NUMERICAL APPROACH TO DOUBLE WELL PROBLEMS

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IMA Preprint Series # 1485

June 1997

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Abstract. This paper deals with two-sided numerical energy estimates of a solution to two-dimensional double well problems. These estimates are obtained by computing the energy appropriate for the polyconvex envelope and an upper estimate of the energy appropriate for the rank-one convex envelope of the energy density. Examples of computed laminated microstructures are shown.

Key words. Calculus of variations, double well problem, microstructure, polyconvex envelope, rank-one convex envelope, Young measures.

AMS subject classifications. 49J35, 73C50

0. Introduction. In this paper we shall treat the following problem:

$$\inf \left\{ I(u) = \int_{\Omega} \Phi(x, u(x), \nabla u(x)) dx; u \in W^{1,p}(\Omega; \mathbb{R}^2), u = u_0 \text{ on } \Gamma \right\} \quad (1)$$

for $\Omega \subset \mathbb{R}^2$, a bounded Lipschitz domain, where $\Gamma \subset \partial\Omega$ is a measurable set with a positive Hausdorff measure, $\Phi : \Omega \times \mathbb{R}^2 \times \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$ is a continuous function such that $\Phi(x, u, \cdot) : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$ is non-quasiconvex, u_0 is a given function and $p > 2$. We also assume that I is coercive on $W^{1,p}(\Omega; \mathbb{R}^2)$, i.e., $\lim_{\|u\|_{W^{1,p}(\Omega; \mathbb{R}^2)} \rightarrow \infty} I(u) = +\infty$. We denote by $E \in \mathbb{R}^{2 \times 2}$ the identity matrix, and by a *rotation* we always mean an element belonging to the set of proper rotations $\text{SO}(2) = \{R \in \mathbb{R}^{2 \times 2}; \det R = 1, RR^T = R^T R = E\}$. We also suppose that

$$\mathcal{A}_{u_0} = \{u \in W^{1,p}(\Omega; \mathbb{R}^2); u = u_0 \text{ on } \Gamma\} \neq \emptyset.$$

If $\Phi(x, u, \cdot)$ is not quasiconvex, the functional I in (1) is not sequentially weakly lower semicontinuous and therefore the problem (1) generally does not have any solution in $\mathcal{A}_{u_0}$. By a solution of (1) we mean $\inf_{v \in \mathcal{A}_{u_0}} I(v)$ and this value will be addressed as $\inf(1)$. A similar notation is used in the sequel.

Let us recall that a function $\tilde{f} : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$ is *quasiconvex* if for any matrix $A \in \mathbb{R}^{2 \times 2}$ and for any smooth function $\varphi : \Omega \rightarrow \mathbb{R}^2$ compactly supported on Ω it holds that

$$\int_{\Omega} \tilde{f}(A + \nabla \varphi(x)) dx \geq \tilde{f}(A) \text{meas}(\Omega).$$

On the other hand, we can introduced a so-called *relaxed* problem:

$$\min \left\{ I_Q(u) = \int_{\Omega} Q\Phi(x, u(x), \nabla u(x)) dx; u \in \mathcal{A}_{u_0} \right\}, \quad (2)$$

where $Q\Phi(x, u, \cdot)$ is the quasiconvex envelope of $\Phi(x, u, \cdot)$ defined by

$$Q\Phi(x, u, \cdot) = \sup \{ \tilde{f} \leq \Phi(x, u, \cdot); \tilde{f} \text{ quasiconvex} \}.$$

In this case, I_Q is sequentially weakly lower semicontinuous and the problem (2) has a solution, i.e., there is $u \in \mathcal{A}_{u_0}$ such that $I_Q(u) = \min_{v \in \mathcal{A}_{u_0}} I_Q(v) \equiv \min (2)$.

The importance of the relaxed problem follows from the relaxation theorem which is due to Dacorogna ([13, Sec.1]) and which says that:

- (i) $\inf (1) = \min (2)$ and
- (ii) if $u \in \mathcal{A}_{u_0}$ is a solution to (2) then there is a minimizing sequence $\{u_k\}_{k \in \mathbb{N}} \subset \mathcal{A}_{u_0}$ converging weakly to u in $W^{1,p}(\Omega; \mathbb{R}^2)$ and $\lim_{k \rightarrow \infty} I(u_k) = I_Q(u)$.

We are going to concentrate on problems of two-dimensional mathematical elasticity, where Φ can be written as

$$\Phi(x, u(x), \nabla u(x)) = W(\nabla u(x)) - f(x)u(x), \quad x \in \Omega,$$

where $u : \Omega \rightarrow \mathbb{R}^2$ is a deformation mapping, $W : \{F \in \mathbb{R}^{2 \times 2}; \det F > 0\} \rightarrow \mathbb{R}$ is a *stored energy density* that is supposed to be nonnegative and $f \equiv (f_1, f_2) : \Omega \rightarrow \mathbb{R}^2$ is a density of outer body forces. We suppose that W satisfies the *frame-indifference principle* (see e.g. [5, ch. 4] and [23])

$$W(F) = W(RF)$$

for any deformation tensor $F \in \mathbb{R}^{2 \times 2}$, $\det F > 0$ and for any arbitrary rotation matrix $R \in \text{SO}(2)$. A value of $I(u)$ physically means the energy of the body with deformation u . Note that the right Cauchy–Green stress tensor $C = F^T F$ is invariant with respect to a rotation of F .

Moreover, we suppose that W has the so-called *double well* structure, or in other words, that (1) is the double well problem. It means that W attains its minimum precisely in two equilibrium states represented by deformation tensors F_1 and F_2 such that $F_2 \neq RF_1$, for any rotation $R \in \text{SO}(2)$. The wells are formed by the orbits $\{RF_i; R \in \text{SO}(2)\}$, $i = 1, 2$. Of course, due to the frame indifference principle W attains its minimum not only on F_1 and F_2 but on the whole orbits. The wells are *rank-one connected* if there exist two rotations $R_1, R_2 \in \text{SO}(2)$ such that $\text{rank}(R_1 F_1 - R_2 F_2) \leq 1$.

This double well (generally multiple well) structure of W typically appears in modeling of martensitic crystals; cf. e.g. [2, 3, 23]. These crystals exist in two phases; in a high-temperature phase called *austenitic* and in a low-temperature phase called *martensitic*. The austenitic phase has only one variant but the martensitic phase appears in several variants. A spatial alternation of these variants forms a microstructure. The number of variants is equal to the number of wells in the structure of W , i.e., we suppose two variants. A material microstructure plays an important role in the development of new technologies, e.g., shape-memory alloys. Hence, the numerical modeling of a microstructure and a relaxation is needed because W is not quasiconvex.

Early computations dealing with microstructures for a rotationally invariant stored energy density appeared in [8]. A numerical analysis of a microstructure was first treated in [10, 11]; cf. also [6, 7, 16, 20, 21, 23, 27]. A numerical analysis of the double well problem studied in this paper has been given in [22].

Quasiconvexity as a non-local property is generally very difficult to be verified except in some special situations. It follows that we almost never can find an analytical expression of the quasiconvex envelope of a particular function. For this reason, it is useful to define

weaker and stronger kinds of convexity than quasiconvexity, i.e., rank-one convexity and polyconvexity, respectively:

a function $\tilde{f} : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$ is

- (i) *polyconvex* if $\tilde{f}(A) = g(A, \det A)$ with $g : \mathbb{R}^5 \rightarrow \mathbb{R}$ convex and
- (ii) *rank-one convex* if

$$\tilde{f}(\lambda A + (1 - \lambda)B) \leq \lambda \tilde{f}(A) + (1 - \lambda) \tilde{f}(B) , \text{ whenever } \text{rank}(A - B) \leq 1 \text{ and } 0 \leq \lambda \leq 1 .$$

REMARK 1. Clearly, all these notions of convexity can be defined for functions $\tilde{f} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$; cf. [13].

In fact, it is still an open question whether or not rank-one convexity implies quasiconvexity for functions $\tilde{f} : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$. See e.g. [14] for some numerical experiments. There is only known the negative answer given by Šverák (cf. [33]) for functions $\tilde{f} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ for $n \geq 2$ and $m \geq 3$.

All of these notions of convexity are identical with usual convexity if $m = 1$ or $n = 1$.

We can also define the rank-one convex envelope $R\Phi$ and the polyconvex envelope $P\Phi$ of Φ . Let us recall that (see [13, Sec.1])

$$\begin{aligned} P\Phi(x, u, \cdot) &= \sup \{ \tilde{f} \leq \Phi(x, u, \cdot); \tilde{f} \text{ polyconvex} \} , \\ R\Phi(x, u, \cdot) &= \sup \{ \tilde{f} \leq \Phi(x, u, \cdot); \tilde{f} \text{ rank-one convex} \} , \end{aligned}$$

and that

$$P\Phi \leq Q\Phi \leq R\Phi \leq \Phi .$$

Using these envelopes, we can state the following problems:

$$\inf \left\{ I_R(u) = \int_{\Omega} R\Phi(x, u(x), \nabla u(x)) \, dx; \quad u \in \mathcal{A}_{u_0} \right\} \quad (3)$$

and

$$\min \left\{ I_P(u) = \int_{\Omega} P\Phi(x, u(x), \nabla u(x)) \, dx; \quad u \in \mathcal{A}_{u_0} \right\} . \quad (4)$$

It follows from Remark 1 that we do not know whether or not (3) has a solution in $\mathcal{A}_{u_0}$.

Alternatively, Dacorogna (cf. [13]) gave a more useful characterization of the polyconvex envelope. We adapt his assertion for $\tilde{f} : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$.

PROPOSITION 1. (see [13, sec. 5.1]) *Let $\tilde{f} : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$. Then for every $A \in \mathbb{R}^{2 \times 2}$,*

$$P\tilde{f}(A) = \inf \left\{ \sum_{i=1}^6 \lambda_i \tilde{f}(A_i); \sum_{i=1}^6 \lambda_i (A_i, \det A_i) = (A, \det A), \lambda_i \geq 0, \sum_{i=1}^6 \lambda_i = 1 \right\} .$$

The rank-one convex envelope is characterized by the following proposition.

PROPOSITION 2. (see [17, II], also [13, sec. 5.1]) *Let $\tilde{f} : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$ be bounded below. Then for every $A \in \mathbb{R}^{2 \times 2}$,*

$$R\tilde{f}(A) = \lim_{k \rightarrow \infty} R_k \tilde{f}(A) \quad (5)$$

where $R_1 \tilde{f} = \tilde{f}$ and

$$\begin{aligned} R_{k+1} \tilde{f}(A) = \inf \Big\{ & \lambda R_k \tilde{f}(A_0) + (1 - \lambda) R_k \tilde{f}(A_1); \ 0 \leq \lambda \leq 1, \\ & A = \lambda A_0 + (1 - \lambda) A_1, \ \text{rank}(A_1 - A_0) \leq 1 \Big\}, \ k \in \mathbb{N}. \end{aligned}$$

It is obvious that $\tilde{f} \geq R_k \tilde{f} \geq R_{k+1} \tilde{f} \geq \dots \geq R\tilde{f}$. Hence, utilizing this characterization of the rank-one convex envelope we can state for any $k \in \mathbb{N}$

$$\inf \left\{ I_k(u) = \int_{\Omega} R_k \Phi(x, u(x), \nabla u(x)) \, dx; \ u \in \mathcal{A}_{u_0} \right\}, \quad (6)$$

where $R_k \Phi$ is an approximation (given in Proposition 2) of the rank-one convex envelope of Φ with respect to the third variable. Due to the relaxation theorem $\inf (1) = \min (2) = \inf (6)$.

Our results below show examples of Φ where we are able to get solutions to (6) for some $k \in \mathbb{N}$ and solutions to (4) which are “near” to each other and due to the relation among the envelopes we get a good estimate of the solution to $\min (2)$. We compute an upper estimate of the rank-one convex envelope by using the representation given in Proposition 2 and the method given in [24] that is based on this representation. We use the method proposed in [29, 30] and based on Proposition 1 for the computation of the polyconvex envelope.

1. The computation of $\inf (6)$ and the solution to (6). We now describe the algorithm for the solution to (6), which gives an upper estimate of the rank-one convex envelope; cf. [17, 24]. The problem is stated as follows:

$$\text{minimize } \bar{I}_L(u, \tilde{\lambda}_1, \dots, \tilde{\lambda}_L, A_1, \dots, A_L) = \int_{\Omega} \sum_{l=1}^L \tilde{\lambda}_l(x) \Phi(x, u(x), A_l(x)) \, dx, \ u \in \mathcal{A}_{u_0} \quad (7a)$$

subject to

$$\nabla u(x) = \sum_{l=1}^L \tilde{\lambda}_l(x) A_l(x), \ L = 2^{k-1}, \ A_l \in L^p(\Omega; \mathbb{R}^{2 \times 2}), \quad (7b)$$

$$\sum_{l=1}^L \tilde{\lambda}_l(x) = 1, \ \tilde{\lambda}_l(x) \geq 0, \ \tilde{\lambda}_l \in L^\infty(\Omega; \langle 0, 1 \rangle), \quad (7c)$$

where (7b-c) holds for almost all $x \in \Omega$. Moreover, there are further restrictions on $(\tilde{\lambda}_l, A_l)$, $l = 1, \dots, L$ coming from Proposition 2. See also the so-called (H_L) condition in [13, Sec. 4.1].

To figure out these restrictions let us start with $L = 2$. Let us write for $L = 2$ a convex combination

$$\nabla u = \lambda A_0 + (1 - \lambda) A_1 .$$

According to Proposition 2 it is necessary that $\text{rank}(A_1 - A_0) \leq 1$ or, equivalently, $A_1 - A_0 = q \otimes r$, where $q, r : \Omega \rightarrow \mathbb{R}^2$ are such that $q \otimes r \in L^p(\Omega; \mathbb{R}^{2 \times 2})$, i.e., $A_0 = \nabla u - (1 - \lambda) q \otimes r$ and $A_1 = \nabla u + \lambda q \otimes r$. We recall that $(q \otimes r)_{ij} = q_i r_j$, $i, j = 1, 2$. Repeating this procedure we obtain the representation for an arbitrary L . For A_0, A_1 given as above, write convex combinations

$$A_0 = \lambda_0 A_{00} + (1 - \lambda_0) A_{01} , \quad A_1 = \lambda_1 A_{10} + (1 - \lambda_1) A_{11} ,$$

where $A_{01} - A_{00} = q_0 \otimes r_0$, and $A_{11} - A_{10} = q_1 \otimes r_1$ with $q_i, r_i : \Omega \rightarrow \mathbb{R}^2$, $q_i \otimes r_i \in L^p(\Omega; \mathbb{R}^{2 \times 2})$, $i = 0, 1$ arbitrary. This construction can be represented by a binary tree (see [24]). We use $L = 4$, i.e. $k = 3$ (keep in mind that $L = 2^{k-1}$) in our computations which enables us to write

$$\begin{aligned} R_3 \Phi(\cdot, \cdot, A) &= \inf \{ \lambda \lambda_0 \Phi(\cdot, \cdot, A_{00}) + \lambda(1 - \lambda_0) \Phi(\cdot, \cdot, A_{01}) \\ &\quad + (1 - \lambda) \lambda_1 \Phi(\cdot, \cdot, A_{10}) + (1 - \lambda)(1 - \lambda_1) \Phi(\cdot, \cdot, A_{11}) \} . \end{aligned}$$

Moreover,

$$\nabla u = \lambda \lambda_0 A_{00} + \lambda(1 - \lambda_0) A_{01} + (1 - \lambda) \lambda_1 A_{10} + (1 - \lambda)(1 - \lambda_1) A_{11} .$$

Thus, we put in the method (7)

$$\tilde{\lambda}_1 := \lambda \lambda_0 , \quad \tilde{\lambda}_2 := \lambda(1 - \lambda_0) , \quad \tilde{\lambda}_3 := (1 - \lambda) \lambda_1 , \quad \tilde{\lambda}_4 := (1 - \lambda)(1 - \lambda_1)$$

and

$$A_1 := A_{00} , \quad A_2 := A_{01} , \quad A_3 := A_{10} , \quad A_4 := A_{11} .$$

Eventually, we can express A_i , $i = 1, \dots, 4$ by means of $q, q_0, q_1, r, r_0, r_1, \lambda, \lambda_0, \lambda_1$ and ∇u

$$A_1 = \nabla u - (1 - \lambda) q \otimes r - (1 - \lambda_0) q_0 \otimes r_0 , \quad A_2 = \nabla u - (1 - \lambda) q \otimes r + \lambda_0 q_0 \otimes r_0$$

and

$$A_3 = \nabla u + \lambda q \otimes r - (1 - \lambda_1) q_1 \otimes r_1 , \quad A_4 = \nabla u + \lambda q \otimes r + \lambda_1 q_1 \otimes r_1 .$$

The spatial discretization of this approach was made in [24] using a continuous piecewise linear approximation of u and a piecewise constant approximation of A_l and $\tilde{\lambda}_l$, $1 \leq l \leq L$. This construction (for $L = 4$ it is known as a 2nd order lamination) is intimately related to a microstructure. This relation is outlined on Figure 1 and it can be found e.g. in [2]. An approximation of a laminated microstructure is analyzed also in [22]. Some relations between laminated microstructures and rank-one convex envelopes are treated in [25].

Figure 1: Relation between optimized parameters and a microstructure.

Proposition 2 shows that for $L \rightarrow \infty$ and a fixed mesh the discrete finite element (FE) solution of (7) converges to a discrete FE solution to (3), and therefore, unfortunately, this method does not approach for $L \rightarrow \infty$ the FE solution of (2) in case that the rank-one convex and quasiconvex envelopes are different to each other.

However, it is shown in [23] that the finite element approximation of (7) for fixed L converges to the solution of (2) as the mesh size approaches zero.

2. The computation of min (4) and a solution to (4). This method is based on Proposition 1., cf. also [28]. We solve the problem:

$$\text{minimize } \bar{I}_L(u, \tilde{\lambda}_1, \dots, \tilde{\lambda}_L, A_1, \dots, A_L) = \int_{\Omega} \sum_{l=1}^L \tilde{\lambda}_l(x) \Phi(x, u(x), A_l(x)) dx, \quad u \in \mathcal{A}_{u_0} \quad (8a)$$

subject to

$$\nabla u(x) = \sum_{l=1}^L \tilde{\lambda}_l(x) A_l(x), \quad A_l \in L^p(\Omega; \mathbb{R}^{2 \times 2}), \quad (8b)$$

$$\det \sum_{l=1}^L \tilde{\lambda}_l(x) A_l(x) = \sum_{l=1}^L \tilde{\lambda}_l(x) \det A_l(x), \quad (8c)$$

$$\sum_{l=1}^L \tilde{\lambda}_l(x) = 1, \quad \tilde{\lambda}_l(x) \geq 0, \quad \tilde{\lambda}_l \in L^\infty(\Omega; \langle 0, 1 \rangle). \quad (8d)$$

Again we suppose that (8b-d) is fulfilled for almost all $x \in \Omega$ and we use the continuous piecewise linear approximation of u and the piecewise constant approximation of A_l and $\tilde{\lambda}_l$. It follows from Proposition 1 (cf. also [30, Proposition 4.3.9]) that it is enough to take $L = 6$ to obtain the minimum of the polyconvex envelope. Therefore, we suppose $L = 6$ in our examples.

The next proposition shows that for $L = 2$ both of the methods (7) and (8) give the same results.

PROPOSITION 3. *Let $A, B \in \mathbb{R}^{2 \times 2}$ and let $0 < \lambda < 1$. Then the following equivalence holds*

$$\det(\lambda A + (1 - \lambda)B) = \lambda \det A + (1 - \lambda) \det B \iff \text{rank}(A - B) \leq 1 .$$

Proof. As the function $A \mapsto \det A$ is polyaffine, it is rank-one affine and therefore the implication “ $\Leftarrow$ ” is obvious even independently of the dimension. (We recall that a function $\tilde{f}$ is polyaffine if $\tilde{f}$ and $-\tilde{f}$ are polyconvex and similarly for rank-one affinity.) We need only to prove the implication “ $\Rightarrow$ ”.

Let us denote by ε the two-dimensional Levi-Civita skew symbol defined by

$$\varepsilon_{ij} = \begin{cases} 1 & \text{if } i < j \\ 0 & \text{if } i = j \\ -1 & \text{if } i > j . \end{cases}$$

Besides, we write $A = \{a_{ij}\}_{i,j=1}^2$ and $B = \{b_{ij}\}_{i,j=1}^2$. One can easily see that e.g. $\det A = \sum_{i,j=1}^2 \varepsilon_{ij} a_{1i} a_{2j}$. We can write

$$\begin{aligned} \det(\lambda A + (1 - \lambda)B) &= \sum_{i,j=1}^2 \varepsilon_{ij} (\lambda a_{1i} + (1 - \lambda)b_{1i})(\lambda a_{2j} + (1 - \lambda)b_{2j}) \\ &= \sum_{i,j=1}^2 \varepsilon_{ij} (\lambda^2 a_{1i} a_{2j} + (1 - \lambda)^2 b_{1i} b_{2j} \\ &\quad + \lambda(1 - \lambda)(a_{1i} b_{2j} + a_{2j} b_{1i})) \\ &= \lambda^2 \det A + (1 - \lambda)^2 \det B + \lambda(1 - \lambda) \sum_{i,j=1}^2 \varepsilon_{ij} (a_{1i} b_{2j} + a_{2j} b_{1i}) . \end{aligned} \tag{9}$$

On the other hand we have

$$\begin{aligned} \det(A - B) &= \sum_{i,j=1}^2 \varepsilon_{ij} (a_{1i} - b_{1i})(a_{2j} - b_{2j}) \\ &= \sum_{i,j=1}^2 \varepsilon_{ij} (a_{1i} a_{2j} + b_{1i} b_{2j} - a_{1i} b_{2j} - a_{2j} b_{1i}) \\ &= \det A + \det B - \sum_{i,j=1}^2 \varepsilon_{ij} (a_{1i} b_{2j} + a_{2j} b_{1i}) . \end{aligned} \tag{10}$$

Expressing $\sum_{i,j=1}^2 \varepsilon_{ij} (a_{1i} b_{2j} + a_{2j} b_{1i})$ from (10) and putting it in (9) we obtain

$$\begin{aligned} \det(\lambda A + (1 - \lambda)B) &= \lambda^2 \det A + (1 - \lambda)^2 \det B \\ &\quad + \lambda(1 - \lambda)(\det A + \det B - \det(A - B)) \\ &= \lambda \det A + (1 - \lambda) \det B - \lambda(1 - \lambda) \det(A - B) . \end{aligned}$$

As $A, B \in \mathbb{R}^{2 \times 2}$ we obtain $\det(A - B) = 0 \iff \text{rank}(A - B) \leq 1$ and the proposition is proved. $\square$

The reader is invited to verify by means of Proposition 3 that a solution obtained by (7) fulfills constraints involved by (8).

3. Remarks on the Young measure representation. Both of the methods (7) and (8) can be equivalently expressed via the Young measure representation. See [18, 24, 29, 30] for the method (7) and [18, 30] for method (8).

There is a general result (see [1, 19, 30, 32, 34]) that for an open bounded set $\tilde{\Omega} \subset \mathbb{R}^n$ and from any bounded sequence $\{w_k\}_{k \in \mathbb{N}} \subset L^p(\tilde{\Omega}; \mathbb{R}^{m \times n})$, $1 \leq p \leq +\infty$ we can extract a subsequence (denoted by the same indices) such that there exists a family of probability measures $\nu = \{\nu_x\}_{x \in \tilde{\Omega}}$ and

$$\lim_{k \rightarrow \infty} v \circ w_k = v_\nu \text{ weakly in } L^1(\tilde{\Omega}) ,$$

for any continuous function $v : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ with the growth lesser than p at infinity, and where $v_\nu(x) = \int_{\mathbb{R}^{m \times n}} v(A) \nu_x(dA)$ for almost all $x \in \Omega$. A family of parameterized probability measures obtained by this way is called a Young measure. In case that $w_k = \nabla \tilde{w}_k$ for all $k \in \mathbb{N}$ and $\{\tilde{w}_k\}_{k \in \mathbb{N}} \subset W^{1,p}(\tilde{\Omega}; \mathbb{R}^m)$ we speak about a *gradient Young measure*; cf. e.g. [4, 15, 29].

Supposing now that $\nu_x = \sum_{l=1}^L \lambda_l(x) \delta_{A_l(x)}$ for almost all $x \in \Omega$ with $\lambda_l \in L^\infty(\Omega; \langle 0, 1 \rangle)$, $\sum_{l=1}^L \lambda_l = 1$, $A_l \in L^p(\Omega; \mathbb{R}^{2 \times 2})$ for $l = 1, \dots, L$ with $\delta_{A_l(x)}$ being a Dirac measure supported at $A_l(x)$ we can reformulate (7a) and (8a) as

$$\text{minimize } I_Y(u, \nu) = \int_{\Omega} \int_{\mathbb{R}^{2 \times 2}} \Phi(x, u(x), A) \nu_x(dA) dx , \quad u \in \mathcal{A}_{u_0} .$$

Note that for (7a) and $L = 4$ the appropriate atomic gradient Young measure is given by

$$\begin{aligned} \nu_x &= \lambda(x) \lambda_0(x) \delta_{A_{00}(x)} + \lambda(x) (1 - \lambda_0(x)) \delta_{A_{01}(x)} \\ &+ (1 - \lambda(x)) \lambda_1(x) \delta_{A_{10}(x)} + (1 - \lambda(x)) (1 - \lambda_1(x)) \delta_{A_{11}(x)} , \quad x \in \Omega . \end{aligned}$$

4. Finite element approximation and remarks on computations. All of the computations were made on an HP 9000 700/RX for the rectangle $\Omega_0 = (0, 6) \times (0, 1)$, $\Gamma_1 = \{0\} \times (0, 1)$ and $\Gamma_2 = \{6\} \times (0, 1)$. Due to the symmetry of problems solved below, we computed in fact only on $\Omega = (0, 3) \times (0, 1)$, and then we verified the results on the whole mesh. Besides we always stated Dirichlet's boundary conditions $u(x) = x$ for $x \in \Gamma_1 \cup \Gamma_2$. The computations of tasks outlined on Figures 3, 5, 7 usually took no more than 20 min. for (7) and 45 min. for (8). Computations related to Figures 4, 6, 8 lasted approximatively 100 min. for (7) and 240 min. for (8). The triangulation $\{\tau_h\}_{h>0}$ of $\tilde{\Omega}$ with the discretization parameter $h > 0$ consists of elements (= triangles) denoted by K and it is outlined on Figure 2.

The element-wise linear approximation of u , u_h , is such that $u_h \in V_h = \{v \in C(\bar{\Omega}; \mathbb{R}^2); v \text{ is linear on each } K \in \tau_h, v(x) = x \text{ for } x \in \Gamma_1 \cup \Gamma_2\}$ and it is known that $\forall u \in W^{1,p}(\Omega)$, $u(x) = x$ for $x \in \Gamma_1 \cup \Gamma_2$ there is $\{u_h\}_{h>0}$ such that $\lim_{h \rightarrow 0} \|u - u_h\|_{W^{1,p}(\Omega)} = 0$. Similarly, $A_l^h \in \{A : \Omega \rightarrow \mathbb{R}^{2 \times 2}; A \text{ is constant on each } K \in \tau_h\}$ and $\lambda_l^h, \tilde{\lambda}_l^h \in \{\lambda : \Omega \rightarrow \langle 0, 1 \rangle; \lambda \text{ is constant on each } K \in \tau_h\}$ for $1 \leq l \leq L$. The discretization parameter h will be

Figure 2: Ω_0 and its triangulation.

omitted in the following part of this paper. Details about the convergence of both of the methods for $h \rightarrow 0_+$ can be found e.g. in [30].

4.1 Description of algorithms. We developed the following procedure for the decomposition of matrices which is needed in Section 1. For simplicity, we choose a fixed element $K \in \tau_h$. Taking $B \in \mathbb{R}^{2 \times 2}$, $0 \leq \gamma \leq 1$, $p_1, p_2 \in \mathbb{R}^2$ we can define

$$(B_1, B_2) = \text{DECOMP}(B, \gamma, p_1, p_2),$$

where $B_1, B_2 \in \mathbb{R}^{2 \times 2}$, and $B_1 = B + \gamma p_1 \otimes p_2$ and $B_2 = B - (1 - \gamma) p_1 \otimes p_2$. As the approximation of u is element-wise linear, i.e., $u(x) = \tilde{A}x + \tilde{B}$, $x \in K$, $\tilde{A} \in \mathbb{R}^{2 \times 2}$ and $\tilde{B} \in \mathbb{R}^2$, ∇u is element-wise constant and $\nabla u(x) = \tilde{A}$ for $x \in K$. To obtain a first lamination, i.e., $L = 2$ we have to evaluate $(A_0, A_1) = \text{DECOMP}(\tilde{A}, \lambda, q, r)$. In our case, for $L = 4$, we have to use DECOMP still twice. Put $(A_{00}, A_{01}) = \text{DECOMP}(A_0, \lambda_0, q_0, r_0)$ and $(A_{10}, A_{11}) = \text{DECOMP}(A_1, \lambda_1, q_1, r_1)$. We emphasize that $\lambda, \lambda_0, \lambda_1$ are arbitrary non-negative numbers not greater than one and $q, q_0, q_1, r, r_0, r_1 \in \mathbb{R}^2$ are arbitrary vectors. The objective function which is minimized and which arises from a discretization of the problem depends on:

- (i) values of a deformation mapping u at mesh nodes,
- (ii) values of a density of body forces f at mesh nodes and
- (iii) $\lambda|_K, \lambda_0|_K, \lambda_1|_K$ and $q|_K, q_0|_K, q_1|_K, r|_K, r_0|_K, r_1|_K$, $\forall K \in \tau_h$

where $\cdot|_K$ denotes a restriction of an appropriate variable on an element $K \in \tau_h$. Note that these restrictions are constant and arbitrary on each element.

The algorithm for the computation of the polyconvex envelope is easier. There is no decomposition similar to that described above. Therefore, the objective function depends directly on:

- (i) values of a deformation mapping u at mesh nodes,
- (ii) values of a density of body forces f at mesh nodes and
- (iii) $\tilde{\lambda}_l|_K, A_l|_K$, $l = 1, \dots, 6$ and $K \in \tau_h$,

where $\tilde{\lambda}_l|_K$ and $A_l|_K$ are restrictions of $\tilde{\lambda}_l$ and A_l on $K \in \tau_h$, respectively. Moreover, the following conditions must be fulfilled on any $K \in \tau_h$: $\tilde{\lambda}_l|_K \geq 0$, $\sum_{l=1}^6 \tilde{\lambda}_l|_K = 1$, $\nabla u|_K = \sum_{l=1}^6 \tilde{\lambda}_l|_K A_l|_K$ and $\det \nabla u|_K = \sum_{l=1}^6 \tilde{\lambda}_l|_K \det A_l|_K$. Also here we use the element-wise linear approximation of u , i.e., ∇u is element-wise constant. Obviously, $\nabla u|_K$ denotes a restriction of ∇u on $K \in \tau_h$.

The Fortran sequential quadratic programming routines NLPQL0 (see [31]) and E04UCF from the NAG-Library are used for minimization of appropriate functions given

by discretization of the problem. Both of the methods (7)-(8) were carried out by NLPQL0 and the method (8) still by E04UCF. Although these routines are universal for solving non-linear constrained problems for our type of problems it should be better to use some special software for sparse problems; cf. [27].

To outline the microstructure on any element, we always calculate the quantity

$$\frac{|A_l^T A_l - F_1^T F_1|}{|A_l^T A_l - F_1^T F_1| + |A_l^T A_l - F_2^T F_2|}, \quad l = 1, \dots, L, \quad (11)$$

which gives the ratio between Euclidean distances of $A_l^T A_l$ from $F_1^T F_1$ and from $F_2^T F_2$. The shade of the grey color is then proportional to a weighted average of these fractions with weights equaled to $\tilde{\lambda}_l$. Also the shades of the second order laminates on Figures 3, 5, 7 are proportional to the above fractions. The well defined by F_1 is colored white and the other well defined by F_2 , is colored black.

Now let us make several remarks on the computations.

4.2. Remarks on computations.

- The basic disadvantage of the method (7) is that we generally do not know the difference between our result and $\inf$ (4). On the other hand, it uses box constraints only.
- The method (8) requires nonlinear constraints but, at least theoretically, we can approach by means of it for $h \rightarrow 0_+$ the polyconvex envelope of $\Phi(x, u, \cdot)$ precisely, which gives the required solution whenever $Q\Phi(x, u, \cdot) = P\Phi(x, u, \cdot)$.
- As we deal with the elasticity problems we should verify that $\det \nabla u > 0$ and that $\det A_l > 0$ for $l = 1, \dots, L$ on any $K \in \tau_h$.
- The main problem is in fact a limitation on the number of variables of a function to be minimized by the optimization procedures. Let us denote this number by N_v , a number of mesh nodes by N_{nodes} and a number of mesh elements by N_e . We remark that the method (7) needs for some L (here L is supposed to be a power of 2)

$$N_v \sim 2N_{\text{nodes}} + 5(L - 1)N_e.$$

The second used the method (8) needs for $L = 6$

$$N_v \sim 2N_{\text{nodes}} + 30N_e$$

and moreover,

$$5N_e$$

of nonlinear constraints and N_e of linear constraints.

- We can use a similar binary (non-symmetric) tree which was used for (7) also for (8). This tree is constructed as it was explained in Section 1 but appropriate differences of matrices on the tree branches are general. This saves 5 variables, a linear constraint and 4 nonlinear constraints on each element in comparison with the direct application. On the other hand, remaining constraints have higher nonlinearities.

- Our experience shows that both mentioned optimization routines are able to work effectively only for $N_V < 400$ so that, we often had to fight with the downright shortage of the CPU memory. This prevented us to make a finer triangulation of Ω , to enlarge L , or to handle three-dimensional tasks.
- It is important to ensure that the constraints are fulfilled with enough precision. For this, we usually had to multiply the nonlinear constraints by some large scaling constant (typically 10^4).
- The important advantage of both of these methods in comparison with a direct application of a finite element method is that they give satisfactory results also for rather coarse grids. For instance, taking the energy density from Example 5.2 below, putting $f = 0$ and imposing boundary conditions $u(x) = x$, i.e., fixing the boundary, we get the zero energy solution independently of a mesh size. Moreover, the computational effort in (7) does not depend on the orientation of the grid with respect to laminates.
- The finite element approach ([23]) with element-wise linear continuous elements is covered by setting $A_l := \nabla u$, $l = 1, \dots, L$ in (7) and (8). In [23] it is shown that in this case the energy of the finite element solutions decreases at least as $\mathcal{O}(\sqrt{h})$, where h is a mesh size; cf. [22, 23] for details. On the other hand, this energy gives an upper bound for the solution obtained by means of (7) because we still have freedom in varying the A_l 's.

5. Sample types of the stored energy densities and the numerical results. In this section we introduce three types of stored energy densities and the numerical results. We recall that $C = F^T F$ and that $|\cdot|$ means the Euclidean norm on $\mathbb{R}^{2 \times 2}$.

5.1 Example: Ericksen-James' stored energy density. The first example is Ericksen-James' stored energy density (see [9])

$$\begin{aligned} W(F) &= a_1(C_{11} + C_{22} - 2)^2 + a_2 C_{12}^2 \\ &+ a_3 \left(\left(\frac{C_{11} - C_{22}}{2} \right)^2 - \epsilon^2 \right)^2, \end{aligned} \quad (12)$$

where a_1, a_2, a_3 are positive constants and $\epsilon \leq 1$. As in [9] we used $a_1 = 10, a_2 = 3, a_3 = 1, \epsilon = 0.1$. This function has been already used e.g. in [9]. Dirichlet's boundary conditions $u(x) = x$ are used on $\Gamma_1 \cup \Gamma_2$. The wells are defined by F_1, F_2 , where

$$F_1 = \begin{pmatrix} \sqrt{1-\epsilon} & 0 \\ 0 & \sqrt{1+\epsilon} \end{pmatrix}, \quad F_2 = \begin{pmatrix} \sqrt{1+\epsilon} & 0 \\ 0 & \sqrt{1-\epsilon} \end{pmatrix}$$

and they are rank-one connected, cf. [9]. The microstructure for one particular loading is shown on Figure 3. On Figure 4 we find the dependence of value of solution to (7) and (8) on the varying loading by body forces. The starting point for the method (7) was the solution for $\epsilon = 0$ and $f = 0$ ($u(x) = x, x \in \Omega$). As to Figure 4, it was obtained

by the successive increasing of the loading of the body and the solution for the previous loading was taken as the starting point for the next loading. In this case the value of ϵ was constantly $\epsilon = 0.1$. The starting points for (8) were the appropriate solutions to (7) and points close to these solutions in the sense of $|\cdot|$.

Figure 3: Loading by the body force $f = (0, 0.013)$. Ericksen-James' stored energy density (12).

Figure 4: Dependence of the solutions (7) and (8) on the body load for the stored energy density (12).

5.2 *Example.* The second stored energy density is the following

$$W(F) = \left| C - \begin{pmatrix} 1 & -\epsilon \\ -\epsilon & 1 + \epsilon^2 \end{pmatrix} \right|^2 \left| C - \begin{pmatrix} 1 & \epsilon \\ \epsilon & 1 + \epsilon^2 \end{pmatrix} \right|^2, \quad \epsilon > 0. \quad (13)$$

The wells are given by

$$F_1 = \begin{pmatrix} 1 & -\epsilon \\ 0 & 1 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 1 & \epsilon \\ 0 & 1 \end{pmatrix}.$$

We remark that a similar density is used in [7]. Note that $\text{rank}(F_1 - F_2) = 1$ for any $\epsilon > 0$ and therefore the wells are rank-one connected.

We suppose $\epsilon = 0.1$ and Dirichlet's boundary conditions $u(x) = x$ on $\Gamma_1 \cup \Gamma_2$. Let us remark that for $f = 0$ and for the above supposed boundary conditions there is the unique solution $u(x) = x$, $x \in \Omega$ and $\nabla u(x) = 0.5F_1 + 0.5F_2$, $x \in \Omega$. This precise solution for $f = 0$ was used as the starting point for (7). The starting points for the method (8) were chosen by the same way as in the previous example.

Note that the solution on Figure 5 creates only a simple laminate microstructure. It means that $\nabla u = A_0 = A_1$ on Figure 1. In other words, $q = 0$ and $\lambda = 0.5$. The computed microstructure is outlined on Figure 5.

On Figure 6 we find the dependence of the solution to (7) and (8) on the loads. This figure was obtained by the successive increasing of loads.

Notice that for $f = 0$ we have a stress-free configuration and that $P\Phi(\cdot, \cdot, E) \equiv Q\Phi(\cdot, \cdot, E) \equiv R\Phi(\cdot, \cdot, E)$, where $E \in \mathbb{R}^{2 \times 2}$ is the identity matrix.

Figure 5: Loading by the body force $f = (0, 0.08)$. Stored energy density (13).

Figure 6: Dependence of solutions obtained by (7) and (8) on the loading by the body force for (13).

5.3 *Example: non rank-one connected wells.* The third example is the stored energy density with wells which are not rank-one connected:

$$W(F) = \left| C - \begin{pmatrix} (1+\epsilon)^2 & 0 \\ 0 & (1+\epsilon)^2 \end{pmatrix} \right|^2 \left| C - \begin{pmatrix} \frac{1}{(1+\epsilon)^2} & 0 \\ 0 & \frac{1}{(1+\epsilon)^2} \end{pmatrix} \right|^2, \quad \epsilon > 0. \quad (14)$$

The wells are given by

$$F_1 = \begin{pmatrix} 1+\epsilon & 0 \\ 0 & 1+\epsilon \end{pmatrix}, \quad F_2 = \begin{pmatrix} \frac{1}{1+\epsilon} & 0 \\ 0 & \frac{1}{1+\epsilon} \end{pmatrix}.$$

To prove the non-rank-one connectivity of wells, note that it suffices to show that $\det(RF_1 - F_2) \neq 0$ for any rotation $R \in SO(2)$. Taking $R_\eta \in SO(2)$ as follows

$$R_\eta = \begin{pmatrix} \cos \eta & \sin \eta \\ -\sin \eta & \cos \eta \end{pmatrix}, \quad 0 \leq \eta < 2\pi$$

we obtain

$$\begin{aligned} \det(R_\eta F_1 - F_2) &= (1+\epsilon)^2 + (1+\epsilon)^{-2} - 2 \cos \eta \\ &\geq (1+\epsilon)^2 + (1+\epsilon)^{-2} - 2 > 0 \quad \text{for } \epsilon > 0. \end{aligned}$$

Again we used Dirichlet's boundary conditions $u(x) = x$ on $\Gamma_1 \cup \Gamma_2$. The microstructure is outlined on Figure 7 for one particular ϵ . Figure 8 shows the dependence of the solutions (7) and (8) on ϵ . Firstly, we took the known precise solution for $\epsilon = 0$, namely $u(x) = x$ for $x \in \Omega$ and then we gradually changed ϵ within $0 - 0.5$. The starting points for (8) were usually the solutions gained by (7) or near these solutions in the sense of the Euclidean norm. In this example, we put $f \equiv 0$.

The wells are not rank-one connected, F_1, F_2 are symmetric and positive-definite and therefore, it follows from [4, Th. 2.2] that if $\nabla u = \sum_{l=1}^L \tilde{\lambda}_l A_l$ in the method (7) and $A_l \in SO(2)F_1 \cup SO(2)F_2$ for $1 \leq l \leq L$ then all these matrices belong only to one orbit. However, due to the imposed boundary conditions it is energetically much more convenient that some of A_l 's do not belong to these orbits. Hence, there is at least one A_l that $A_l \notin SO(2)F_1 \cup SO(2)F_2$ and we obtain a mixture of both of the phases on particular elements. The outlined microstructure is given by a relation (11). As A_l 's are rather "far away" from the orbits in comparison with two previous examples the laminated microstructure is drawn gray.

Likewise in the previous case we have for $\epsilon = 0$ and $f = 0$ a stress-free state and, clearly, in this case $P\Phi(\cdot, \cdot, E) \equiv Q\Phi(\cdot, \cdot, E) \equiv R\Phi(\cdot, \cdot, E)$.

Figure 7: $\epsilon = 0.08$. Stored energy (14).

Figure 8: Dependence of the solutions (7) and (8) on ϵ for (14).

On the last figure we plot the distance of the matrices A_l , $l = 1, \dots, L$ from the wells against ϵ for (7) and (8). More precisely, for a given ϵ we evaluate

$$D = \sum_{K \in \tau_h} \sum_{l=1}^L \tilde{\lambda}_l |_K \min(|(A_l^T A_l)|_K - F_1^T F_1|, |(A_l^T A_l)|_K - F_2^T F_2|) ,$$

where “ $|_K$ ” denotes the restriction on an element $K \in \tau_h$. Note that $D = 0$ if and only if any matrix A_l on any element $K \in \tau_h$ belongs to one of the orbits.

Figure 9: Dependence of D on ϵ for (14).

Acknowledgment: I would like to thank Professor Tomáš Roubíček for many fruitful discussions, comments and for his constant encouragement. I am also indebted to Professor Mitchell Luskin whose remarks have contributed to a more readable form of the paper. The revised version of this paper has been prepared during my stay in the Institute for mathematics and its applications, University of Minnesota. This stay has been supported by the IMA and by the Fulbright commission grant No. 15964027.

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