Relaxation and the computation of effective energies and microstructures in solid mechanics

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Summary. We address the numerical analysis of relaxed formulations for scalar and vectorial nonconvex variational problems originating from models for solid-solid phase transitions and crystal plasticity. We discuss algorithms for the approximation of the quasiconvex envelope using laminates, rank-one convexity, and polyconvexity, and present some numerical applications to benchmarks problems, and to a model for single-slip crystal plasticity.

1 Introduction

Variational models based on nonlinear elasticity, and their mathematical analysis, have proved useful for the study of phase transitions and microstructures in elastic solids, starting with the seminal work of Ball & James [BJ87, BJ92]. The methods of relaxation have in some cases lead to new understandings on the mesoscopic phase diagram [DSD02], on the microscopic origin of complex domain patterns [KM94], and on geometrical conditions relevant for the design of new devices and materials [Bha03].

Mathematically, one minimizes the functional

$$E(u) = \int_\Omega W(Du)\,dx \tag{1}$$

over the set of admissible deformations $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$, with $u \in W^{1,p}(\Omega;\mathbb{R}^m)$, $u = u_D$ on $\partial\Omega$, and W the energy density of the crystal. Here $W^{1,p}(\Omega;\mathbb{R}^m)$ denotes standard Sobolev spaces with $p \in (1,\infty)$ related to the growth of W, and (1) may include lower-order terms representing external forces.

One says that the functional E predicts a microstructure if a minimum does not exist, and gradients of infimizing sequences exhibit oscillations on finer and finer scales. Objective of the research is the analysis and numerical simulation of those infimizing sequences and/or their most relevant features.

The determination of low-energy states of such functionals E by standard finite element methods will typically yield mesh dependent results with oscillations in Du_h on a length scale comparable with the mesh size. Further, the computations can be very sensitive to mesh orientation and miss completely the description of the real microstructural configuration. For instance, the precise characterization of the minimizers of a non-convex problem in [BP04] shows that they develop complicated branching structures and are therefore difficult to detect numerically. One is therefore interested in alternative approaches, which do not attempt a direct numerical minimization, and is lead to the concept of relaxation.

From a physical point of view, relaxation focuses on macroscopic features and on the average material behaviour, rather than on the details of the microstructure. This means that one operates a separation of scales, and tries to extract from the microscale all information that is relevant for the macroscale, and no more. The macroscopic deformation is then determined by studying a problem which contains an effective energy density, which automatically accounts for the optimal local microstructure.

From a mathematical point of view, relaxation theory aims to replace an ill posed problem with a well posed one (at least as far as existence is concerned), preserving the essential features of the original problem. This can be achieved following basically two approaches. The first option is to enlarge the class of the competing functions, allowing for measure-valued solutions [You80, Ped97, Rou96]. The second one is to focus on the weak limits of infimizing sequences. Weak convergence, which qualitatively corresponds to convergence of averages, eliminates the fine-scale oscillations and gives a limit which only contains information on the macroscopic scale. The idea is, therefore, to study the behaviour of infimizing sequences by characterizing their limit points as minimizers of a new functional [But89, Dac89, Mue99].

Lack of strong convergence of infimizing sequences, and lack of existence of a minimizer, is strictly related to the lack of weak lower semicontinuity of the functional (1) on the space $W^{1,p}(\Omega;\mathbb{R}^m)$, which in turn is equivalent to quasiconvexity of W, under suitable continuity and growth conditions [Dac89, Mue99]. Precisely, if W is coercive then weak sequential lower semicontinuity (and hence quasiconvexity) is a sufficient condition for the existence of minimizers. If instead W is not quasiconvex, then one must expect fine-scale oscillations in the gradients of infimizing sequences. The relaxation of $E(u)$ is achieved in this case by replacing W with its quasiconvex envelope W^{qc}, the largest quasiconvex function bounded from above by W. Knowledge of W^{qc} would permit an accurate simulation of the macroscopic features of E. Unfortunately, analytical formulas for the quasiconvex envelope are known only for very few energy densities W. Consequently, one is interested to nu-

merical relaxation, which aims at an efficient approximation of W^{qc}. This will be illustrated and discussed below, considering model examples of microstructures in phase transitions and in elastoplasticity described by scalar and vector nonconvex variational problems. We call the minimization of (1) scalar if $n \wedge m := \min\{n, m\} = 1$, vector otherwise.

The remaining part of the paper is organized as follows. Section 2 analyzes generalized and relaxed formulations of a scalar nonconvex minimization problem for a two-well energy density. Section 3 deals, instead, with nonconvex vector variational problems by introducing the notions of quasiconvexity, rank-one convexity, and polyconvexity. Section 4 describes numerical algorithms for the evaluation of the rank-one convex and polyconvex envelope as approximation of the quasiconvex envelope. Applications to models for microstructure in phase transitions and plasticity are given in Section 5. Finally, Section 6 concludes the paper with some observations.

2 The scalar double-well problem and its relaxation

We consider in this section the anti-plane shear simplification of the Ericksen-James energy density

$$W(F) := |F - F_1|^2 |F - F_2|^2 \quad \text{for } F \in \mathbb{R}^2, \tag{2}$$

with $F_1, F_2 \in \mathbb{R}^2$, $F = Du$, and $u : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$, as a typical example of a scalar nonconvex minimization problem. This reads as follows.

Problem 1. Seek $u \in \mathcal{A}$ that minimizes

$$E(u) = \int_\Omega W(Du)\, dx + \alpha \int_\Omega |u - f|^2\, dx, \tag{P}$$

over the set of admissible functions $\mathcal{A} := u_D + W_0^{1,4}(\Omega; \mathbb{R})$, with $u_D \in W^{1,4}(\Omega; \mathbb{R})$ prescribed, $\alpha \geq 0$, and $f \in L^2(\Omega; \mathbb{R})$.

As discussed in the Introduction, direct minimization of (P) is difficult [Lus96]. The rest of this section discusses alternative approaches. Precisely, in Subsection 2.1 we introduce the concept of Young measures, and in Subsections 2.2 and 2.3 generalizations of (P) with Young measures (problem (GP)) and by convexification (problem (CP)) are discussed. Convergence of adaptive mesh refinement algorithms is discussed in the Subsection 2.4, whereas Subsection 2.5 summarizes the main results for the formulations (CP) and (GP) for an *ad hoc* extension to 2D of the broken Tartar problem [NW93] developed in [CJ03].

2.1 Young measures capture oscillations

Infimizing sequences (u_ℓ) for (P) are typically weakly but not strongly convergent in $W^{1,p}(\Omega;\mathbb{R})$ and the corresponding weak limits are in general not solutions of (P), because of the lack of weak lower semicontinuity. Young measures provide the mathematical tool for representing the weak-$*$ limit, whenever it exists, of sequences $(f(u_\ell)) \subset L^\infty(\Omega;\mathbb{R})$ with $f \in C_0(\mathbb{R};\mathbb{R})$. Here $C_0(\mathbb{R}^m;\mathbb{R})$ for $m \geq 1$ is the space of the functions $f \in C(\mathbb{R}^m;\mathbb{R})$ such that $\lim_{|x|\to\infty} f(x) = 0$. Definitions and properties of Young measures are given next in relation to their use for sequences $(u_\ell) \subset L^\infty(\Omega \subset \mathbb{R}^n;\mathbb{R}^m)$.

Definition 2 ([Mue99]). *Denote with $\mathcal{M}(\mathbb{R}^m)$ the set of all finite signed Radon measures supported in $\mathbb{R}^m$, and with $L^\infty_w(\Omega;\mathcal{M}(\mathbb{R}^m))$ the space of functions $\nu = (\nu_x)_{x\in\Omega}$ defined in $\Omega \subset \mathbb{R}^n$ and with values in $\mathcal{M}(\mathbb{R}^m)$ such that*

$$\langle \nu; g\rangle : \Omega \to \mathbb{R}, \quad x \mapsto \langle \nu_x; g\rangle := \int_{\mathbb{R}^m} g\, d\nu_x$$

are measurable for all $g \in C_0(\mathbb{R}^m;\mathbb{R})$. Let $YM(\Omega;\mathbb{R}^m)$ be the set of all $\nu \in L^\infty_w(\Omega;\mathcal{M}(\mathbb{R}^m))$ which are probability measures, i.e. $\nu_x \geq 0$ and $\nu_x(\mathbb{R}^m)$=1 for almost all $x \in \Omega$. The elements of $YM(\Omega;\mathbb{R}^m)$ are called Young measures.

Theorem 3 (Existence theorem for Young measures [Mue99]). *Assume the sequence (u_ℓ) bounded in $L^\infty(\Omega;\mathbb{R}^m)$. Then there exists a compact set $K \subset \mathbb{R}^m$, a subsequence $(u_{\ell_j}) \subset (u_\ell)$, and a Young measure $\nu = (\nu_x)_{x\in\Omega} \in L^\infty_w(\Omega;\mathcal{M}(\mathbb{R}^m))$ such that:*

(i) supp $\nu_x \subseteq K$ a.e. in Ω

(ii)for each $f \in C_0(\mathbb{R}^m;\mathbb{R})$ we have

$$\int_\Omega f(u_{\ell_j})h\, dx \to \int_\Omega \bar{f}h\, dx \text{ for every } h \in L^1(\Omega;\mathbb{R}), \tag{3}$$

where

$$\bar{f}(x) = \langle \nu_x; f\rangle := \int_{\mathbb{R}^m} f d\nu_x \text{ for a.e. } x \in \Omega. \tag{4}$$

Definition 4. *We call $\nu = (\nu_x)_{x\in\Omega}$ in Theorem 3 the Young measure associated with (or generated by) the sequence (u_{ℓ_j}).*

Remark 5. (i) From Theorem 3 one obtains a criterion for strong convergence, and consequently a criterion to decide on the occurrence or not of oscillations. Given $u_\ell \overset{*}{\rightharpoonup} u$ in $L^\infty(\Omega;\mathbb{R}^m)$, then $u_\ell \to u$ strongly in $L^p(\Omega;\mathbb{R}^m)$ with $p < \infty$ if and only if $\nu_x = \delta_{u(x)}$ a.e. in Ω [Mue99].
(ii) By making specific choices for f, we can read off certain information regarding the structure of the Young measures. For instance, if $u_\ell \overset{*}{\rightharpoonup} u$ in $L^\infty(\Omega;\mathbb{R}^m)$ and $f = \mathrm{id}$ in a neighbourhood of supp ν, then

$$u(x) = \int_{\mathbb{R}^m} \lambda d\nu_x(\lambda)$$

where $(\nu_x)_{x\in\Omega}$ is the Young measure associated with (u_ℓ).

Since microstructures are associated with oscillations in the gradients of infimizing sequences, one is mainly interested in understanding what are the Young measures associated with the sequence (Du_ℓ). These are called gradient Young measures.

Definition 6 ([Mue99]). *An element $\nu \in L^\infty_w(\Omega; \mathcal{M}(\mathbb{R}^m))$ is called a $W^{1,\infty}$-gradient Young measure generated by (u_ℓ) if it is the Young measure generated by the sequence of gradients (Du_ℓ) with (u_ℓ) weakly-$*$ convergent in $W^{1,\infty}(\Omega;\mathbb{R}^m)$.*

Remark 7. (i) From equation (3) with $f = \mathrm{id}$ in a neighbourhood of supp ν, the weak-$*$ limit Du of a sequence of gradients (Du_ℓ) for an infimizing sequence (u_ℓ) for (P) is related to the gradient Young measure generated by (u_ℓ) by

$$Du(x) = \int_{\mathbb{R}^2} F d\nu_x(F) = \langle \nu_x; \mathrm{id}\rangle \text{ a.e. in } \Omega. \tag{5}$$

Therefore the gradient Young measure ν permits to compute the macroscopic strain Du. Analogously, specifying $f = DW$ around supp ν in (3), if $(DW(Du_\ell))$ is weakly-$*$ convergent to some σ, one obtains

$$\sigma(x) = \int_{\mathbb{R}^2} DW(F) d\nu_x(F) = \langle \nu_x; DW\rangle \text{ a.e. in } \Omega. \tag{6}$$

(ii) Specifying then $f = W$ around supp ν in (3) one has

$$\lim_{\ell\to\infty} \int_\Omega W(Du_\ell)\, dx = \int_\Omega \langle \nu_x; W\rangle\, dx. \tag{7}$$

2.2 Relaxation with Young measures and their numerical approximation

Equation (7) along with (5) motivate the following generalized problem.

Problem 8. Seek a minimizer $(u,\nu) \in \mathcal{B}$ of

$$GE(u,\nu) := \int_\Omega \langle \nu_x, W\rangle\, dx + \alpha \int_\Omega |u - f|^2\, dx \tag{GP}$$

over $\mathcal{B} := \{(u,\nu) \in \mathcal{A} \times YM(\Omega;\mathbb{R}^2) : Du(x) = \langle \nu_x; \mathrm{id}\rangle \text{ for a.e. } x \in \Omega\}$.

The relevance of problem (GP) follows from relaxation theory.

Theorem 9 ([Rou96, Theorem 5.2.1][Ped97, Theorem 4.4]). *Problem* (GP) *has a solution and there holds*

$$\inf_{u\in\mathcal{A}} E(u) = \min_{(u,\nu)\in\mathcal{B}} GE(u,\nu).$$

Moreover, if (u_ℓ) *is a weakly convergent infimizing sequence for* (P)*, with weak limit* u*, that generates the gradient Young measure* ν*, then* (u,ν) *is a minimizer for* (GP)*. Vice versa, if* (u,ν) *is a solution of* (GP) *then there is a weakly convergent infimizing sequence* (u_ℓ) *such that its weak limit is* u *and* ν *is the Young measured generated by* (u_ℓ)*.*

Remark 10. Given $\nu \in L^\infty_w(\Omega;\mathcal{M}(\mathbb{R}^2)$, the compatibility condition $\langle \nu_x;\mathrm{id}\rangle = Du(x)$ with $u \in W^{1,\infty}(\Omega;\mathbb{R})$, and $\operatorname{supp}\nu_x \subseteq K$ compact subset of $\mathbb{R}^2$, characterize in the scalar case completely the gradient Young measures associated with sequences.

Numerical approximations of (GP) have been proposed in [NW93, CR98, Rou96a, Ped95]. Those involve a discretization of the admissible set $\mathcal{A}\times YM(\Omega;\mathbb{R}^2)$ and care of the differential constraint.

Within a finite element scheme, denote with $\mathcal{T}$ a regular triangulation of Ω, and by $\mathcal{E}$ and $\mathcal{N}$ the set of all edges and vertices, respectively. Then introduce the following finite dimensional spaces

$$\begin{aligned}\mathcal{S}^1(\mathcal{T}) :=& \{v_h \in C(\bar\Omega) : \forall T\in\mathcal{T},\, v_h|_T \text{ is affine}\},\\ \mathcal{S}^1_0(\mathcal{T}) :=& \{v_h \in \mathcal{S}^1(\mathcal{T}) : v_h = 0 \text{ on } \partial\Omega\}.\end{aligned}$$

Let $\mathcal{K} := \mathcal{N}\cap\Omega$ denote the set of free nodes, the Dirichlet boundary conditions u_D are discretized by nodal interpolation, i.e. $u_{D,h}\in\mathcal{S}^1(\mathcal{T})$ with

$$u_{D,h}(z) = u_D(z) \text{ if } z\in\mathcal{K} \text{ and } u_{D,h}(z) = 0 \text{ if } z\in\mathcal{N}\setminus\mathcal{K}.$$

A conforming finite element method of (GP) is obtained by replacing the space $\mathcal{A}$ with $\mathcal{A}_h := u_{D,h} + \mathcal{S}^1_0(\mathcal{T})$ whereas the set of Young measures $YM(\Omega;\mathbb{R}^2)$ is approximated by element-wise constant measures, i.e. homogeneous Young measures ν_T expressed as a convex combination of Dirac measures supported at the nodes of a triangulation τ of a convex polygonal domain $\omega\subset\mathbb{R}^2$ with mesh size d. That is, denote by $\mathcal{N}_d(\omega)$ the set of nodes of the triangulation τ of ω, we assume

$$\nu_{T,d} = \sum_{F_{T,j}\in\mathcal{N}_d(\omega)} a_{F_{T,j}}\delta_{F_{T,j}} \tag{8}$$

with known atoms $F_{T,j}\in\mathcal{N}_d(\omega)$, and unknown coefficients $a_{T,j}$. We denote this set with $\mathcal{L}^0(\mathcal{T};\mathcal{PM}_{h,d})$ where $\mathcal{PM}_{h,d}$ is the set of probability measures expressed as in (8). Consider the set

$$\mathcal{B}_{h,d} = \{(v_h,\mu_{h,d})\in\mathcal{A}_h\times\mathcal{L}^0(\mathcal{T};\mathcal{PM}_{h,d}) : \forall T\in\mathcal{T},\, Dv_h|_T = \langle\mu_{h,d}|_T;\mathrm{id}\rangle\}, \tag{9}$$

the discrete generalized problem reads

Problem 11. Seek $(u_h, \nu_{h,d}) \in \mathcal{B}_{h,d}$ such that

$$\text{Minimize } GE(u_h, \nu_{h,d}) \text{ over } \mathcal{B}_{h,d}. \tag{GP$_{h,d}$}$$

An existence result for (GP$_{h,d}$) follows as for (GP). Let $\mathcal{L}^0(\mathcal{T};\mathbb{R}^2)$ be the set of piecewise constant functions on $\mathcal{T}$ with values in $\mathbb{R}^2$, W^{**} the convex envelope of W (defined in Section 2.3) and $W_d^c = (\mathcal{P}_\tau W)^{**}$ the convex envelope of $\mathcal{P}_\tau W$, the nodal interpolation of W associated with the triangulation τ of ω. Let $\sigma = DW^{**}(Du)$ for a solution $u \in \mathcal{A}$ of (CP) (see Problem 13), then we have the following a-priori and a-posteriori error bounds

Theorem 12 ([Bar04, Theorem 4.6 & Theorem 4.8]). *Assume $u \in \mathcal{A}$ solution of* (CP)*, $(u_h, \nu_{h,d}) \in \mathcal{B}_{h,d}$ solution of* (GP$_{h,d}$)*, and $\lambda_{h,d} \in \mathcal{L}^0(\mathcal{T};\mathbb{R}^2)$ the Lagrange multiplier associated with the constraint $Dv_h|_T = \langle \mu_{h,d}|_T; \mathrm{id}\rangle$. Then, there holds*

$$\begin{aligned} \|\sigma - \lambda_{h,d}\| \le{}& C \inf_{v_h \in \mathcal{A}_h} (\|\nabla(u - v_h)\| + \alpha\|u - v_h\|) \\ &+ C\|\partial W_d^c - DW^{**}\|_{L^\infty(\omega)}\,; \end{aligned} \tag{10}$$

$$\begin{aligned} \|\sigma - \lambda_{h,d}\|^2 \le{}& C\Big\{ (\sum_{T\in\mathcal{T}} h_T^2 \|f + \mathrm{div}\lambda_{h,d} + 2\alpha(f - u_h)\|)^{1/2} \\ &+ (\sum_{E\in\mathcal{E}} h_E \|[\lambda_{h,d}\cdot n_E]\|^2)^{1/2} + \|\partial W_d^c - DW^{**}\|_{L^\infty(\omega)} \\ &+ \|h_{\mathcal{E}}^{3/2} \partial_{\mathcal{E}}^2 u_D/\partial s^2\|_{L^2(\Gamma_D)} \Big\}. \end{aligned} \tag{11}$$

Since $\|\partial W_d^c - DW^{**}\|$ can be bounded from above in terms of grid size d and D^2W^{**}, together with the density of the finite element spaces in $\mathcal{A}$, from (10) one proves $\lambda_{h,d} \to \sigma$ in L^2 as $h, d \to 0$, whereas (11) represents a basic ingredient of the multilevel adaptive scheme for the definition of the support of the Young measures developed by [Bar04].

2.3 Relaxation via convex envelopes

By minimizing the two contributions in (GP) separately one obtains another relaxation of (P). For fixed $F = Du$ one can find a probability measure $\nu = (\nu_x)_{x\in\Omega}$ such that ν minimizes the expression $\langle \mu; W\rangle$ among all the probability measures μ satisfying $\langle \mu; \mathrm{id}\rangle = F$. In some cases, it is also possible to obtain an explicit expression for the convex hull of W, defined by

$$W^{**}(F) = \min_{\substack{\mu \in YM(\Omega;\mathbb{R}^2) \\ \langle \mu; \mathrm{id}\rangle = F}} \langle \mu, W\rangle. \tag{12}$$

The notation is motivated by the fact that for continuous W the convex envelope coincides with the bipolar function. We recall that, since we are in the scalar case, convexity and quasiconvexity coincide.

Problem (GP) and (12) motivate to consider the convexified problem.

Problem 13. Seek $u \in \mathcal{A}$ that minimizes

$$E^c(u) := \int_\Omega W^{**}(Du)\,dx + \alpha \int_\Omega |u-f|^2\,dx. \tag{CP}$$

Likewise problem (GP), the importance of problem (CP) follows from relaxation theory.

Theorem 14 ([Dac89]). *Problem* (CP) *has a solution and there holds*

$$\inf_{u\in\mathcal{A}} E(u) = \min_{u\in\mathcal{A}} E^c(u). \tag{13}$$

Moreover, if (u_ℓ) *is a weakly convergent minimizing sequence of* (P) *and* u *is its weak limit, then* u *is a solution of* (CP)*. Vice versa, if* u *is a solution of* (CP) *then there exists a weakly convergent minimizing sequence of* (P) *having* u *as weak limit. The stress field* $\sigma = DW^{**}(u)$ *is unique and independent of* u *among the solutions of* (CP) *[Fri94].*

Remark 15. Whenever $\alpha > 0$ in (P), problem (CP) admits a unique solution u. If $\alpha = 0$, however, the numerical treatment of (CP) requires the introduction of a perturbation in E^c, usually in the form of a strictly convex functional scaled by a small quantity. The introduction of the stabilized term finds its justification in the need of including some kind of 'selection mechanism' in the model which (i) ensures uniqueness on discrete level, (ii) is necessary for the design of convergent iterative solvers [BCHH04], and (iii) with some stabilizations terms for standard low-order finite element methods yields strong convergence of the gradients [BCPP04]. The same happens when dealing with quasiconvex envelopes in the vectorial case, see, e.g., [CDD02].

2.4 Adaptive finite element methods for relaxed formulations

An h-finite element adaptive algorithm consists of successive loops of the form

$$\text{SOLVE} \to \text{ESTIMATE} \to \text{MARK} \to \text{REFINE} \tag{14}$$

designed to produce with less computational effort more efficient meshes by targeted local refinements. The use of such algorithms for the direct finite element minimization, however, does not always lead to an improved convergence rate in the stress error and also unclear is its convergence. For degenerately convex problems with C^1 energy density W characterized for some constants p, r, s by the conditions

$$\begin{aligned} |DW(A) - DW(B)|^r &\le c(1+|A|^s+|B|^s)(W(B)-W(A) \\ &\qquad -DW(A)\cdot(B-A))\,, \\ c_l(|A|^p-1) \le W(A) &\le c_u(|A|^p+1)\,, \end{aligned} \tag{15}$$

to hold for all $A, B \in \mathbb{R}^n$, [Car06] proves the convergence of the stress fields $\sigma_0, \sigma_1, \ldots$ produced by (14) to $\sigma = DW^{**}(Du)$ in $L^{r/(1+s/p)}(\Omega;\mathbb{R}^2)$. In the

algorithm (14), the step `MARK` is realized by the criterion introduced by [Dor96] where one marks the edges $E \in \mathcal{M} \subset \mathcal{E}$ such that $\Theta \sum_{E\in\mathcal{E}} \eta_E^2 \leq \sum_{E\in\mathcal{M}} \eta_E^2$ with η_E the edge contribution to the global error estimator. In the step `REFINE`, on the other hand, one refines each triangle T with an edge in $\mathcal{M}$ such that an inner node is created, with possible further refinements that guarantee that $\|h_j Df\|_{L^2(\Omega;\mathbb{R}^2)}$ tends to zero as $j \to \infty$ and the resulting triangulation is regular.

2.5 A 2D scalar benchmark problem

In this section we report on the analysis of (P) in the particular case of $\alpha = 1$, f and u_D given in [CJ03], $\Omega = (0,1) \times (0,3/2)$, and the two wells $F_1 := -(3,2)/\sqrt{13}$ and $F_2 = -F_1$. The convex envelope W^{**} was computed in [CP97], and is

$$W^{**}(F) = ((|F|^2 - 1)_+)^2 + 4(|F|^2 - ((3,2)\cdot F)^2) \tag{16}$$

with $(\cdot)_+ := \max\{0, \cdot\}$ and the symbol $\cdot$ the inner product in $\mathbb{R}^2$. From relaxation theory, we have the following result.

Theorem 16 ([CJ03]). *The problem* (CP) *has a unique solution* $u \in \mathcal{A}$

$$\inf_{v\in\mathcal{A}} E(v) = \min_{v\in\mathcal{A}} E^{**}(v) = E^{**}(u), \tag{17}$$

characterized as the solution of the Euler-Lagrange equation

$$\int_\Omega \sigma \cdot Dv\, dx + 2\int_\Omega (u - f)v\, dx = 0 \text{ for all } v \in W_0^{1,4}(\Omega;\mathbb{R}), \tag{18}$$

where $\sigma := DW^{**}(Du)$. *Furthermore, any infimizing sequence* (u_ℓ) *of* (P) *is bounded in* $W^{1,4}(\Omega;\mathbb{R})$ *and generates a sequence of stresses* $\sigma_\ell := DW(Du_\ell)$ *convergent in measure toward* $\sigma = DW^{**}(Du)$.

For this problem, moreover, one obtains an analytical expression for the gradient Young measure which is unique and is given by

$$\nu_x = \lambda(F)\delta_{S_+(F)} + (1 - \lambda(F))\delta_{S_-(F)}, \tag{19}$$

with $F = Du$ and

$$\lambda(F) = \frac{1}{2}(1 + F_2 \cdot F(1 - |\mathbb{P}F|^2)^{-1/2}) \in [0,1], \tag{20}$$

$$S_\pm(F) = \begin{cases} \mathbb{P}F \pm F_2(1 - |\mathbb{P}F|^2)^{-1/2} & \text{for } |F| < 1, \\ F & \text{for } 1 < |F|, \end{cases} \tag{21}$$

where $\mathbb{P} = \mathbb{I} - F_2 \otimes F_2$ (with $\otimes$ tensor product of vectors of $\mathbb{R}^2$).

Remark 17. Since σ_ℓ converges toward σ, from (6) the stress field $\sigma = DW^{**}(Du)$ can then be represented as

$$\sigma(x) = \int_{\mathbb{R}^2} DW \, d\nu_x, \tag{22}$$

with ν given in (19) [Fri94].

With the notation of Section 2.2 the Galerkin discretization of (18) reads

Problem 18. Seek $u_h \in \mathcal{A}_h$ such that

$$\int_\Omega \sigma_h \cdot Dv_h \, dx + 2\int_\Omega (u_h - f)v_h \, dx = 0 \text{ for all } v_h \in \mathcal{S}^1_0(\mathcal{T}) \tag{CP$_h$}$$

with $\sigma_h := DW^{**}(Du_h)$

Strong convergence in $L^{4/3}(\Omega;\mathbb{R}^2)$ of the stress fields σ_h results from the a priori error estimate [CP97]

$$\|\sigma - \sigma_h\|_{L^{4/3}(\Omega;\mathbb{R}^2)} \le c_1 \inf_{v_h \in \mathcal{A}_h} \|u - v_h\|_{W^{1,4}(\Omega;\mathbb{R})}. \tag{23}$$

This is obtained using the condition

$$|DW^{**}(A) - DW^{**}(B)|^2 \le c(1+|A|^2+|B|^2)(DW^{**}(B) - DW^{**}(A)) : (B-A) \tag{24}$$

that holds for any $A, B \in \mathbb{R}^2$ together with some $p = 4$ and $q = 3$ growth conditions on W and on DW^{**}, respectively. Another application of (24) also shows the reliability of residual and averaging based error estimates whereas the efficiency follows from standard arguments; that is, one has also

$$c_2\eta_M - h.o.t. \le \|\sigma - \sigma_h\|_{L^{4/3}(\Omega;\mathbb{R}^2)} \le c_2\eta_M^{1/2} + h.o.t. \tag{25}$$

The minimal averaging error estimator η_M that enters (25) is defined by

$$\eta_M = \Big(\sum_{T\in\mathcal{T}} \eta_T^{4/3}\Big)^{3/4} \text{ for } \eta_T = \|\sigma_h - \sigma_h^*\|_{L^{4/3}(T;\mathbb{R}^2)},$$

with $\sigma^* \in \mathcal{S}^1(\mathcal{T})^2$ that minimizes

$$\|\sigma_h - \tau_h\|_{L^{4/3}(\Omega;\mathbb{R}^2)} \text{ among } \tau_h \in \mathcal{S}^1(\mathcal{T})^2.$$

Figure 1 displays experimental convergence rates for $\|\sigma - \sigma_h\|_{L^{4/3}(\Omega;\mathbb{R}^2)}$ and the error estimators η_M and $\eta_M^{1/2}$ for uniform and adaptive mesh refinement. The adaptive refinement strategy leads to significantly reduced error and improved experimental convergence rates.

Remark 19. The two-sided estimates (25) shows that lower bounds are no valid upper bounds and vice versa, due to the different exponents for η_M in the reliability and efficiency estimate. This miss balance is referred to as reliability-efficiency gap [CJ03].

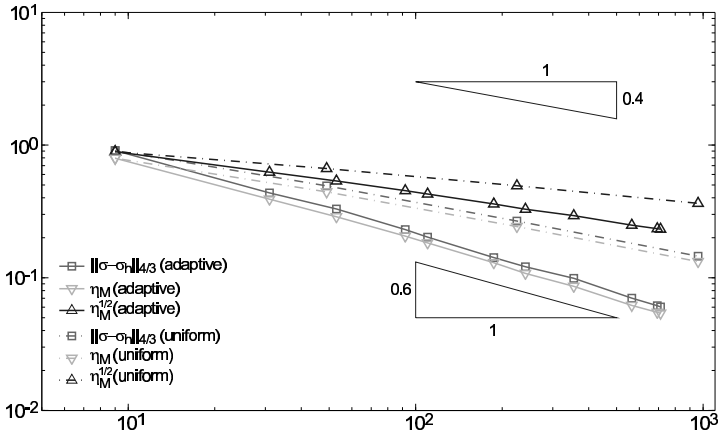


Fig. 1. The 2D benchmark problem. Experimental convergence rates for $\|\sigma - \sigma_h\|_{L^{4/3}(\Omega;\mathbb{R}^2)}$ and the error estimators η_M and $\eta_M^{1/2}$ plotted against degrees of freedom N with a logarithmic scale for uniform and adaptive mesh refinement.

3 Nonconvex vector variational problems

For scalar nonconvex variational problems the convexity of $W(Du)$ with respect to $F = Du$ ensures the weak (weak-$*$) sequential lower semicontinuity of the functional $E(u) = \int_\Omega W(Du)$ on $W^{1,p}(\Omega;\mathbb{R}^m)$ for $1 \le p < \infty$ (resp. $p = \infty$). Along with suitable growth conditions on W, one can prove the existence of minimizers using the direct method of the calculus of variations. In the vectorial case a weaker condition is sufficient, namely, quasiconvexity.

3.1 Quasiconvexity and effective energy density

Quasiconvexity was introduced by Morrey in 1952 as a condition on the energy density W which is equivalent, under appropriate growth conditions, to weak sequential lower semicontinuity of the functional E [Mor52].

Definition 20. *Given a function $W : \mathbb{R}^{3\times3} \to \mathbb{R}$, we say that W is quasiconvex at $F \in \mathbb{R}^{3\times3}$ if for every open and bounded set $\omega \subseteq \mathbb{R}^3$ one has*

$$\int_\omega W(F + Dy(x))\,dx \ge \int_\omega W(F)\,dx = |\omega|W(F) \text{ for each } y \in W_0^{1,\infty}(\omega;\mathbb{R}^3). \tag{26}$$

Quasiconvexity lies at the heart of the relaxation theory for functionals of the type $E(u) = \int_\Omega W(Du)\,dx$. An instrumental role is played by the quasiconvex envelope of W defined as the pointwise supremum of the quasiconvex functions that are bounded from above by W, i.e., for each $F \in \mathbb{R}^{3\times3}$,

$$W^{qc}(F) = \sup\{f(F) : f \le W \text{ with } f \text{ quasiconvex}\}. \tag{27}$$

Under suitable growth conditions on W, the weakly (weakly-$*$ for $p = \infty$) sequentially lower semicontinuous envelope of the functional

$$E(u) = \int_\Omega W(Du)\,dx + \mathcal{L}(u), \tag{28}$$

has the following integral representation

$$E^{qc}(u) = \int_\Omega W^{qc}(Du)\,dx + \mathcal{L}(u). \tag{29}$$

Here $\mathcal{L}(u)$ is a linear term representing external forces.

The link between the minimization of (28) and (29) is given by relaxation theory.

Theorem 21 ([Dac89, Mue99]). *Let $u_D \in W^{1,p}(\Omega;\mathbb{R}^3)$ be fixed, $\mathcal{A} = u_D + W_0^{1,p}(\Omega;\mathbb{R}^3)$, and assume W to have p-growth and be p-coercive. Then the relaxed problem*

$$\text{Minimize } E^{qc}(u) \text{ amongst } u \in \mathcal{A}, \tag{QP}$$

has a solution and there holds

$$\min_{u\in\mathcal{A}} E^{qc}(u) = \inf_{u\in\mathcal{A}} E(u). \tag{30}$$

Furthermore, any solution u of (QP) *is the weak limit of an infimizing sequence for* (28).

The quasiconvex envelope of W at F can be characterized equivalently as [Dac89, Mue99]

$$W^{qc}(F) = \inf_{\substack{y\in W^{1,\infty}(\omega;\mathbb{R}^3)\\ y=Fx \text{ on } \partial\omega}} \frac{1}{|\omega|}\int_\omega W(Dy(x))\,dx. \tag{31}$$

Inequality (26) states that the deformation $u(x) = Fx$ is a minimizer of $\int_\Omega W(Dy)\,dx$ subject to its own boundary values. As such $W^{qc}(F)$ represents the infimum of the average energy taken over all possible microstructures $y = y(x)$ that satisfy the boundary condition $y(x) = Fx$ on $\partial\Omega$, with the least energy achieved by the deformation $y = Fx$ itself.

Remark 22. (*i*) For $n \geq 2$, $m \geq 3$ it has been shown in [Kri99] that there does not exist a local characterization of (26), that is, there is no set of inequalities on W and its derivatives at an arbitrary matrix F which is necessary and sufficient for W to be quasiconvex. As a result, quasiconvexity is a very difficult property to verify in practice. Only few examples of analytical expressions of quasiconvex envelopes of particular functions are known with notable examples reported in [KS86, Koh91, DSD02, CT05, CO05].
(*ii*) The generalized formulation with gradient Young measures does not circumvent the quasiconvexification. The set of admissible gradient Young measures, besides the conditions listed in Remark 10, is characterized by the fact that Jensen's inequality should hold for any quasiconvex function, i.e. [KP91]

$$f(\langle \nu_x; \mathrm{id}\rangle) \le \langle \nu_x; f\rangle \text{ a.e. } x \in \Omega, \text{ for all quasiconvex functions } f. \tag{32}$$

For the constructive characterization and evaluation of W^{qc} for general W one is, therefore, faced with a direct minimization of a nonconvex functional with linear boundary conditions and no lower order terms on an arbitrary domain ω, whose solution may be, however, very difficult to tackle with. Necessary or sufficient conditions for quasiconvexity have been, therefore, introduced providing some insight for the analysis of microstructures.

3.2 Rank-one convexity and laminated microstructures

A necessary condition for quasiconvexity is rank-one convexity, stating convexity of the function W along all rank-one directions.

Definition 23. *A function $W : \mathbb{R}^{3\times 3} \to \mathbb{R}$ is rank-one convex if for all $A, B \in \mathbb{R}^{3\times 3}$ such that $\mathrm{rank}(A-B) \le 1$ and all $\lambda \in (0,1)$,*

$$W(\lambda A + (1-\lambda)B) \le \lambda W(A) + (1-\lambda)W(B). \tag{33}$$

Equivalently, W is rank-one convex if for all $A \in \mathbb{R}^{3\times 3}$ and all $a, n \in \mathbb{R}^3$ the function $\lambda \mapsto W(A + \lambda a \otimes n)$ is convex on $\mathbb{R}$. This is in turn equivalent to

$$W(A + \lambda a \otimes n) \le \lambda W(A + a \otimes n) + (1-\lambda)W(A), \tag{34}$$

for all $\lambda \in (0,1)$, and all A, a and n.

The following considerations illustrate the relevance of rank-one convexity in the analysis of microstructures. By letting $y \in W^{1,\infty}(\Omega;\mathbb{R}^3)$ with $y(x) = Fx$ on $\partial\omega$, $W^{qc}(F)$ provides a macroscopic description of all possible microstructures with average deformation F. In the evaluation of the infimum (31) it may be convenient to restrict $y = y(x)$ to a subclass of $W^{1,\infty}(\Omega;\mathbb{R}^3)$ corresponding only to certain microstructure patterns. For example, one can consider the deformations $y_\ell = y_\ell(x)$ describing first order laminates, and with $y_\ell(x) = Fx$ on $\partial\omega$. The corresponding sequence of gradients will, therefore, oscillate between two phases

$$F_0 = F + (1-\lambda)a \otimes n \text{ and } F_1 = F - \lambda a \otimes n \tag{35}$$

with some $a, n \in \mathbb{R}^{3\times 3}$, $\lambda \in (0,1)$, and $F_0 - F_1 = a \otimes n$. The gradient Young measure associated with (y_ℓ) will be homogeneous and equal to

$$\nu = \lambda\delta_{F_0} + (1-\lambda)\delta_{F_1}.$$

For such infimizing sequences (y_ℓ) one has [Dac89, Mue99]

$$\lim_{\ell\to\infty} \frac{1}{|\omega|} \int_\omega W(Dy_\ell(x))\,dx = \lambda W(F_0) + (1-\lambda)W(F_1). \tag{36}$$

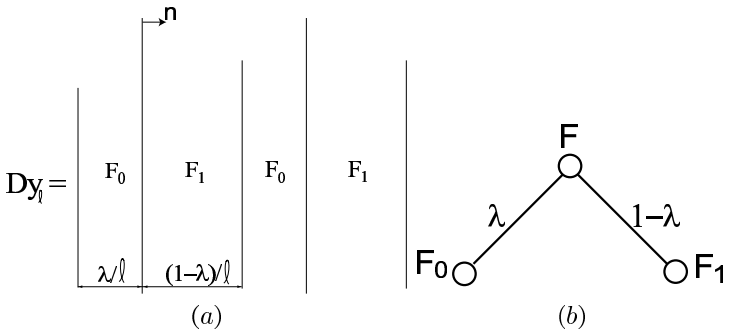


Fig. 2. (a) Microstructural patterns in first order laminates. (b) Graph representation.

In the class of the first order laminates defined by (35), those that realize the lowest energetic content will therefore be solution of the problem

$$R^{(1)}W(F) = \inf\{\lambda W(\underbrace{F + (1-\lambda)a \otimes n}_{F_0}) + (1-\lambda)W(\underbrace{F - \lambda a \otimes n}_{F_1})) : \\ 0 \leq \lambda \leq 1 \text{ and } a, n \in \mathbb{R}^3\}. \tag{37}$$

If $\lambda = 0$ or $\lambda = 1$ then no microstructure will occur. The graphical interpretation of condition (35) and the corresponding microstructure pattern are depicted in Figure 2.

For F_0 and F_1 given as above, consider the convex combination

$$F_0 = \lambda_0 F_{00} + (1-\lambda_0)F_{01} \text{ and } F_1 = \lambda_1 F_{10} + (1-\lambda_1)F_{11}, \tag{38}$$

with

$$F_{00} - F_{01} = a_0 \otimes n_0 \text{ and } F_{10} - F_{11} = a_1 \otimes n_1. \tag{39}$$

By replacing (38) into (35) one obtains

$$F = \lambda\lambda_0 F_{00} + \lambda(1-\lambda_0)F_{01} + (1-\lambda)\lambda_1 F_{10} + (1-\lambda)(1-\lambda_1)F_{11}. \tag{40}$$

The graphical interpretation of this decomposition and the corresponding microstructure pattern are shown in Figure 3.

Microstructures defined by (40) are called second order laminates. One can therefore inquire on the second order laminates (if they exist) that minimize $1/|\omega| \int_\omega W(Du)\,dx$. Those will be solution of the following global nonlinear optimization problem

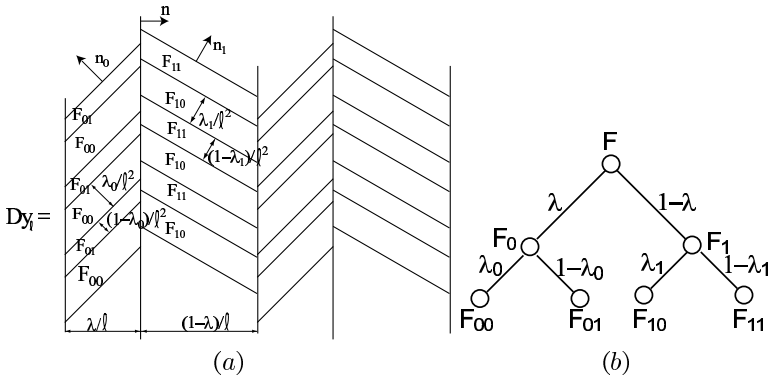


Fig. 3. (a) Microstructural patterns in second order laminates. (b) Graph representation.

$$R^{(2)}W(F) = \inf\Big\{\lambda\lambda_0 W(F_{00}) + \lambda(1-\lambda_0)W(F_{01}) + (1-\lambda)\lambda_1 W(F_{10}) + (1-\lambda)(1-\lambda_1)W(F_{11}) \,:\, 0 \le \lambda, \lambda_0, \lambda_1 \le 1, \text{ and } a, n, a_0, n_0, a_1, n_1 \in \mathbb{R}^3\Big\}. \tag{41}$$

It can be shown that it is also

$$R^{(2)}W(F) = \inf\big\{\lambda R^{(1)}W(F_0) + (1-\lambda)R^{(1)}W(F_1) \,:\, 0 \le \lambda \le 1,\ a, n \in \mathbb{R}^3\big\} \tag{42}$$

with F_0, F_1 defined as in (35). The iteration of (42) produces laminates of order $k \in \mathbb{N}$ such that [KS86]

$$W^{rc}(F) = \lim_{k\to\infty} R^{(k)}W(F), \tag{43}$$

and there holds

$$W^{qc} \le W^{rc} \le \cdots \le R^{(k)}W \le \cdots \le R^{(2)}W \le R^{(1)}W \le W. \tag{44}$$

In (43), W^{rc} denotes the rank-one convex envelope of W defined by (27) with rank-one convex functions.

3.3 A lower bound to W^{qc}: polyconvex envelope

Polyconvexity was introduced by Ball in [Bal77] as a structural condition on W compatible with some physical requirements that simple convexity would violate, and that was sufficient to ensure existence of minimizers for nonlinear finite strain elasticity. Both polyconvexity and convexity provide sufficient conditions for quasiconvexity.

Definition 24 ([Bal77]). *The function $W : \mathbb{R}^{3\times 3} \to \mathbb{R}$ is polyconvex if there exists a convex function $g : \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \times \mathbb{R} \to \mathbb{R}$ such that*

$$W(F) = g(T(F)) \text{ for each } F \in \mathbb{R}^{3\times 3}. \tag{45}$$

Here

$$T : F \in \mathbb{R}^{3\times 3} \to T(F) = (F, \operatorname{cof} F, \det F) \in \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \times \mathbb{R}. \tag{46}$$

The function g is not defined uniquely from W. Using Carathéodory theorem it can be shown that one possible choice is [Dac89]

$$\begin{aligned} g(T(F)) = \inf_{\substack{A_i \in \mathbb{R}^{3\times 3} \\ \lambda_i \in \mathbb{R}}} \{ \sum_{i=1}^{19} \lambda_i W(A_i) \, : & \lambda_i \geq 0, \sum_{i=1}^{19} \lambda_i = 1, \\ & \sum_{i=1}^{19} \lambda_i T(A_i) = T(F) \} \, . \end{aligned} \tag{47}$$

The value of the polyconvex envelope W^{pc} at $F \in \mathbb{R}^{3\times 3}$, can be, therefore, characterized equivalently as solution of the following minimization problem.

$$\begin{aligned} W^{pc}(F) = \inf_{\substack{A_i \in \mathbb{R}^{3\times 3} \\ \lambda_i \in \mathbb{R}}} \{ \sum_{i=1}^{19} \lambda_i W(A_i) \, : & \lambda_i \geq 0, \sum_{i=1}^{19} \lambda_i = 1, \\ & \sum_{i=1}^{19} \lambda_i T(A_i) = T(F) \}. \end{aligned} \tag{48}$$

The semiconvex notions introduced so far reduce to convexity in the scalar case, whereas in the vector case, their relation is represented in the following diagram

$$W \text{ convex } \Rightarrow W \text{ polyconvex } \Rightarrow W \text{ quasiconvex} \Rightarrow W \text{ rank-one convex}, \tag{49}$$

with the converse not holding in general [Mue99]. In view of (49) one has

$$W^c \leq W^{pc} \leq W^{qc} \leq W^{rc} \leq \cdots \leq R^{(k)}W \leq \cdots \leq R^{(2)}W \leq R^{(1)}W \leq W, \tag{50}$$

with W^{pc} and W^{rc} providing lower and upper bound to W^{qc}, respectively.

From Theorem 21 it follows

$$\begin{aligned} \min_{u\in\mathcal{A}} \int_\Omega W^{qc}(Du)\,dx = \inf_{u\in\mathcal{A}} \int_\Omega W^{rc}(Du)\,dx = \cdots = \inf_{u\in\mathcal{A}} \int_\Omega R^{(k)}W(Du)\,dx \\ \cdots = \inf_{u\in\mathcal{A}} \int_\Omega R^{(1)}W(Du)\,dx = \inf_{u\in\mathcal{A}} \int_\Omega W(Du)\,dx. \end{aligned} \tag{51}$$

4 Numerical relaxation

The evaluation of rank–one convex and polyconvex envelopes for a characterization of the quasiconvex hull is an extremely complex task since the energy density W is defined on four– or nine–dimensional matrix spaces in the space dimension $n = m = 2$ or $n = m = 3$ but can be reduced using invariance under rotations. Furthermore, the definition of an envelope is typically not local, that is, the value at a given $F \in \mathbb{R}^{n\times n}$ depends, in general, on the values of W on the whole space $\mathbb{R}^{n\times n}$ and not just on a bounded neighborhood of F.

In view of the difficulty involved in checking analytically the previous notions, one tries to resort to efficient numerical algorithms for the approximation to rank–one convex and polyconvex envelope, referred to as numerical relaxation, exploiting growth conditions and qualitative properties of W.

4.1 Numerical polyconvexification

For $F \in \mathbb{R}^{3\times 3}$ the value of the polyconvex envelope at F, $W^{pc}(F)$, given by equation (48) involves a nonlinear optimization problem whose solution may be very difficult. Given a finite set of nodes $\mathcal{N}_{\delta,r} = \delta\mathbb{Z}^{3\times 3} \cap \overline{B_r(0)} \subseteq \mathbb{R}^{3\times 3}$, δ mesh size such that $0 \leq \delta \leq r$ and r large enough so that $F \in \operatorname{co}\mathcal{N}_{\delta,r}$, convex hull of $\mathcal{N}_{\delta,r}$, an approximation to $W^{pc}(F)$ can be obtained by solving the following linear optimization problem over the space $\mathbb{R}^{\#\mathcal{N}_{\delta,r}}$ with $\#\mathcal{N}_{\delta,r}$ the cardinality of the discrete set $\mathcal{N}_{\delta,r}$.

$$W^{pc}_{\delta,r}(F) = \inf_{\theta_A\in\mathbb{R}^{\#\mathcal{N}_{\delta,r}}} \Big\{ \sum_{A\in\mathcal{N}_{\delta,r}} \theta_A W(A) \ : \theta_A \geq 0, \sum_{A\in\mathcal{N}_{\delta,r}} \theta_A = 1, \sum_{A\in\mathcal{N}_{\delta,r}} \theta_A T(A) = T(F) \Big\}. \tag{52}$$

Under the assumption that $W \in C^{1,\alpha}_{loc}(\mathbb{R}^{3\times 3};\mathbb{R})$ with $\alpha \in [0,1]$ [Bar04a] shows that there exists $r' < r$ such that the following estimates holds

$$|W^{pc}_{\delta,r}(F) - W^{pc}(F)| \leq c\delta^{1+\alpha}|W|_{C^{1,\alpha}_{loc}(B_{r'}(0))} \tag{53}$$

obtained by constructing a continuous piecewise multilinear approximation to W^{pc}. Furthermore, let $\lambda^F_{\delta,r} \in \mathbb{R}^{19}$ denote the Lagrangian multiplier associated with the constraints

$$\sum \theta_A A = F, \quad \sum \theta_A \mathrm{cof}A = \mathrm{cof}F, \text{ and } \sum \theta_A \det A = \det F. \tag{54}$$

If additionally $\alpha > 0$ and $W^{pc} \in C^{1,\alpha}_{loc}(\mathbb{R}^{3\times 3};\mathbb{R})$ then an approximation to $\sigma := DW^{pc}(F)$ is given by $\lambda^F_{\delta,r} \circ DT(F)$, where $DT(F)$ is the Gateaux derivative of T, and $\circ$ denotes the composition operator between $\lambda^F_{\delta,r} \in \mathcal{L}(\mathbb{R}^{19};\mathbb{R})$ and $DT \in \mathcal{L}(\mathbb{R}^9;\mathbb{R}^{19})$ (with $\mathcal{L}(\mathbb{R}^m;\mathbb{R}^n)$ space of linear operators of $\mathbb{R}^m$ into $\mathbb{R}^n$).

The solution of (52) involves a large number of unknowns equal to the cardinality of the discrete set $\mathcal{N}_{\delta,r}$. The combination of an active set strategy with local grid refinement and coarsening to avoid checking a Weierstrass-type maximum principle in all the nodes of $\mathcal{N}_{\delta,r}$ leads to a very efficient but still reliable algorithm that computes $W^{pc}_{\delta,r}(F)$ [Bar04a].

4.2 Numerical finite lamination

Approximations to the rank-one convex envelope W^{rc} can be realized by $R^{(k)}W$ by iterating the construction described in Section 3 and motivated by the condition (43). The algorithm proposed by [Dol99, Dol03], on the other hand, performs convexification along rank-one directions until the function is stable under this operation. A pseudo-algorithm for the approximation of W^{rc} would therefore have the following main ingredients:

Algorithm 4.1 (Numerical lamination)
(a) $k = 0$*;* $R^{(k)}W = W$*.*
(b) For certain F*, and for* $a, n \in \mathbb{R}^3$*,* $g(t) =$*convexify* $R^{(k)}W(F + ta \otimes n)$*.*
(c) $R^{(k+1)}W(F) = g(0)$ *and compare with* $R^{(k)}W(F)$ *to stop, otherwise set* $k = k + 1$ *and go to (b).*

Approximations are, therefore, introduced in step (a), by restricting the space $\mathbb{R}^{3\times 3}$ where to evaluate W, and in step (b) where only discrete set of rank-one directions will be considered.

With the notation of Section 4.1, introduce the discrete set of rank-one directions

$$\mathcal{R}^1_\delta = \{\delta R \in \mathbb{R}^{3\times 3} : R = a \otimes n, \text{ with } a, n \in \mathbb{Z}^3\},$$

and for $R \in \mathcal{R}^1_\delta$ the following set $\ell_{R,\delta} := \{\ell \in \mathbb{Z} : F + \ell\delta R \in \overline{\mathrm{co}\mathcal{N}_{\delta,r}}\}$. For assigned $R \in \mathcal{R}^1_\delta$, the elements of $\ell_{R,\delta}$ identify the intersection of the grid $\overline{\mathrm{co}\mathcal{N}_{\delta,r}}$ with the direction $F + tR$. In step (a) of the Algorithm 4.1, one set $R^{(0)}W = I_{\delta,r}W$ as nodal interpolation of W in $\mathrm{co}\mathcal{N}_{\delta,r}$ whereas at step (c) one solves the following optimization problem

$$R^{(k+1)}_{\delta,r}W(F) = \inf_{R\in\mathcal{R}^1_\delta} \inf_{\theta\in\mathbb{R}^{\#\ell_{R,\delta}}} \left\{ \sum_{\ell\in\ell_{R,\delta}} \theta_\ell R^{(k)}_{\delta,r}W(F+\delta\ell R) : \theta_\ell \geq 0, \sum_{\ell\in\ell_{R,\delta}} \theta_\ell = 1 \right\},$$

with $R^{(k)}_{\delta,r}W := \infty$ in $\mathbb{R}^{3\times 3}$ and nodal interpolation of $R^{(k)}_{\delta,r}W$ in $\overline{\mathrm{co}\mathcal{N}_{\delta,r}}$ at variance of the algorithm proposed in [Dol99].

Assuming $W \in C^{1,1}(\mathbb{R}^{3\times 3};\mathbb{R})$ and equal to W^{rc} in $\mathbb{R}^{3\times 3}\setminus B_r(0)$ with some r, bounds on a and b in the definition of $\mathcal{R}^1_\delta$, and that there exists a lamination level L such that $R^{(L)}_{\delta,r}W = W^{rc}$, [Bar04b] improves the estimate of [DW00]

$$\|R^{(k+1)}_{\delta,r}W - W^{rc}\|_{L^\infty(\mathrm{co}\mathcal{N}_{\delta,r};\mathbb{R})} \leq c\delta\,. \tag{55}$$

Even if one does not know L and r, $R^{(k+1)}_{\delta,r}W$ provides, however, an upper bound to W^{rc} for all $k \geq 0$, $r \geq \delta > 0$ and $F \in \mathrm{co}\mathcal{N}_{\delta,r}$.

5 Phase transitions and plasticity as vector nonconvex minimization problems

This section discusses the numerical analysis and approximation of relaxed formulations for two types of nonconvex vector stored energy densities. In the first example the quasiconvex envelope is known whereas for the other one no analytical expression of any semiconvex envelope is available. In the latter case, therefore, we proceed to numerical relaxation by computing the polyconvex and lamination convex envelope.

5.1 Compatible phase transitions in elastic solids

We consider a solid with two phases, whose energy density takes the form

$$W(F) = \min\{W_1(F), W_2(F)\}. \tag{56}$$

In a geometrically linear context, the energy of each phase is

$$W_j = \frac{1}{2}\,\mathbb{C}(F - F_j)\colon (F - F_j)\,, \tag{57}$$

where $\mathbb{C}$ is the linear elasticity tensor, the symbol : the inner product in $\mathbb{R}^{n\times n}$, $n = 2, 3$, and F_j the stress-free configuration of phase j.

Since W is not rank-one convex, thus neither quasiconvex, the functional E in (28) is not sequentially weakly lower semicontinuous. Assuming that the two wells F_1 and F_2 are rank-one connected, then there exists an affine function that equals W at the two wells and is elsewhere a strict lower bound of W and, therefore, there is no attainment of minimizer.

The quasiconvex envelope of W is given by [Koh91]

$$W^{qc} = \begin{cases} W_2(F) & \text{if } W_2(F) + \gamma \le W_1(F), \\ \dfrac{1}{2}(W_1(F) + W_2(F)) & \\ \quad -\dfrac{1}{4\gamma}(W_2(F) - W_1(F))^2 - \dfrac{\gamma}{4} & \text{if } |W_2(F) - W_1(F)| \le \gamma, \\ W_1(F) & \text{if } W_1(F) + \gamma \le W_2(F), \end{cases} \tag{58}$$

with $\gamma = 1/2\langle F_2 - F_1, \mathbb{C}(F_2 - F_1)\rangle$ for rank-one connected wells. In this case, W^{qc} belongs to $C^1(\mathbb{R}^{n\times n}; \mathbb{R})$ and is convex. Further, from a result of [CP00], one can show that the following conditions hold true for W^{qc} and are, in fact, equivalent [HL93, CHO06]

$$|DW^{qc}(E) - DW^{qc}(F)| \le L|E - F|\,, \tag{59}$$

$$\frac{1}{L}|DW^{qc}(E) - DW^{qc}(F)|^2 \le (DW^{qc}(E) - DW^{qc}(F))\colon (E - F)\,, \tag{60}$$

$$\frac{1}{2L}|DW^{qc}(E) - DW^{qc}(F)|^2 \le W^{qc}(E) - W^{qc}(F) - DW^{qc}(F)\colon (E - F)\,, \tag{61}$$

for any $E, F \in \mathbb{R}^{n\times n}$. Given the functional

$$\mathcal{H}(u) := \int_\Omega W^{qc}(\varepsilon(u))\,dx + \int_\Omega f u\,dx + \|u\|^2_{L^2(\Omega;\mathbb{R}^n)} \tag{62}$$

with $\varepsilon(u) = \operatorname{sym} Du$, using (59)–(61), and the following condition

$$W^{qc}(E) - W^{qc}(F) - DW^{qc}(F) : (E-F) \le (DW^{qc}(F) - DW^{qc}(E)) : (F-E) \tag{63}$$

that holds for any $E, F \in \mathbb{R}^{n\times n}$ for the convexity of W^{qc}, [CHO06] prove the convergence of (14) for the minimization of (62) over $\mathcal{A} := u_D + W^{1,2}_0(\Omega;\mathbb{R}^n)$ and the preasymptotic convergence rate of the energy. More precisely, let $\delta_h := \mathcal{H}(u_h) - \mathcal{H}(u)$, with u and u_h minimizers of $\mathcal{H}$ over $\mathcal{A}$ and $\mathcal{A}_h$, respectively. Then, there holds

$$\delta_\ell + \|\sigma - \sigma_\ell\|^2_{L^2(\Omega;\mathbb{R}^{n\times n})} + \|u - u_\ell\|^2_{L^2(\Omega;\mathbb{R}^n)} \le C\big((\delta_\ell - \delta_{\ell+1})^{1/2} + \operatorname{osc}_\ell\big) \tag{64}$$

with $\sigma := DW^{qc}(\varepsilon(u))$, $C > 0$ depending on the mesh regularity and material parameters, and osc_ℓ a node-patchwise definition of the data oscillations. The observation that $(\mathcal{H}_\ell)$ is a Cauchy sequence yields, finally, that

$$\sigma_h \to \sigma \text{ in } L^2(\Omega;\mathbb{R}^{n\times n}), \quad \text{and} \quad u_h \to u \text{ in } L^2(\Omega;\mathbb{R}^n), \tag{65}$$

provided that one controls also the data oscillations.

5.2 Single-slip elastoplasticity

We consider here a simplified model for plastic deformation in ductile single crystals. We focus on two spatial dimensions, and on the case that only a single slip system is active, which is described by an orthonormal pair of vectors s and n, with $s \in \mathbb{S}^1$ (where $\mathbb{S}^1 = \{x \in \mathbb{R}^2 : |x| = 1\}$) the slip direction on the slip plane and $n \in \mathbb{S}^1$ the normal to the slip plane. In a geometrically nonlinear context, we assume the multiplicative decomposition of the deformation gradient $F = F_e F_p$ with $F_p = I + \gamma s \otimes n$, where $\gamma \in \mathbb{R}$ is referred to as plastic slip. Hardening is included through a single internal variable $p \in \mathbb{R}$. Within the framework of rate-independent processes [Mie02, Mie02a, Mie05], we consider monotonic loading, or equivalently the first time step in a time-discrete scheme, and, set equal to zero the initial values of the internal variables (γ, p). Minimizing out locally the internal variables leads to a variational formulation analogous to (1), which can again be analysed using the discussed methods of the calculus of variations. The analogy with the study of martensitic microstructures via continuum models based on nonlinear elasticity, and the study via a variational problem expressed only in terms of the deformation gradient $F = D\phi$, was advanced for the first time in [OR99].

The constitutive behaviour of the single crystal can be described in terms of two potentials: the free energy density $W(F_e, p)$ and the dissipation potential

$J(\gamma, p)$. The free energy density is sum of an elastic and a plastic contribution as follows

$$W(F_e, p) = W_e(F_e) + W_p(p)\,, \tag{66}$$

with

$$W_e(F_e) = U(F_e) + \frac{\mu}{2}(|F_e|^2 - 2)\,, \quad W_p(p) = \frac{h}{2}p^2\,, \tag{67}$$

and $U(F_e)$ a polyconvex function defining a Neo-Hookian material, such as

$$U(F_e) = \begin{cases} \dfrac{\kappa}{4}((\det F_e)^2 - 1) - \dfrac{\kappa + 2\mu}{2}\log(\det F_e) & \text{if } \det F_e > 0 \\ +\infty & \text{else,} \end{cases} \tag{68}$$

with μ, κ material constants and h the hardening moduli. The dissipation potential $J(\gamma, p)$ is

$$J(\gamma, p) = \begin{cases} \tau_{cr}|\gamma| & \text{if } |\gamma| + p \leq 0 \\ \infty & \text{else}\,, \end{cases} \tag{69}$$

with τ_{cr} the critical shear stress. This is the same model considered in [CHM02, BCHH04, MLG04].

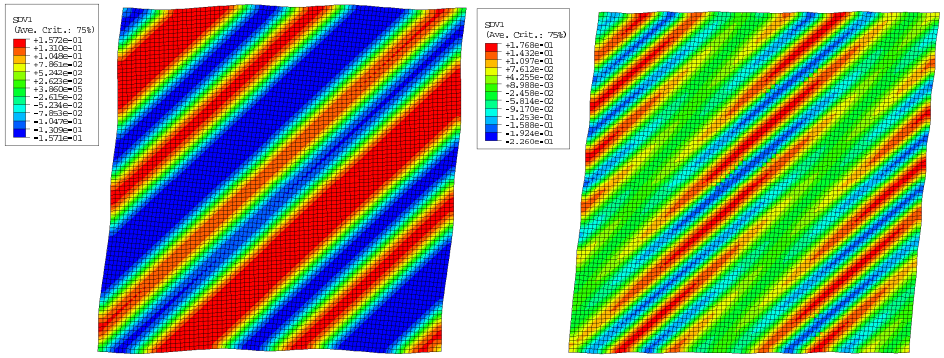
For this particular example, by minimizing with respect to the internal variables (γ, p), we obtain a closed form of the condensed energy $W_{\text{cond}}(F)$ as

$$W_{\text{cond}}(F) = U(F) + \frac{\mu}{2}(|F|^2 - 2) - \frac{1}{2}\frac{(max(0, \mu|Cs \cdot n| - \tau_{cr}))^2}{\mu Cs \cdot s + h}\,, \tag{70}$$

with $C = F^T F$. The energy density (70) is not rank-one convex and, hence, not quasiconvex. As a result, one may expect non attainment of minimizers for the corresponding functional, and developments of oscillations in the gradients of low-energy deformations. For the case under consideration, the occurrence of such microstructures can be shown by a direct finite element simulation using representative volume elements under periodic boundary conditions, cf. [HH02]. Figure 4 shows two typical results of these simulations: Oscillations in the plastic slip field γ, forming first and second order laminates. These oscillations are highly mesh-dependent with the number of oscillations growing towards infinity when the mesh becomes finer and finer.

The macroscopic material behaviour can be, however, understood by minimizing out locally the possible microstructures and defining the quasiconvex envelope of W_{cond}. Unfortunately, a closed form for condensed energies of the kind of W_{cond} is known only in few simplified cases [Con03, CT05, CO05]. We therefore resort to an approximation to the rank-one convex envelope $W^{rc}_{\text{cond}}(F)$ (Sect. 4) based on laminates.

Let $a, b \in \mathbb{S}^1$ with $a = (\cos\alpha, \sin\alpha)$ and $b = (\cos\beta, \sin\beta)$, then all the rank one matrices can be expressed in $\mathbb{R}^{2\times 2}$ as $\rho a \otimes b$ for α, β, $\rho \in \mathbb{R}$. Considering first order laminates, the average energy is given by



(a) (b)

Fig. 4. Single-slip plasticity (a) First order laminates and (b) Second order laminates as from (37) and (41) respectively, assuming periodic boundary conditions.

$$\begin{aligned} E^{lc(1)}(F;\alpha,\beta,\lambda,\rho) = \lambda W_{\mathrm{cond}}(F+(1-\lambda)\rho a\otimes b) \\ +(1-\lambda)W_{\mathrm{cond}}(F-\lambda\rho a\otimes b) \end{aligned} \tag{71}$$

with the microscopic energy $W_{\mathrm{cond}}(F)$ defined in (70). Let $q=(\alpha,\beta,\lambda,\rho)$ and introduce the feasible set

$$\Sigma = \{q\in\mathbb{R}^4 :\ \alpha,\beta,\rho\in\mathbb{R},\quad \lambda\in[0,1]\}\,,$$

the first order laminate envelope is obtained by solving the following global optimization problem

$$R^{(1)}W_{\mathrm{cond}}(F) = \min_{q\in\Sigma} E^{lc(1)}(F;q)\,, \tag{72}$$

under the constraints

$$\det(F+(1-\lambda)\rho a\otimes b)>0\,,\quad \det(F-\lambda\rho a\otimes b)>0\,. \tag{73}$$

Following the definitions in (40) corresponding minimization problems can be set up for higher order laminates. The growing number of optimization variables, however, strongly limits a practical application. Already for low order laminates the numerical search for the minimizer of (72) turns out to be difficult, because the objective function may present an exponential number of nearby optimal local minima [Car01].

Within the techniques of global optimization for the solution of (72), probabilistic global search procedures are the one commonly adopted. Applying a local search several times starting from randomly chosen sampling points leads, however, to an inefficient global search, because the same local minimum may be identified over and over. As an improvement, clustering methods attempt to avoid this inefficiency by carefully selecting points at which the local search is initiated.

Algorithm 5.1 (Clustering method)
Input F, initial population $q_i \in \Sigma$ of n starting points, tolerance ε.
(a) (Sampling and reduction): Sample the objective function $E^{lc(1)}$ at q_i and reduce population taking the m best points giving the least value.
(b) (Clustering): Identify clusters, such that the points inside a cluster are 'close' to each other, and the clusters are 'separated' from each other.
(c) (Center of attraction): Identify a center of attraction in each cluster.
(d) (Local search): Start a local search from the center of attraction and stop when a minimum is reached within the tolerance ε.
Output the value of $R^{(1)}W_{cond}(F)$.

The final local search step is done by using sequential quadratic programming methods with simple bounds [NW99]. Since in a finite element framework the above algorithm has to be performed at every material point (e.g. Gauss point), for real applications it is important to develop fast techniques for the numerical relaxation. In the literature the computational effort related to the global search is usually reduced by fixing some laminate related parameters on the basis of conjectures motivated by physical considerations [ORS00, AFO03, ML03, MLG04].

Mixed analytical-numerical relaxation

A different approach to the relaxation of W_{cond} over laminates has been pursued in [CCO06]. Rather than attacking the global minimization by a brute-force global optimization algorithm that is anyway computationally very expensive, [CCO06] exploit the structure of the problem both to achieve a fundamental understanding on the optimal microstructure and, in parallel, to design an efficient numerical relaxation scheme. Inspired by results based on the global optimization [BCHH04] and on analytical relaxation in the case of rigid elasticity and no self-hardening [CT05], we determine analytically a second order laminate which has 'good' energy and furnishes an upper bound to the relaxed energy.

We consider first an elastically rigid problem where the elastic part of the deformation is assumed to be a rotation, and only the contribution from the plastic free energy is considered, i.e., dissipation is neglected. The condensed energy for this case is then given by

$$W'(F) = \begin{cases} \frac{h}{2}\gamma^2 \text{ if } F = Q(I + \gamma s \otimes m) \quad Q \in SO(2)\,, \\ \infty \quad \text{else}\,, \end{cases} \tag{74}$$

with the quasiconvex envelope obtained as follows

Theorem 25 ([Con03, Con05]). *The quasiconvex, rank-one convex, and polyconvex envelope of $W'(F)$ are equal and given by*

$$W'_{qc}(F) = \begin{cases} \frac{h}{2}(|Fm|^2 - 1) \text{ if } \det F = 1 \text{ and } |Fs| \leq 1\,, \\ \infty \qquad\qquad \text{else}\,. \end{cases} \tag{75}$$

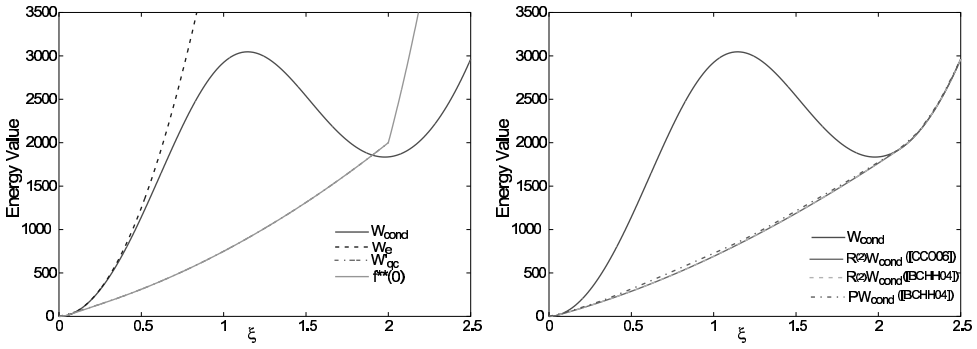


Fig. 5. (a) Bounds to the quasiconvex envelope of the condensed energy for zero dissipation; (b) Polyconvex and second-order laminate envelope for the condensed energy density in single-slip plasticity.

The optimal energy is given by a first-order laminate, which is supported on two matrices which have plastic deformation γ of the same magnitude and opposite sign.

We then construct a more refined model by assuming the microstructure to have the form of a laminate of second order, which is supported either on rigid-plastic deformations or on purely elastic ones. In this case, assuming volume-preserving deformations, the relaxation is reduced to a global minimization of a function of only one variable which defines the orientation of the laminate. Using this solution and the splitting of F_p from Theorem 25, we obtain an approximate second order laminate. The latter is then used as a starting point for the local minimization of the full energy density, including dissipation, and removing the kinematic constraint.

Figure 5(a) depicts the condensed energy W_{cond} (see eq. (70)) together with W_e (see eq (67)), W'_{qc} (see eq (75)) and the value of the energy over the approximate second order laminate (which we denote by $f^{**}(0)$) for the case of a pure shear strain $F = I + \xi r \otimes r^{\perp}$ with $r = (1, 0)$, $r^{\perp} = (0, 1)$ and for the material constants $\mu = 1.0 \cdot 10^4$MPa, $\kappa = 1.5 \cdot 10^4$ MPa, $h = 1.0 \cdot 10^3$ MPa and $\tau_{cr} = 10$ MPa.

Figure 5(b) shows a very good quantitative agreement for the values of the relaxed energy with those in [BCHH04] which had required a significantly higher numerical effort and compares approximations of the polyconvex hull $W^{pc}_{\delta,r}(F)$, realized with the procedure described in Section 4.1. A finer analysis at small deformations reveals however some differences, which will be discussed elsewhere [CCO06].

Figure 6 depicts finally the value of the volume fractions λ and λ_1 whereas $\lambda_0 = 1$. Initially, the material is in a homogeneous elastic state. Then an elastic state and a mixture of two opposite–slip plastic states appears. The volume fraction of the elastic phase starts at 100% and then decreases continuously

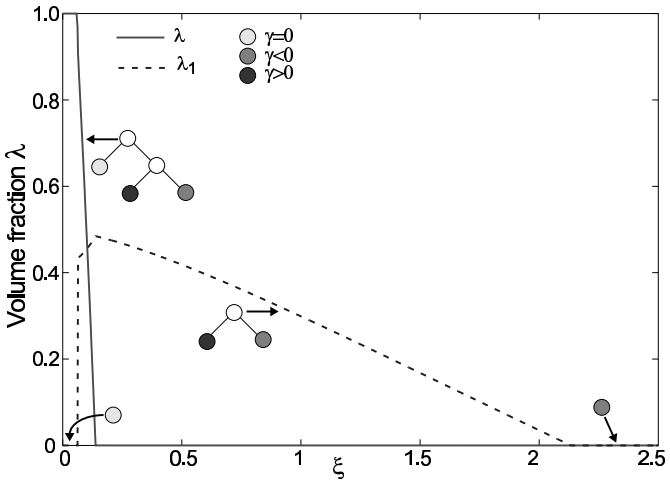


Fig. 6. Volume fractions λ and λ_1 for different values of ξ

until it vanishes at a shear $\xi = 0.13$. Both plastic phases then progress with slowly varying volume fractions until the homogeneous phase F is stable.

6 Conclusions

In this paper we have considered the numerical analysis of relaxed formulations for variational formulations lacking lower semicontinuity, and discussed algorithms for the approximation of the quasiconvex envelope of energy densities, in cases where it is not known in closed form. Relaxed solutions convey important information on the macroscopic behaviour of the microstructure, summarized by the relaxation theory. A resulting benefit is that the approximation of macroscopic quantities does not pose severe difficulties and classical algorithms for numerical optimization can be efficiently employed.

Acknowledgments

This work has been supported by the DFG Priority Program 1095 'Analysis, Modeling and Simulation of Multiscale Problems' under projects Ca 151/13 and Co 304/1.

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