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Modelling of microstructure governed by non-quasiconvex variational problems

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Abstract

This contribution surveys various numerical approximation techniques applicable to relaxed vectorial variation problems describing, e.g., a steady-state configuration of cristalline martensitic materials.

Keywords

Non-quasiconvexconvex vectorial variational problems, fast oscillations, relaxation, Young measures, numerical approximation.

1 THE ORIGINAL PROBLEM

A steady-state configuration of elastic both geometrically and meterially nonlinear solid bodies occupying a bounded domain $\Omega \subset \mathbb{R}^n$ with a Lipschitz boundary Γ is governed by a vectorial variational problem

$$\text{(VP)} \qquad \int_\Omega \varphi(x, y(x), \nabla y(x))\mathrm{d}x \ + \int_\Gamma \varphi_1(x, y(x))\mathrm{d}S \to \ \inf, \qquad y \in W^{1,p}(\Omega; \mathbb{R}^m) \ ,$$

where $y : \Omega \to \mathbb{R}^m$ is a displacement, $\varphi : \Omega \times \mathbb{R}^m \times \mathbb{R}^{m\times n} \to \mathbb{R}$ is a potential-energy density and $\varphi_1 : \Gamma \times \mathbb{R}^n \to \mathbb{R}$ is a surface energy density, $1 < p < +\infty$. We admit also $n \neq m$ though in elasticity $n = m$ except some symmetrical situations like, e.g., the anti-plane deformation where $m = 1$. We are especially interested in crystalline materials composed from several phases (typically several lower-symmetry martensitic phase and possibly also higher-symmetry austenite) which may exhibit a microstructure. In this situation, the potential $\varphi(x, r, \cdot)$ has several rotationally invariant wells, each of them corresponds to one phase. Therefore, we must admit a certain nonconvexity of $\varphi(x, r, \cdot) : \mathbb{R}^{m\times n} \to \mathbb{R}$ (more precisely, $\varphi(x, r, \cdot)$ need not be quasiconvex) and then (VP) need not possess any solution so that its extension (=relaxation) must be done. Recall that a function $v : \mathbb{R}^{m\times n} \to \mathbb{R}$ is called quasiconvex if $v(A) \leq \text{meas}(\Omega)^{-1} \int_\Omega v(A + \nabla y(x))\mathrm{d}x$ for any $A \in \mathbb{R}^{m\times n}$ and any $y \in W_0^{1,p}(\Omega; \mathbb{R}^m)$, cf. [7].

2 THE RELAXED PROBLEM

We will treat a continuous extension of (VP), which preserves a detailed "limit" information about the possible fine oscillations of the gradient of minimizing sequences for (VP), i.e. the so-called microstructure. Neglecting some technicalities, the continuously extended relaxed problem involves Young measures in place of ∇y (cf. e.g. [1, 2, 4]):

$$
\text{(RP)} \qquad \left\{ \begin{array}{ll} \text{Minimize} & \int_\Omega \int_{\mathbb{R}^{m\times n}} \varphi(x, y(x), A)\nu_x(\mathrm{d}A)\mathrm{d}x + \int_\Gamma \varphi_1(x, y(x))\mathrm{d}S \ , \\ \text{subject to} & \int_{\mathbb{R}^{m\times n}} A\nu_x(\mathrm{d}A) \ = \ \nabla y(x) \ \text{ for a.a. } x \in \Omega, \\ & y \in W^{1,p}(\Omega; \mathbb{R}^m), \quad \nu \in \mathcal{G}^p(\Omega; \mathbb{R}^{m\times n}), \end{array} \right.
$$

where $\mathcal{G}^p(\Omega; \mathbb{R}^{m\times n}) = \{\nu = \{\nu_x\}_{x\in\Omega};\ \exists \{y_k\}_{k\in\mathbb{N}} \subset W^{1,p}(\Omega; \mathbb{R}^m)$ bounded & $\forall h \in L^1(\Omega; C_0(\mathbb{R}^{m\times n})) : \lim_{k\to\infty} \int_\Omega h(x, \nabla y_k) = \int_\Omega \int_{\mathbb{R}^{m\times n}} h(x, A)\nu_x(\mathrm{d}A)\mathrm{d}x\}$ denotes the set of all so-called gradient L^p-Young measures. The continuous relaxation yields a detailed information about a microstructure described by a Young measure (= a weakly measurable collection of probability measures parametrized by $x \in \Omega$) ν and also avoids a necessity to evaluate the quasiconvex envelope of $\varphi(x, r, \cdot)$, which arises within lower-semicontinuous relaxation, but creates inevitably another difficulty because the set $\mathcal{G}^p(\Omega; \mathbb{R}^{m\times n})$ is not effectively defined.

We assume the following data qualification: φ and φ_1 are Carathéodory functions with a suitable growth and coercivity, namely

$$
c_0|A|^p \leq \varphi(x, r, A) \leq a_0(x) + c_1(|r|^p + |A|^p) \ , \quad b(x)|r|^\beta \leq \varphi_1(x, r) \leq a_1(x) + c_1|r|^p \quad (1)
$$

with $a_0 \in L^1(\Omega)$, $a_1 \in L^1(\Gamma)$, $c_0, c_1, \beta > 0$, $b \geq 0$ nonvanishing on Γ, $1 < p < +\infty$, and such that $\varphi(x, \cdot, A)$ is Lipschitz continuous in the sense

$$
|\varphi(x, r_1, A) - \varphi(x, r_2, A)| \leq (a(x) + c|r_1|^{p-1} + c|r_2|^{p-1} + c|A|^{p-1})|r_1 - r_2| \qquad (2)
$$

with some $a \in L^{p/(p-1)}(\Omega)$ and $c > 0$. Then it is possible to show that (RP) is a correct relaxation of the original problem (VP) in the sense that (RP) always posseses a solution, the set of all solutions to (RP) is stable (more precisely, upper semicontinuous) with respect to a suitable data perturbations, every minimizing sequence for (VP) has a weak* cluster point which solves (RP) and, conversely, every solution to (RP) is attainable by a minimizing net for (VP), for details see [18].

3 APPROXIMATION OF THE RELAXED PROBLEM

The main aim of this contribution is to present a state of art in approximation theory of the relaxed vectorial variational problem (RP); due to the restricted scope, the results will be presented without proofs, referring to the references, especially to [17, 18].

We will not consider a direct finite-element approximation of (VP) (cf. a series of works by Chipot, Collins, Gremaud, Luskin, Kinderlehrer Nicolaides, Riordan, and Wang [3, 5, 6, 8, 10, 13, 14]) which always converges to (RP) but expectedly very slowly.

Rather we can make a direct finite-element approximation of (RP) by making a triangulation $\mathcal{T}_d$ of Ω such that all elements (=simplexes) from $\mathcal{T}_d$ have diameter less than $d > 0$, and then by restriction of (RP) to y element-wise affine and ν element-wise constant; let us denote the resulted problem by (RP_d). It is known that, for $d \to 0$, the solution of (RP_d) converges to a solution of (RP) in the sense that

$$\lim_{d\to 0} \min(\mathsf{RP}_d) = \min(\mathsf{RP}) \tag{3}$$

and every cluster point of every sequence of solutions to (RP_d) solves (RP), which can be written shortly in terms of the Kuratowski upper limit "Limsup" as

$$\operatorname*{Limsup}_{d\to 0}\ \mathrm{Argmin}(\mathsf{RP}_d) \subset \mathrm{Argmin}(\mathsf{RP}), \tag{4}$$

where "Argmin" denotes the set of all solutions to the indicated problem; we refer to [17] or also to [18, Proposition 6.3.7] for details. For $\varphi(x, r, A)$ independent of x and r the scheme (RP_d) has been also proposed by Pedregal [16].

Anyhow, the problem how to describe effectively the set $\mathcal{G}^p(\Omega; \mathbb{R}^{m\times n})$ still remains. Therefore, further approximation is needed. The general philosophy is to replace $\mathcal{G}^p(\Omega; \mathbb{R}^{m\times n})$ by another set (either smaller or larger) which can be defined effectively.

As to the former case, one can take all 2^k-atomic pair-wise rank-one connected Young measures, the resulted set being denoted by $\mathcal{G}^p_k(\Omega; \mathbb{R}^{m\times n})$ and the resulted problem by (RP^k_d); i.e. this problem consists in minimization of the same functional as in (RP) but for $y \in W^{1,p}(\Omega; \mathbb{R}^n)$ element-wise affine on the triangulation $\mathcal{T}_d$ and ν element-wise constant on $\mathcal{T}_\lceil$ and of the form

$$\nu_x \ = \ \sum_{l=1}^{2^k} a_l(x)\delta_{A_l(x)} \tag{5}$$

with $a_l = a_l(x)$ and $A_l = A_l(x)$ satisfying the following recursive conditions invented by Dacorogna [7] and called (H_N)-condition:

$$\left.\begin{array}{l}
a_l = \prod_{j=1}^k c_{[(l-1)2^{j-k}]+1,j}\ , \qquad A_l = A_{l,k}\ , \qquad l = 1, ..., 2^k \\
c_{2i,j}A_{2i,j} + c_{2i-1,j}A_{2i-1,j} = A_{i,j-1}, \\
c_{2i,j} + c_{2i-1,j} = 1, \quad c_{2i,j}, c_{2i-1,j} \geq 0, \quad \mathrm{Rank}(A_{2i,j} - A_{2i-1,j}) \leq 1, \\
i = 1, ..., 2^{j-1}, \quad j = 1, ..., k, \qquad A_{1,0} = \nabla y \in \mathbb{R}^{m\times n}.
\end{array}\right\} \tag{6}$$

where $[\cdot]$ denotes the integer part. The scheme (RP^k_d) has been proposed by Nicolaides and Walkington [9], see also [19], using basically the same ideas as Dacorogna [7, Section 5.1.1.2] and Kohn and Strang [11, Section 5C].

As to the latter case, one can take all L^p-Young measures which satisfy the Jensen inequality for all quasiconvex functions from a prescibed finite set X, the resulted set being denoted by $\mathcal{G}^p_X(\Omega;\mathbb{R}^{m\times n})$ and the resulted problem by $(\mathsf{RP}_{d,X})$; i.e. this problem consists in minimization of the same functional as in (RP) but for $y\in W^{1,p}(\Omega;\mathbb{R}^n)$ element-wise affine on the triangulation $\mathcal{T}_d$ and ν element-wise constant on $\mathcal{T}_\lceil$ and satisfying

$$\forall v\in X:\qquad \int_{\mathbb{R}^{m\times n}} v(A)\nu_x(\mathrm{d}A)\geq v\Big(\int_{\mathbb{R}^{m\times n}} A\nu_x(\mathrm{d}A)\Big)\ . \tag{7}$$

As $\mathcal{G}^p_k(\Omega;\mathbb{R}^{m\times n})\subset\mathcal{G}^p(\Omega;\mathbb{R}^{m\times n})\subset\mathcal{G}^p_X(\Omega;\mathbb{R}^{m\times n})$, we have always the two-side estimate

$$\min(\mathsf{RP}^k_d)\geq\min(\mathsf{RP}_d)\geq\min(\mathsf{RP}_{d,X}) \tag{8}$$

provided X contains all linear functions, or (which is basically equally effective) all functions $A\mapsto\pm[A]_{ij}$.

The convergence of the scheme (RP^k_d) is based on the results by Dacorogna [7] and Kohn and Strang [11]: if the rank-one convex envelope of $\varphi_d(x,r,\cdot)$, where φ_d denotes the potential φ averaged over the particular elements of $\mathcal{T}_d$, coincide with the quasiconvex one (cf. [7] for definitions of these envelopes), then

$$\lim_{k\to\infty}\min(\mathsf{RP}^k_d)=\min(\mathsf{RP}_d),\qquad\text{and} \tag{9}$$

$$\operatorname*{Limsup}_{k\to\infty}\ \mathrm{Argmin}(\mathsf{RP}^k_d)\subset\mathrm{Argmin}(\mathsf{RP}_d). \tag{10}$$

If the rank-one and the quasi-convex envelopes differ from each other less than $\varepsilon/|\Omega|$ or if

$$\min(\mathsf{RP}^k_d)-\min(\mathsf{RP}_d)\leq\varepsilon, \tag{11}$$

then we can say at least that any solution to (RP^k_d) with k large enough is an ε-approximate solution to (RP_d). The difference (11) is actually often rather small and can be justified experimentally by using the two-side estimate (8).

The character of convergence of $(\mathsf{RP}_{d,X})$ is a bit different. We have always the convergence

$$\lim_{X\to X_\infty}\min(\mathsf{RP}_{d,X})=\min(\mathsf{RP}_d) \tag{12}$$

where $X\to X_\infty$ indicates that X ranges the collection of all finite subsets of the set X_∞ of the quasiconvex functions with a growth less than p; of course, this collection is considered as directed by the inclusion. Then we have also

$$\operatorname*{Limsup}_{X\to X_\infty}\ \mathrm{Argmin}(\mathsf{RP}_{d,X})\subset\mathrm{Argmin}(\mathsf{RP}_d). \tag{13}$$

However, X_∞ is not effectively defined so that this convergence is purely theoretical only. Taking X all $\pm$subdeterminants (and $p>\min(n,m)$), then $G^p_X(\Omega;\mathbb{R}^{m\times n})$ is composed from the so-called polyconvex Young measures (cf. Pedregal [15]) and immediately $\min(\mathsf{RP}_{d,X})=\min(\mathsf{RP}_d)$ if the quasiconvex envelope of $\varphi_d(x,r,\cdot)$ coincides with the polyconvex one; for the definition of the polyconvex envelope see, e.g., [7]. If they differ from each other by no more than $\varepsilon/|\Omega|$ or if

$$\min(\mathsf{RP}_d)-\min(\mathsf{RP}_{d,X})\leq\varepsilon, \tag{14}$$

then solutions to $(\mathsf{RP}_{d,X})$ are in a suitable sense also ε-approximate solutions to (RP_d). More precisely, if (y,ν) solves $\min(\mathsf{RP}_{d,X})$, then there is a modified Young measure $\tilde\nu$ such that the pair $(y,\tilde\nu)$ is an ε-approximate solution to (RP_d), i.e.

$$\left.\begin{array}{l}(y,\tilde\nu)\in W^{1,p}(\Omega;\mathbb{R}^m)\times G^p_H(\Omega;\mathbb{R}^{m\times n}),\\ \int_{\mathbb{R}^{m\times n}}A\tilde\nu(\mathrm{d}A)=\nabla y(x),\quad \tilde\nu \text{ element-wise constant on } \mathcal{T}_d,\\ \int_{\bar\Omega}\int_{\mathbb{R}^{m\times n}}\varphi(x,y(x),A)\tilde\nu(\mathrm{d}A)\,\mathrm{d}x+\int_\Gamma\varphi_1(x,y(x))\mathrm{d}S\le\min(\mathsf{RP}_d)+\varepsilon,\end{array}\right\}\tag{15}$$

and certain momenta of ν and $\tilde\nu$ coincide with each other, namely

$$\forall v \text{ subdeterminant}:\qquad \int_{\mathbb{R}^{m\times n}}v(A)\nu_x(\mathrm{d}A)=\int_{\mathbb{R}^{m\times n}}v(A)\tilde\nu_x(\mathrm{d}A)\ .\tag{16}$$

This fact can be proved by taking $\tilde\nu\in G^p(\Omega;\mathbb{R}^{m\times n})$ element-wise constant such that $\int_{\mathbb{R}^{m\times n}}A\tilde\nu(\mathrm{d}A)=\nabla y(x)$ and $\int_\Omega\int_{\mathbb{R}^{m\times n}}\varphi_d(x,y,A)\tilde\nu(\mathrm{d}A)\mathrm{d}x=\varphi_d(x,y,\nabla y(x))^{\mathrm{qc}}\mathrm{d}x$, where $(\cdot)^{\mathrm{qc}}$ denotes the quasiconvex hull; such $\tilde\nu$ always exists due to the assumed coercivity of φ, cf. (1). The pair $(y,\tilde\nu)$ apparently satisfies (13). Moreover, since X contains $\pm\mathrm{adj}_k$ (here adj_k denotes some subdeterminant of the order k, we have $\int_{\mathbb{R}^{m\times n}}\mathrm{adj}_k(A)\nu(\mathrm{d}A)=\mathrm{adj}_k(\nabla y(x))$. Also we have $\int_{\mathbb{R}^{m\times n}}A\nu(\mathrm{d}A)=\nabla y(x)$ at our disposal. Then every $\tilde\nu\in G^p(\Omega;\mathbb{R}^{m\times n})$ such that $\int_{\mathbb{R}^{m\times n}}A\tilde\nu(\mathrm{d}A)=\nabla y(x)$ satisfies also $\int_{\mathbb{R}^{m\times n}}\mathrm{adj}_k(A)\tilde\nu(\mathrm{d}A)=\mathrm{adj}_k(\nabla y(x))$ from which (16) already follows.

To implement the scheme $\min(\mathsf{RP}_{d,X})$ with X consisting from $\pm$subdeterminants, we can always consider ν as a convex combination of a finite number (namely $1+\sum_{k=1}^{\min(m,n)}\binom{m}{k}\binom{n}{k}$ Dirac measures. The tolerance ε from (14) can be again justified experimentally by means of the two-side estimate (8).

Let us still remark that, by introducing suitable envelopes, these results can be generalized for larger X which contains, beside all $\pm$subdeterminants, also a finite number of some quasiconvex (but not polyconvex) functions.

Let us also note that the scheme (RP^k_d) results (after a suitable transformation) to a nonconvex mathematical-programming problem with several box-constraints only, while the scheme $(\mathsf{RP}_{d,X})$ with X containing all $\pm$determinants yields a nonconvex mathematical-programming problem with $mn+1$ linear but also $\sum_{k=2}^{\min(m,n)}\binom{m}{k}\binom{n}{k}$ nonlinear equality constraints on each element. This makes the latter scheme a bit more delicate for calculations but we cannot rely only on the former scheme because no other estimate of the energy error than (8) does not exist in general situations. Numerical examples for model two-dimensional problems with two rotationally invariant wells describing materials having two phases (tetragonal, monoclinic, or cubic) which are or are not rank-one connected have been calculated by Kružík [12], where a detailed numerical experience can be found.

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