

CONCURRENT MULTISCALE COMPUTING OF DEFORMATION MICROSTRUCTURE BY RELAXATION AND LOCAL ENRICHMENT WITH APPLICATION TO SINGLE-CRYSTAL PLASTICITY

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Abstract. This paper is concerned with the effective modeling of deformation microstructures within a *concurrent multiscale computing* framework. We present a rigorous formulation of concurrent multiscale computing based on relaxation; we establish the connection between concurrent multiscale computing and enhanced-strain elements; and we illustrate the approach in an important area of application, namely, single-crystal plasticity, for which the explicit relaxation of the problem is derived analytically. This example demonstrates the vast effect of microstructure formation on the macroscopic behavior of the sample, e. g., on the force/travel curve of a rigid indenter. Thus, whereas the unrelaxed model results in an overly stiff response, the relaxed model exhibits a proper limit load, as expected. Our numerical examples additionally illustrate that ad-hoc element enhancements, e. g., based on polynomial, trigonometric or similar representations, are unlikely to result in any significant relaxation in general.

1. Introduction. The problem addressed in this paper concerns the effective modeling of deformation microstructures within a *concurrent multiscale computing* framework. In many applications of interest, materials develop fine macrostructure on multiple length and time scales in response to loading [6, 54, 59, 49]. Examples of such microstructures include: martensite; subgrain dislocation structures; dislocation walls and networks; ferroelectric domains; shear bands; spall planes; and others. In addition, materials such as polycrystalline metals may exhibit processing microstructure from the outset, prior to the onset of deformation. The macroscopic behavior of such materials is too complex to be amenable to modeling based on simple representational schemes, such as afforded by continuum thermodynamics, symmetry groups, linearization, polynomial approximations, empirical fitting and calibration, and other similar schemes. Indeed, empirical models are a major source of error and uncertainty in engineering applications, and the empirical paradigm does not offer a systematic means of reducing such error and uncertainty.

Multiscale modeling aims to eliminate empiricism and uncertainty from material models by systematically identifying the rate-controlling mechanisms at all scales; the fundamental laws that govern those mechanisms; and by bridging the relevant space and time length scales through a mathematically rigorous determination of laws of effective or macroscopic behavior. The ultimate aim is to formulate parameter (or 'knob') free macroscopic models of material behavior based solely on fundamental laws of physics and rigorous approximation theory. However, the practical implementation of this program remains an outstanding challenge of our time in materials science, computational science and mathematics.

From a mathematical point of view, the formation of microstructure is a manifestation of the phenomenon of *lack of attainment* [24, 49]. Thus, the minimum principles that govern incremental behavior involve functionals that are often non-convex and lack lower-semicontinuity, with the result that their infima is not attained by any classical solution. The infima can nevertheless be approached arbitrarily close by sequences of fields that exhibit increasingly fine microstructure, or *minimizing se-*

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quences. These sequences give mathematical expression to the concept of microstructure. Therefore, the central computational problem concerns the calculation of solutions that exhibit very fine oscillations on the scale of the domain of analysis.

For problems such as nonlinear elasticity or plasticity whose energies are invariant under rescaling of the domain, thus resulting in a strict separation of the microscopic and macroscopic length scales, the standard mathematical device for the solution of multiscale problems is *relaxation* [35, 36, 24, 25, 49, 10]. The process of relaxation produces a new effective or 'relaxed' problem that is well-posed in the sense of existence of solutions and that implicitly accounts for the formation of microstructure. Indeed, the relaxed problem is fashioned by identifying *optimal microstructures*, i. e., minimizing sequences of fields whose energies converge to the infimum of the energy. Conversely, optimal microstructures can be reconstructed, at no loss of information, from the solutions of the relaxed problem, which however are themselves free of fine oscillations.

The finite element method provides an ideal framework for the implementation of the method of relaxation: the oscillation-free solutions of the relaxed problem are approximated by finite-element interpolation; and microstructure is accounted for at the sub-grid level. Such schemes conform to the *concurrent* multiscale computing paradigm in that both the macroscopic solution and the attendant microstructures are computed *simultaneously* as part of the same calculation. The earliest realizations of this general strategy were concerned with the effective simulation of shear bands resulting from unstable plastic deformation. To this end, Ortiz *et al.* [52, 43, 45, 50, 44] embedded a *discontinuous mode* of deformation carrying a strain discontinuity into finite elements, which they treated as *incompatible elements*. The detection of the point of local instability and the orientation of the resulting strain discontinuities were determined by a local Hadamard stability analysis. Numerous variations of this basic scheme were proposed subsequently, and the resulting elements have been generally referred to as *enhanced-strain elements*.

From the standpoint of relaxation the local strain fields in enhanced-strain elements represent simple microstructures. The precise structure of the strain enhancement is immaterial as regards the effective behavior of the element, only the so-called Young-measure generated by the strain enhancement matters. This Young measure keeps track of the volume fractions occupied by the different strains introduced by the local enhancement. This observation was made by Leroy *et al.* [45], who showed that the original element of Ortiz *et al.* [52] and the embedded-band element of Belytschko *et al.* [8] are indeed identical. In addition, the local Hadamard stability analysis underlying enhanced-strain elements is often based on a linearization of the constitutive relations, leading to the so-called Hill's equivalent solid, and the resulting local enhancements fail to fully exploit the strongly nonlinear multi-well structure of the energy landscape.

More general concurrent multiscale computing schemes based on modern calculus of variations tools have been proposed recently [14, 54, 55, 28, 9, 26, 21, 5, 13, 46, 56]. These schemes allow a fully nonlinear analysis of the energy to be performed at the sub-grid scale and generate microstructures 'on-the-fly' by a variety of algorithms such as sequential lamination [41] and recursive faulting [56]. While this approach conforms strictly to the multiscale modeling paradigm, i. e., it involves no empirical modeling of the macroscopic or effective behavior, the generation of sub-grid microstructure requires the solution of a complex non-convex optimization problem and is often computationally costly. Considerable gains in performance are achieved when

the relaxation of the constitutive relations *is known analytically*. Thus, when the relaxation of the problem is known explicitly, the construction of sub-grid microstructures is bypassed entirely, and yet the behavior of the elements is optimal, i. e., as compliant as possible, and optimal microstructures can be re-constructed *a posteriori* at no loss of information. Unfortunately, explicit relaxations are only known for a handful of material models, though the list of such models continues to grow at a steady rate.

In this paper we present a rigorous formulation of the concurrent multiscale computing paradigm just described; we establish the connection between concurrent multiscale computing and enhanced-strain elements; and illustrate the approach in an important area of application, namely, single-crystal plasticity, for which the explicit relaxation of the problem is derived analytically. Our relaxation theorem extends an earlier result of Conti and Ortiz [22] to the hardening case. The paper is organized as follows. Fundamental results of the direct method in the calculus of variations concerning existence of minimizers and relaxation are briefly reviewed in Section 2. Section 3 is concerned with the convergence of conforming discrete approximations to the relaxed functional in the nonlinear range. Section 4 discusses relaxation in a model of crystal plasticity. Section 5 is devoted to establishing the connection of enrichment techniques and partial relaxation. Section 6 provides an example of application of the relaxation approach to multiscale computations in single crystal plasticity. Finally, closing remarks and outlook are collected in Section 7.

2. Infimization and Relaxation. We review below some results on the existence of a minimizer for a functional on a topological space, as well as the fundamental results concerning relaxation of functionals defined on Sobolev spaces (see for instance [25, 24, 49] for broader presentations). We shall consider functionals $J : X \rightarrow \overline{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\}$, where X is a metric space (a topological space would suffice for most results, see [25]; we shall not need this generality). Typically, X will be a subset of a Sobolev space $W^{1,p}(\Omega; \mathbb{R}^n)$.

The direct method of the calculus of variations permits to establish existence of minimizers for J over X by establishing that any minimizing sequence, i.e., any sequence $u_i \in X$ such that $J(u_i) \rightarrow \inf_X J$, has a subsequence which converges to a minimum. The key ingredients are coercivity and lower semicontinuity. One says that the functional J is coercive in X if for any $t \in \mathbb{R}$, the closure of the set

$$\{J \leq t\} := \{v \in X, \quad J(v) \leq t\}$$

is compact in X . This immediately implies that any sequence u_i for which $J(u_i)$ is bounded has a subsequence converging to some $u \in X$. The second step is then to show that the limit minimizes J . In order to do so it suffices to prove that $J(u) \leq \liminf_{i \rightarrow \infty} J(u_i) = \inf J$, which is implied by lower semicontinuity of J . We recall that J is said to be lower semicontinuous if for every $u \in X$ and every sequence $u_i \rightarrow u$ one has

$$J(u) \leq \liminf_{i \rightarrow \infty} J(u_i).$$

Not all interesting functionals are, however, lower semicontinuous, and in particular those describing materials which spontaneously generate microstructure are not. We are specially interested here in functionals lacking lower semicontinuity, and in their relaxation. A key notion in the theory of relaxation is that of lower semicontinuous envelope. The lower semicontinuous envelope $sc^- J : X \rightarrow \overline{\mathbb{R}}$ of J is defined as

the supremum among all lower semicontinuous functions below J ,

$$sc^- J(u) = \sup \{ G(u) : G : X \rightarrow \overline{\mathbb{R}} \text{ lower semicontinuous, } G(v) \leq J(v) \ \forall v \in X \} .$$

It is easy to see that $sc^- J$ is lower semicontinuous, and that

$$sc^- J(u) = \inf \left\{ \liminf_{i \rightarrow \infty} J(u_i) : u_i \in X, \ u_i \rightarrow u \right\} . \quad (2.1)$$

For any coercive functional J the following holds [25, p.30]:

1. $sc^- J$ is coercive and lower semicontinuous.
2. $sc^- J$ admits at least a minimum point.
3. $\min_{u \in X} sc^- J(u) = \inf_{u \in X} J(u)$.
4. If u is the limit of a minimizing sequence for J , then u is a minimum point for $sc^- J$.
5. If u is a minimum point for $sc^- J$, then u is the limit of a minimizing sequence of J .

We shall focus on functionals J given under integral form over a Lipschitz domain $\Omega \subset \mathbb{R}^n$ by

$$J(u) = \int_{\Omega} W(Du(x)) \, dx, \quad \forall u \in X, \quad (2.2)$$

where Du stands for the weak derivative of u , and

$$X = \{v \in W^{1,p}(\Omega; \mathbb{R}^m), \ v = 0 \text{ on } \Gamma_D\}, \quad 1 < p < +\infty. \quad (2.3)$$

Here $\Gamma_D \subset \partial\Omega$ is the part of the boundary of Ω on which we impose Dirichlet boundary conditions. Even with strong growth conditions on W , these functionals are not coercive with respect to the topology given by the Sobolev norm. They can be however coercive with respect to the weak topology. We recall that for $1 < p < \infty$ a sequence $(f_i)_{i \in \mathbb{N}}$ in $L^p(\Omega; \mathbb{R}^m)$ converges weakly to $f \in L^p(\Omega; \mathbb{R}^m)$, $f_i \rightharpoonup f$, if

$$\lim_{i \rightarrow \infty} \int_{\Omega} f_i \cdot g = \int_{\Omega} f \cdot g,$$

for every $g \in L^{p'}(\Omega; \mathbb{R}^m)$ where $p' = p/(p-1)$. Analogously, a sequence $(u_i)_{i \in \mathbb{N}}$ converges to u weakly in $W^{1,p}(\Omega; \mathbb{R}^m)$ if u_i converges weakly to u in $L^p(\Omega; \mathbb{R}^m)$, and Du_i converges weakly to Du in $L^p(\Omega; \mathbb{R}^{m \times n})$.

The main property of weak convergence of interest here is that bounded sequences have weakly converging subsequences. Precisely, since the spaces $W^{1,p}$ for $1 < p < \infty$ are separable and reflexive, any bounded subset is compact with respect to the weak topology [58] (further, recall that bounded subsets of the same Sobolev spaces are metrizable with respect to the weak topology [58, Th. 3.16], hence it is no loss of generality to focus on metric spaces). Therefore coercivity of J is equivalent to the fact that its sublevel sets are bounded in $W^{1,p}$.

The coercivity of the functional J can be determined from of the growth of W . Precisely, if for some $1 < p < \infty$ we have

$$\frac{1}{C}|F|^p - C \leq W(F) \quad \forall F \in \mathbb{R}^{m \times n}, \quad (2.4)$$

then one immediately obtains

$$\frac{1}{C} \int_{\Omega} |Du|^p \leq J(u) + C|\Omega|,$$

hence Du is bounded in $L^p(\Omega; \mathbb{R}^{m \times n})$ whenever J is bounded. If additionally the set Γ_D has positive $n-1$ dimensional measure, then by the Poincaré-Wirtinger inequality u is also bounded in $L^p(\Omega; \mathbb{R}^m)$. Hence u is bounded in $W^{1,p}$, and this implies coercivity of J with respect to the weak $W^{1,p}$ topology.

Equation (2.4) shows that coercivity depends only on the behavior of W at infinity. Weak lower semicontinuity instead depends on the behavior of W on the entire space of matrices. In one spatial dimension weak lower semicontinuity is equivalent to convexity of the energy density W . In general, weak lower semicontinuity of the energy J given by (2.2) is closely related to the notion of quasiconvexity introduced by Morrey [47, 48]. One says that $W : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ is quasiconvex if for every open bounded domain $\omega \subset \mathbb{R}^n$,

$$\int_{\omega} W(F + Dv) \geq \int_{\omega} W(F), \quad \forall v \in W_0^{1,\infty}(\omega; \mathbb{R}^m). \quad (2.5)$$

The relation between quasiconvexity and lower semicontinuity can be enounced as follows (see, e. g., [49, Th. 4.4]).

THEOREM 2.1. *Let $W : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ be continuous, and assume that there exists a constant $C > 0$ and $1 < p < \infty$ such that*

$$0 \leq W(F) \leq C(1 + |F|^p), \quad \forall F \in \mathbb{R}^{m \times n}, \quad (2.6)$$

and let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain. Then J defined by (2.2) is weakly lower semicontinuous on $W^{1,p}(\Omega; \mathbb{R}^m)$ if and only if W is quasiconvex.

In the case that W is not quasiconvex, and correspondingly J not lower semicontinuous, the quasiconvex envelope of W permits to determine the lower semicontinuous envelope of J . Precisely, the following holds [24, Theorem 2.1, p.228], [49, Theorem 4.5]

THEOREM 2.2. *Let $J : X \rightarrow \overline{\mathbb{R}}$ be the functional defined in (2.2),(2.3). Let $W : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ be continuous and such that*

$$\frac{1}{C}|F|^p - C \leq W(F) \leq C + C|F|^p, \quad \forall F \in \mathbb{R}^{m \times n}, \quad (2.7)$$

for some $1 < p < +\infty$ and $C > 0$. Then, the lower semicontinuous envelope of J for the weak topology of $W^{1,p}(\Omega; \mathbb{R}^m)$ is given by

$$sc^- J(u) = \int_{\Omega} \mathcal{Q}W(Du).$$

Here $\mathcal{Q}W : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ denotes the quasiconvex envelope of W , which can be computed by

$$\mathcal{Q}W(F) = \inf_{v \in W_0^{1,\infty}(\omega; \mathbb{R}^m)} \frac{1}{|\omega|} \int_{\omega} W(F + Dv), \quad \forall F \in \mathbb{R}^{m \times n}. \quad (2.8)$$

Expression (2.8) is independent of the choice of the open bounded domain $\omega \subset \mathbb{R}^n$, provided that its boundary has zero Lebesgue measure.

The computation of quasiconvex envelopes is, in general, exceedingly difficult. There are however some cases where an explicit result is known. For example, in scalar or one-dimensional problems (i.e., if $m = 1$ or $n = 1$) then the quasiconvex envelope is the same as the convex envelope, which is easily computable. In higher dimension only some special cases are known, we mention some of them below.

Example: The Pipkin formula. Consider functions W of the form

$$W(F) = \overline{W}(F^\top F), \quad \forall F \in \mathbb{R}^{m \times n},$$

with \overline{W} convex and $m \geq n$. An explicit formula for $\mathcal{Q}W$ was obtained by Pipkin [57] in the case $m > n$, and extended by Le Dret and Raoult [29] to the case $m = n$. The result is

$$\mathcal{Q}W(F) = \inf_{S \in \mathbb{S}_n^+} \overline{W}(F^\top F + S) \quad \forall F \in \mathbb{R}^{m \times n}, \quad (2.9)$$

where \mathbb{S}_n^+ is the set of symmetric semi-definite positive matrices in $\mathbb{R}^{n \times n}$. Le Dret and Raoult have also shown that formula (2.9) does not hold for $m < n$.

Example: Relaxation in models for membranes. Sometimes, the nonconvexity leading to the necessity of relaxing the energy does not only come from the material properties, but from the geometry. A typical example is thin-film elasticity, in the membrane regime. For this case LeDret and Raoult have shown that taking the quasiconvex envelope of the three-dimensional energy density, which, e.g., for the Saint-Venant Kirchhoff model can be obtained by the mentioned Pipkin formula, is not sufficient to obtain a relaxed membrane model [42]. An additional step of relaxation needs to be carried out, by relaxing the resulting energy density resulting after dimension reduction, which is defined on $\mathbb{R}^{3 \times 2}$; in practice, the first relaxation can be skipped, since the second one automatically includes it. A practical application of this method is illustrated in [31].

Example: Relaxation in liquid-crystal elastomers. Liquid crystal elastomers display a number of interesting mechanical and optical properties due to the coupling between the liquid crystal ordering phase transition and rubber elasticity. Presence of the phase transition leads to nonquasiconvexity of the energy, and to microstructure formation. The explicit computation of the quasiconvex envelope of the energy by DeSimone and Dolzmann [26] in the isotropic model permitted efficient macroscopic finite-element simulations [21]. For a more refined anisotropic model, including an anisotropy term, the relaxation could only be obtained in two dimensions [20]; numerical simulations were then performed in a suitable membrane geometry. The microstructure could be locally reconstructed, inverting the quasiconvexification procedure. Comparison with experiment has shown very good agreement with both macroscopic and microscopic properties computed through the relaxed functional, in particular for the anisotropic model. The quasiconvex envelope of the anisotropic model in three dimensions could not yet be determined.

Example: Sequential faulting in confined brittle samples. When fractures arise in confined brittle materials, distributed damage instead of localised isolated cracks can be expected (cf the experiments of Chen and Ravichandran [17, 18, 15, 16]). Such a distribution of damage can be understood as the occurrence of microstructure, and the energy to be minimized indeed lacks of lower-semicontinuity. In order to provide numerical partial relaxation, Pandolfi *et al.* [56] propose to introduce distributions of cracks, or recursive-faulting, which share several characteristics with—but also differs in significant respects from—sequential lamination. In the particular

case of purely cohesive frictionless fracture, the sequential faulting construction can be shown to deliver the relaxation of the energy [56]. The relaxed energy exhibits a marked tension-compression asymmetry. Thus, whereas in hydrostatic tension the fault microstructure is capable of fully relaxing the energy, under hydrostatic tension–or ‘confinement’–the microstructure can only relax shear and the material behaves as a compressible fluid in hydrostatic equilibrium.

Examples in crystal plasticity will be discussed in Section 4 below.

3. Convergence of approximations. In this section, considering an arbitrary functional J to infimize over X , we consider the successive approximation of infima over finer and finer conforming finite-dimension spaces $(X_i)_{i \geq 0} \subset X$. Under natural assumptions, we show that subsequences of successive minima over X_i , $i \geq 0$, converge to minima of the relaxed energy sc^-J as $i \rightarrow \infty$. The arguments use Γ -convergence theory [35, 36, 25, 10], whose basic ingredients are recalled in Section 3.1 following [25].

3.1. Elements of Γ -convergence. Let $(J_i)_{i \in \mathbb{N}}$ be a sequence of functionals from X to $\overline{\mathbb{R}}$. One says that J_i Γ -converges to $J : X \rightarrow \overline{\mathbb{R}}$ if the following two properties hold:

1. For every $u \in X$, and every sequence $u_i \rightarrow u$, one has

$$J(u) \leq \liminf_{i \rightarrow \infty} J_i(u_i);$$

2. For every $u \in X$, there is a sequence $u_i \rightarrow u$ such that

$$J(u) = \lim_{i \rightarrow \infty} J_i(u_i).$$

The Γ -limit J is automatically lower semicontinuous. Further, a constant sequence $J_i = J$ always has a Γ -limit, which coincides with the lower semicontinuous envelope sc^-J of J .

Extension of the direct method to a family of functionals requires some uniform coercivity assumption. In particular, a sequence $(J_i)_{i \in \mathbb{N}}$ is equi-coercive in X if for any $t \in \mathbb{R}$ there exists a compact set $K_t \subset X$ in (X, T) such that for all $i \in \mathbb{N}$,

$$\{u \in X, \quad J_i(u) \leq t\} \subseteq K_t.$$

It is here crucial that the set does not depend on i .

Consider now a sequece J_i which is equicoercive, and which Γ -converges to some functional J . Then J is necessarily also coercive. Since any Γ -limit is lower semicontinuous, one immediately obtains that the Γ -limit of any equicoercive sequence has a minimizer. Even more, their minimizers are accumulation points of minimizing sequences of the family J_i . Precisely, if $J_i(u_i) = \inf J_i$, then the sequence u_i has a subsequence which converges to a minimizer of J . The converse cannot be true, since J_i need not have a minimizer - it is however true, if approximate minimizers are considered. Assume for definiteness $J_i \geq 0$, and J not identically $+\infty$. Then the set of minimizers of J coincides with the set of accumulation points of the set of minimizing sequences *of the family* J_i . In formulas,

$$\{u : J(u) = \inf J\} = \text{accumulation points of } \left\{ u_i : \lim_{i \rightarrow \infty} [J_i(u_i) - \inf J_i] = 0 \right\}.$$

3.2. Approximation and convergence analysis in the conforming case.

Let $(X_i)_{i \in \mathbb{N}} \subset X$ be a sequence of finite-dimension approximation spaces.

DEFINITION 3.1. *A sequence $(X_i)_{i \in \mathbb{N}} \subset X$ is dense in X if for any $u \in X$, there exists a sequence $(u_i)_{i \in \mathbb{N}}$ converging to u in X such that for every $i \in \mathbb{N}$, $u_i \in X_i$.*

We formulate our result with two abstract topologies; in practice, T will be the strong topology of $W^{1,p}$, and S the weak one. We shall denote by (X, T) and (X, S) the space X endowed with the strong and with the weak topology, respectively. As elsewhere in this paper we assume all topologies to be metrizable, which is not a restriction for the applications we are considering; a first-countability assumption would suffice.

PROPOSITION 3.2. *The set X is assumed to be endowed with two metrizable topologies S and T , and T is finer (any converging sequence for T converges for S). Let $J : X \rightarrow \overline{\mathbb{R}}$ be a coercive functional in (X, S) , and continuous in (X, T) . Let $(X_i)_{i \in \mathbb{N}} \subset X$ be a dense sequence of sets in (X, T) , and $(J_i)_{i \in \mathbb{N}} : X \rightarrow \overline{\mathbb{R}}$ be the sequence defined by*

$$J_i(u) = \begin{cases} J(u), & \text{if } u \in X_i, \\ +\infty, & \text{otherwise,} \end{cases} \quad (3.1)$$

for every $i \in \mathbb{N}$ and every $u \in X$. Then the sequence $(J_i)_{i \in \mathbb{N}}$ Γ -converges to $sc^- J$ in (X, S) and is equicoercive in (X, S) . Here $sc^- J$ is the lower semicontinuous envelope of J in (X, S) .

Proof. Let $u \in X$, and $u_i \rightarrow u$ with respect to S . Since $J_i \geq J$ on X for every $j \in \mathbb{N}$, we have

$$sc^- J(u) \leq \liminf_{i \rightarrow \infty} J(u_i) \leq \liminf_{i \rightarrow \infty} J_i(u_i). \quad (3.2)$$

This proves the first inequality in the definition of Γ -convergence.

Consider now some $u \in X$. By (2.1) there is a sequence $u^k \rightarrow u$ in S such that

$$\lim_{k \rightarrow \infty} J(u^k) = sc^- J(u).$$

By the density of the sequence X_i , for any k there is a sequence $u_i^k \in X_i$, with $u_i^k \rightarrow u^k$ with respect to T . Since J is continuous in the same topology, and $J_i = J$ on X_i ,

$$\lim_{i \rightarrow \infty} J_i(u_i^k) = \lim_{i \rightarrow \infty} J(u_i^k) = J(u^k).$$

Taking a diagonal subsequence the concludes the proof of Γ -convergence.

The equi-coercivity of the sequence is immediate from the coercivity of J , since $J_i \geq J$. \square

Assume for instance that J is of the form (2.2), with $W : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ continuous, and such that

$$c|F|^p - C \leq W(F) \leq C(1 + |F|^p), \quad \forall F \in \mathbb{R}^{m \times n}. \quad (3.3)$$

for some $c, C > 0$, $p \in (1, \infty)$. If Ω is a bounded Lipschitz domain, and $\Gamma_D \subset \partial\Omega$ has positive $n - 1$ -dimensional measure, then J is coercive in the weak topology of $W^{1,p}$. Further, by Lebesgue's dominated convergence theorem, J is continuous in the strong topology of $W^{1,p}$. Therefore Proposition 3.2 applies, for any dense sequence $X_i \subset W^{1,p}$. Typical finite-element spaces, such as piecewise affine functions on finer and finer grids, constitute a dense sequence (provided the boundary data are compatible with the discretization).

4. Relaxation in single-slip plasticity. For a simple single-slip plastic model, Conti and Ortiz have shown the possibility of explicit relaxation [22]. We briefly review their result for the limiting case of infinite latent hardening, and show that it can be extended to situations with finite latent hardening. Let $\Omega \subset \mathbb{R}^3$ represent the reference configuration of a ductile single crystal, and denote by u the displacement field. Under the hypothesis of small deformation, we adopt the following additive decomposition of the gradient $\beta = Du$ into an elastic and a plastic contribution:

$$\beta = Du = \beta^e + \beta^p.$$

Notice that β needs to be a gradient field, i.e., $\nabla \times \beta = 0$; this does not necessarily hold for the individual components β^e and β^p . Plastic deformation in single crystals is crystallographic in nature and, for monotonic deformation, the plastic contribution β^p can be expressed as

$$\beta^p(\gamma) = \sum_{i=1}^N \gamma_i s_i \otimes m_i.$$

The single crystal has N slip systems characterized by the slip directions $(s_i)_{1 \leq i \leq N}$ and the normal vectors $(m_i)_{1 \leq i \leq N}$, the plastic state of the crystal being described by the set of plastic variables $(\gamma_i)_{1 \leq i \leq N}$. Plastic deformations are assumed to be isochoric ($s_i \cdot m_i = 0$ for all $1 \leq i \leq N$). For example, in fcc crystals one has $N = 12$ and the set of slip systems $\mathcal{S} = \{s_i \otimes m_i; 1 \leq i \leq N\}$ is given by

$$\mathcal{S}_{\text{fcc}} = \{(0, 1, 1) \otimes (\pm 1, 1, -1), (0, 1, -1) \otimes (\pm 1, 1, 1), \text{ and cyclic permutations}\};$$

for bcc crystals one instead has $N = 24$ and

$$\mathcal{S}_{\text{bcc}} = \{(\pm 1, 1, 1) \otimes (0, 1, -1), (\pm 1, 1, -1) \otimes (0, 1, 1), \\ (1, -1, \mp 1) \otimes (2, 1, \pm 1), (1, 1, \mp 1) \otimes (2, -1, \pm 1), \text{ and cyclic permutations}\}.$$

Neglecting self-hardening and assuming an infinite latent hardening, the energy density associated to the gradient of displacements β , and with a given amount of plastic slip $\gamma \in \mathbb{R}^N$, can be written as

$$A(\beta, \gamma) = \frac{1}{2} (\beta^{\text{sym}} - [\beta^p(\gamma)]^{\text{sym}}) : \mathbf{E} (\beta^{\text{sym}} - [\beta^p(\gamma)]^{\text{sym}}) + W^p(\gamma),$$

where $W^p : \mathbb{R}^N \rightarrow [0, \infty]$ contains hardening and dissipation terms. The amount of plastic slip $\gamma : \Omega \rightarrow \mathbb{R}^N$ enters the energy locally, and does not need to obey any differential constraint (this corresponds to the fact that $\beta^p(\gamma)$ need not be a gradient field). Therefore we can minimize out γ locally, and define the condensed energy

$$W(\beta) = \min_{\gamma \in \mathbb{R}^N} \left[\frac{1}{2} (\beta^{\text{sym}} - [\beta^p(\gamma)]^{\text{sym}}) : \mathbf{E} (\beta^{\text{sym}} - [\beta^p(\gamma)]^{\text{sym}}) + W^p(\gamma) \right]. \quad (4.1)$$

This condensed energy already takes into account the optimal distribution of the total displacement gradient β into an elastic and a plastic part, at each material point.

The analysis in [22] focussed on the case of infinite latent hardening. Precisely, it was assumed that W^p coincides with the plastic energy function W_∞^p , which prohibits multislip deformation at any material point,

$$W_\infty^p(\gamma) := \begin{cases} \tau_i |\gamma_i| & \text{if } \gamma_j = 0 \text{ for all } j \neq i, \\ +\infty & \text{otherwise.} \end{cases}$$

Here $\tau_i > 0$ are parameters corresponding to the critical stresses along the different slip systems. Its convex envelope $[W_\infty^p]^{**}$ coincides with the energy density W_0^p describing multislip plasticity, i.e., with a model where no latent hardening at all is included:

$$[W_\infty^p]^{**}(\gamma) = W_0^p(\gamma) := \sum_i \tau_i |\gamma_i|.$$

In [22] it was shown that under a kinematic assumption on the set of slip systems the energy W_0^p coincides not only with the convex envelope, but also with the quasiconvex envelope of W_∞^p . We show here that this holds also for all models with finite latent hardening, which are in a sense intermediate between W_∞^p and W_0^p . We remark that, as in classical works on geometrically linear plasticity [60, 3, 61], the natural space in which coercivity is achieved is

$$U(\Omega) := \{u \in BD(\Omega; \mathbb{R}^3); \operatorname{div} u \in L^2(\Omega)\}.$$

We recall that BD is the space of functions of bounded deformation, i.e., the set of L^1 functions such that the symmetric part of the distributional gradient is a bounded measure [60, 3, 61, 1]:

$$BD(\Omega) := \left\{ u \in L^1(\Omega; \mathbb{R}^3) : \sup \left\{ \left| \int_\Omega u \otimes \nabla \phi + \nabla \phi \otimes u \right| : u \in C_0^1(\Omega; \mathbb{R}^3) \right\} < \infty \right\}.$$

We recall that, much as in the case of BV functions, the symmetrized distributional gradient of any function $u \in BD$ can be decomposed as follows:

$$Eu := \frac{Du + (Du)^T}{2} = \mathcal{E}u dx + E^s u.$$

Here Du is the (matrix-valued) distributional gradient of u ; $\mathcal{E}u$ the absolutely continuous part of Eu with respect to the Lebesgue measure, and E^s the rest. Further, it can be shown that E^s is absolutely continuous with respect to the 2-dimensional Hausdorff measure \mathcal{H}^2 (one dimension less than the space, in general). In turn, E^s contains a part which is absolutely continuous with respect to \mathcal{H}^2 , and which represent jumps in u , and a remainder, which is called Cantor part and which is, in some sense, intermediate between a two and three dimensional measure.

The relevant topology is the weak topology of U , i.e., weak convergence of u in BD and weak convergence of $\operatorname{div} u$ in L^2 . Analogously to the case of Sobolev spaces, on bounded sets this is equivalent to the strong L^1 topology, which is metrizable. Hence we shall use the latter.

THEOREM 4.1. *Let $\Omega \subset \mathbb{R}^3$ be an open set, and the set of slip systems $\{s_i \otimes m_i; 1 \leq i \leq N\}$ be \mathcal{S}_{bcc} or \mathcal{S}_{fcc} . Assume that plastic energy $W^p : \mathbb{R}^N \rightarrow [0, \infty]$ fulfills*

$$W_0^p(\gamma) \leq W^p(\gamma) \leq W_\infty^p(\gamma) \quad \text{for all } \gamma \in \mathbb{R}^N, \quad (4.2)$$

and let W be as in (4.1). Then, the relaxation of the functional $J : U(\Omega) \rightarrow [0, \infty]$ defined by

$$J(u) = \begin{cases} \int_\Omega W(Du) & \text{if } u \in W^{1,2}(\Omega; \mathbb{R}^3), \\ +\infty & \text{otherwise,} \end{cases}$$

with respect to the strong L^1 topology is

$$\mathcal{J}(u) = \begin{cases} \int_{\Omega} W^{**}(\mathcal{E}u) dx + \int_{\Omega} W^{\infty} \left(\frac{E_s u}{|E_s u|} \right) d|E_s u| & \text{if } u \in U(\Omega), \\ +\infty & \text{otherwise.} \end{cases} \quad (4.3)$$

In the above expression, W^{**} stands for the convex envelope of W and is obtained from W by replacing the plastic energy W^p by its convex hull $[W^p]^{**} = W_0^p$. The corresponding regression function is defined as $W^{\infty}(F) = \lim_{t \rightarrow \infty} W^{**}(t\beta)/t$. *Proof.* Let J^{∞} denote the functional obtained in the case $W^p = W_0^p$. In [22, Theorem 3.3] it was shown that $sc^{-} J^{\infty} = \mathcal{J}$, with respect to the strong L^1 topology. This implies, in particular, that \mathcal{J} is lower semicontinuous. We claim that $\mathcal{J}(u) \leq J(u)$ for all u . Since the right-hand side is ∞ for $u \notin W^{1,2}$, it suffices to consider the case $u \in W^{1,2}$. But then $\mathcal{J}(u)$ equals the integral of $W^{**}(\nabla u)$, and since by assumption $W^{**} = W_0^p \leq W^p$, the claim follows. From the definition of the lower semicontinuous envelope it follows that

$$\mathcal{J} \leq sc^{-} J. \quad (4.4)$$

We now prove the converse inequality. By [22, Theorem 3.3] for any $u \in U(\Omega)$ there is a sequence $u_i \in W^{1,2}(\Omega; \mathbb{R}^3)$ such that $u_i \rightarrow u$ in L^1 , and $J^{\infty}(u_i) \rightarrow \mathcal{J}(u)$. Since $J \leq J^{\infty}$, we have

$$\limsup_{i \rightarrow \infty} J(u_i) \leq \limsup_{i \rightarrow \infty} J^{\infty}(u_i) = \mathcal{J}(u).$$

In turn, $sc^{-} J$ is lower semicontinuous and below J , hence

$$sc^{-} J(u) \leq \liminf_{i \rightarrow \infty} sc^{-} J(u_i) \leq \limsup_{i \rightarrow \infty} sc^{-} J(u_i) \leq \limsup_{i \rightarrow \infty} J(u_i).$$

Comparing these two relations it is clear that

$$sc^{-} J \leq \mathcal{J}$$

which, together with (4.4), implies the thesis. \square

REMARK 1. *The same proof used in [22] establishes that additional kinematical condition can be prescribed on the original model and are not affected by the relaxation process. It is the case*

- when a slipping boundary condition $(u - u_0) \cdot \nu = 0$ is prescribed over $\Gamma \subset \partial\Omega$, ν denoting a normal vector on Γ ;
- for the linearized incompressibility constraint $\operatorname{div} u = 0$.

PROPOSITION 4.2. *If the plastic energy W^p fulfills, in addition to (4.2), also*

$$W^p(\gamma) \leq M|\gamma| \quad \text{for all } \gamma \in \mathbb{R}^N, \quad (4.5)$$

for some $M \in \mathbb{R}$, then Theorem 4.1 holds for any set of slip systems $\{s_i \otimes m_i; 1 \leq i \leq N\}$ such that their symmetric parts span the set of traceless symmetric matrices. The key point in this proof is the following extension of Lemma 3.5 of [22].

LEMMA 4.3. *Let $\mathcal{S} = \{s_i \otimes m_i; 1 \leq i \leq N\}$ be a set of slip systems such that their symmetric parts span the set of traceless symmetric matrices. Then there is c such that for any $\beta \in \mathbb{R}^{3 \times 3}$ one has*

$$W(\beta) \leq c(|\beta + \beta^T| + |\operatorname{Tr} \beta|^2).$$

REMARK 2. In comparing with Lemma 3.5 of [22] one should consider the degenerate laminate $\nu = \delta_\beta$.

Proof. Consider the linear map $T : \mathbb{R}^N \rightarrow \mathbb{R}^{3 \times 3}$ defined by

$$T\gamma = \sum_{i=1}^N \gamma_i \frac{s_i \otimes m_i + s_i \otimes m_i}{2}.$$

By assumption, $T\mathbb{R}^N = \mathbb{R}_{\text{sym},0}^{3 \times 3}$, where $\mathbb{R}_{\text{sym},0}^{n \times n} = \{F \in \mathbb{R}^{n \times n} : F^T = F, \text{Tr } F = 0\}$ is the set of symmetric, traceless matrices. Therefore T has a linear inverse $S : \mathbb{R}_{\text{sym},0}^{3 \times 3} \rightarrow \mathbb{R}^N$ (not necessarily uniquely defined). Consider now a generic $\beta \in \mathbb{R}^{3 \times 3}$, and define

$$\beta_{\text{sym}}^D = \frac{\beta + \beta^T}{2} - \frac{1}{3}(\text{Tr } \beta)\text{Id} \in \mathbb{R}_{\text{sym},0}^{3 \times 3}.$$

We set $\gamma = S\beta_{\text{sym}}^D$. Then,

$$\beta = \omega + \sum_{i=1}^N \gamma_i s_i \otimes m_i + \frac{1}{3}(\text{Tr } \beta)\text{Id},$$

with ω antisymmetric, and $|\gamma| \leq C|\beta_{\text{sym}}^D| \leq C|\beta + \beta^T|$, with a constant depending on \mathcal{S} but not on β . Therefore, recalling (4.5),

$$W(\beta) \leq c|\text{Tr } \beta|^2 + |\beta + \beta^T|C \max_i \tau_i,$$

with a constant depending on the elastic moduli \mathbf{E} and on \mathcal{S} . The thesis follows. \square

5. Algorithmic relaxation. In the absence of an explicit knowledge of the relaxed energy, a fall back strategy is to approximate the relaxation by the consideration of *special microstructures*. These microstructures can be evaluated *a priori*, and the relaxed energy tabulated for subsequent use; or they can be generated 'on the fly', simultaneously with the full scale simulation.

5.1. Sequential lamination. Given the variational structure of the problems under consideration, upper bounds are particularly useful: if W is replaced by any function \tilde{W} such that $\mathcal{Q}W \leq \tilde{W} \leq W$, then sc^-J is not changed. However, if \tilde{W} is a good approximation to $\mathcal{Q}W$, the numerical behavior of the functional might be largely improved. Practically all available approximations to $\mathcal{Q}W$ from above are obtained through the following result, which is (under slightly more stringent assumptions) due to Morrey [47, 48]. The present version is proven in [32], see also [49, Lemma 4.3].

LEMMA 5.1. *If $W : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ is quasiconvex, it is rank-1 convex. This means that for all $A, B \in \mathbb{R}^{m \times n}$ with $\text{rank}(B - A) = 1$, and every $\lambda \in [0, 1]$, one has*

$$W(\lambda A + (1 - \lambda)B) \leq \lambda W(A) + (1 - \lambda)W(B).$$

The converse assertion is false, as proved by the counterexample of Šverák [62]. To characterize the rank-1 convex envelope, we follow the approach of Kohn and Strang [40, 41].

LEMMA 5.2. Let $W : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$. The rank-1 convex envelope $\mathcal{R}W$ of W , i.e., the greatest rank-1 convex function below W , is characterized for every $F \in \mathbb{R}^{m \times n}$ by $\mathcal{R}W(F) = \lim_{k \rightarrow \infty} \mathcal{R}_k W(F)$ with

$$\begin{aligned} \mathcal{R}_0 W(F) &= W(F), \\ \mathcal{R}_{k+1} W(F) &= \inf \left\{ \lambda \mathcal{R}_k W(F_1) + (1 - \lambda) \mathcal{R}_k W(F_2) : \lambda F_1 + (1 - \lambda) F_2 = F, \right. \\ &\quad \left. \lambda \in [0, 1], \text{ and } \text{rank}(F_1 - F_2) \leq 1 \right\}, \quad \forall k \in \mathbb{N}^*. \end{aligned}$$

Additionally, for every $F \in \mathbb{R}^{m \times n}$ and all k , we have $\mathcal{Q}W(F) \leq \mathcal{R}W(F) \leq \mathcal{R}W_k(F) \leq W(F)$.

This iterative characterization is particularly useful if the rank-1 envelope is reached after a *finite number* K of steps, so that $\mathcal{R}W(F) = \mathcal{R}_K W(F)$. This is however in general not true, see the discussion accompanying [24, theorem 1.1, p.201]. From a numerical point of view, in [27, 28] an algorithm for the global determination of rank-one convex envelopes has been developed, and uniform convergence estimates have been proven.

Due to the computable character of $\mathcal{R}_K W(F)$, it is tempting to replace the quasiconvex envelope $\mathcal{Q}W(F)$, unaccessible in general, by the sequential lamination $\mathcal{R}_K W(F)$ where K is fixed to a small value (typically $K = 1$). Then, the energy which will be minimized over finite dimensional spaces is

$$\int_{\Omega} \mathcal{R}_K W(Du). \quad (5.1)$$

Of course, the sequentially laminated energy (5.1) is not guaranteed to have a minimum over X , but the approach has proven useful in elasto-plasticity [54, 55, 5, 22, 13].

5.2. Local enrichment and Partial relaxation. In this section, we illustrate the relation between local enrichment and relaxation in computational hyperelasticity within the finite element framework. Let us consider J of the form (2.2) defined on the space X given by (2.3). We denote by \mathcal{T}_h a mesh of the polygonal domain Ω , and by X_h the associated discrete space of displacements defined as

$$X_h := \{v \in X, \quad v|_T \in [\mathbf{R}_q(T)]^n, \quad \forall T \in \mathcal{T}_h\},$$

where $\mathbf{R}_q(T)$ is the space of polynomials of total (resp. partial) order less than q on the simplex (resp. parallelootope) T . For each element $T \in \mathcal{T}_h$, one can choose a finite-dimension space $E_h(T) \subset W_0^{1,\infty}(T; \mathbb{R}^m)$ of local enrichments. The space E_h of enrichments over Ω can then be defined as

$$E_h := \{v \in W^{1,\infty}(\Omega; \mathbb{R}^m), \quad v|_T \in E_h(T), \quad \forall T \in \mathcal{T}_h\}.$$

The enriched space of approximation being now $X_h \oplus E_h$, one is interested in infimizing

$$\begin{aligned} & \inf_{v_h = \bar{v}_h + v'_h \in X_h \oplus E_h} \int_{\Omega} W(D\bar{v}_h + Dv'_h) \\ &= \inf_{\bar{v}_h \in X_h} \left(\sum_{T \in \mathcal{T}_h} \inf_{v'_h \in E_h(T)} \left(\int_T W(D\bar{v}_h + Dv'_h) \right) \right) \\ &= \inf_{\bar{v}_h \in X_h} \sum_{T \in \mathcal{T}_h} \mathcal{E}_T W(D\bar{v}_h), \end{aligned}$$

where the partially relaxed energy $\mathcal{E}_T W$ on T is defined by the integral relation

$$\mathcal{E}_T W(F) = \inf_{v \in E_h(T)} \int_T W(F + Dv), \quad \forall F \in L^p(T; \mathbb{R}^{m \times n}). \quad (5.2)$$

Assume now that F is constant, i.e., that one is working with piecewise affine functions on simplexes. Recall the definition of the quasiconvex envelope in (2.8),

$$\int_T \mathcal{Q}W(F) = \inf_{v \in W_0^{1,\infty}(T; \mathbb{R}^m)} \int_T W(F + Dv), \quad \forall F \in \mathbb{R}^{m \times n}. \quad (5.3)$$

Since $E_h(T) \subset W_0^{1,\infty}(T; \mathbb{R}^m)$ we have

PROPOSITION 5.3. *Let us consider J of the form (2.2) defined on the space X given by (2.3). With above notation, for every $T \in \mathcal{T}_h$ and every $F \in \mathbb{R}^{m \times n}$, one has*

$$\int_T \mathcal{Q}W(F) \leq \mathcal{E}_T W(F) \leq \int_T W(F). \quad (5.4)$$

This implies immediately that, if X_h consists of functions which are affine on each $T \in \mathcal{T}_h$, then

$$\inf_{\bar{v}_h \in X_h} \sum_{T \in \mathcal{T}_h} \int_T \mathcal{Q}W(D\bar{v}_h) \leq \inf_{\bar{v}_h \in X_h} \sum_{T \in \mathcal{T}_h} \mathcal{E}_T W(D\bar{v}_h) \leq \inf_{\bar{v}_h \in X_h} \sum_{T \in \mathcal{T}_h} \int_T W(D\bar{v}_h). \quad (5.5)$$

As a consequence, the local enrichment of finite element formulations by bubbles as in the Variational Multiscale Method [38, 39] can be interpreted as a partial relaxation of the formulation in the case of minimization problems, at least for $q = 1$ and simplexes. Such an approach extends the early idea of bubble function introduced in [23]. As we will see nevertheless, enriched formulations provide poor advantages in the case of interest here.

REMARK 3. *The preceding conclusion is not at odds with the notable improvements provided by local enrichments in problems where the lack of lower semicontinuity is not an issue, for instance advection-diffusion problems [33, 11, 34, 12] – which can also be rewritten as the minimization of a residual in H^{-1} (see [51]) – or recovering the inf-sup condition for kinematically constrained systems (e. g. incompressibility [4], mortar methods [7, 37]).*

REMARK 4. *We show with two counterexamples that the first inequality in Proposition 5.3 does not hold for higher-order elements, not even for convex energy densities. The first example concerns the case $n = m = 1$, with $W(F) = F^2$, so that $\mathcal{Q}W(F) = W(F)$. We take quadratic elements, i.e., $q = 2$, $T = (-1, 1)$, and consider for definiteness the function $\bar{v}_h(x) = x^2$. Then*

$$\int_{-1}^1 \mathcal{Q}W(2x) dx = 2 \int_{1/2}^1 (2x)^2 dx = \frac{7}{3} > 0.$$

However, if $\tilde{v}_j = 1 - x^2 \in E_h$, then

$$\mathcal{E}_T W(F) \leq \int_{-1}^1 W(\tilde{v}'_h + \tilde{v}'_j) = \int_{-1}^1 W(0) = 0.$$

In the second example we take $n = 2$, $m = 1$, and $W(F) = (F_1 + F_2)^2 + \varepsilon|F|^2$. This is convex and coercive for any $\varepsilon > 0$, the precise value will be chosen at the end.

Therefore $\mathcal{Q}W = W$. Assume $T = (0, 1)^2$, use componentwise affine functions, and let the boundary values be $u(0, 0) = u(0, 1) = u(1, 0) = 0$, $u(1, 1) = 1$. Then the finite element function in T is $u(x) = x_1x_2$, and the corresponding energy

$$\int_T W(Du) = \int_T \mathcal{Q}W(Du) = \int_T (x_1 + x_2)^2 + \varepsilon(x_1^2 + x_2^2) = \frac{7}{6} + \frac{2}{3}\varepsilon.$$

Assume now that the function $v(x) = \min(x_1, x_2) - x_1x_2 \in W_0^{1,\infty}(T)$ is contained in the enrichment set. Then the enriched problem can achieve the energy

$$\int_T W(Du + Dv) = \int_T W(D \min(x_1, x_2)) = \int_T 1 + \varepsilon = 1 + \varepsilon.$$

If $\varepsilon < 1/2$, this energy is lower than the one computed above with the quasiconvex envelope.

6. Numerical examples. In this section we present an application of the concurrent multiscale computing methodology described in the foregoing to single crystal plasticity. Specifically, for computational purposes we take advantage of the knowledge of the exact relaxed energy \mathcal{J} given by theorem 4.1. The discretization should be chosen in order to match the functional form, and the coercivity, of \mathcal{J} . As is evident from the expression given in theorem 4.1, the functional \mathcal{J} is finite not only on continuous deformations, but also on those with jump discontinuities, and with a distributed singular part in the gradient. Precisely, the singular part $E_s u$ of the strain is the sum of a jump term $E_j u = [u] \otimes n \delta_S$ distributed over a 2-dimensional manifold \mathcal{S} inside Ω , and a Cantor part $E_c u$ (see [2]) which is difficult to represent. Moreover, the jump part $E_j u$ might include “high density regions” with high level of branching in micro-fractures. Assuming that fractures remain at the macroscopic level in the relaxed model, it would be possible to allow them within a Finite Element representation by using cohesive elements [53, 19] endowed with the cohesive energy $\int_{\Omega} W^\infty \left(\frac{E_j u}{|E_j u|} \right) d|E_j u|$. Here instead, we work with continuous discretizations. Since smooth functions are dense in BD , this choice of interpolation suffices to achieve the relaxation of the functional.

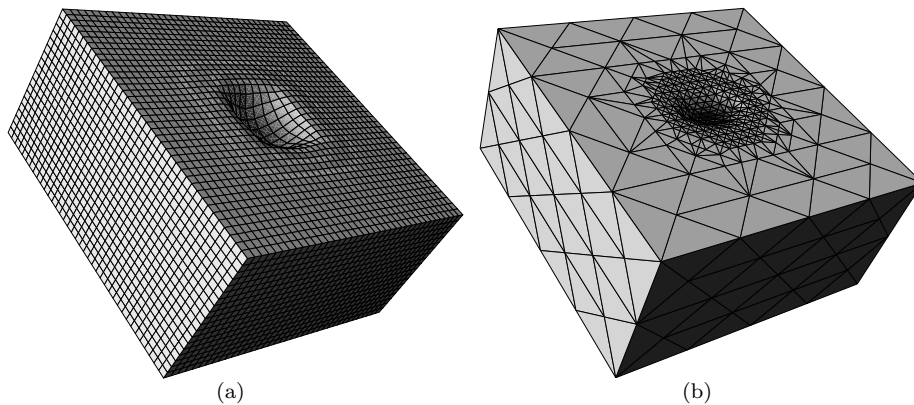


FIG. 6.1. Two models of a BCC single crystal deforming under a rigid indenter. a) Hexahedral mesh with 32000 nodes, 6859 elements; b) Tetrahedral mesh with 5424 nodes, 30779 elements. The vertical displacements are constrained on the base of the crystal, which is otherwise unconstrained.

The particular problem under consideration concerns the indentation of a (100) surface of a BCC crystal, Fig. 6.1. For simplicity, the elastic moduli of the crystal are assumed to be isotropic with Young's modulus $E = 2000$ MPa and Poisson's ratio $\nu = 0.29$. The crystal is assumed to slip on the $\{211\}[111]$ and $\{110\}[111]$ families of systems, and the critical resolved shear stress is taken to be $\tau_0 = 1.0$ MPa for all systems. Two discretizations of the domain are considered: a hexahedral mesh consisting of 32000 nodes and 6859 elements, Fig. 6.1b; and a tetrahedral mesh consisting of 5424 nodes, 30779 elements. The vertical displacements are constrained on the base of the crystal, which is otherwise unconstrained.

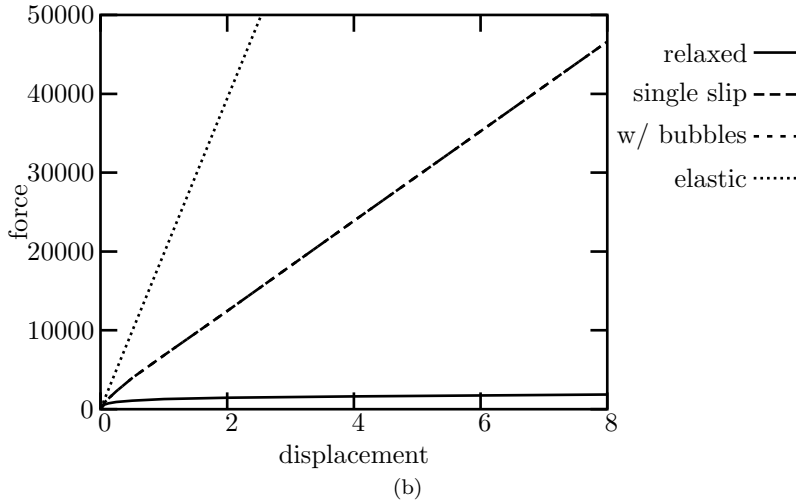
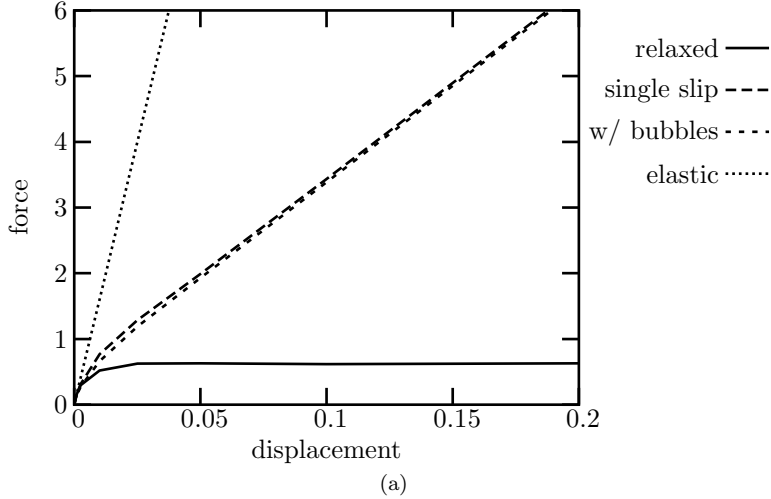


FIG. 6.2. Displacement/force response of the hexahedral (top) and tetrahedral (bottom) models during the nano-indentation process. The curves illustrating single-slip computations with or without bubble enrichment prove to be almost confounded.

The computed indenter force/travel curves for the hexahedral and tetrahedral meshes are shown in Figs. 6.2a and 6.2b, respectively. The figures show the curves computed in the elastic regime; with the unrelaxed, strong latent hardening, single-

crystal plasticity model; a conventional bubble enhancement [23]; and the fully relaxed model. As may be seen from the figures, the behavior of the unrelaxed response is much stiffer than the relaxed response, which attains a limit load. The bubble enhancement affords an ostensibly imperceptible gain in compliance with respect to the unrelaxed model.

Finally, we proceed to demonstrate how the optimal microstructures can be reconstructed *a posteriori* from the solution of the relaxed model. To this end, we begin by recalling the following lemma.

LEMMA 6.1 (Lemma 3.6 of [22]). *Under the assumptions of Theorem 4.1, for any $F \in \mathbb{R}^{3 \times 3}$ and any $\varepsilon > 0$, there exists a laminate ν of finite order such that*

$$\langle \nu, Id \rangle := \int_{\mathbb{R}^{3 \times 3}} \beta \, d\nu(\beta) = F,$$

$$\langle \nu, W \rangle := \int_{\mathbb{R}^{3 \times 3}} W(\beta) \, d\nu(\beta) \leq W^{**}(F) + \varepsilon,$$

where ν is understood as a probability measure on the set $\mathbb{R}^{3 \times 3}$ of matrices.

Considering that for any $F \in \mathbb{R}^{3 \times 3}$ the rank-one envelope is defined by $\mathcal{R}W(F) = \inf\{\langle \nu, W \rangle; \langle \nu, Id \rangle = F\}$, lemma 6.1 ensures that rank-one and convex envelopes coincide, i.e. $\mathcal{R}(F) = W^{**}(F)$. Consequently, due to the inequality $\mathcal{R}W \leq \mathcal{Q}W \leq W^{**}$, it follows that the quasiconvex envelope is also equal to the other two, $\mathcal{Q}W = \mathcal{R}W = W^{**}$. The proof of lemma 6.1 given in [22] is based on the explicit construction of the laminate ν . The precise algorithm for reconstructing optimal microstructures from the solutions of the relaxed problem is as follows:

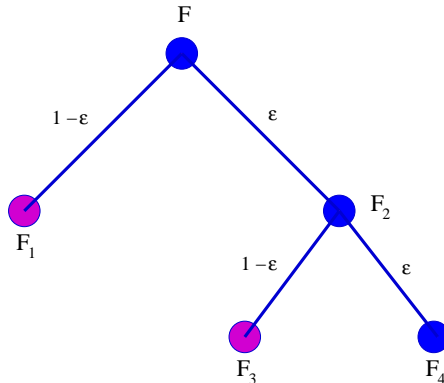
- i) Let $F = F^e + F^p$ be the macroscopic strain. Choose a possible decomposition $F^p = \sum_{i=1}^I \gamma_i s_i \otimes m_i$. One natural choice criterion to enforce is to make I as small as possible; but in general this does not suffice to make the choice unique.
- ii) If $0 \leq I \leq 1$, the laminate $\nu = \delta_F$ is satisfactory (even with $\varepsilon = 0$).
- iii) If $I \geq 2$, a recursive construction can be performed. Precisely, assume that a criterion is given to decompose sums of $I - 1$ slips into laminates, and consider F as above.
 - iii.a) Let $F_1 = F^e + \sum_{i=1}^{I-1} \gamma_i s_i \otimes m_i$ and $F_2 = F_1 + \frac{1}{\varepsilon} \gamma_I s_I \otimes m_I$, so that $(1 - \varepsilon) \delta_{F_1} + \varepsilon \delta_{F_2}$ is a laminate with average F .
 - iii.b) Let $F_3 = F^e + \sum_{i=2}^{I-1} \gamma_i s_i \otimes m_i + \frac{1}{\varepsilon} \gamma_I s_I \otimes m_I$ and $F_4 = F_3 + \frac{1}{\varepsilon} \gamma_1 s_1 \otimes m_1$, so that $(1 - \varepsilon) \delta_{F_3} + \varepsilon \delta_{F_4}$ is a laminate with average F_2 .
 - iii.c) Compose the two mentioned steps, and obtain the laminate

$$\nu = (1 - \varepsilon) \delta_{F_1} + \varepsilon(1 - \varepsilon) \delta_{F_3} + \varepsilon^2 \delta_{F_4} \quad (6.1)$$

with average F .

- iii.d) F_1 and F_3 involve $I - 1$ systems, hence δ_{F_1} and δ_{F_3} can be replaced by appropriate laminates by the inductive assumption.

The laminate described by equation (6.1) can be represented by the following tree:



In this diagram each node is the average of its two daughter nodes weights probabilities specified on the bonds, and each pair of daughter nodes is rank-one compatible.

REMARK 5. *It should be carefully noted that the preceding algorithm, while delivering a laminate with the optimal energy (up to an arbitrarily small error ε), it does not always return the simplest possible laminate. In particular, the algorithm never gives a first-order laminate, even when the average plastic strain is the average of a simple laminate supported on two different slip systems (cf the discussion in Section 3.6 of [22], in particular Lemma 3.10).*

It can be shown ([22], lemma 3.5) that there exists a laminate ν_4 such that

$$\langle \nu_4, Id \rangle = F_4, \quad \langle \nu, W \rangle \leq c(|F_4^{\text{sym}}| + |\text{Tr } F_4|^2).$$

Since this part of the laminate involves (as $\varepsilon \rightarrow 0$) a negligible volume fraction, and a negligible part of the energy, we do not include it in the visualizations of the microstructures. Additionally, in practice, the slip systems are relabeled such that γ_i increases with $1 \leq i \leq I$. Doing so, our algorithm starts by representing the contribution of the highest components of the plastic variable.

As an illustration of the construction just described, Figs.6.3 and 6.4 show the microstructures reconstructed from the solution of the relaxed problem on the hexahedral and tetrahedral meshes, respectively. The software used for the visualization of the laminates is due to Fago [30]. The complexity the optimal microstructures is striking. This complexity makes it unlikely that ad-hoc strain enhancements, based on polynomial, trigonometric or similar representations, may come near to being optimal. Indeed, an enhancement must necessarily account for the physical mechanisms of deformation in order to be effective.

7. Concluding remarks. Concurrent multiscale computing provides a powerful means of accounting for the development of deformation microstructures in situations in which there is a strict separation of scales. In these cases, the macroscopic behavior is accurately described by the relaxed problem, which in turn can be solved numerically by standard methods such as finite elements, and the deformation microstructures take place at the sub-grid level. The particular example presented in this paper, concerned with single crystals possessing strong latent hardening, demonstrates the vast effect of microstructure formation on the macroscopic behavior of the sample, e. g., on the force/travel curve of a rigid indenter. Thus, whereas the unrelaxed model results in an overly stiff response, the relaxed model exhibits a proper limit load, as

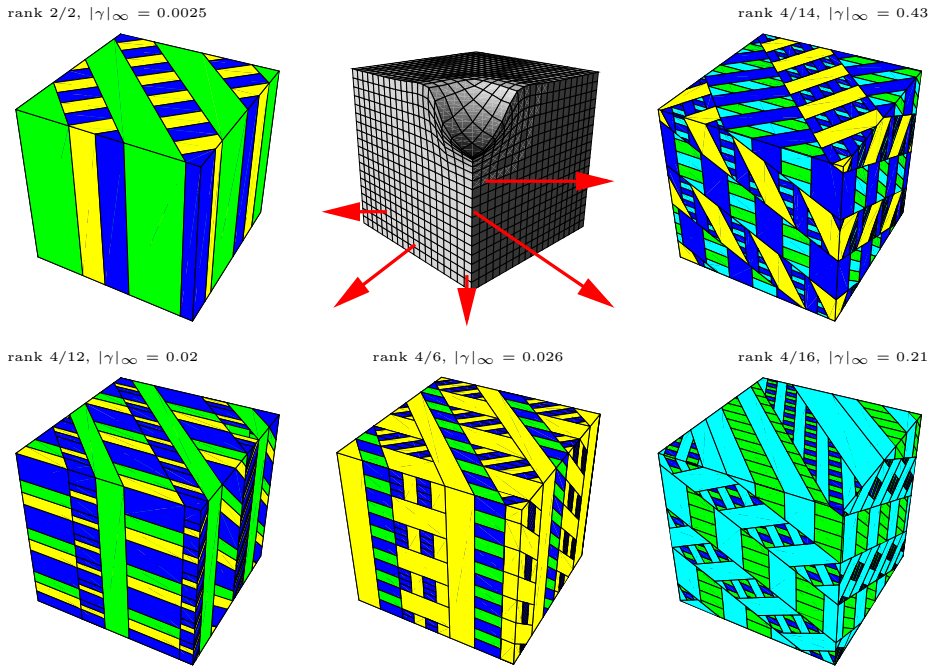


FIG. 6.3. Reconstruction at selected Gauss-points of optimal microstructures from the solution of the relaxed problem on the hexahedral mesh. The order of the laminate as well as the maximum slip strain magnitude are indicated. The reconstruction is performed for $\varepsilon = 0.5$.

expected. The numerical examples reported in this paper also illustrate that ad-hoc element enhancements are unlikely to result in any significant relaxation. The application to single crystals also demonstrates an evident but nevertheless compelling fact: the explicit knowledge of the relaxation of a problem results in an enormous reduction of computational cost, and a correspondingly vast improvement in performance, with respect to methods that construct sub-grid microstructures numerically 'on the fly' (e.g., [5]). This strongly suggests that explicit relaxation results such as collected in Section 4 will inevitably play a decisive role in rendering multiscale computing feasible.

We close by pointing some of the limitations of the framework presented in this paper. Strict separation of scales is an idealization which is never completely realized in nature. In actual materials, the process of microstructural refinement described by a minimizing sequence is checked by physical phenomena unaccounted for in the original model. For instance, in single crystals the interfaces between the variants of a laminate are dislocation walls that carry a well-defined energy per unit area [54]. Consideration of this additional energy has the effect of introducing an intrinsic lengthscale commensurate with the Burgers vector and is responsible for scaling laws such as the Hall-Petch effect [55, 22]. The dislocation wall energy has the additional effect of radically changing the geometry of the optimal microstructures, which tend to exhibit self-similar refinement towards the boundary [22]. Under these conditions, the relaxed energy of, e.g., a grain is no longer local, i.e. described by an effective energy density depending solely on the deformation gradient. To the best of our knowledge, the formulation of multiscale numerical methods capable of dealing with

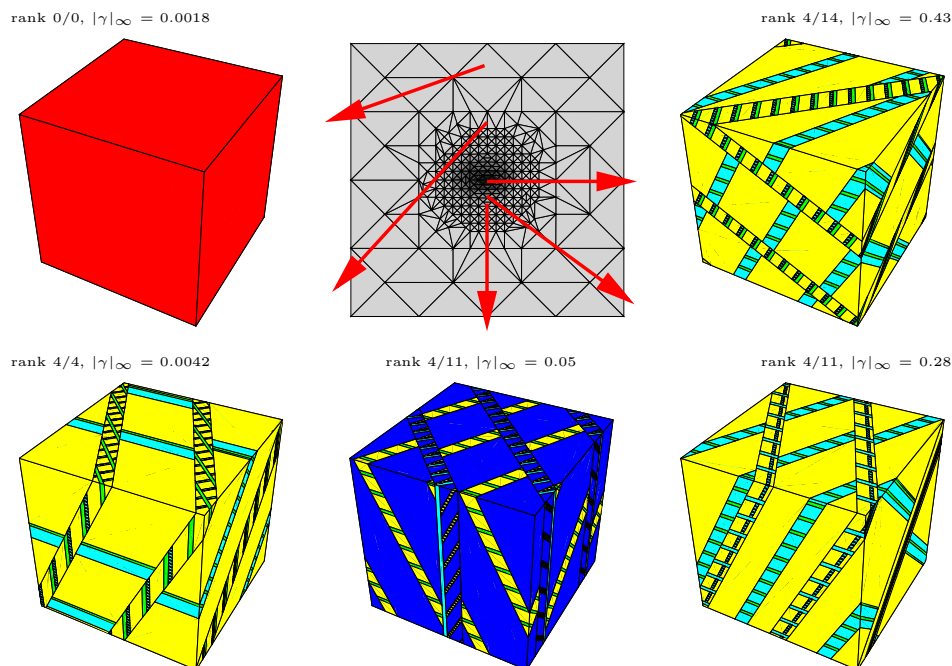


FIG. 6.4. Reconstruction at selected Gauss-points of optimal microstructures from the solution of the relaxed problem on the tetrahedral mesh. The order of the laminate as well as the maximum slip strain magnitude are indicated. The reconstruction is performed for $\varepsilon = 0.2$.

nonlocal effective energies remains an open question at present.

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