Finite Element Computation of Macroscopic Quantities in Nonconvex Minimisation Problems and Applications in Materials Science

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Summary. Many physical processes can be modelled by minimising a given energy functional $E(u)$ amongst a class of admissable displacements. Convexity conditions guarantee sequential lower semicontinuity of E and then accumulation points of infimising seqences are minimisers, i.e., the minimum of E is attained. For some important problems involving phase transitions in nonlinear elasticity or ferromagnetic bodies, these convexity properties are not valid and so E is not sequential lower semicontinuous; in general the minimum is not attained. Typical features of infimising sequences include their weak accumulation points regarded as a macroscopic displacement of a (generalised) solution or their oscillations in terms of Young measures to describe the phases of the strains. Those macroscopic quantities can be described within relaxed formulations. This article focuses on the numerical treatment of relaxed problems where an analytic formula of the relaxed, (quasi-) convexified energy density is known.

1. Introduction

The minimisation of nonconvex functionals in applied physics leads to highly oscillating microstructures in the solution. Two examples will be adressed in this article: the scalar double-well problem and a problem from nonlinear elasticity.

Numerical schemes for these problems have to find a global minimiser (in a discrete subspace) amongst a huge number of local ones. Classical iteration methods fail to work properly here; a few thousand starting values are needed before a scheme finds a global minimiser. To avoid these severe difficulties and since one is mainly interested in the macroscopic quantities, we consider different forms of convexifications of the related functionals. This enables efficient implementation and a priori as well as a posteriori error estimates. In all the three examples the most important microscopic quantities can be recovered from the solution of the relaxed problem.

The generic example in microstructure is due to L.C. Young [18].

Problem (P_α). Minimise

$$E(u) := \int_0^1 (u'^2 - 1)^2 + \alpha u^2 \, dx$$

amongst the space $\mathcal{A}$ of all Lipschitz-continuous functions $u : (0,1) \to \mathbb{R}$ with $u(0) = u(1) = 0$.

For $\alpha = 0$, the infimum of E over $\mathcal{A}$ equals zero and there are infinitely many minimisers. Indeed, every Lipschitz-function with slopes ± 1 almost everywhere that satisfies the boundary conditions is a minimiser. For instance, $u(x) = \min\{x, 1-x\}$ is a solution and Fig. 1.1 shows other examples.

For $\alpha = 1$, the infimum of E over $\mathcal{A}$ is also zero since there exist functions with slope ± 1 almost everywhere and with arbitrary small amplitude. The infimum is not attained because there is no admissable function satisfying $u \equiv 0$ with slopes ± 1. Some functions u_j satisfying $E(u_j) = 4^{-(j+1)}/3$ are depicted in Fig. 1.1; note that they are also solutions for (P_0). The sequence

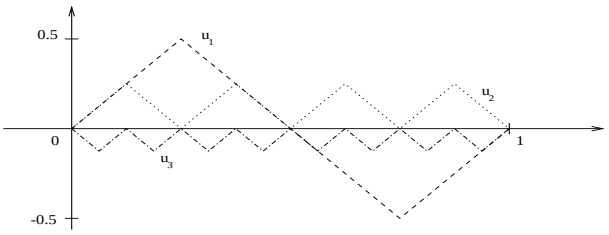

Fig. 1.1. First few members of a possible minimising sequence for (P_1)

(u_j) infimises E and converges strongly to zero in $L^\infty(0,1)$, but the sequence (u_j') only converges weakly to zero in $L^4(0,1)$. Obviously, $u \equiv 0$ is no minimiser but describes the macroscopic quantities of a (nonclassical) minimiser. The lacking strong convergence is caused by oscillations of (u_j') which can be described within a statistical notion by Young measures as follows: Let $\nu^j_{x,\delta}$ denote the probability distribution of $u_j'(y)$ where y is taken uniformly at random from the ball $B(x,\delta)$ of radius δ around x. Then, for a subsequence,

$$\nu_x := \lim_{\delta\to 0} \lim_{j\to\infty} \nu^j_{x,\delta} \quad \text{(weak* in measure)}$$

defines a probability measure, the related Young measure. It can be shown (cf. [14]) that for (P_1), any minimising sequence generates the Young measure

$$\nu_x = \tfrac{1}{2}\delta_{-1} + \tfrac{1}{2}\delta_1, \tag{1.1}$$

where $\delta_{\pm 1}$ denotes the Dirac measure with mass at $+1$ resp. -1. The representation (1.1) corresponds to the fact that we need half the slopes to be one and half of the slopes to be -1 to obtain a macroscopic slope zero. In this sense, (1.1) describes the microscopic mechanism, they do both lower the double-well energy $(u'^2-1)^2$ and have a macroscopic limit $u = 0$. The fact that $\nu_x \neq \delta_{u'(x)}$ causes microstructure and excludes strong convergence of infimising sequences.

A relaxation of (P_1) considers the functional E^{**} in which the nonconvex energy density $W(x) = (x^2-1)^2$ is replaced its convexification CW.

Problem (RP_1). Seek a minimiser $u \in \mathcal{A}$ of the functional

$$E^{**}(u) := \int_0^1 CW(u') + u^2\,dx.$$

One easily verifies that CW is given by $CW(x) = 0$ for $|x| \leq 1$ and $CW(x) = W(x)$ for $|x| > 1$. Obviously, $u \equiv 0$ is the unique solution for (RP_1).

The advantage in considering problem (RP_1) instead of (P_1) is that E^{**} is a convex functional so that any classical minimisation algorithm can be used to compute an approximation of a minimiser of E^{**}. This is not the case for E and one can show that classical algorithms fail to compute a minimiser of E in a finite-dimensional space.

The remaining part of this survey article treats more-dimensional and more applied examples and is organised as follows. Section 2 starts with a scalar model problem to illustrate the most important results from relaxation in modern theory of calculus of variations and gives an error analysis for the numerical solution. We consider a problem from nonlinear elasticity in Section 3.

2. Scalar double-well problem and its numerical solution

In a variational model for phase transitions in certain crystalline alloys, fine mixtures of phases are described by oscillating infimising sequences of the stored elastic energy [2, 3]. The variational framework is based on the minimisation of an energy functional with a non-convex energy density. In the double-well problem for two distinct given vectors $F_1, F_2 \in \mathbb{R}^d$ this energy density is defined by

$$W(F) := |F - F_1|^2 |F - F_2|^2, \tag{2.1}$$

for $F \in \mathbb{R}^d$. The variational problem (P) reads as follows.

Problem (P). Find a function $u \in \mathcal{A}$ that minimises the energy functional

$$E(u) := \int_\Omega \big(W(\nabla u) + |u - f|^2\big)\,dx \quad .$$

in a body Ω, a bounded Lipschitz-domain in $\mathbb{R}^d$ with boundary Γ. The non-physical term $|u-f|^2$ for a given function $f \in L^2(\Omega)$ serves as regularisation term. The set of admissible functions is $\mathcal{A} := u_D + W_0^{1,p}(\Omega)$ for given $u_D \in W^{1,p}(\Omega)$ and $W_0^{1,p}(\Omega) = \{v \in W^{1,p}(\Omega) : v|_\Gamma = 0\}$.

As shown in the introduction and depending on the given data, (P) may have infinitely many or no solutions at all. The direct method of the calculus of variations does not give the existence of solutions since due to the non-convex nature of W the functional E is not weakly lower semicontinuous. Nevertheless, one is interested in information on minimising sequences.

A finite element method replaces the space of admissible functions $\mathcal{A}$ by a discrete subspace $\mathcal{A}_h \subset \mathcal{A}$ and seeks a minimiser in $\mathcal{A}_h$ which exists since $\mathcal{A}_h$ is finite-dimensional and E satisfies certain growth conditions. For an

overview of approximation results in model examples we refer to [8, 9, 13]. Since local minimisers cluster around global ones, it requires a huge amount of computational work to minimise E directly over $\mathcal{A}_h$ (cf. [4]) and numerical solutions are strongly dependent on starting values.

Relaxation utilising Young measures. Minimising sequences (∇u_j) for (P) are typically weakly but *not* strongly convergent and their weak limits are in general not solutions of (P). The reason for this is their oscillatory nature. To describe this behaviour by a generalized limit, one is led to measure-valued strains: The bounded sequence (∇u_j) generates a family of probability measures $(\nu_x)_{x\in\Omega}$ on $\mathbb{R}^d$, the *gradient Young measure* $\nu \in YM(\Omega;\mathbb{R}^d)$, such that, for all $g \in C(\mathbb{R}^d)$ that vanish at infinity, there holds

$$(g(\nabla u_j)) \rightharpoonup^* \int_{\mathbb{R}^d} g(F)\, d\nu(F) \quad \text{in } L^\infty(\Omega). \tag{2.2}$$

We refer to [1, 14, 15, 16] for details.

The weak limit ∇u of a sequence of gradients (∇u_j) for a minimising sequence (u_j) for (P) is related to a Young measure by the identity

$$\nabla u(x) = \int_{\mathbb{R}^d} F\, d\nu_x(F) =: \langle \nu_x, id\rangle \quad \text{a.e. in } \Omega \tag{2.3}$$

which follows from (2.2) with $g = id$ in a neighbourhood of $\operatorname{supp}\nu$, and gives a connection between the macroscopic strain ∇u and the gradient Young measure ν. Since one is often interested only in the macroscopic quantities ∇u, $DW(\nabla u)$, and the generated Young measure, relation (2.3) motivates **Problem (GP).** Seek a minimiser of

$$GE(u,\nu) := \int_\Omega \langle \nu_x, W\rangle\, dx + \int_\Omega |u-f|^2\, dx \tag{2.4}$$

amongst all $(u,\nu) \in \mathcal{B} := \{(v,\mu) \in \mathcal{A} \times YM(\Omega;\mathbb{R}^d); \nabla v(x) =< \mu_x, id > \text{ for a.a. } x \in \Omega\}$.

Note that in contrast to (P), (GP) always has solutions and $\inf_{\mathcal{A}} E = \min_{\mathcal{B}} GE$ by construction of $\mathcal{B}$. Moreover, if (∇u_j) is a minimising sequence for (P) that generates the gradient Young measure ν and which converges weakly to ∇u, then (u,ν) is a minimiser for (GP) (cf. [15]). This situation is more involved in the vectorial case (cf. [14, 17]).

A numerical scheme for (GP) would replace the set $\mathcal{A}$ by a finite element space $\mathcal{A}_h$ and the space $YM(\Omega;\mathbb{R}^d)$ by elementwise convex-combinations of Dirac measures (cf. [7]). This approach results in a very high number of degrees of freedom.

Relaxation by convexification. Another relaxation of (P) can be obtained from (GP) by minimising the two contributions in (2.4) seperately. For fixed $F = \nabla u(x)$ one can find a probability measure ν_x such that ν_x minimises the expression $\langle \mu, W\rangle$ amongst all probability measures μ satisfying $\langle \mu, id\rangle = F$. Sometimes it is even possible to calculate an explict formula for a function QW that satisfies

$$QW(F) = \min_{\langle \mu, id\rangle = F} \langle \mu, W\rangle. \tag{2.5}$$

In the scalar case QW is given by the second Legendre transform W^{**} of W which equals the lower convex hull CW of W. Equations (2.5) and (2.4) motivate **Problem (*RP*).** Find a minimiser $u \in \mathcal{A}$ for the functional

$$E^{**}(u) = \int_\Omega W^{**}(\nabla u)\, dx + \int_\Omega |u - f|^2\, dx. \tag{2.6}$$

The map W^{**} is constructed in [5] and given by the formula

$$W^{**}(F) = \Big(\big(|F-B|^2 - |A|^2\big)_+ \Big)^2 + 4\Big(|A|^2 |F-B|^2 - \big(A^T \cdot (F-B)\big)^2 \Big),$$

where $A := (F_2 - F_1)/2 \neq 0$, $B := (F_1 + F_2)/2$, and $(\cdot)_+ := \max\{\cdot, 0\}$.

Note that (RP) always has a solution and that $\inf_{\mathcal{A}} E = \min_{\mathcal{A}} E^{**}$. Moreover, if (∇u_j) is a minimising sequence for (P) which converges weakly to ∇u, then u is a solution for (RP) (cf. [15]).

The convexified problem (RP) plays an important role in the scalar case since the most relevant information concerning (P) such as the Young measure and the macroscopic displacement and stress field can be recovered from a minimiser u of E^{**}. Since two different energy densities might have the same lower convex envelope, one loses information on the actual problem, in general. In the vectorial case one has to consider the quasiconvex hull of W which is harder to compute than and in general different from CW.

Numerical analysis of the convexified problem allowing microstructure. In this subsection we outline the numerical analysis of the relaxation (RP) of problem (P) and seek a minimiser for E^{**} in a discrete subspace $\mathcal{A}_h \subset \mathcal{A}$ based on a *regular triangulation* $\mathcal{T}$ of Ω into closed triangles and parallelograms in the sense of [10]. We allow energy densities more general than (2.1). As mentioned before, problems like (P) may have infinitely many or no solutions at all but there usually exists a Young measure solution ν from which one can calculate the macroscopic stress field

$$\sigma := \int_{\mathbb{R}^d} DW(A)\, d\nu(A) \stackrel{!}{=} DW^{**}(\nabla u) =: \sigma^{**} \tag{2.7}$$

where a solution u of the convexified problem (RP) defines σ^{**} which actually equals σ in (2.7) and is independent of the choice of the minimiser u. Similarly, a discretisation of (RP) gives a solution $u_h \in \mathcal{A}_h$ and again, the associated stress field σ_h is independent of the choice of the minimiser.

For W given in (2.1) the gradient Young measure ν can be calculated as soon as one knows a solution of (RP): Define $A_0 := A/|A|$ and let $P = 1 - A_0 \cdot A_0^T$ denote the orthogonal projection in $\mathbb{R}^d$ onto $\mathrm{span}\{A\}^\perp$. Let

$$\begin{aligned} \lambda(F) &:= \big(1 + A_0^T \cdot (F-B)\big(|A|^2 - |P\cdot(F-B)|^2\big)^{-1/2}\big)/2, \\ S_\pm(F) &:= B + P\cdot(F-B) \pm \big(|A|^2 - |P\cdot(F-B)|^2\big)^{1/2} A_0, \end{aligned}$$

and define the map $\tilde{\mu}$, that maps a vector $F \in \mathbb{R}^d$ to a probability measure $\tilde{\mu}(F)$, by

$$\tilde{\mu}(F) := \begin{cases} \delta_F & \text{if } |A| \leq |F-B|, \\ \lambda(F)\,\delta_{S_+(F)} + (1-\lambda(F))\,\delta_{S_-(F)} & \text{if } |F-B| < |A|. \end{cases}$$

Then, $\mu : u \mapsto \tilde{\mu}(\nabla u)$ defines a map $\mu : W^{1,p}(\Omega) \to YM(\Omega;\mathbb{R}^d)$ such that, if (∇u_j) is a minimising sequence for E in $\mathcal{A}$ which converges weakly to $u \in \mathcal{A}$ and which generates the Young measure ν, then $\nu_x = \mu(\nabla u(x))$ for a.a. $x \in \Omega$ (cf. [5]). The map also allows us to calculate discrete Young measures $\nu_x^h := \mu(\nabla u_h(x))$ for solutions u_h of (RP_h), thus recovering microscopic information from averaged quantities.

A priori error estimates. The following results hold for minimising problems related to more general energy densities than W from (2.1). We refer to [5] for a more general version of the subsequent theorem in which $\mathcal{A}_h \subset \mathcal{A}$ is a discrete subspace.

Theorem 2.1 ([5]). *There exist minimisers u and u_h of (2.6) in $\mathcal{A}$ resp. $\mathcal{A}_h$. The stress $\sigma := DW^{**}(\nabla u)$ and the discrete stress $\sigma_h := DW^{**}(\nabla u_h)$ are determined in a unique way. Furthermore, if $u, u_h \in W^{1,4}(\Omega)$*

$$\begin{aligned} \|\sigma - \sigma_h\|^2_{L^{4/3}(\Omega)} \quad &+ \quad \|u - u_h\|^2_{L^2(\Omega)} \\ &\leq \quad c_1 \inf_{v_h \in \mathcal{A}_h} \big(\|u - v_h\|^2_{L^2(\Omega)} + \|\nabla u - \nabla v_h\|^2_{L^4(\Omega)} \big). \end{aligned}$$

Since no higher regularity results are known for problems of the form (RP), the error estimate is of limited use for error control in practice. Therefore, a posteriori error estimates, which allow us to estimate the error in terms of the computed approximation, are of particular interest.

A posteriori error estimates. Given a regular triangulation $\mathcal{T}$ of Ω we can define the lowest order finite element space $\mathcal{S}^1(\mathcal{T})$ which consists of all continuous functions $v : \Omega \to \mathbb{R}$ such that $v|_T$ is affine for all $T \in \mathcal{T}$. For the numerical treatment of (RP) we set $\mathcal{S}^1_0(\mathcal{T}) := \mathcal{S}^1(\mathcal{T}) \cap W^{1,4}_0(\Omega)$ and define $\mathcal{A}_h := u_D + \mathcal{S}^1_0(\mathcal{T})$. Let $\mathcal{E}$ be the set of all edges appearing in $\mathcal{T}$ and note that $\cup\mathcal{E}$, the union of all edges, is the skeleton of edges in $\mathcal{T}$. We denote by $h_T := \operatorname{diam}(T)$, $T \in \mathcal{T}$, and $h_E = \operatorname{diam}(E)$, $E \in \mathcal{E}$, the diameters of elements and edges in $\mathcal{T}$.

Given a solution $u_h \in \mathcal{A}_h$ of (RP_h), let $\sigma_h := DW^{**}(\nabla u_h)$. For all $T \in \mathcal{T}$ the *error indicator* η_T^R is defined by

$$\eta_T^R := h_T^{4/3} \int_T |2(f - u_h) + \operatorname{div} \sigma_h|^{4/3} dx + \sum_{E \subseteq \partial T \setminus \Gamma} h_E \int_E |[\sigma_h \cdot n_E]|^{4/3} ds. \quad (2.8)$$

The integrand $[\sigma_h \cdot n_E]$ denotes the jump of the discrete stresses $\sigma_h \cdot n_E$ along a face E of two neighbouring elements, n_E is a unit normal vector of a fixed orientation along E, and the summation in (2.8) is over all such faces of T.

Theorem 2.2 ([5]). *There exists a constant $c_2 > 0$ which is independent of $h_{\mathcal{T}}$, such that*

$$\|\sigma - \sigma_h\|^2_{L^{4/3}(\Omega)} + \|u - u_h\|^2_{L^2(\Omega)} \leq c_2 \Big(\sum_{T \in \mathcal{T}} \eta_T^R \Big)^{3/8} =: c_2\, \eta_R.$$

The proof of the theorem requires the use of the rough estimate $\|u - v_h\|_{W^{1,4}(\Omega)} \leq c_3$ for an approximation $v_h \in \mathcal{A}_h$ of u, and so loses efficiency when keeping reliability.

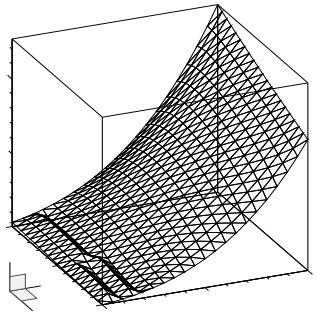

Fig. 2.1. Solution for the double-well problem. The figure shows a solution for the problem (P_h) on the unit square. Microstructure can be observed close to the left lower edge

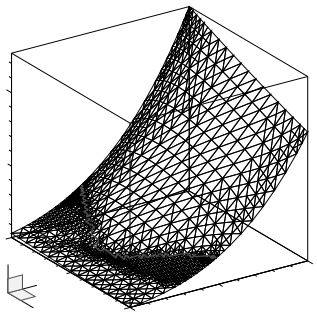

Fig. 2.2. Solution for the relaxed double-well problem using the adaptive Algorithm 1. Note that in contrast to the (discrete) solution for (P_h) no microstructure can be observed

The local error indicators η_T^R can be used in the following algorithm for adaptive mesh refinement.

Adaptive Algorithm (A). (a) Start with a coarse mesh $\mathcal{T}_0$, $k = 0$.
(b) Compute a minimiser $u_h \in \mathcal{A}_h$ of E^{**} with respect to the mesh $\mathcal{T}_k$.
(c) Compute η_T^R for each T in $\mathcal{T}$.
(d) Compute the error bound η_R and decide to terminate or to continue and then go to (e).
(e) Refine, i.e., halve the largest edge of, $T \in \mathcal{T}$ provided $\eta_T^R \geq \frac{1}{2} \max_{T' \in \mathcal{T}} \eta_{T'}^R$.

(f) Refine further elements to avoid hanging nodes and thereby define a new mesh $\mathcal{T}_{k+1}$, update k, and go to (a).

For a numerical example let $d = 2$, $\Omega = (0,1)^2$, $F_{1,2} := \mp(\cos\frac{\pi}{6}, \sin\frac{\pi}{6})$, and define $f(x,y) := f_0(x\cos\frac{\pi}{6} + y\sin\frac{\pi}{6})$ in Ω, $u_D(x,y) := f_1(x\cos\frac{\pi}{6} + y\sin\frac{\pi}{6})$ on $\partial\Omega$, for $f_0(s) := -\frac{3}{128}(s-0.5)^5 - \frac{1}{3}(s-0.5)^3$ and $f_1(s) := f_0(s)$ if $0 \le s \le 0.5$, $f_1(s) := \frac{1}{24}(s-0.5)^3 + (s-0.5)$ if $0.5 < s \le 1$.

Then, the discrete deformations for (P_h) and (RP_h) are shown Fig. 2.1 and Fig. 2.2 respectively. The microstructure seen in the solution for (P_h) vanishes in the solution for (RP_h).

3. Numerical analysis of linearised phase transitions in elastic solids

The variational model of an elastic body which occupies a bounded Lipschitz-domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, with two distinct zero-stress strain phases F_1 and F_2 in $\mathbb{R}^{d\times d}_{sym} := \{F \in \mathbb{R}^{d\times d} : F = F^T\}$ defines a double-well problem similar to the scalar one discussed above. For each well F_j, $j = 1, 2$, with minimal energy $W_j^0 \in \mathbb{R}$ one has a quadratic elastic energy which is, for $F \in \mathbb{R}^{d\times d}_{sym}$, defined by (cf. [12])

$$W_j(F) := \tfrac{1}{2}\langle F - F_j, \mathbb{C}(F - F_j)\rangle + W_j^0,$$

where $\mathbb{C}$ is a fourth-order elasticity tensor and $\langle\cdot,\cdot\rangle$ denotes the scalar product in $\mathbb{R}^{d\times d}$. Energy minimisation balances the configuration of the two phases and so the strain energy density W is modelled by the minimum of W_1 and W_2 (cf. [12]), i.e.,

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

The displacement $u \in \mathcal{A}$ minimises the energy functional

$$E(u) := \int_\Omega W(\epsilon(u))\,dx + \int_\Omega f\cdot u\,dx - \int_{\Gamma_N} g\cdot\,ds, \quad \epsilon(u) = \tfrac{1}{2}(\nabla u + \nabla u^T),$$

amongst all admissible displacements. The given functions $f \in L^2(\Omega)$ and $g \in L^2(\Gamma_N)$, $\Gamma_N \subset \partial\Omega$, describe lower order body forces. The space of admissible functions includes the Dirichlet data $u_D \in W^{1,2}(\Omega)$ and is defined by $\mathcal{A} := u_D + W^{1,2}_D(\Omega)$, where $W^{1,2}_D(\Omega) = \{v \in W^{1,2}(\Omega)^d : v|_{\Gamma_D} = 0\}$ for $\Gamma_D \subseteq \partial\Omega$ with positive surface measure.

Problem (P). Find a minimiser of E in $\mathcal{A}$.

As in the scalar case for (P) from Section 2, we do not have weak lower semicontinuity for E so that we cannot expect the existence of a minimiser. A relaxation allowing gradient Young measures generalising the approach in (GP) is possible but for computational reasons it is preferable to follow the ideas that led to (RP) in Section 2. The appropriate choice for the relaxed energy density is the quasiconvex envelope QW of W (cf. [11]).

Quasiconvexity is the right form of convexity to obtain weak lower semicontinuity for functionals like E to guarantee the existence of a minimiser $u \in \mathcal{A}$ of

$$QE(u) = \int_\Omega QW(\epsilon(u))\,dx + \int_\Omega f \cdot u\,dx - \int_{\Gamma_N} g \cdot u\,ds.$$

Problem (*RP*). Find a minimiser of QE in $\mathcal{A}$.

The connection between (P) and (RP) is that (RP) has solutions which are weak limits of minimising sequences for E and there holds $\inf_{\mathcal{A}} E = \min_{\mathcal{A}} QE$ (cf. [15]). Since all the important macroscopic quantities can be recovered from a solution u for (RP) it is relevant to consider this relaxed problem. For the problem at hand, the quasiconvex envelope of W is known explicitly from [12],

$$QW(F) = \begin{cases} W_2(F) & \text{if } W_2(F) + \gamma \le W_1(F), \\ \frac{1}{2}\big(W_2(F) + W_1(F)\big) - & \frac{1}{4\gamma}\big(W_2(F) - W_1(F)\big)^2 - \frac{\gamma}{4} \\ & \quad \text{if } |W_2(F) - W_1(F)| \le \gamma, \\ W_1(F) & \text{if } W_1(F) + \gamma \le W_2(F), \end{cases}$$

where γ is given by a certain projection onto the space of symmetric matrices. In case $\operatorname{rank}(F_1 - F_2) \le 1$ we have $\gamma = \frac{1}{2}\langle F_2 - F_1, \mathbb{C}(F_2 - F_1)\rangle$.

Note that in general, the quasiconvex hull of an energy density is not known explicitly.

A discretisation of (RP) consists in replacing $\mathcal{A}$ by a discrete subspace $\mathcal{A}_h$ and leads to the problem (RP_h) which has a minimiser $u_h \in \mathcal{A}_h$.

The relaxed problem and its approximation. For the numerical analysis of problem (RP) we assume that the energy wells F_1, F_2 are compatible, i.e., the difference $F_1 - F_2$ has rank one. This condition is satisfied in some applications and allows us to exploit the Galerkin-orthogonality but also implies that QW is convex.

Theorem 3.1 ([6]). *Suppose* $\operatorname{rank}(F_1 - F_2) = 1$*, and that* u *solves* (RP) *while* u_h *solves* (RP_h)*. Then, for the stress fields* $\sigma := DQW(\epsilon(u))$ *and* $\sigma_h := DQW(\epsilon(u_h))$ *we have the a priori error estimate*

$$\|\mathbb{C}^{-1/2}(\sigma - \sigma_h)\|^2_{L^2(\Omega)} \le \inf_{v_h \in \mathcal{A}_h} \|\mathbb{C}^{1/2}\nabla(u - v_h)\|^2_{L^2(\Omega)}. \tag{3.1}$$

Note that u and u_h are in general not unique but (3.1) holds independent of the choice of the minimisers.

Finite element approximation and a posteriori error control. In order to derive a computable a posteriori error estimate, let $\mathcal{T}$ denote a regular triangulation of the domain Ω and suppose that $\operatorname{rank}(F_1 - F_2) = 1$.

The volume and edge residuals $R \in L^2(\Omega)^d$ and $J \in L^2(\cup\mathcal{E})^d$ are defined as residuals from the strong form of the Euler-Lagrange equations by

$$R|_T := (f + \operatorname{div}\sigma_h)|_T \quad \text{and} \quad J|_E := \begin{cases} [\sigma_h \cdot n_E] & \text{if } E \not\subseteq \Gamma, \\ g - \sigma_h \cdot n & \text{if } E \subseteq \overline{\Gamma}_N, \\ 0 & \text{if } E \subseteq \Gamma_D, \end{cases} \tag{3.2}$$

for $T \in \mathcal{T}$ and $E \in \mathcal{E}$, respectively. Moreover, we denote by $h_{\mathcal{T}}$ and $h_{\mathcal{E}}$ the functions satisfying $h_{\mathcal{T}}|_T = h_T$ and $h_{\mathcal{E}}|_E = h_E$ for all $T \in \mathcal{T}$ and $E \in \mathcal{E}$, respectively.

Theorem 3.2 ([6]). *There exists a positive constant c_4, which only depends on the shape and not on the size of the elements in $\mathcal{T}$, such that*

$$\|\mathbb{C}^{-1/2}(\sigma - \sigma_h)\|^2_{L^2(\Omega)} \le c_4 \|u\|_{W^{1,2}(\Omega)} \big(\|h_{\mathcal{T}} R\|_{L^2(\Omega)} + \|h_{\mathcal{E}}^{1/2} J\|_{L^2(\cup\mathcal{E})}\big).$$

As in Theorem 2.2, one faces a loss of efficiency due to lacking smoothness properties of u but the estimate of the theorem still allows us to define local error indicators which can be used in Algorithm (A) for adaptive mesh refinement strategies.

Remarks on microstructures. The relaxed energy density can be seen as a convex combination of the two energies W_1 and W_2. We interpret the volume fraction θ of the area in which the material has elastic properties defined by W_1. A formula for the calculation of θ in terms of the exact strain $\epsilon(u)$ is given in [12]. A numerical approximation u_h for u thus allows us to compute an approximation θ_h of θ, although theoretical bounds are lacking.

The left plot of Fig. 3.1 shows the deformation and the modulus of the stress fields on the deformed unit square with fixed lower side and load in the vertical direction on the upper side. The material is defined through the elasticity tensor $\mathbb{C}$ and the matrices F_1, F_2 (cf. [6]). The corresponding volume fraction θ_h is shown in the right plot of Fig. 3.1.

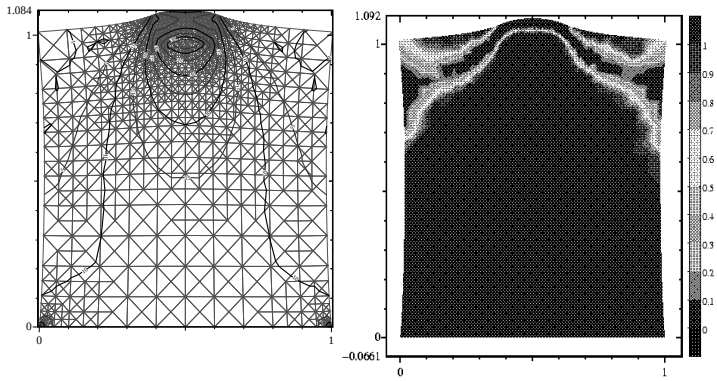

Fig. 3.1. Deformation u_h, stress field $|\sigma_h|$ (left), and volume fraction θ_h (right)

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