic cells that have a Lipschitz boundary.

Periodic homogenization aims at studying problems for which the energy density W_ϵ is of the form

$$W_\epsilon(x, A) = W\left(\frac{x}{\epsilon}, A\right),$$

where W is periodic in space. This heterogeneous energy density is commonly used to model composite materials.

The limit $\epsilon \rightarrow 0$ of the minimization problem (2) with W_ϵ is described by

Theorem 2 [5] *Let $W : \mathbb{R}^3 \times \mathcal{M}_3(\mathbb{R}) \rightarrow [0, +\infty)$ be a standard energy density satisfying the periodicity assumption*

$$W(\cdot, A) \text{ is 1-periodic for all } A \in \mathcal{M}_3(\mathbb{R})$$

and the growth condition (1) of order $p \geq 1$.

For Ω a bounded open set of \mathbb{R}^3 , $u \in W^{1,p}(\Omega, \mathbb{R}^3)$ and $\epsilon > 0$, we set

$$J_\epsilon(u) = \int_{\Omega} W\left(\frac{x}{\epsilon}, \nabla u(x)\right) dx$$

Then, for all $\bar{u} \in W^{1,p}(\Omega, \mathbb{R}^3)$,

$$\lim_{\epsilon \rightarrow 0} \inf \{J_\epsilon(u + \bar{u}) \mid u \in W_0^{1,p}(\Omega)\} = \inf \{J_{\text{homog}}(u + \bar{u}) \mid u \in W_0^{1,p}(\Omega)\}, \quad (3)$$

where $J_{\text{homog}}(u) = \int_{\Omega} W_{\text{homog}}(\nabla u(x)) dx$ and $W_{\text{homog}} : \mathcal{M}_3(\mathbb{R}) \rightarrow [0, +\infty)$ is a standard energy density functional defined by the asymptotic homogenization formula

$$W_{\text{homog}}(A) = \lim_{N \rightarrow \infty} \frac{1}{N^3} \inf \left\{ \int_{(0,N)^3} W(x, A + \nabla v(x)) dx \mid v \in W_0^{1,p}((0, N)^3, \mathbb{R}^3) \right\} \quad (4)$$

for all $A \in \mathcal{M}_3(\mathbb{R})$. The function W_{homog} satisfies in particular condition (1) of order p .

In addition, if u_ϵ is a minimizing sequence of $J_\epsilon(\cdot + \bar{u})$ on $W_0^{1,p}(\Omega, \mathbb{R}^3)$ weakly converging to some u in $W_0^{1,p}(\Omega, \mathbb{R}^3)$, then u is a minimizer of $J_{\text{homog}}(\cdot + \bar{u})$ on $W_0^{1,p}(\Omega, \mathbb{R}^3)$.

Remark 1 *The asymptotic homogenization formula (4) can be replaced by*

$$W_{\text{homog}}(A) = \lim_{N \rightarrow \infty} \frac{1}{N^3} \inf \left\{ \int_{(0,N)^3} W(x, A + \nabla v(x)) dx \mid v \in W_{\#}^{1,p}((0, N)^3, \mathbb{R}^3) \right\} \quad (5)$$

where $W_{\#}^{1,p}((0, N)^3, \mathbb{R}^3)$ is the set of N -periodic functions v of $W^{1,p}((0, N)^3, \mathbb{R}^3)$ such that $\int_{\Omega} v = 0$. Note that the limit $N \rightarrow \infty$ can be replaced by an infimum on $N \in \mathbb{N}$ in (4) and (5).

2.3 Homogenization for connected media

Connected media are defined as follows.

Definition 6 *Let E be an infinite 1-periodic, connected, open subset of \mathbb{R}^3 (that is in particular a periodic replication of a subset of $(0, 1)^3$) with a Lipschitz boundary, and Ω be a bounded open subset of \mathbb{R}^3 . Given $\epsilon \in \mathbb{R}_+$, $\Omega \cap \epsilon E$ is called a connected medium.*

Theorem 2 also holds in a weaker form for connected media:

Theorem 3 *Let E and Ω be as in Definition 6. Given a standard energy density $W : E \times \mathcal{M}_3(\mathbb{R}) \rightarrow \mathbb{R}$ with $W(\cdot, A)$ 1-periodic for every $A \in \mathcal{M}_3(\mathbb{R})$, satisfying condition (1) with $1 < p < +\infty$, let $J_\epsilon : L^p(\Omega; \mathbb{R}^3) \rightarrow [0, +\infty]$ be the functional defined for every $\epsilon > 0$ by*

$$J_\epsilon(u) = \begin{cases} \int_{\Omega \cap \epsilon E} W\left(\frac{x}{\epsilon}, \nabla u(x)\right) dx & \text{if } u|_{\Omega \cap \epsilon E} \in W^{1,p}(\Omega \cap \epsilon E; \mathbb{R}^3), \\ +\infty & \text{otherwise.} \end{cases}$$

Then there exist a constant $k_1 > 0$ depending on E and p , and a standard energy density functional $W_{homog} : \mathcal{M}_3(\mathbb{R}) \rightarrow \mathbb{R}$ satisfying

$$\frac{c}{k_1} |A|^p \leq W_{homog}(A) \leq C |(0, 1)^3 \cap E| (1 + |A|^p),$$

for all $A \in \mathcal{M}_3(\mathbb{R})$, and such that, defining the functional $J_{homog} : L^p(\Omega; \mathbb{R}^3) \rightarrow [0, +\infty]$ by

$$J_{homog}(u) = \begin{cases} \int_{\Omega} W_{homog}(\nabla u(x)) dx & \text{if } u \in W^{1,p}(\Omega; \mathbb{R}^3), \\ +\infty & \text{otherwise,} \end{cases}$$

we have, for all $\bar{u} \in W^{1,p}(\Omega)$,

$$\lim_{\epsilon \rightarrow 0} \inf \{ J_\epsilon(u + \bar{u}) \mid u \in W_0^{1,p}(\Omega) \} = \inf \{ J_{homog}(u + \bar{u}) \mid u \in W_0^{1,p}(\Omega) \}.$$

The functional W_{homog} is given by the asymptotic homogenization formula

$$W_{homog}(A) = \lim_{N \rightarrow \infty} \inf \left\{ \frac{1}{N^3} \int_{(0,N)^3 \cap E} W(x, \nabla v(x) + A) dx \mid v \in W_0^{1,p}((0,N)^3; \mathbb{R}^3) \right\}$$

for all $A \in \mathcal{M}_3(\mathbb{R})$.

In addition, if u_ϵ is a minimizing sequence of $J_\epsilon(\cdot + \bar{u})$ on $W_0^{1,p}(\Omega, \mathbb{R}^3)$ weakly converging to some u in $W_0^{1,p}(\Omega, \mathbb{R}^3)$, then u is a minimizer of $J_{homog}(\cdot + \bar{u})$ on $W_0^{1,p}(\Omega, \mathbb{R}^3)$.

2.4 Homogenization of elliptic operators in divergence form

If W is differentiable and the minimization problems (2) for W_ϵ and W_{homog} , and (5) or (4) are attained, the minimizers satisfy the Euler-Lagrange equations. In that case we denote by

$$a(x, \xi) = \frac{\partial W}{\partial \xi}(x, \xi).$$

Keeping the notation of Theorem 2, the Euler-Lagrange equation for the minimization of J_ϵ reads

$$\begin{cases} -\operatorname{div} \left(a\left(\frac{x}{\epsilon}, \nabla u_\epsilon\right) \right) = f & \text{in } \Omega \\ u_\epsilon = \bar{u} & \text{on } \partial\Omega. \end{cases} \quad (6)$$

On the other hand, if $W_\epsilon(x, \cdot)$ is strictly convex for almost every $x \in \Omega$, the one for J_{homog} is

$$\begin{cases} -\operatorname{div} \left(a_{homog}(\nabla u) \right) = f & \text{in } \Omega \\ u = \bar{u} & \text{on } \partial\Omega, \end{cases} \quad (7)$$

where a_{homog} is defined by $\mathcal{M}_3(\mathbb{R}) \ni \xi \mapsto a_{homog}(\xi) = \int_{(0,1)^3} a(y, \nabla v_\xi(y) + \xi) dy$ and v_ξ is the periodic solution in $W_{\#}^{1,p}((0,1)^3, \mathbb{R}^3)$ of

$$-\operatorname{div} (a(y, \nabla v_\xi(y) + \xi)) = 0, \quad (8)$$

the latter equation being called the *cell-problem* (see [5]).

It may be noticed that (8) is the Euler-Lagrange equation of (5) for $N = 1$. In fact the infimum in (5) is attained for $N = 1$, due to convexity. We abusively say that $N = 1$ in the cell-problem (8).

Considering non-symmetric operators a , monotonicity assumptions (see [18] and [23]) extend the results of Theorem 2 and provide more precise results on the homogenized operator, as stated in the following theorem.

Theorem 4 [23] *Assume $p \geq 2$. Let $a : \mathbb{R}^3 \times \mathcal{M}_3(\mathbb{R}) \rightarrow \mathcal{M}_3(\mathbb{R}), (x, \xi) \mapsto a(x, \xi)$ be Carathéodory and 1-periodic in x . Assume also that $a(\cdot, 0)$ is bounded and that the following continuity and monotonicity properties hold*

$$\begin{aligned} \exists 0 \leq \alpha \leq p-1, C > 0 \quad | \quad \text{for ae } x \in \mathbb{R}^3, \forall \xi_1, \xi_2 \in \mathcal{M}_3(\mathbb{R}) \\ |a(x, \xi_1) - a(x, \xi_2)| \leq C(1 + |\xi_1| + |\xi_2|)^{p-1-\alpha} |\xi_1 - \xi_2|^\alpha, \end{aligned} \quad (9)$$

$$\begin{aligned} \exists 2 \leq \beta < +\infty, c > 0 \quad | \quad \text{for ae } x \in \mathbb{R}^3, \forall \xi_1, \xi_2 \in \mathcal{M}_3(\mathbb{R}) \\ (a(x, \xi_1) - a(x, \xi_2), \xi_1 - \xi_2) \geq c(1 + |\xi_1| + |\xi_2|)^{p-\beta} |\xi_1 - \xi_2|^\beta. \end{aligned} \quad (10)$$

Then, given $f \in L^{p'}(\Omega, \mathbb{R}^3)$, the solution $u_\epsilon \in W_0^{1,p}(\Omega, \mathbb{R}^3)$ of

$$-\operatorname{div} \left(a\left(\frac{x}{\epsilon}, \nabla u_\epsilon\right) \right) = f$$

weakly converges in $W_0^{1,p}(\Omega, \mathbb{R}^3)$ to the solution $u \in W_0^{1,p}(\Omega, \mathbb{R}^3)$ of

$$-\operatorname{div} (a_{homog}(\nabla u)) = f,$$

where $a_{\text{homog}} : \mathcal{M}_3(\mathbb{R}) \rightarrow \mathcal{M}_3(\mathbb{R})$ is defined by

$$a_{\text{homog}}(A) = \int_{(0,1)^3} a(y, A + \nabla u_A(y)) dy$$

and $u_A \in W_{\#}^{1,p}((0,1)^3, \mathbb{R}^3)$ is the solution of

$$-\text{div} (a(y, A + \nabla u_A(y))) = 0.$$

In addition a_{homog} satisfies (10) with the same coefficients as a and (9) with $\gamma = \alpha/(\beta - \alpha)$ instead of α .

The existence of a corrector, which allows to obtain a strong convergence instead of the weak convergence of Theorem 4, is given by

Theorem 5 [23] *Under the hypotheses and notation of Theorem 4, let $(M_\epsilon)_\epsilon$ be the set of mean operators defined by*

$$M_\epsilon : L^p(\Omega) \rightarrow L^p(\Omega), \quad \phi(x) \mapsto M_\epsilon \phi(x) = 1/\epsilon^3 \int_{(\epsilon[Y, (Y+1)])^3} \phi(y),$$

with $Y \in \mathbb{Z}^3$ such that $x \in (\epsilon[Y, (Y+1)])^3$. The set $\{M_\epsilon \phi\}_\epsilon$ is a set of piecewise constant functions strongly converging to ϕ in $L^p(\Omega)$.

The corrector v_ϵ associated to u is then given by

$$v_\epsilon : \Omega \rightarrow \mathbb{R}^3, \quad x \in (\epsilon[Y, (Y+1)])^3 \mapsto v_\epsilon(x) = v_{\epsilon, Y}\left(\frac{x}{\epsilon}\right),$$

where $v_{\epsilon, Y} \in W_{\#}^{1,p}((0,1)^3, \mathbb{R}^3)$ is the periodic solution of

$$-\text{div} a(y, M_\epsilon \nabla u(x) + \nabla v_{\epsilon, Y}(y)) = 0. \quad (11)$$

And the following strong convergence in $W^{1,p}(\Omega, \mathbb{R}^3)$ holds,

$$\|(u + \epsilon v_\epsilon) - u_\epsilon\|_{1,p,\Omega} \rightarrow 0,$$

$\|\cdot\|_{1,p,\Omega}$ standing for the norm of $W^{1,p}(\Omega)$.

In the remainder of the article all the monotonic operators considered will be symmetric and associated to a strictly convex energy density.

2.5 Some open issues

The conclusions of Theorem 2 are specific to the growth condition (1) and the minimization space $W_0^{1,p}(\Omega, \mathbb{R}^3)$. They can be extended to Neumann boundary conditions and mixed Dirichlet and Neumann boundary conditions in weak form. However, two open questions

Type		Homogenized	Existence of correctors	Number of cells N to consider in	
Operator		Operator		problem (8)	
Linear	+cc ^a	Linear+cc	True	1	
Monotone	+(10)+(9)	Monotone+(10)+(9)	True	1	
Energy density		Energy density		formula (4)	formula (5)
Convex	+sgc ^b	Convex+sgc	True	∞	1
Quasiconvex	+sgc	Quasiconvex+sgc	? ^c	∞	∞
	+polyconvex +sgc	Quasiconvex+sgc	?	∞	∞
	+polyconvex	?	?	?	?

Table 1: Summary of some homogenization results available to date

^acoercive and continuous on $W^{1,2}$, in order to apply Lax-Milgram lemma

^bstandard growth condition of order p

^cunknown today

prevent from applying rigorously the above results to general nonlinear elasticity whose energy densities do not satisfy (1), e.g. general polyconvex energies.

First, it is not known whether Theorem 2 holds if $W_0^{1,p}(\Omega)$ is replaced by the set $\{u \in W_0^{1,p}(\Omega) \mid \det(\nabla u + \nabla \bar{u}) = 1 \text{ ae}\}$. This variational set models incompressible materials.

The second open question deals with the more general problem of Γ -convergence of sequentially lower semicontinuous functionals. The Γ -convergence is an approach which can be applied to prove Theorem 2 (see e.g. [5]). In this case, it requires the growth condition (1), which is also used to prove the lower semicontinuity of the integral functional J_ϵ of Theorem 2. Given that other mathematical properties than the growth condition (1) can ensure the lower semicontinuity of the functional (typically the polyconvexity), a natural issue would be to try to generalize the application of the Γ -convergence theory to general sequentially lower semicontinuous functionals, which is still an open issue today.

The answers to several questions related to what has been recalled in this section for different types of energies and operators in divergence form are collected in Table 1. The number N of cells to consider in (4) and (5) to attain convergence depends on the problem at stake and on the functional space. The question relative to the existence of correctors is of importance since it allows to recover strong convergence of minimizers. The existence of correctors is extensively used to derive error estimates for numerical methods, such as e.g. the multiscale finite element method proposed by Hou and co-authors ([14],[9]).

3 Approximation result for the standard homogenization problem

Two results of approximation are recalled in details for nonlinear elasticity boundary problems in the standard case. They show that isolated minimizers u of (2) can be approximated by minimizers u_h of

$$\inf \left\{ \int_{\Omega} W(x, \nabla(u_h + \bar{u})) dx \mid u \in V_h \right\},$$

where (V_h) are finite dimensional subspaces of $W_0^{1,p}(\Omega, \mathbb{R}^3)$. Under an assumption on the form of the energy density W (Theorem 6) or up to adding a vanishing perturbing term to the energy density (Theorem 7), u_h converges to u in $W_0^{1,p}(\Omega, \mathbb{R}^3)$. In Section 3.2 a similar result is proven for the standard homogenization problem (Theorem 8), in the context of Theorem 2. In Section 3.3 an error estimate is derived for a nonlinear elasticity problem with a strictly convex energy density in the context of Section 2.4.

3.1 Approximation theory for standard energy densities

The first result of this section is classical. The proof, given for completeness, is simpler than that of Le Tallec in [17] due to the restricted class of energies considered. The second result exploits the idea of Pedregal in [24] to get rid of the assumption on the form of the energy density, by adding a vanishing perturbing term.

Definition 7 *Let $W : \Omega \times \mathcal{M}_3(\mathbb{R}) \rightarrow \mathbb{R}$ be a standard energy density. The integral functional J is defined by*

$$\begin{aligned} J : W^{1,p}(\Omega) &\rightarrow \mathbb{R} \\ v &\mapsto \int_{\Omega} W(x, \nabla v(x)) dx \end{aligned}$$

Given $\bar{u} \in W^{1,p}(\Omega)$, we consider an isolated minimizer u of

$$\inf \{ J(v + \bar{u}), v \in W_0^{1,p}(\Omega) \}$$

on $B(u, \bar{r})$, $\bar{r} > 0$, that is a minimizer such that

$$J(u + \bar{u}) < J(v + \bar{u}) \quad \forall v \in W_0^{1,p}(\Omega, \mathbb{R}^3) \quad | \quad \|u - v\|_{1,p} < \bar{r} \text{ and } v \neq u$$

In the remainder of the paper, for $v \in W^{1,p}(\Omega)$ and $\rho > 0$, the open ball centered at v and of radius ρ in $W^{1,p}(\Omega)$ is denoted by $B(v, \rho)$.

The following lemma on Carathéodory functions will be used in the proofs of the approximation results.

Lemma 2 [16] *Let Φ be a function of the type*

$$\Phi(y)(x) = \zeta(x, y(x)),$$

where ζ is Carathéodory and such that Φ sends $L^p(\Omega)$ into $L^q(\Omega)$. Then Φ is continuous from $L^p(\Omega)$ into $L^q(\Omega)$.

Theorem 6 *Let W , \bar{u} , J , u and $B(u, \bar{r})$ be as in Definition 7. Let W satisfy:*

$$W(x, A) = c(x)|A|^p + W_1(x, A) \quad (12)$$

with $c(x) \geq c/2$ a.e. in Ω and W_1 a standard energy density. Assume that there exist discrete spaces $V_h \subset W_0^{1,p}(\Omega, \mathbb{R}^3)$ and a sequence $\{w_h\}_h$, $w_h \in V_h \cap B(u, \bar{r})$, satisfying $u = \lim_{h \rightarrow 0} w_h$ in $W^{1,p}(\Omega, \mathbb{R}^3)$.

Then the minimization problems

$$\inf\{J(v_h + \bar{u}) \mid v_h \in V_h \cap B(u, \bar{r})\} \quad (13)$$

are attained, and any sequence u_h of minimizers of (13) converges to u in $W^{1,p}(\Omega)$.

Proof

As J is continuous on $W^{1,p}(\Omega)$ (Lemma 2) and $V_h \cap B(u, \bar{r}) \ni w_h$ is compact in $W^{1,p}(\Omega)$ since it is a non empty, bounded and closed subset, $J(\cdot + \bar{u})$ attains its minimum on $V_h \cap B(u, \bar{r})$. Denote by u_h one of the minimizers.

The sequence u_h is bounded by $\|u\|_{1,p} + \bar{r}$ in $W^{1,p}(\Omega)$. Thus there exists an extracted sequence, still denoted by u_h , that converges weakly in $W^{1,p}(\Omega)$ to some $u_\infty \in B(u, \bar{r})$.

By definition of u_h ,

$$J(u_h + \bar{u}) \leq J(w_h + \bar{u}) \text{ for all } h.$$

As J is lower semi-continuous for the weak topology (Lemma 1) and continuous for the strong topology of $W^{1,p}(\Omega)$, the inequalities

$$\begin{aligned} J(u_\infty + \bar{u}) &\leq \liminf J(u_h + \bar{u}) \\ &\leq \lim J(w_h + \bar{u}) \\ &= J(u + \bar{u}) \end{aligned}$$

hold.

Since u is the unique minimizer of $J(\cdot + \bar{u})$ on $B(u, \bar{r})$, the latter inequality implies

$$u_\infty = u \text{ and } \lim J(u_h + \bar{u}) = J(u + \bar{u})$$

The limit $u_\infty = u$ being independent from the extraction, the whole original sequence u_h converges weakly to u in $W^{1,p}(\Omega)$.

Next, the strong convergence comes from the particular form of the energy functional: since $(x, A) \mapsto c(x)|A|^p$ and $(x, A) \mapsto W_1(x, A)$ are quasiconvex for almost every $x \in \Omega$ and satisfy (1), the integral functionals associated to these two energies are lower semi-continuous (Lemma 1), which implies

$$\int_{\Omega} c(x)|\nabla(u(x) + \bar{u}(x))|^p dx \leq \liminf \int_{\Omega} c(x)|\nabla(u_h(x) + \bar{u}(x))|^p dx$$

and

$$\int_{\Omega} W_1(x, u(x) + \bar{u}(x)) dx \leq \liminf \int_{\Omega} W_1(x, u_h(x) + \bar{u}(x)) dx.$$

As in addition $\lim J(u_h + \bar{u}) = J(u + \bar{u})$, necessarily

$$\lim \int_{\Omega} c(x) |\nabla(u_h(x) + \bar{u}(x))|^p dx = \int_{\Omega} c(x) |\nabla(u(x) + \bar{u}(x))|^p dx \quad (14)$$

Since Ω is bounded, combining the weak convergence of $\nabla(\bar{u} + u_h)$ to $\nabla(\bar{u} + u)$ in $L^p(\Omega)$ with (14), the strong convergence of $\nabla(\bar{u} + u_h)$ holds, and consequently:

$$\|u - u_h\|_{1,p} \rightarrow 0$$

□

Energy densities satisfying (12) are indeed the ones that are most encountered in practice. If an energy density does not satisfy (12), the addition of a vanishing term allows to recover strong convergence, as stated by

Theorem 7 *Let W , \bar{u} , J , u and $B(u, \bar{r})$ be as in Definition 7. Assume that there exist discrete spaces $V_h \subset W_0^{1,p}(\Omega, \mathbb{R}^3)$ and a sequence $\{w_h\}_h$, $w_h \in V_h \cap B(u, \bar{r})$, satisfying $u = \lim_{h \rightarrow 0} w_h$ in $W^{1,p}$. Let $\{J_\eta\}$ be the set of perturbed energy functionals defined by*

$$J_\eta(v) = J(v) + \eta \int_{\Omega} |\nabla(v)|^p, \quad (15)$$

for $\eta > 0$ and $v \in W^{1,p}(\Omega)$.

The minimization problems

$$\inf \{J_\eta(v_h + \bar{u}) \mid v_h \in V_h \cap B(u, \bar{r})\} \quad (16)$$

are attained and minimizers of $J_\eta(\bar{u} + \cdot)$ on $V_h \cap B(u, \bar{r})$ are denoted by $u_{\eta,h}$.

For any extracting function ϕ_η such that $u_{\eta,\phi_\eta(h)}$ weakly converges in $W^{1,p}(\Omega, \mathbb{R}^3)$ as h goes to zero, the convergence is actually strong and

$$\lim_{\eta \rightarrow 0} \lim_{h \rightarrow 0} u_{\eta,\phi_\eta(h)} = u \quad \text{in } W^{1,p}(\Omega, \mathbb{R}^3).$$

Proof

Following [24] the perturbed energy density is obtained by adding the term $\eta \int_{\Omega} |\nabla v|^p$ to J ,

for $\eta \in \mathbb{R}^+$,

$$J_\eta(v) = J(v) + \eta \int_{\Omega} |\nabla v|^p.$$

The following three assertions hold:

- (i) $J_\eta(\cdot + \bar{u})$ has at least a minimizer u_η in $B(u, \bar{r})$
- (ii) u_η is a minimizing sequence of $J(\cdot + \bar{u})$ on $B(u, \bar{r})$
- (iii) $u_\eta \rightarrow u$ strongly in $W^{1,p}(\Omega)$ as $\eta \rightarrow 0$

Assertion (i) is a consequence of the lower semi-continuity of J_η , as the sum of two lower semi-continuous functionals.

Assertion (ii) follows from the inequalities

$$J(u + \bar{u}) \leq J(u_\eta + \bar{u}) \leq J_\eta(u_\eta + \bar{u}) \leq J_\eta(u + \bar{u}), \quad (17)$$

where have been successively used that u minimizes $J(\cdot + \bar{u})$ and u_η minimizes $J_\eta(\cdot + \bar{u})$ on $B(u, \bar{r})$. Next, for all $v \in W^{1,p}(\Omega)$, $\lim_{\eta \rightarrow 0} J_\eta(v) = J(v)$, thus (17) implies that $J(u_\eta + \bar{u}) \rightarrow J(u + \bar{u})$ as $\eta \rightarrow 0$, that is (ii).

To prove (iii), it may first be noticed that (ii) implies that

$$u_\eta \rightharpoonup u \quad \text{in } W^{1,p}(\Omega), \quad (18)$$

arguing as in the proof of Theorem 6 since u is the unique minimizer of $J(\cdot + \bar{u})$ on $B(u, \bar{r})$.

The following observation

$$\begin{aligned} \eta \int_{\Omega} |\nabla u_\eta + \nabla \bar{u}|^p &\leq \eta \int_{\Omega} |\nabla u_\eta + \nabla \bar{u}|^p + \frac{1}{\eta} (J(u_\eta + \bar{u}) - J(u + \bar{u})) \\ &= \frac{1}{\eta} J_\eta(u_\eta + \bar{u}) - \frac{1}{\eta} J(u + \bar{u}) \\ &\leq \frac{1}{\eta} J_\eta(u + \bar{u}) - \frac{1}{\eta} J(u + \bar{u}) \\ &= \eta \int_{\Omega} |\nabla u + \nabla \bar{u}|^p, \end{aligned} \quad (19)$$

combined with (18), implies (iii).

As in the proof of Theorem 6, the set of minimizers $\{u_{\eta,h}\}$ of $J_\eta(\bar{u} + \cdot)$ on $V_h \cap B(u, \bar{r})$ is weakly compact. Thus there exists a subsequence $\{u_{\eta,\phi_\eta(h)}\}_h$ which weakly converges to some $u_\eta \in B(u, \bar{r})$. Due to the perturbing term $\eta \int_{\Omega} |\nabla v|^p$, J_η satisfies (12) and (14) holds with $c(x) = \eta$. This implies the strong convergence of the subsequence in $W^{1,p}(\Omega)$. Combined with assertion (iii), it proves

$$\lim_{\eta \rightarrow 0} \lim_{h \rightarrow 0} u_{\eta,\phi_\eta(h)} = u \quad \text{in } W^{1,p}(\Omega).$$

□

3.2 Approximation result for a homogenized energy density

This section is devoted to the proof of a result of approximation for a problem of type (2) with the energy density (4), when $W_0^{1,p}(\Omega, \mathbb{R}^3)$ in (2) and $W_0^{1,p}((0, N)^3, \mathbb{R}^3)$ in (4) are replaced by finite dimensional subspaces.

Definition 8 For $N \in \mathbb{N}$, $\{V_{N,h}\}$ is a family of finite dimensional subspaces of $W_0^{1,p}((0, N)^3, \mathbb{R}^3)$ satisfying

$$h_2 \leq h_1 \implies V_{N,h_1} \subset V_{N,h_2},$$

and such that $\overline{\cup_h V_{N,h}} = W_0^{1,p}((0, N)^3, \mathbb{R}^3)$.

Similarly, $\{V_{\Omega,H}\}$ is a family of finite dimensional subspaces of $W_0^{1,p}(\Omega, \mathbb{R}^3)$ such that $\overline{\cup_H V_{\Omega,H}} = W_0^{1,p}(\Omega, \mathbb{R}^3)$.

Given a standard energy density W and the homogenized energy density W_{homog} associated by formula (4), for any (N, h) the approximate homogenized energy density $W^{N,h} : \mathcal{M}_3(\mathbb{R}) \rightarrow \mathbb{R}$ is defined by

$$A \mapsto W^{N,h}(A) = \frac{1}{N^3} \inf \left\{ \int_{(0,N)^3} W(x, A + \nabla v(x)) dx : v \in V_{N,h} \right\}. \quad (20)$$

Its associated approximate energy functional is

$$J^{N,h}(v) = \int_{\Omega} W^{N,h}(\nabla v) \quad \text{on } W^{1,p}(\Omega). \quad (21)$$

The approximation result is given by

Theorem 8 Let W , W_{homog} , $V_{N,h}$, $V_{\Omega,H}$ and $J^{N,h}$ be as in Definition 8. Assume that W_{homog} also satisfies (12) (see however Remark 2 below). Given $\bar{u} \in W^{1,p}(\Omega)$, u is defined as an isolated minimizer of

$$\inf \left\{ \int_{\Omega} W_{homog}(\nabla(v + \bar{u})) dx \mid v \in W_0^{1,p}(\Omega) \right\}. \quad (22)$$

The minimization problems

$$\inf \{ J^{N,h}(v + \bar{u}) \mid v \in V_{\Omega,H} \cap B(u, \bar{r}) \} \quad (23)$$

are attained and let $\{u_H^{N,h}\}_{H,N,h}$ denote sequences of minimizers of (23). Then, for all extracted sequences in N and h , still denoted by $u_H^{N,h}$, such that $\lim_{N \rightarrow \infty} \lim_{h \rightarrow 0} u_H^{N,h}$ exists,

$$\lim_{H \rightarrow 0} \lim_{N \rightarrow \infty} \lim_{h \rightarrow 0} u_H^{N,h} = u \quad \text{in } W^{1,p}(\Omega). \quad (24)$$

Proof

Step 1: convergence in H

In view of Theorem 2, W_{homog} is a quasiconvex function satisfying (1). In addition, W_{homog} satisfies (12) by assumption. The application of Theorem 6 to the minimization problem (22) implies that any sequence u_H of minimizers of

$$\inf \left\{ \int_{\Omega} W_{homog}(\nabla(v + \bar{u})) dx \mid v \in V_{\Omega, H} \cap B(u, \bar{r}) \right\}, \quad (25)$$

converges to u :

$$\lim_{H \rightarrow 0} u_H = u \quad \text{in } W_0^{1,p}(\Omega). \quad (26)$$

Step 2: convergence in N

In the limit taken in (4), let us consider the approximate energy density

$$W^N(A) = \inf \left\{ \frac{1}{N^3} \int_{(0, N)^3} W(x, \nabla v(x) + A) dx : v \in W_0^{1,p}((0, N)^3, \mathbb{R}^3) \right\}, \quad (27)$$

and define an approximation of problem (25) by replacing W_{homog} by W^N :

$$\inf \left\{ \int_{\Omega} W^N(\nabla(v + \bar{u})) \mid v \in V_{\Omega, H} \cap B(u, \bar{r}) \right\}. \quad (28)$$

In the sequel, $J^N(v) = \int_{\Omega} W^N(\nabla v) dx$.

The second step consists in proving that for all $N \in \mathbb{N}^*$ the minimization problem (28) is attained and that any converging subsequence of minimizers u_H^N of (28) converges in $W^{1,p}(\Omega)$ to a minimizer u_H of (25) as N goes to infinity.

Let us prove that W^N is a continuous function on $\mathcal{M}_3(\mathbb{R})$. Let $(A_i)_{i \in \mathbb{N}} \in (\mathcal{M}_3(\mathbb{R}))^{\mathbb{N}}$ satisfy $A_i \rightarrow A \in \mathcal{M}_3(\mathbb{R})$ and let $(u_{A_i})_i$ and u_A be minimizers of

$$\inf \left\{ \frac{1}{N^3} \int_{(0, N)^3} W(x, \nabla v(x) + B) dx : v \in W_0^{1,p}((0, N)^3, \mathbb{R}^3) \right\},$$

with $B = A_i$ and $B = A$ respectively.

From Theorem 1 such minimizers exist. Thanks to (1), $(u_{A_i})_i$ is bounded in $W_0^{1,p}((0, N)^3)$. There exists a subsequence, still denoted by u_{A_i} , which weakly converges to some $u_{A_\infty} \in W_0^{1,p}((0, N)^3)$. Lemma 2 ensures that $v \mapsto \int_{\Omega} W(x, \nabla v)$ is continuous on $W^{1,p}(\Omega)$, which implies

$$\int_{(0, N)^3} W(x, A + \nabla u_A) = \lim_{i \rightarrow \infty} \int_{(0, N)^3} W(x, A_i + \nabla u_{A_i}). \quad (29)$$

By definition of u_{A_i} and after taking the inferior limit, we have

$$\liminf_{i \rightarrow \infty} \int_{(0,N)^3} W(x, A_i + \nabla u_A) \geq \liminf_{i \rightarrow \infty} \int_{(0,N)^3} W(x, A_i + \nabla u_{A_i}). \quad (30)$$

The lower semi-continuity of $v \mapsto \int_{(0,N)^3} W(x, \nabla v)$ for the weak topology of $W^{1,p}((0,N)^3)$ implies

$$\liminf_{i \rightarrow \infty} \int_{(0,N)^3} W(x, A_i + \nabla u_{A_i}) \geq \int_{(0,N)^3} W(x, A + \nabla u_{A_\infty}). \quad (31)$$

Combining (29), (30) and (31) gives

$$\int_{(0,N)^3} W(x, A + \nabla u_A) \geq \int_{(0,N)^3} W(x, A + \nabla u_{A_\infty}). \quad (32)$$

The definition of u_A and (32) then imply

$$W^N(A) = \int_{(0,N)^3} W(x, A + \nabla u_A) = \int_{(0,N)^3} W(x, A + \nabla u_{A_\infty}).$$

Therefore $\lim_{i \rightarrow \infty} W^N(A_i) = W^N(A)$ does not depend either on the sequence A_i nor on the subsequence u_{A_i} considered, which proves the continuity of W^N . Consequently, W^N is Carathéodory and satisfies (1). The same result and proof hold for $W^{N,h}$.

Lemma 2 implies that J^N and $J^{N,h}$ are continuous on $W^{1,p}(\Omega)$. The same property holds for J_{homog} since W_{homog} is also a Carathéodory function satisfying (1) (Theorem 2). As $V_{\Omega,H} \cap B(u, \bar{r})$ is a compact set of $W_0^{1,p}(\Omega)$ and J^N is continuous, the minimization problem (28) is attained.

Let $\{u_H^N\}_N$ be a sequence of minimizers of (28). As $V_{\Omega,H}$ is compact, there exists a subsequence $u_H^{\phi_H(N)}$ which converges to some u_H^∞ in $W^{1,p}(\Omega)$. To prove that u_H^∞ is a minimizer of (25), it suffices to show that J^N converges to J_{homog} uniformly on $V_{\Omega,H} \cap B(u, \bar{r})$.

For all $\chi \in W_0^{1,p}((0, 2^N)^3)$, let χ^* denote the periodization of χ in $W_0^{1,p}((0, 2^{N+1})^3)$. Consequently, $W^{2^{N+1}}(A) \leq W^{2^N}(A)$ for all $A \in \mathcal{M}_3(\mathbb{R})$, which implies $J^{2^{N+1}}(v) \leq J^{2^N}(v)$ for all $v \in W^{1,p}(\Omega)$. As J^{2^N} is a decreasing sequence of continuous functions which converges to a continuous function J_{homog} on the compact set $V_{\Omega,H} \cap B(u, \bar{r})$, Dini's theorem implies that J^{2^N} converges uniformly to J_{homog} on $V_{\Omega,H} \cap B(u, \bar{r})$. Actually this shows that the whole sequence J^N converges uniformly on $V_{\Omega,H} \cap B(u, \bar{r})$, as proved below.

For all $\epsilon > 0$, there exists $I \in \mathbb{N}$ such that for all $v \in V_{\Omega,H} \cap B(u, \bar{r})$,

$$|J^{2^I}(v) - J_{homog}(v)| \leq \epsilon. \quad (33)$$

For all $M \geq 2^I$ and $v \in V_{\Omega,H} \cap B(u, \bar{r})$, either $J^M(v) \leq J^{2^I}(v)$ and

$$|J^M(v) - J_{homog}(v)| \leq \epsilon, \quad (34)$$

since $J_{homog} \leq J^N$ for all $N \in \mathbb{R}$ (Remark 1), or

$$0 \leq J^M(v) - J^{2^I}(v). \quad (35)$$

For all $\chi \in W_0^{1,p}((0, 2^I)^3)$, let $\chi^{**} \in W_0^{1,p}((0, M)^3)$ be defined by $\left[\frac{M}{2^I}\right]^3$ replications of χ on $\left(0, \left[\frac{M}{2^I}\right] 2^I\right)^3$ and be extended by zero elsewhere in $(0, M)^3$, where $[\cdot]$ stands for the integer part. Thus

$$\int_{(0,M)^3} W(x, A + \chi^{**}(x)) = \left[\frac{M}{2^I}\right]^3 \int_{(0,2^I)^3} W(x, A + \chi(x)) + \int_{([\frac{M}{2^I}]2^I, M)^3} W(x, A),$$

which implies, using (1),

$$J^M(v) - J^{2^I}(v) \leq \frac{M^3 - ([\frac{M}{2^I}] 2^I)^3}{M^3} C(1 + \|v\|_{1,p}^p). \quad (36)$$

As $\|v\|_{1,p} \leq \|u\|_{1,p} + \bar{r}$, the right hand side of (36) converges to zero uniformly on $V_{\Omega,H} \cap B(u, \bar{r})$ when M goes to infinity. Therefore, there exists $N^* \geq 2^I$ such that for all $v \in V_{\Omega,H} \cap B(u, \bar{r})$ and $M \geq N^*$ either (34) holds or

$$|J^M(v) - J_{homog}(v)| \leq |J^{2^I}(v) - J_{homog}(v)| + |J^{2^I}(v) - J^M(v)| \leq 2\epsilon,$$

by combining (33), (35) and (36). This implies the uniform convergence of J^N to J_{homog} on $V_{\Omega,H} \cap B(u, \bar{r})$.

We are now in position to prove that u_H^∞ is a minimizer of J_{homog} on $V_{\Omega,H} \cap B(u, \bar{r})$. The triangle inequality implies

$$\begin{aligned} |J^{\phi_H(N)}(u_H^{\phi_H(N)}) - J_{homog}(u_H^\infty)| &\leq |J^{\phi_H(N)}(u_H^{\phi_H(N)}) - J_{homog}(u_H^{\phi_H(N)})| \\ &\quad + |J_{homog}(u_H^{\phi_H(N)}) - J_{homog}(u_H^\infty)|. \end{aligned}$$

The first term goes to zero independently of $u_H^{\phi_H(N)}$ thanks to the uniform convergence of $J^{\phi_H(N)}$ whereas the second term goes to zero thanks to the continuity of J_{homog} .

Thus, $\lim_{N \rightarrow \infty} J^{\phi_H(N)}(u_H^{\phi_H(N)}) = J_{homog}(u_H^\infty)$. In addition, for all $v \in V_{\Omega,H} \cap B(u, \bar{r})$ and $N \in \mathbb{N}$, $J^{\phi_H(N)}(v) \geq J^{\phi_H(N)}(u_H^{\phi_H(N)})$. Passing to the limit, we obtain $J_{homog}(v) \geq J_{homog}(u_H^\infty)$, which implies that u_H^∞ is a minimizer of J_{homog} on $V_{\Omega,H} \cap B(u, \bar{r})$.

For any extraction function ϕ_H such that the sequence $u_H^{\phi_H(N)}$ of minimizers of (28) converges as N goes to infinity, (26) then shows

$$\lim_{H \rightarrow 0} \lim_{N \rightarrow \infty} u_H^{\phi_H(N)} = u \quad \text{in } W^{1,p}(\Omega). \quad (37)$$

Step 3: convergence in h

Step 3 consists in determining an adequate approximation of u_H^N by restricting (25) to a finite dimensional subspace as prescribed by Definition 8.

For $h_1 \geq h_2$, $V_{N,h_1} \subset V_{N,h_2}$, thus, for all $A \in \mathcal{M}_3(\mathbb{R})$, $W^{N,h_2}(A) \leq W^{N,h_1}(A)$, showing that $\{J^{N,h}\}_h$ is a decreasing sequence of functions. As $J^{N,h}$ and J^N are continuous on $W^{1,p}(\Omega)$, hypotheses of Dini's theorem hold and $J^{N,h}$ converges uniformly to J^N on $V_{\Omega,H} \cap B(u, \bar{r})$. Arguing as in *Step 2*, there exists a subsequence $u_H^{N,\psi_{N,H}(h)}$ of minimizers of (23) which converges to a minimizer $u_H^{N,0}$ of (28) in $W^{1,p}(\Omega)$ as h goes to zero.

For any extraction function $\psi_{N,H}$ such that the sequence $u_H^{N,\psi_{N,H}(h)}$ of minimizers of (22) converges as h goes to zero, (37) finally shows

$$\lim_{H \rightarrow 0} \lim_{N \rightarrow \infty} \lim_{h \rightarrow 0} u_H^{\phi_H(N), \psi_{\phi_H(N), H}(h)} = u \quad \text{in } W^{1,p}(\Omega). \quad (38)$$

□

Let err be an error range, Theorem 8 implies that there exist N , H and h depending on err such that

$$\|u - u_H^{N,h}\|_{1,p} \leq err. \quad (39)$$

Whereas minimizers u_H of (25) cannot be computed directly (W_{homog} is not available analytically), $u_H^{N,h}$ can **actually** be computed by a finite element method.

Remark 2 *The energy density W_{homog} does not satisfy (12) in general (see [12]), even if $W(x, \cdot)$ does satisfy it almost everywhere in x . Theorem 8 has been stated this way for the sake of simplicity. In general the homogenized energy density has to be modified as in (15), which leads to a straightforward adaptation of Theorem 8; Theorem 7 then allows to pass to the limit as η goes to zero, showing, with obvious notation,*

$$\lim_{\eta \rightarrow 0} \lim_{H \rightarrow 0} \lim_{N \rightarrow \infty} \lim_{h \rightarrow 0} u_{\eta,H}^{N,h} = u. \quad (40)$$

The question of the existence of an isolated minimizer u is partly discussed in Section 6 in view of [12].

Remark 3 *Theorem 8 has been stated and proved in the framework of formula (4). The proofs and result also hold with formula (5) and straightforward adaptations, replacing $W_0^{1,p}((0,N)^3)$ by $W_{\#}^{1,p}((0,N)^3)$. In particular, when dealing with a convex energy density and $W_{\#}^{1,p}((0,N)^3)$, the limit in N in (38) can be skipped.*

3.3 Error estimates in the convex case

Theorem 8 does not provide the explicit dependence of H , N and h upon err in (39). For general quasiconvex energy densities, no error estimate can be derived to complement the approximation result since there is no general error estimate related to Theorem 6.

Theorem 8 remains thus abstract. However, in some particular cases, it turns out to be possible to give an error estimate.

The analysis is more difficult for N than for H and h , as N is indeed closely linked to buckling phenomena (see [12] and [22]) in the cell-problem and strongly depends on the load A in (4) and not only on err . This issue is investigated numerically in Section 6.

In the example of a convex energy density treated here, the general analysis for N need not be handled, since formula (5) applies with $N = 1$ (see Table 1). It is thus enough to deal with $W^{1,h}$ and $J^{1,h}$ defined by (20) and (21), where $V_{1,h}$ is a subspace of $W_{\#}^{1,p}((0,1)^3, \mathbb{R}^3)$ (see Remark 3). With the notation of Theorem 8 and Remark 2, (40) is replaced by

$$\lim_{\eta \rightarrow 0} \lim_{H \rightarrow 0} \lim_{h \rightarrow 0} u_{\eta,H}^{1,h} = u \quad \text{in } W^{1,p}(\Omega, \mathbb{R}^3). \quad (41)$$

It will be seen next that modifying the homogenized energy as in Remark 2 is indeed unnecessary in this case.

Two different error estimates for convex energy densities associated to symmetric monotonic operators are presented: one relying on the continuity property (9) with $\alpha > 0$ and another one also valid for $\alpha = 0$ (see Theorems 9 and 10 below). The proofs of these theorems are based on regularity properties of the solutions to monotonic elliptic systems.

Optimal regularity results of Savaré ([26]) and of Ebmeyer et al. ([8]) are recalled for symmetric monotonic systems on Lipschitz and convex domains. An error estimate is then obtained for the cell-problem and finally a global error estimate is derived for problem (23).

Hypotheses 1 *The energy density $W : \mathbb{R}^3 \times \mathcal{M}_3(\mathbb{R}) \ni (y, \xi) \mapsto W(y, \xi) \in \mathbb{R}$ is a continuous function, 1-periodic in y and convex in ξ for almost every $y \in (0,1)^3$ that satisfies (1) with $p \geq 2$. The operator $a := \frac{\partial W}{\partial \xi}$ is monotonic and continuous in the sense of (10) and (9), and $a(y, 0) = 0$ for all $y \in (0,1)^3$ (without loss of generality). In addition W enjoys the following uniform Lipschitz property with respect to y ,*

$$\exists L > 0 : |W(y_1, \xi) - W(y_2, \xi)| \leq L|y_1 - y_2|(1 + |\xi|^p), \quad \forall y_1, y_2 \in \mathbb{R}^3, \quad \forall \xi \in \mathcal{M}_3(\mathbb{R}).$$

Lemma 3 *Under Hypotheses 1 and for $p > 2$, let \mathcal{O} be an open bounded domain of \mathbb{R}^3 , $\bar{u} \in W^{1+2/p,p}(\mathcal{O}, \mathbb{R}^3)$ and $u \in W_0^{1,p}(\mathcal{O}, \mathbb{R}^3)$ be the solution of*

$$-\operatorname{div} a(x, \nabla(u + \bar{u})) = 0.$$

Then,

- *if \mathcal{O} is Lipschitz, $u \in W_0^{1+\lambda/p,p}(\mathcal{O}, \mathbb{R}^3)$ for all $\lambda \in [0, 1[$ (see [26]),*
- *if \mathcal{O} is convex, $u \in W_0^{1+\lambda/p,p}(\mathcal{O}, \mathbb{R}^3)$ for all $\lambda \in [0, 2[$ (see [8]).*

Remark 4 Lemma 3 also holds when $W_0^{1,p}$ and $W_0^{1+\lambda/p,p}$ are respectively replaced by $W_{\#}^{1,p}$ and $W_{\#}^{1+\lambda/p,p}$.

For simplicity, in the remainder of the section, Ω is supposed to be convex.

Definition 9 With the notation of Hypotheses 1 and for all $A \in \mathcal{M}_3(\mathbb{R})$, u_A is defined as the unique solution in $W_{\#}^{1,p}((0,1)^3, \mathbb{R}^3)$ of

$$-\operatorname{div} a(x, \nabla u_A + A) = 0. \quad (42)$$

Given a family $\{V_h\}_h$ of finite dimensional subspaces of $W_{\#}^{1,p}((0,1)^3, \mathbb{R}^3)$ such that $\overline{\cup_h V_h} = W_{\#}^{1,p}((0,1)^3, \mathbb{R}^3)$, u_A^h denotes an approximation of u_A in V_h defined as the unique solution in V_h of the variational problem

$$\int_{(0,1)^3} a(x, \nabla u_A^h + A) \cdot \nabla v_h = 0 \quad \forall v_h \in V_h. \quad (43)$$

Lemma 4 Assume Hypotheses 1 and in addition $\alpha \geq 0$ in (9) and $\beta \geq 2$ in (10), and let $A \in \mathcal{M}_3(\mathbb{R})$, $u_A \in W_{\#}^{1,p}((0,1)^3, \mathbb{R}^3)$ be the solution of (42) and u_A^h be the solution of (43). Then there exists a constant $C > 0$ independent of h such that

$$\|u_A - u_A^h\|_{1,p} \leq C \inf \left\{ \|u_A - v_h\|_{1,p}^s, v_h \in V_h \right\}, \quad (44)$$

with $s = (\alpha + 1)/\beta$.

Proof

Since u_A and u_A^h are solutions to (42) and (43), for any $v_h \in V_h$,

$$\begin{aligned} & \int_{(0,1)^3} (a(x, A + \nabla u_A) - a(x, A + \nabla u_A^h)) \cdot (u_A - u_A^h) \\ &= \int_{(0,1)^3} (a(x, A + \nabla u_A) - a(x, A + \nabla u_A^h)) \cdot (u_A - v_h) \\ &\leq C(1 + 2|A| + \|u_A\|_{1,p} + \|u_A^h\|_{1,p})^{p-1-\alpha} \|u_A - v_h\|_{1,p}^{\alpha+1}, \end{aligned} \quad (45)$$

using (9).

The monotonicity property (10) also implies

$$\begin{aligned} & \int_{(0,1)^3} (a(x, A + \nabla u_A) - a(x, A + \nabla u_A^h)) \cdot (u_A - u_A^h) \\ &\geq c(1 + \|A + \nabla u_A\|_{0,p} + \|A + \nabla u_A^h\|_{0,p})^{p-\beta} \|u_A - u_A^h\|_{1,p}^{\beta}. \end{aligned} \quad (46)$$

Combining (45) with (46) and taking the infimum on $v_h \in V_h$, (44) follows. \square

Lemmata 3 and 4 allow to prove the

Theorem 9 *Assume Hypotheses 1 and in addition $\alpha > 0$ in (9) and $\beta \geq 2$ in (10). Let \mathcal{T}_h be a regular triangulation of $(0, 1)^3$, \mathcal{T}_H be a regular triangulation of Ω and V_h and V_H be linear finite element subspaces of $W_{\#}^{1,p}((0, 1)^3, \mathbb{R}^3)$ and of $W_0^{1,p}(\Omega, \mathbb{R}^3)$ respectively associated to \mathcal{T}_h and \mathcal{T}_H . Let $\bar{u} \in W^{1+2/p,p}(\Omega, \mathbb{R}^3)$ and u be the minimizer of (22). Theorem 8 and formula (41) provide a minimizer $u_H^h = u_H^{1,h}$ of (23).*

Then there exist positive constants C_1 and C_2 independent of h and H , such that

$$\|u - u_H^h\|_{1,p} \leq C_1 h^{\frac{2(\alpha+1)}{p\beta} - \frac{\alpha}{\beta-1}} + C_2 H^{\frac{2}{p(\beta-\alpha)}}. \quad (47)$$

Proof

Theorems 2, 4 and 6, Remark 3 and property (41) ensure the existence and uniqueness of u and u_H^h , minimizers of (22) and (23).

For $A \in \mathcal{M}_3(\mathbb{R})$, let us introduce the notation:

$$a_{homog}(A) = \frac{\partial W_{homog}}{\partial \xi}(A), \quad (48)$$

and

$$a_h(A) = \frac{\partial W^h}{\partial \xi}(A). \quad (49)$$

Functions a_{homog} and a_h may be shown to be well-defined respectively using the homogenization theory of elliptic operators and the implicit function theorem (see Section 4.2 for details).

The proof is divided in two steps, which aim at estimating $a_{homog}(A) - a_h(A)$ for $A \in \mathcal{M}_3(\mathbb{R})$ and $\int_{\Omega} (a_{homog}(\nabla v) - a_h(\nabla v)) \cdot \nabla v$ for $v \in W^{1,p}(\Omega, \mathbb{R}^3)$ and $w \in W_0^{1,p}(\Omega, \mathbb{R}^3)$ respectively. The concluding argument uses monotonicity.

Step 1

By definition,

$$W_{homog}(A) = \inf \left\{ \int_{(0,1)^3} W(x, \nabla v(x) + A) dx : v \in W_{\#}^{1,p}((0, 1)^3, \mathbb{R}^3) \right\}, \quad (50)$$

$$W^h(A) = \inf \left\{ \int_{(0,1)^3} W(x, \nabla v(x) + A) dx : v \in V_h \right\}. \quad (51)$$

As W is strictly convex, both minima are uniquely attained at v_A and v_A^h . Inequality (9) then implies

$$|a_{homog}(A) - a_h(A)| \leq \left| \int_{(0,1)^3} a(x, A + \nabla v_A) - a(x, A + \nabla v_A^h) \right| \quad (52)$$

$$\leq C \|\nabla v_A - \nabla v_A^h\|_{0,p}^{\alpha} (1 + \|A + \nabla v_A\|_{0,p} + \|A + \nabla v_A^h\|_{0,p})^{p-1-\alpha}. \quad (53)$$

On one hand, as v_A is the minimizer of (50) and $\{x \mapsto 0\} \in W_{\#}^{1,p}((0,1)^3, \mathbb{R}^3)$, (1) implies

$$C(1 + |A|^p) \geq \int_{(0,1)^3} W(x, A) \geq \int_{(0,1)^3} W(x, A + \nabla v_A) \geq c \|A + \nabla v_A\|_{0,p}^p.$$

Thus

$$\frac{C}{c}(1 + |A|^p) \geq \|A + \nabla v_A\|_{0,p}^p. \quad (54)$$

The same inequality holds for v_A^h .

On the other hand, Lemma 4 applied to v_A and v_A^h with the regularity given by Lemma 3 provides the error estimate

$$\|v_A - v_A^h\|_{1,p} \leq Ch^{s\lambda/p}, \quad (55)$$

for all $\lambda \in [0, 2[$ and for $s = \frac{\alpha + 1}{\beta}$, using the interpolation theory for P1-finite elements.

Combining inequalities (52), (54) and (55) gives

$$|a_{homog}(A) - a_h(A)| \leq Ch^{s\alpha\lambda/p}(1 + |A|^{p-1-\alpha}). \quad (56)$$

Step 2

For all $v \in W^{1,p}(\Omega, \mathbb{R}^3)$ and $w \in W_0^{1,p}(\Omega, \mathbb{R}^3)$, (56) and the Hölder inequality imply

$$\begin{aligned} \left| \int_{\Omega} \left(a_{homog}(\nabla v) - a_h(\nabla v) \right) \cdot \nabla w \right| &\leq Ch^{s\alpha\lambda/p} \int_{\Omega} (1 + |\nabla v(x)^{p-1-\alpha}|) |\nabla w| dx \\ &\leq Ch^{s\alpha\lambda/p} (1 + \|\nabla v\|_{0,p}^{p-1}) \|\nabla w\|_{0,p}. \end{aligned} \quad (57)$$

Let u_H be the unique solution in V_H of

$$\int_{\Omega} a_{homog}(\nabla u_H + \nabla \bar{u}) \cdot \nabla v_H = 0 \quad \forall v_H \in V_H, \quad (58)$$

and recall that u_H^h is the minimizer of (23), which thus satisfies the Euler-Lagrange equation

$$\int_{\Omega} a_h(\nabla u_H^h + \nabla \bar{u}) \cdot \nabla v_H = 0 \quad \forall v_H \in V_H. \quad (59)$$

Taking $v = u_H^h + \bar{u}$, inequality (57) reads

$$\begin{aligned} \left| \int_{\Omega} \left(a_{homog}(\nabla(u_H^h + \bar{u})) - a_h(\nabla(u_H^h + \bar{u})) \right) \cdot \nabla w \right| \\ \leq Ch^{s\alpha\lambda/p} (1 + \|\nabla(u_H^h + \bar{u})\|_{0,p}^{p-1}) \|\nabla w\|_{0,p}. \end{aligned}$$

The same arguments as in the proof of (54) show

$$\left| \int_{\Omega} \left(a_{homog}(\nabla(u_H^h + \bar{u})) - a_h(\nabla(u_H^h + \bar{u})) \right) \cdot \nabla w \right| \leq Ch^{s\alpha\lambda/p} (1 + \|\nabla \bar{u}\|_{0,p}^{p-1}) \|\nabla w\|_{0,p}. \quad (60)$$

As u_H solves (58), u_H^h solves (59) and $u_H - u_H^h \in V_H$ is an admissible test function for both problems,

$$\int_{\Omega} \left(a_{homog}(\nabla(u_H + \bar{u})) - a_h(\nabla(u_H^h + \bar{u})) \right) \cdot \nabla(u_H - u_H^h) = 0. \quad (61)$$

The monotonicity (10) of a_{homog} given by Theorem 4 implies

$$\left| \int_{\Omega} \left(a_{homog}(\nabla(u_H + \bar{u})) - a_{homog}(\nabla(u_H^h + \bar{u})) \right) \cdot \nabla(u_H - u_H^h) \right| \geq c \|\nabla u_H - \nabla u_H^h\|_{0,p}^{\beta} (1 + \|\nabla(\bar{u} + u_H)\|_{0,p} + \|\nabla(\bar{u} + u_H^h)\|_{0,p})^{p-\beta},$$

whereas inequalities (60) and (61) give

$$\begin{aligned} & \left| \int_{\Omega} \left(a_{homog}(\nabla(u_H + \bar{u})) - a_{homog}(\nabla(u_H^h + \bar{u})) \right) \cdot \nabla(u_H - u_H^h) \right| \\ & \leq \left| \int_{\Omega} \left(a_{homog}(\nabla(u_H + \bar{u})) - a_h(\nabla(u_H^h + \bar{u})) \right) \cdot \nabla(u_H - u_H^h) \right| \\ & \quad + \left| \int_{\Omega} \left(a_h(\nabla(u_H^h + \bar{u})) - a_{homog}(\nabla(u_H^h + \bar{u})) \right) \cdot \nabla(u_H - u_H^h) \right| \\ & \leq Ch^{s\alpha\lambda/p} (1 + \|\nabla \bar{u}\|_{0,p}^{p-1}) \|\nabla u_H - \nabla u_H^h\|_{0,p}. \end{aligned}$$

The Poincaré inequality shows that there exists a constant C_1 depending only on $c, C, \alpha, \beta, |\Omega|, \bar{u}$ and p , such that,

$$\begin{aligned} \|u_H - u_H^h\|_{1,p} & \leq \frac{C_1 h^{\alpha\lambda s/(p(\beta-1))}}{(1 + \|\nabla(\bar{u} + u_H)\|_{0,p} + \|\nabla(\bar{u} + u_H^h)\|_{0,p})^{(p-\beta)/(\beta-1)}} \\ & \leq C_1 h^{\alpha\lambda s/(p(\beta-1))}. \end{aligned} \quad (62)$$

As a_{homog} satisfies (9) with $\gamma = \frac{\alpha}{\beta - \alpha}$ instead of α , a variant of Lemma 4 implies the existence of a constant C_2 such that $\|u - u_H\|_{1,p} \leq C_2 H^{\frac{\lambda}{p(\beta-\alpha)}}$. The latter inequality, combined with (62) for $\lambda = 2$, implies

$$\|u - u_H^h\|_{1,p} \leq C_1 h^{\frac{2(\alpha+1)}{p\beta} \frac{\alpha}{\beta-1}} + C_2 H^{\frac{2}{p(\beta-\alpha)}}.$$

□

This result is also true for scalar monotonic equations as the Laplace equation, for which $p = 2$, $\alpha = 1$ and $\beta = 2$. In this case, $\frac{2(\alpha+1)}{p\beta} \frac{\alpha}{\beta-1} = 1$ and $\frac{2}{p(\beta-\alpha)} = 1$. According to Theorem 9, an optimal error is obtained for $h \simeq H$ in (47). This is in agreement with the analysis performed by Allaire in [1]. In the general setting of monotonic operators for which the continuity assumption (9) is only assumed for $\alpha = 0$, the previous analysis is no longer valid. However the following more general result holds.

Theorem 10 *With the notation of Theorem 9, assume Hypotheses 1 with $\alpha \geq 0$ in (9) and $\beta \geq 2$ in (10). Then there exist positive constants C_1 and C_2 independent of h and H , such that*

$$\|u - u_H^h\|_{1,p} \leq C_1 h^{\frac{2(\alpha+1)}{p\beta} \frac{1}{\beta}} + C_2 H^{\frac{2}{p(\beta-\alpha)}}. \quad (63)$$

Proof

Let us follow the proof of Theorem 9 and focus on W instead of a . As the continuity property (9) implies

$$\begin{aligned} |W(y, \xi_2) - W(y, \xi_1)| &= \left| \int_0^{|\xi_2 - \xi_1|} a(y, \xi_1 + t \frac{\xi_2 - \xi_1}{|\xi_2 - \xi_1|}) dt \right| \\ &\leq C |\xi_2 - \xi_1| (1 + |\xi_1|^{p-1} + |\xi_2 - \xi_1|^{p-1}) \\ &\leq C |\xi_2 - \xi_1| (1 + |\xi_1|^{p-1} + |\xi_2|^{p-1}), \end{aligned}$$

(57) can be replaced by

$$\left| \int_{\Omega} W_{homog}(\nabla v) - W^h(\nabla v) \right| \leq Ch^{s\lambda/p} (1 + \|\nabla v\|_{0,p}^{p-1}), \quad (64)$$

(60) by

$$\left| \int_{\Omega} W_{homog}(\nabla(u_H^h + \bar{u})) - W^h(\nabla(u_H^h + \bar{u})) \right| \leq Ch^{s\lambda/p} (1 + \|\nabla \bar{u}\|_{0,p}^{p-1}), \quad (65)$$

and (61) by

$$\left| \int_{\Omega} W_{homog}(\nabla(u_H + \bar{u})) - W^h(\nabla(u_H^h + \bar{u})) \right| \leq Ch^{s\lambda/p} (1 + \|\nabla \bar{u}\|_{0,p}^{p-1}). \quad (66)$$

Inequality (66) is a direct consequence of the control of $W_{homog} - W^h$ close to the minima on V_H of W_{homog} and W^h :

$$\begin{aligned} \left| \inf_v \left\{ \int_{\Omega} W_{homog}(\nabla(v + \bar{u})) \right\} - \int_{\Omega} W^h(\nabla(u_H + \bar{u})) \right| &\leq Ch^{s\lambda/p} (1 + \|\nabla \bar{u}\|_{0,p}^{p-1}), \\ \left| \inf_v \left\{ \int_{\Omega} W^h(\nabla(v + \bar{u})) \right\} - \int_{\Omega} W_{homog}(\nabla(u_H^h + \bar{u})) \right| &\leq Ch^{s\lambda/p} (1 + \|\nabla \bar{u}\|_{0,p}^{p-1}). \end{aligned}$$

The following consequence of the monotonicity (10) of a_{homog} (Theorem 1 in [26]) allows to conclude: since u_H is a minimizer of $\int_{\Omega} W_{homog}(\nabla(\bar{u} + \cdot))$ on V_H and $u_H^h \in V_H$,

$$\begin{aligned} & \left| \int_{\Omega} W_{homog}(\nabla(u_H + \bar{u})) - W_{homog}(\nabla(u_H^h + \bar{u})) \right| \\ & \geq c(1 + \|\nabla(u_H + \bar{u})\|_{0,p} + \|\nabla(u_H^h + \bar{u})\|_{0,p})^{p-\beta} \|\nabla u_H - \nabla u_H^h\|_{0,p}^{\beta} \\ & \geq c \|\nabla u_H - \nabla u_H^h\|_{0,p}^{\beta}. \end{aligned} \quad (67)$$

Formula (63) is then obtained by combining (64), (65), (66) and (67). \square

Depending on how $\frac{1}{\beta}$ compares with $\frac{\alpha}{\beta-1}$, either formula (47) or formula (63) gives a better estimate. However Theorem 10 is more general. The worst case is $\alpha = 0$ and $\beta = p$, and then $h \simeq H^p$ yields the optimal error in (63).

For the general quasiconvex case, we are not able to have a similar result. We may however suppose that the optimal meshsize h for the cell problem given the meshsize H for the homogenized problem could depend on p , the order of the growth condition (1).

4 Numerical method

In this section, a direct approach to numerical homogenization in the framework of non-linear elasticity is introduced. The numerical resolution of (3)-(22) is directly tackled by solving (23).

The method is presented in the convenient case of zero body force and Dirichlet boundary conditions. The numerical tests of Section 6 are also performed in this setting. However the method adapts straightforwardly to more general body forces and boundary conditions provided classical adaptations of the energy density and of the variational spaces.

4.1 Presentation

The numerical analysis performed above makes use of a ball $B(u, \bar{r})$ where the minimizer u of (22) is isolated. The minimizer u , and consequently the ball $B(u, \bar{r})$, being unknown in practice, the numerical approach consists in considering, instead of (23), the problem

$$\inf \{ J^{N,h}(v + \bar{u}) dx \mid v \in V_{\Omega,H} \}, \quad (68)$$

for N and h fixed, using the notation (20)-(21).

This minimization problem is attained since $J^{N,h}$ is continuous on $W^{1,p}(\Omega)$, $J^{N,h}(v) \rightarrow \infty$ when $\|v\|_{1,p} \rightarrow \infty$ and $V_{\Omega,H}$ is a finite dimensional space.

In the remainder of Section 4.1 the energy density $W^{N,h}$ defined by (20) is supposed to be twice continuously differentiable. In this case, if u is a minimizer of (68) then u satisfies the Euler-Lagrange equation in the following weak form: for all $v \in V_{\Omega,H}$,

$$\int_{\Omega} \frac{\partial W^{N,h}}{\partial \xi} (\nabla(u + \bar{u})) \cdot \nabla v = 0. \quad (69)$$

The nonlinear equation (69) is solved by an iterative Newton-Raphson method. Knowing u^n at step n , the associated linearized problem at step $n+1$ reads: find u^{n+1} such that for all $v \in V_{\Omega,H}$,

$$\int_{\Omega} \left(\frac{\partial W^{N,h}}{\partial \xi} (\nabla(\bar{u} + u^n)) + \frac{\partial^2 W^{N,h}}{\partial \xi^2} (\nabla(\bar{u} + u^n)) \cdot (\nabla u^{n+1} - \nabla u^n) \right) \cdot \nabla v = 0, \quad (70)$$

and iterate until convergence.

To perform the Newton-Raphson method, an explicit expression of the stress tensor $\frac{\partial W^{N,h}}{\partial \xi}$ and the stiffness matrix $\frac{\partial^2 W^{N,h}}{\partial \xi^2}$ is needed. This is the matter of the following section.

4.2 Computation of the stress tensor and the stiffness matrix

Let

$$\begin{aligned} I : \mathcal{M}_3(\mathbb{R}) \times W_{\#}^{1,p}((0,N)^3) &\rightarrow \mathbb{R} \\ (\xi, \phi) &\mapsto \int_{(0,N)^3} W(y, \xi + \nabla \phi(y)) dy, \end{aligned}$$

and $\{\psi_i\}_i$ be a basis of $V_{N,h}$.

The following hypotheses are made so that I be regular.

Hypotheses 2 *The function $W(y, \cdot)$ is three times continuously differentiable on $\mathcal{M}_3(\mathbb{R})$ and satisfies (1) and the following growth properties*

$$\max \left\{ \left| \frac{\partial W}{\partial \xi}(x, \xi) \right|, \left| \frac{\partial^2 W}{\partial \xi^2}(x, \xi) \right|, \left| \frac{\partial^3 W}{\partial \xi^3}(x, \xi) \right| \right\} \leq C(1 + |\xi|^p) \quad (71)$$

In addition $V_{N,h} \subset W^{1,\infty}((0,N)^3)$.

Let us first study the differentiability of I .

Lemma 5 *If W and $V_{N,h}$ satisfy Hypotheses 2, then $I \in C^3(\mathcal{M}_3(\mathbb{R}) \times V_{N,h}, \mathbb{R})$.*

Proof

This proof is classical (see [17] e.g.) and is only sketched for the first derivative.

As $\nabla\psi \in L^\infty((0, N)^3) = L^1((0, N)^3)'$ and $\frac{\partial W}{\partial \xi}(y, \cdot)$ sends $L^p((0, N)^3)$ on $L^1((0, N)^3)$ thanks to (71), Lemma 2 implies that for all $\psi \in V_{N,h}$ and $\zeta \in \mathcal{M}_3(\mathbb{R})$,

$$\chi \mapsto \int_{(0,N)^3} \frac{\partial W}{\partial \xi}(y, \zeta + \nabla\chi) \cdot \nabla\psi$$

is continuous on $V_{N,h}$.

Next, for all $\psi \in V_{N,h}$ and $\zeta \in \mathcal{M}_3(\mathbb{R})$, $\sigma_{\psi, \zeta}$ is defined by

$$\sigma_{\psi, \zeta} : (t, y) \mapsto \frac{1}{t} \left(W(y, \zeta + \nabla\chi(y) + t\nabla\psi(y)) - W(y, \zeta + \nabla\chi(y)) \right).$$

The Fréchet derivative of W at $\zeta + \nabla\chi(y)$ in the direction $\nabla\psi(y)$ is given by

$$\lim_{t \rightarrow 0} \int_{(0,N)^3} \sigma_{\psi, \zeta}(t, y) dy.$$

Pointwise, $\lim_{t \rightarrow 0} \sigma_{\psi, \zeta}(y, t) = \frac{\partial W}{\partial \xi}(y, \zeta + \nabla\chi(y)) \cdot \nabla\psi(y)$.

As $W(y, \cdot)$ is C^1 , for all $t \in (0, 1)$ there exists $\theta \in (0, 1)$ such that

$$\sigma_{\psi, \zeta}(y, t) = \frac{\partial W}{\partial \xi}(y, \zeta + \nabla\chi(y) + \theta\nabla\psi(y)) \cdot \nabla\psi(y).$$

Using (71), $\sigma_{\psi, \zeta}(y, t)$ is uniformly dominated in t by the integrable function

$$(y, t) \mapsto C(1 + (|\nabla\chi(y)| + |\nabla\psi(y)| + |\zeta|)^p) \|\psi\|_{1, \infty}.$$

The Lebesgue dominated convergence theorem shows

$$\frac{\partial I}{\partial \phi}(\zeta, \chi) \cdot \psi = \int_{(0,N)^3} \frac{\partial W}{\partial \xi}(y, \zeta + \nabla\chi) \cdot \nabla\psi. \quad (72)$$

Similarly,

$$\frac{\partial I}{\partial \xi}(\zeta, \chi) = \int_{(0,N)^3} \frac{\partial W}{\partial \xi}(y, \zeta + \nabla\chi) \cdot Id, \quad (73)$$

where Id is the fourth order identity tensor. As the right hand sides are continuous in (72) and (73), I is C^1 on $\mathcal{M}_3(\mathbb{R}) \times V_{N,h}$.

Repeating the same arguments, I is proved to be three times continuously differentiable. \square

Definition 10 For all $A \in \mathcal{M}_3(\mathbb{R})$, $\phi \in V_{N,h}$ is said to be a local minimizer of $I(A, \cdot)$ on $V_{N,h}$ if there exists $r > 0$ such that for all $\psi \in B(\phi, r) \cap V_{N,h}$, $I(A, \phi) \leq I(A, \psi)$.

A local minimizer ϕ is global on $V_{N,h}$ if for all $\psi \in V_{N,h}$, $I(A, \phi) \leq I(A, \psi)$.

A minimizer ϕ on $V_{N,h}$ is isolated if there exists $\rho > 0$ and if for all $\psi \in B(\phi, \rho) \cap V_{N,h}$ such that $\psi \neq \phi$, $I(A, \phi) < I(A, \psi)$.

Hypotheses 3 Given $A \in \mathcal{M}_3(\mathbb{R})$, there exists a minimizer ϕ of $I(A, \cdot)$ on $V_{N,h}$, satisfying

- ϕ is an isolated global minimizer on $V_{N,h}$
- the Hessian matrix $\left(\int_{(0,N)^3} \nabla \psi_i(y)^T \cdot \frac{\partial^2 W}{\partial \xi^2}(y, A + \nabla \phi(y)) \cdot \nabla \psi_j(y) dy \right)_{i,j}$ is positive definite.

Theorem 11 Let W and $V_{N,h}$ satisfy Hypotheses 2 and $(A, \phi) \in \mathcal{M}_3(\mathbb{R}) \times V_{N,h}$ satisfy Hypotheses 3, then there exist two open balls $B_A \subset \mathcal{M}_3(\mathbb{R})$ and $B_\phi \subset V_{N,h}$, and there exists a function $g_\phi \in C^2(B_A, B_\phi)$, such that for all $\xi \in B_A$, $g_\phi(\xi)$ is an isolated local minimizer of $I(\xi, \cdot)$ on $V_{N,h}$.

In addition, for $\{e_i\}_{1 \leq i \leq 9}$ a basis of $\mathcal{M}_3(\mathbb{R})$,

$$\frac{\partial \nabla g_\phi(\xi)}{\partial \xi} \Big|_{\xi=A} \cdot e_i = \nabla v_i,$$

where v_i is the solution in $V_{N,h}$ of

$$\int_{\Omega} \left(\frac{\partial^2 W(y, \xi)}{\partial \xi^2} \Big|_{\xi=A+\nabla \phi(y)} \cdot (e_i + \nabla v_i) \right) \cdot \nabla \psi = 0 \quad \forall \psi \in V_{N,h}; \quad (74)$$

and

$$\frac{\partial^2 \nabla g_\phi(\xi)}{\partial \xi^2} \Big|_{\xi=A} : e_j \otimes e_i = \nabla w_{ij},$$

where w_{ij} is the solution in $V_{N,h}$ of

$$\int_{\Omega} \left(\frac{\partial^2 W(y, \xi)}{\partial \xi^2} \Big|_{\xi=A+\nabla \phi(y)} \cdot \nabla w_{ij} + \frac{\partial^3 W(y, \xi)}{\partial \xi^3} \Big|_{\xi=A+\nabla \phi(y)} \cdot (e_i + \nabla v_i) \cdot (e_j + \nabla v_j) \right) \cdot \nabla \psi = 0 \quad \forall \psi \in V_{N,h}. \quad (75)$$

Proof

In this proof, ν and $\{\Psi_i\}_{1 \leq i \leq \nu}$ denote the dimension and a basis of $V_{N,h}$. Theorem 11 is a direct application of the implicit function theorem to

$$\begin{aligned} \pi : \mathcal{M}_3(\mathbb{R}) \times V_{N,h} &\rightarrow \mathbb{R}^\nu \\ (\zeta, \chi) &\mapsto \pi(\zeta, \chi), \end{aligned}$$

where

$$\pi(\zeta, \chi) = \begin{pmatrix} \int_{(0,N)^3} \frac{\partial W}{\partial \xi}(y, \zeta + \nabla \chi(y)) \cdot \nabla \psi_1(y) dy \\ \vdots \\ \int_{(0,N)^3} \frac{\partial W}{\partial \xi}(y, \zeta + \nabla \chi(y)) \cdot \nabla \psi_\nu(y) dy \end{pmatrix}.$$

As I is C^3 , $\pi \in C^2(\mathcal{M}_3(\mathbb{R}) \times V_{N,h}, \mathbb{R}^\nu)$ and by definition of ϕ , $\pi(A, \phi) = 0$. As $\frac{\partial \pi}{\partial \chi}(A, \phi)$ is invertible since it is the Hessian matrix of Hypotheses 3, the implicit function theorem shows that there exist two open balls $\tilde{B}_A \ni A$ and $B_\phi \ni \phi$ and a function $g_\phi : \tilde{B}_A \rightarrow B_\phi$ such that for all $\zeta \in \tilde{B}_A$, $g_\phi(\zeta)$ is the unique solution in B_ϕ of $\pi(\zeta, \cdot) = 0$. In addition, g_ϕ is twice continuously differentiable.

As $\frac{\partial \pi}{\partial \chi}(\zeta, g_\phi(\zeta))$ is continuous and $\frac{\partial \pi}{\partial \chi}(A, \phi)$ is positive definite, there exists a non empty open ball $B_A \subset \tilde{B}_A$ such that for all $\zeta \in B_A$, $\frac{\partial \pi}{\partial \chi}(\zeta, g_\phi(\zeta))$ is also positive definite, which implies that $g_\phi(\zeta)$ is an isolated local minimizer of $I(\zeta, \cdot)$ on $V_{N,h}$.

Equations (74) and (75) are then obtained by differentiating once and twice respectively $\zeta \mapsto \pi(\zeta, g_\phi(\zeta))$ at $\zeta = A$.

□

Theorem 12 *Assume that W satisfies Hypotheses 2 and that (A, ϕ) satisfies Hypotheses 3, then, with the notation of Theorem 11, the function $\xi \mapsto I(\xi, g_\phi(\xi))$ is twice continuously differentiable on B_A at $\xi = A$ and its derivatives are given by*

$$\frac{d}{d\xi} I(\xi, g_\phi(\xi)) \Big|_{\xi=A} = \int_{(0,N)^3} \frac{\partial W(y, \xi)}{\partial \xi} \Big|_{\xi=A+\nabla\phi(y)} dy, \quad (76)$$

$$\frac{d^2}{d\xi^2} I(\xi, g_\phi(\xi)) \Big|_{\xi=A} = \quad (77)$$

$$\int_{(0,N)^3} \left(Id + \frac{\partial \nabla g_\phi(\xi)}{\partial \xi} \Big|_{\xi=A} \right)^T \cdot \frac{\partial^2 W(y, \xi)}{\partial \xi^2} \Big|_{\xi=A+\nabla\phi(y)} \cdot \left(Id + \frac{\partial \nabla g_\phi(\xi)}{\partial \xi} \Big|_{\xi=A} \right) dy,$$

where Id is the fourth order identity tensor.

Proof

The function $\xi \mapsto I(\xi, g_\phi(\xi))$ is twice continuously differentiable on B_A at $\xi = A$ as the composition of two differentiable functions. A direct calculus shows

$$\frac{d}{d\xi} I(\xi, g_\phi(\xi)) \Big|_{\xi=A} = \int_{(0,N)^3} \frac{\partial W(y, \xi)}{\partial \xi} \Big|_{\xi=A+\nabla\phi(y)} \cdot \left(Id + \frac{\partial \nabla g_\phi(\xi)}{\partial \xi} \Big|_{\xi=A(y)} \right) dy.$$

As ϕ satisfies $\pi(A, \phi) = 0$ and $\frac{\partial \nabla g_\phi(\xi)}{\partial \xi} \in V_{N,h}$,

$$\int_{(0,N)^3} \frac{\partial W(y, \xi)}{\partial \xi} \Big|_{\xi=A+\nabla\phi(y)} \cdot \frac{\partial \nabla g_\phi(\xi)}{\partial \xi} \Big|_{\xi=A(y)} dy = 0,$$

which proves (76).

An analogous calculus leads to formula (77). □

In general, whereas $W^{N,h}(\xi)$ is only defined by (20), $I(\xi, g_\phi(\xi))$ is the only quantity that can be computed. If the global minimizer defining $W^{N,h}(\xi)$ is unique and depends continuously on ξ then $W^{N,h}(\xi) = I(\xi, g_\phi(\xi))$. This is indeed the case for strictly convex energy densities as stated in

Theorem 13 *In addition to Hypotheses 2 and 3, assume, with the notation of Theorem 11, that $W(y, \cdot)$ is strictly convex for almost every y . Then, for all $A \in \mathcal{M}_3(\mathbb{R})$, the minimizer ϕ of $I(A, \cdot)$ on $V_{N,h}$ is unique, $W^{N,h}$ is twice differentiable, $W^{N,h}(\xi) = I(\xi, g_\phi(\xi))$ and its derivatives are given by the right hand sides of (76) and (77) respectively.*

Proof

Thanks to strict convexity, the minimizer ϕ is unique and the Hessian is positive definite for all couples $(A, \phi(A))$. The function g_ϕ does not depend on ϕ and is denoted by g . It is defined on $\mathcal{M}_3(\mathbb{R})$ and for all $\xi \in \mathcal{M}_3(\mathbb{R})$, $g(\xi)$ is the unique global minimizer of $I(\xi, \cdot)$ on $V_{N,h}$, which implies $W^{N,h}(\xi) = I(\xi, g(\xi))$. □

When dealing with nonconvex energy densities, the simple analysis performed above does not apply. We however use the derivatives of $I(\xi, g_\phi(\xi))$ in practice in order to compute the stress tensor and the stiffness matrix for the homogenized constitutive law. The assumption on the stiffness matrix is not severe since its validity can be inferred a posteriori from the convergence of the Newton algorithm. In contrast, the assumption on the stress tensor is really strong since a failure in the validity of this assumption cannot be detected, even if the algorithm converges. If the Newton algorithm converges, we have found a critical point of a numerical energy, that is expected to be close to the homogenized energy.

Following the work of Geymonat, Müller and Triantafyllidis in [12], this section can be rewritten in a variational setting. More precise results can be obtained assuming the exclusion of discontinuous bifurcations in the minimization of the cell-problems and making other assumptions hard to verify in practice. Our presentation is restricted to what the algorithm can actually perform and is therefore limited to local minimizers in general. If the computed minimizer happens to be global, then the results of [12] (Section 5.2) apply and justify the numerical approach.

4.3 Implementation of the algorithm in a nonlinear elasticity software

The direct approach to numerical homogenization presented here can be used in a nonlinear elasticity solver by using the right hand sides of (76) and (77) as derivatives for the stress tensor and the stiffness matrix in (70). This method has the important advantage not to modify the structure of the existing solver.

This method has been implemented within a classical finite element code (Modulef, INRIA, see [27] and [20]). The call of an analytical formula giving the stress tensor and the stiffness matrix at each Gauss point has been replaced by a subroutine solving itself a nonlinear elasticity cell problem (20) and providing the main program with (76) and (77). The global structure of the code remains therefore unchanged. Any sophisticated technique already used in the code directly adapts without modification: mixed finite elements, augmented Lagrangians, arc-length continuation and parallelization (see [27] and [17]). Numerical tests are reported on in the last section.

The major part of the computational cost comes from the computation of the homogenized constitutive law, as opposed to a classical nonlinear elasticity problem for which this is a simple evaluation of an analytical formula. For the computation of this homogenized constitutive relation itself, the main cost comes from solving the cell-problem (20). The resolution of linear systems is performed by direct inversions, such as Cholesky factorization, because of the large condition number and the lack of efficient preconditioners for nonlinear elasticity problems. Once the cell-problem is solved, the computation of (76) and (77) is obtained by solving a linear system with nine different right hand sides. This linear system is indeed the same as in the last iteration of the Newton algorithm solving the cell-problem, it is therefore already factorized.

On a PC with 2GB of memory, a three dimensional elasticity problem with 40 000 degrees of freedom can be solved without domain decomposition methods, which means for Q2-finite elements a mesh with 12 nodes per dimension in the cell-problem. In that sense, the cell-problems are a limiting factor. On the other hand the global CPU time does not vary too much with respect to the number of degrees of freedom of the macroscopic problem provided efficient domain decomposition methods and parallel computing for the macroscopic problem are used.

A simple way to reduce the cost of computation of the homogenized constitutive law is not to recompute it at each step if the strain gradient has not changed too much and to use the solution at the previous step or at a neighboring Gauss point as an initial guess in the cell-problem.

5 Alternative method: multiscale finite elements (Ms-FEM)

It is interesting to relate the direct method with more elaborate approaches, such as the multiscale finite element method.

5.1 Description of the method

We refer to the work of Hou, Efendiev and coauthors ([14],[9],[23]) for the detailed description of the MsFEM in the linear and nonlinear settings.

This method has primarily been designed in [14] to solve efficiently the linear elliptic equation arising in porous media flows in heterogeneous materials. It has been then extended from the linear case to the monotone case in [9] and [23]. This method is proved to converge in the periodic setting. It has also been used in a more general context and turns out to be quite efficient in the cases reported on by the authors.

Basically, the MsFEM is a Galerkin method for which the solution is searched in a specific space associated to the elliptic operator. Its convergence is then proved thanks to the homogenization theory. Conversely, in (23), a classical Galerkin space (classical finite elements) is used but the original elliptic operator is approximated by its homogenized operator. Although the methods seem to be different at first sight, they turn out to be identical under some hypotheses.

In the setting of periodic homogenization, Hou and coworkers exploit the periodicity of the operator to compute the multiscale finite element manifold on one periodic cell instead of one element (triangle or tetrahedra), which drastically reduces the size of the problems. In this case, the MsFEM exactly consists in solving (23) as shown in the next paragraph and coincides with the direct approach. This observation allows to apply Theorem 9, which thus provides with some insight in the choice of the meshsize of the fine triangulation used in the MsMFEM. In their analysis, Hou and coauthors have focused on the resonance error linked to the boundary condition used to build the multiscale finite elements. They have not addressed the question of the influence on the global error of the approximation by a Galerkin method of the multiscale map itself. This has been answered by Allaire in [1] in the linear case. The result may indeed be different in the nonlinear setting as shown by Theorem 9.

5.2 Comparison of the two methods in the periodic setting

The analysis of the MsFEM requires a corrector result. In order to compare the two methods a monotonic operator is considered in the setting of periodic homogenization of Section 2.4. The notation of Theorems 4 and 5 is used.

We suppose that the macroscopic mesh perfectly fits to the underlying periodic structure so that there is no mismatch (triangular mesh with equilateral triangles and periodic structure with equilateral triangle in 2D e.g.). This technical requirement allows to use a single periodic cell in order to compute the multiscale map (i.d. basis functions in the linear case), as pointed out in [9]. In this case, there is no resonance error due to the boundary conditions.

Let us give some details on the computation of the multiscale finite element map in the P1-Lagrange case. The triangulation \mathcal{T}_H and the finite element space V_H introduced in Theorem 9 are used. Given an element $T \in \mathcal{T}_H$ and a function $u \in V_H$, the associated multiscale function w is defined on T by

$$w(x) = u(x) + \epsilon \nabla v_{u_T} \left(\frac{x}{\epsilon} \right),$$

where v_{u_T} is the solution in $W_{\#}^{1,p}((0,1)^3)$ of

$$-\operatorname{div} (a(y, \nabla u_T + \nabla v_{u_T}(y))) = 0 \quad \text{in } (0,1)^3, \quad (78)$$

and ∇u_T is the gradient of u , which is constant on T since $u \in V_H$. As $u \in V_H$ implies $M_\epsilon \nabla u = \nabla u$, (78) is exactly (11) and the multiscale function w is thus exactly the sum of a classical part, the finite element function u , and of its associated corrector given by Theorem 5. In order to compare the formulation (7), completed by the corrector, to the MsFEM, we just have to compare the classical parts of the solutions.

Consider the multiscale finite element solution w_{MsFEM} of problem (6) in the sense of a Petrov-Galerkin formulation, see [9]. By definition of the MsFEM, for all P1-Lagrange shape functions $\{u_j\}_j$ on \mathcal{T}_H , we have with obvious notation:

$$\begin{aligned} & \int_{\Omega} a\left(\frac{x}{\epsilon}, \nabla w_{MsFEM}(x)\right) \cdot \nabla u_j(x) \\ &= \sum_T \int_T a\left(\frac{x}{\epsilon}, \nabla u_{MsFEM}(x) + \epsilon \nabla v_{u_T}\left(\frac{x}{\epsilon}\right)\right) \cdot (\nabla u_j)_T \\ &= \sum_T \int_T a_{homog}\left((\nabla u_{MsFEM})_T\right) \cdot (\nabla u_j)_T \\ &= \int_{\Omega} a_{homog}\left(\nabla u_{MsFEM}(x)\right) \cdot \nabla u_j(x). \end{aligned}$$

Therefore, w_{MsFEM} is the MsFEM solution to (6) if and only if u_{MsFEM} is the (classical) finite element solution u_H to (7).

In the previous analysis, (78) is solved exactly. Suppose from now on that (78) is solved on V_h as in Theorem 9. Denoting by w_{MsFEM}^h the approximate multiscale solution, the same calculation as above shows

$$\int_{\Omega} a\left(\frac{x}{\epsilon}, \nabla w_{MsFEM}^h(x)\right) \cdot \nabla u_j(x) = \int_{\Omega} a_h\left(\nabla u_{MsFEM}^h(x)\right) \cdot \nabla u_j(x),$$

where a_h is given by (49). Thus, $u_{MsFEM}^h = u_H^h$, where u_H^h is the solution of (23) in the particular case of Theorem 9. Therefore the error analysis of Section 3.3 can be applied to the MsFEM, providing an a priori indication for the order of magnitude of the meshsize h of the fine triangulation in function of the meshsize H of the rough triangulation and of the continuity and monotonicity properties (9) and (10) of the operator a .

6 Numerical tests

This section is dedicated to numerical tests in nonlinear elasticity. The numerical tests of the first paragraph confirm the simple analysis presented above for convex energy densities. In the subsequent paragraphs, some issues of theoretical and practical interest are investigated with the use of numerical experiments:

- buckling in the cell-problem;
- instability of the homogenized energy;
- application of the method to a wider class of energy densities.

6.1 The convex case

Problem (22) is considered with the following energy density:

$$\begin{aligned} W : (0, 1)^3 \times \mathcal{M}_3(\mathbb{R}) &\rightarrow \mathbb{R} \\ (y, \xi) &\mapsto \gamma_1(y)|\xi|^4 + \gamma_2(y)|\xi|^2, \end{aligned}$$

where $\gamma_1, \gamma_2 \geq 1$ is Lipschitz and 1-periodic on \mathbb{R}^3 . Theorem 9 and Lemma 4 apply with $p = 4$, $\alpha = 1$, $\beta = 2$ so that the error estimate (47) reads

$$\|u - u_H^h\|_{1,p} \leq C_1 h^{1/2} + C_2 H^{1/2}. \quad (79)$$

In this case, the algorithm indeed converges, the result does not depend on the number of periodic cells N considered. The numerical tests performed so far seem to show that the rate of convergence (79) is not sharp. Definite conclusions on this optimality issue are yet to be obtained (see [13]).

6.2 Buckling of the cell-problem in the standard case

In the convex case, the infimum in (5) is attained on one periodic cell, for $N = 1$. In [22], S. Müller gives an example in two dimensions for which the infimum in (5) is strictly smaller than the infimum on one single periodic cell. This example relies on the mechanical concept of buckling of a rigid bar in compression: there is a bifurcation and the equilibrium state with the lowest energy breaks the symmetry of the problem.

In three dimensions, the corresponding energy density reads

$$\begin{aligned} \tilde{W} : \mathcal{M}_3(\mathbb{R}) &\rightarrow \mathbb{R} \\ \xi &\mapsto |\xi|^4 + h(\det(\xi)), \end{aligned}$$

where h is given by

$$\begin{aligned} h : \mathbb{R} &\rightarrow \mathbb{R} \\ r &\mapsto \begin{cases} \frac{12(1+a)^2}{r+a} - 12(1+a) - 9 & \text{if } r > 0, \\ \frac{12(1+a)^2}{r+a} - 12(1+a) - 9 - \frac{12(1+a)^2}{a^2}r & \text{if } r \leq 0, \end{cases} \end{aligned}$$

with $a \in]0, 1/2[$.

Period	1 ^a	3	5	9	13	17	23
Energy	5.819	5.388	4.319	3.736	3.587	3.530	3.495
Ratio ^b	0	-7.4%	-25.8%	-35.8%	-38.3%	-39.3%	-39.9%
Stress tensor ^c	-0.0623	-0.0461	-0.0541	-0.0621	-0.0620	-0.0597	-0.0553
	-9.25	-4.30	-1.78	-0.693	-0.426	-0.319	-0.246
	-36.8	-16.1	-6.41	-2.45	-1.50	-1.12	-0.867

Table 2: Numerical tests on S. Müller's example

^areference^bdifference with the reference energy^cthis tensor turns out to be diagonal

In the numerical tests, $a = 0.25$ and the following energy density has been used in the periodic cell $(0, 1)^3$: $W(y, \xi) = C(y)\bar{W}(\xi)$, where $C(y) = 0.01$ if $y \in (0, 1/2) \times (0, 1)^2$ and $C(y) = 10$ if $y \in (1/2, 1) \times (0, 1)^2$. This models a layered material, whose energy density satisfies the hypotheses of Theorem 2.

The cell-problem (20) has been solved for

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0.8 \end{pmatrix}$$

and different numbers of periodic cells. The computations have been made using a finite meshsize, however the differences between the energies are large enough with respect to the convergence error to be meaningful. The solutions reported on are obtained by a Newton algorithm and, theoretically, minima are only known to be local. From mechanical arguments and given the initial guesses, these minima may actually be considered global. The results are collected in Table 2. The energies of the solutions and the associated stress tensors are displayed versus the periods of the solutions. As the periods of the solutions increase, the energies of the solutions decrease and the material relaxes its stress. Therefore, several periodic cells have to be taken into account to reach the limit in (5). This is not an easy task since tracking bifurcations is quite hard in practice with a Newton method. In addition, even in the cases presented above, for which the form of the bifurcation is intuitive, the solution is very sensitive to the initial guess. This makes the automation of the procedure quite tricky.

We have also checked on an example the influence of the buckling of the cell-problem on the solution of the macroscopic problem itself. The test consists in the compression of 20% of a cube in the vertical direction, it is simple enough to allow us to find automatically the buckling in the cell-problems and complex enough not to have a trivial solution. The result shows that the minimizers of the numerical homogenized energies are also very different, even when the test is quite simple. The resolution of the macroscopic problem does not simplify or reduce the influence of buckling of the cell-problem. This test has been performed

$\ u_H^{1,h}\ _{1,4}$	$\ u_H^{3,h} - u_H^{1,h}\ _{1,4} / \ u_H^{1,h}\ _{1,4}$
0.2620	14.12%

Table 3: Influence of N on $u_H^{N,h}$

for 1-periodic (no buckling) and 3-periodic solutions (buckling) of the cell-problems. The norm of the difference between the two macroscopic solutions is reported on in Table 3. Qualitatively both macroscopic solutions respect the anisotropy of the heterogenous material in the $(0x)$ direction. However, more the solutions of the cell-problems get relaxed, smaller the macroscopic deformation is.

6.3 Shear band instabilities

In [12], Geymonat et. al. have studied the stability of homogenized energy densities and have suggested that, under some hypotheses, the homogenized material can develop *shear band instabilities*, that is no resistance of the material in one shear direction at least.

These shear band instabilities are linked to a loss of strict rank-one convexity of the homogenized energy density: there exist two vectors $a, b \in \mathbb{R}^3$ such that for all $A \in \mathcal{M}_3(\mathbb{R})$ the function $\mathbb{R} \rightarrow \mathbb{R}, t \mapsto W_{homog}(A + ta \otimes b)$ is convex but not strictly convex.

We have performed numerical tests and have obtained several corresponding shear bands, strongly depending on the mesh. The problem considered is of type (68) and is posed on a cube submitted to:

- $u(x) = -0.2 x_3 e_3$ on the faces $x_3 = 0$ and $x_3 = 1$;
- homogeneous natural boundary conditions elsewhere.

The cell-problem has been posed on one single periodic cell. The deformed solutions showing the shear bands are plotted on Figure 1.

This shear band instability is the cause of two major difficulties: the approximation result of Section 3 is not valid any more since the minimizer is not isolated and the Newton algorithm fails to converge. Mechanically speaking this quality of the homogenized energy density is an artefact due to the homogenization procedure: the real layered material with $\epsilon > 0$ is strictly rank-one convex and does not have shear band instabilities. Therefore, the homogenized energy has non-mechanical minimizers, which makes the direct numerical practice impossible. In order to be able to compute minimizers and to recover an approximation result we can stabilize the approximate energy density by adding a small strictly rank-one convex perturbation.

This stabilization procedure, which is naive and may certainly be improved in many ways, can also be seen as a filtering procedure which allows to get rid of a range of meaningless minimizers. In numerical tests, stabilizing in such a way is not always sufficient to

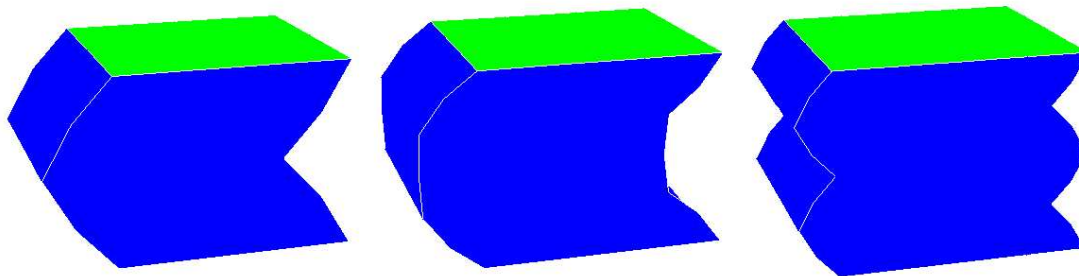


Figure 1: Two, three and four shear bands

guarantee the convergence of the Newton algorithm as the macroscopic mesh gets finer. We are indeed also limited by the ratio between the mesh of the cell-problem and the mesh of the macroscopic domain to go further in the numerical study.

Buckling is clearly a limit of the numerical approach developed throughout the paper. We have thus tried to determine numerically, for specific periodic cells, the occurrence of buckling in the cell-problem for a given range of loads A . With the constitutive law of S. Müller and a ratio of 1000, as for $C(y)$, we have not been able to make cell-problems buckle within a wide range of loads for the following simple geometry: a cubic soft inclusion in a matrix. This is no proof that we have reached a solution with the lowest energy but it allows us to deal with numerically stable cases.

6.4 Tests on a wider class of energies

Cases of practical interest do not usually satisfy the growth condition (1) and the homogenization formula (4) has not been proved in this framework. We have however tested the numerical method in such a case. The basic example of a polyconvex energy density dealt with models an ideal rubber foam, that is a material made of a rubber matrix with air bubbles of a few microns at a given concentration. Several constitutive laws have been proposed in the literature to model rubber foams. They are however more likely to give a coarse description than provide with quantitative results ([3],[4]).

The material considered is obtained by the periodic replication of a unit cell. This cell is composed of a rubber matrix and a bubble of air. The rubber matrix is a cube and the bubble is supposed spherical as in Figure 2. The proportion of air ranges from 5% to 15% in the numerical experiments.

A classical constitutive law for rubber-like materials is the Ciarlet-Geymonat constitutive law. Its stored energy function W is polyconvex and depends on the three invariants of the

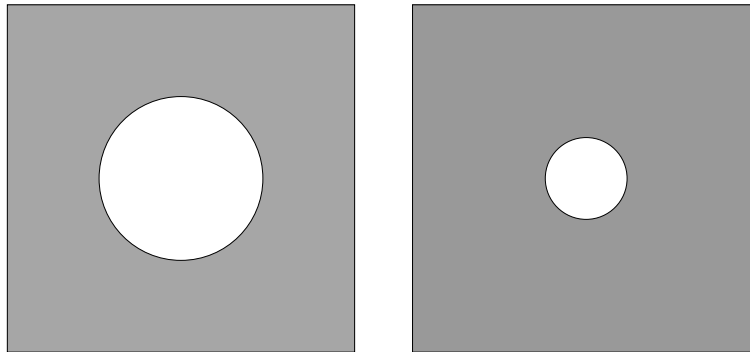


Figure 2: Two examples of unit cell (in 2D)

strain tensor ∇u , it is characterized by three positive constants C_1 , C_2 , a , and is given by

$$W(F) = C_1(I_1 - 3) + C_2(I_2 - 3) + a(I_3 - 1) - (C_1 + 2C_2 + a)\ln I_3,$$

where $I_1 = \text{Tr}(C)$, $I_2 = 1/2(\text{Tr}(C)^2 - \text{Tr}(C^2))$ and $I_3 = \det(C)$, with $C = {}^T (Id + \nabla u) \cdot (Id + \nabla u)$. The term $\ln(I_3)$ does not satisfy (1).

The numerical values of the above constants are typically

$$\begin{cases} C_1 = 0.5 \text{ MPa}, \\ C_2 = 0.0056 \text{ MPa}. \end{cases}$$

W is compressible for finite a , typically of the order of C_1 . In the limit $a \rightarrow \infty$ the material becomes incompressible. Quasi-incompressible materials are materials with a finite but quite important a . In the quasi-incompressible case, numerical difficulties arise (locking) if the volumetric part of W (that is the part depending on I_3) is not treated correctly ([17]). In Modulf, this difficulty is overcome thanks to a mixed formulation ([27]).

Numerical tests are positive since the algorithm is quite stable for a wide range of tests and has not encountered the convergence difficulties linked to the loss of strict rank-one convexity discussed in Section 6.3.

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