

COMPUTATION OF LOWER SEMICONTINUOUS ENVELOPE OF INTEGRAL FUNCTIONALS AND NON-HOMOGENEOUS MICROSTRUCTURES

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ABSTRACT. A numerical method is established to compute the weakly lower semicontinuous envelope of integral functionals with non-quasiconvex integrands. The convergence of the method is proved and it is shown that the method is capable of capturing curved and non-homogeneous microstructures. Numerical examples are given to show the effectiveness of the method to capture curved and non-homogeneous laminated microstructures.

1. INTRODUCTION

Consider the problem of minimizing an integral functional

$$F(u; \Omega) = \int_{\Omega} f(x, u(x), \nabla u(x)) dx \quad (1.1)$$

with nonquasiconvex integrand $f : \Omega \times R^m \times R^{mn} \rightarrow R^1$ in a set of admissible functions

$$\mathbb{U}(u_0; \Omega) = \{u \in W^{1,p}(\Omega; R^m) : u = u_0, \text{ on } \partial\Omega\}, \quad (1.2)$$

where $\Omega \subset R^n$ is a bounded open set with Lipschitz continuous boundary $\partial\Omega$ and $1 < p < \infty$. To solve the problem, the Γ^- -limit of the functional $F(\cdot; \Omega)$ in $\mathbb{U}(u_0; \Omega)$, which is identified by

$$\Gamma^- \text{-lim } F(u; \Omega) = \min\{\liminf_{\alpha \rightarrow \infty} F(u_{\alpha}; \Omega) : u_{\alpha} \in \mathbb{U}(u_0; \Omega), \\ u_{\alpha} \rightharpoonup u \text{ in } W^{1,p}(\Omega; R^m)\}, \quad (1.3)$$

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(where ' $\rightharpoonup$ ' means 'converges weakly to') plays an important role, since it is the sequentially weakly lower semicontinuous envelope of $F(\cdot; \Omega)$ in $\mathbb{U}(u_0; \Omega)$, *i.e.*, the greatest sequentially weakly semicontinuous functional defined on $\mathbb{U}(u_0; \Omega)$ less than or equal to $F(\cdot; \Omega)$ (see [7, 13]).

The main purpose of this paper is to establish a numerical method to evaluate Γ -lim $F(u; \Omega)$ for a given $u \in \mathbb{U}(u_0; \Omega)$ under the hypotheses

(H1): $f : \Omega \times R^m \times R^{mn} \rightarrow R^1$ is continuous and

$$0 \leq f(x, s, \xi) \leq a + b(|s|^p + |\xi|^p), \quad (1.4)$$

where $a \in R^1$ and $b > 0$.

(H2): $Qf : \Omega \times R^m \times R^{mn} \rightarrow R^1$, the quasiconvex envelope of f respect to the last variable [3, 13, 32], is continuous.

(H3): Γ -lim $F(\cdot; \Omega)$ defined by (1.3) has an integral representation

$$\Gamma\text{-lim } F(u; \Omega) = QF(u; \Omega) \equiv \int_{\Omega} Qf(x, u(x), \nabla u(x)) \, dx. \quad (1.5)$$

Remark 1.1. It is well known that (H3) is satisfied under certain general hypotheses on the growth and coerciveness of f [1, 7, 13, 22, 31]. For example, let f be continuous and such that

$$\textbf{(h1): } \max\{0, a_1 + b_1(|s|^p + |\xi|^p)\} \leq f(x, s, \xi) \leq a_2 + b_2(|s|^p + |\xi|^p),$$

$$\textbf{(h2): } |f(x, s, \xi) - f(x, t, \eta)| \leq K(1 + |s|^{p-1} + |t|^{p-1} + |\xi|^{p-1} + |\eta|^{p-1})(|s - t| + |\xi - \eta|),$$

$$\textbf{(h3): } |f(x, s, \xi) - f(y, s, \xi)| \leq \beta(|x - y|)(1 + |s|^p + |\xi|^p),$$

where $a_1 \in R^1$, $a_2 > 0$, $b_2 \geq b_1 > 0$, $K > 0$, $\beta : R^1 \rightarrow R^1$ is continuous and increasing and $\beta(0) = 0$. Then, (H1)-(H3) are satisfied [13].

Since the minimizing sequences of $F(\cdot; \Omega)$ in $\mathbb{U}(u_0; \Omega)$ often consist of finer and finer oscillations and lead to microstructures [4, 13, 20, 23], and since for non-homogeneous integrand f or for nonlinear boundary data the microstructures are in general non-homogeneous and not necessarily being flat laminated, the method to be established should be capable of capturing non-homogeneous and curved microstructures.

Many numerical methods have been developed for the computation of (flat) laminated microstructures, for example, gradient iterative methods [11, 12], methods utilizing simulated annealing and Monte Carlo techniques [17, 29],

rotational transformation method and mesh transformation type methods [24, 25, 27], numerical methods using quasi-convex envelope [8], the Young measure relaxation [9] and rank-one convex envelope [14, 26], more references can be found in [16, 30]. Numerical methods for the computation of non-homogeneous microstructures in homogeneous materials have also been developed, see for example [2, 28]. As is known that for homogeneous materials, the interfaces of laminated microstructures are always flat, since the gradients on both sides of an interface are constants. However, for non-homogeneous materials the interfaces of laminated microstructures can be non-flat or, in other word, curved, since the gradients in a laminate may no longer be constant in such cases, and as far as what is known to the author, there still lack a practical numerical method designed for the computation of non-homogeneous and curved laminated microstructures.

In the present paper, aimed at computing non-homogeneous and curved laminated microstructures, a numerical method for the evaluation of Γ - $\lim F(u; \Omega)$ is given. The basic idea is to approximate the value by the solutions to a set of subproblems defined on a finite element subdivision of Ω (see Sec. 2), the subproblems, each of which concerns with homogeneous integrand and boundary data, are then solved parallelly by any available numerical methods, for example the rotational transformation method combined with the incremental crystallization method [24] (see Sec. 3). In Sec. 4, the finite element solutions to the subproblems are used to construct minimizing sequences of the original problem (see (1.3)) and the convergence of the method is proved. In Sec. 5, numerical examples are given to show the effectiveness of the method in the computation of curved and non-homogeneous laminated microstructures.

2. SEMI-DISCRETIZATION AND HOMOGENEOUS SUBPROBLEMS

For simplicity, let Ω be a polyhedron, let $\mathfrak{T}_h(\Omega)$ be regular triangulations of Ω [10] and let u_0 and $\mathfrak{T}_h(\Omega)$ be such that

$$u_0|_{\partial\Omega \cap \partial K} \in (P_1(\partial\Omega \cap \partial K))^m, \quad \forall K \in \mathfrak{T}_h(\Omega), \quad (2.1)$$

where $P_1(E)$ is the set of all affine functions defined on E . Define

$$\begin{aligned} U_h(u_0; \Omega) = \{u \in (C(\bar{\Omega}))^m : u|_K \in (P_1(K))^m, \forall K \in \mathfrak{T}_h(\Omega); \\ u = u_0, \text{ on } \partial\Omega\}. \end{aligned} \quad (2.2)$$

Let $u \in U(u_0; \Omega)$. By the finite element approximation theory [10], there exist finite element functions $u_h \in U_h(u_0; \Omega)$ such that

$$u_h \rightarrow u \quad \text{in } W^{1,p}(\Omega; \mathbb{R}^m). \quad (2.3)$$

Lemma 2.1. *Let $f : \Omega \times \mathbb{R}^m \times \mathbb{R}^{mn} \rightarrow \mathbb{R}^1$ satisfy the hypotheses (H1)-(H3). Then*

$$\lim_{h \rightarrow 0} \Gamma\text{-}\lim F(u_h; \Omega) = \Gamma\text{-}\lim F(u; \Omega). \quad (2.4)$$

Proof. By (H1) and (H2), $Qf : \Omega \times \mathbb{R}^m \times \mathbb{R}^{mn} \rightarrow \mathbb{R}^1$ is continuous and satisfies [13]

$$0 \leq Qf(x, s, \xi) \leq a + b(|s|^p + |\xi|^p). \quad (2.5)$$

Thus (2.4) follows from (H3), (2.3) and the dominated convergence theorem [15]. $\square$

Let $h_i > 0$, $i = 1, 2, \dots$ be a sequence of numbers such that

$$\lim_{i \rightarrow \infty} h_i = 0, \quad (2.6)$$

and

$$\mathfrak{T}_{h_{i+1}}(\Omega) \succ \mathfrak{T}_{h_i}(\Omega), \quad \forall i, \quad (2.7)$$

i.e., for all i , $\mathfrak{T}_{h_{i+1}}(\Omega)$ is a refinement of $\mathfrak{T}_{h_i}(\Omega)$.

Lemma 2.2. *Let the hypotheses (H1) and (H2) be satisfied. Then*

$$\int_{\Omega} Qf(x, u_{h_i}(x), \nabla u_{h_i}(x)) dx = \lim_{j \rightarrow \infty} \sum_{K \in \mathfrak{T}_{h_{i+j}}(\Omega)} \int_{\Omega} Qf(x_K, u_{h_i}(x_K), A_K) dx \quad (2.8)$$

for all i , where

$$\begin{cases} x_K \in K, & \forall K \in \mathfrak{T}_{h_{i+j}}(\Omega), \\ A_K = \nabla u_{h_i}|_K, & \forall K \in \mathfrak{T}_{h_{i+j}}(\Omega). \end{cases} \quad (2.9)$$

Proof. (2.8) follows as a consequence of the continuity of Qf and u_{h_i} , (2.5) and the dominated convergence theorem [15]. $\square$

For each $K \in \mathfrak{T}_{h_{i+j}}(\Omega)$, define $f_{i,K} : \mathbb{R}^{mn} \rightarrow \mathbb{R}^1$ by

$$f_{i,K}(\xi) = f(x_K, u_{h_i}(x_K), A_K + \xi). \quad (2.10)$$

Then, by the definition of quasiconvex envelope [3, 13, 32], we have

$$Qf_{i,K}(\xi) = Qf(x_K, u_{h_i}(x_K), A_K + \xi). \quad (2.11)$$

Lemma 2.3. *Let f satisfy (H1). Then, for all $i \geq 1$ and $K \in \mathfrak{T}_{h_{i+j}}(\Omega)$, we have*

$$Qf_{i,K}(0) \text{meas}(K) = \inf_{v \in U(0; K)} \int_K f_{i,K}(\nabla v(x)) dx. \quad (2.12)$$

Proof. By (H1), $f_{i,K}$ is continuous and satisfies

$$0 \leq f_{i,K}(\xi) \leq c_i + c_2|\xi|^p, \quad (2.13)$$

where $c_i \in R^1$ and $c_2 > 0$. Thus (2.12) follows [1, 7, 13]. $\square$

Summing up the above analyses, we obtain the following semidiscretization result.

Theorem 2.1. *Let f satisfy (H1)-(H3). Then*

$$\Gamma\text{-}\lim F(u; \Omega) = \lim_{i \rightarrow \infty} \lim_{j \rightarrow \infty} \sum_{K \in \mathfrak{T}_{h_{i+j}}(\Omega)} \inf_{v \in U(0; K)} \int_K f_{i,K}(\nabla v(x)) dx, \quad (2.14)$$

where $f_{i,K}$ is defined by (2.10).

Proof. (2.14) is a direct consequence of lemma 2.1- 2.3, (2.6) and (2.11). $\square$

This motivates us to evaluate $\Gamma\text{-}\lim F(u; \Omega)$ and to find a minimizing sequence to the right-hand side of (1.3) by solving numerically the subproblems

$$\inf_{v \in U(0; K)} \int_K f_{i,K}(\nabla v(x)) dx, \quad (2.15)$$

for all $K \in \mathfrak{T}_{h_{i+j}}(\Omega)$. Notice here that for each subproblem both the integrand (see (2.10)) and the boundary data ($v = 0$ on ∂K) are homogeneous.

Theorem 2.2. *Let f satisfy (h1)-(h3). Let $\{\tilde{u}_\alpha^{i,K}\}_{\alpha=1}^\infty$ be minimizing sequences of (2.15) satisfying*

$$\tilde{u}_\alpha^{i,K} \rightharpoonup 0, \quad \text{in } W^{1,p}(K; R^m) \text{ as } \alpha \rightarrow \infty. \quad (2.16)$$

Let the functions $u_\alpha^{i,j} \in U(u_0; \Omega)$ be defined by

$$u_\alpha^{i,j}(x) = u_{h_i}(x) + \tilde{u}_\alpha^{i,K}(x), \quad \text{if } x \in K, \forall K \in \mathfrak{T}_{h_{i+j}}(\Omega). \quad (2.17)$$

Then, we have

$$\Gamma\text{-}\lim F(u; \Omega) = \lim_{i \rightarrow \infty} \lim_{j \rightarrow \infty} \lim_{\alpha \rightarrow \infty} F(u_\alpha^{i,j}; \Omega). \quad (2.18)$$

Furthermore, there exist nondecreasing functions $J(i)$ and $A(i, j)$ such that the sequence $\{u^i\}$ defined by

$$u^i(x) = u_\alpha^{i,j}(x), \quad \forall x \in \Omega, \quad \forall i \text{ and } j \geq J(i), \quad \alpha \geq A(i, j)$$

is a minimizing sequence of $\Gamma\text{-}\lim F(u; \Omega)$, that is

$$u^i \rightharpoonup u \quad \text{in } W^{1,p}(\Omega; \mathbb{R}^m), \quad (2.19)$$

$$\Gamma\text{-}\lim F(u; \Omega) = \lim_{i \rightarrow \infty} F(u^i; \Omega). \quad (2.20)$$

Proof. By the minimizing property of $\{\tilde{u}_\alpha^{i,K}\}_{\alpha=1}^\infty$ and the hypothesis (h1), it is easily seen that $u_\alpha^{i,j}$ are uniformly bounded in $W^{1,p}(\Omega; \mathbb{R}^m)$, that is

$$\|u_\alpha^{i,j}\|_{1,p} \leq C, \quad \forall i, j, \alpha, \quad (2.21)$$

for a constant C . By (2.16), (2.17) and the Kondrakov compactness theorem [6], we have

$$\lim_{\alpha \rightarrow \infty} \|u_\alpha^{i,j}\|_{0,p} = 0, \quad \forall i, j. \quad (2.22)$$

Since $\{\tilde{u}_\alpha^{i,K}\}_{\alpha=1}^\infty$ are minimizing sequences of (2.15), it follows from (2.9), (2.10) and theorem 2.1 (see also remark 1.1) that

$$\Gamma\text{-}\lim F(u; \Omega) = \lim_{i \rightarrow \infty} \lim_{j \rightarrow \infty} \lim_{\alpha \rightarrow \infty} \sum_{K \in \mathfrak{T}_{h_i+j}(\Omega)} \int_K f(x_K, u_{h_i}(x_K), \nabla u_\alpha^{i,j}(x)) dx.$$

Thus, by (h2) and (h3), there is a constant $C > 0$ such that

$$\begin{aligned} & |\Gamma\text{-}\lim F(u; \Omega) - \lim_{i \rightarrow \infty} \lim_{j \rightarrow \infty} \lim_{\alpha \rightarrow \infty} F(u_\alpha^{i,j}; \Omega)| \\ & \leq \lim_{i \rightarrow \infty} \lim_{j \rightarrow \infty} \lim_{\alpha \rightarrow \infty} C \{ (\text{meas}(\Omega))^{\frac{p-1}{p}} + \|u_{h_i}\|_{1,p}^{\frac{p-1}{p}} + \|u_\alpha^{i,j}\|_{1,p}^{\frac{p-1}{p}} \|u_{h_i} - u_\alpha^{i,j}\|_{0,p} \\ & \quad + \beta(h_{i+j})(\text{meas}(\Omega) + \|u_{h_i}\|_{1,p}^p + \|u_\alpha^{i,j}\|_{1,p}^p) \}. \end{aligned} \quad (2.23)$$

In view of (2.3), (2.6), (2.21), (2.22) and $\lim_{t \rightarrow 0} \beta(t) = 0$ (see (h3)), (2.23) gives (2.18). (2.19) and (2.20) follows from (2.3), (2.16), (2.18) and a standard diagonal process. $\square$

3. NUMERICAL SOLUTIONS TO THE HOMOGENEOUS SUBPROBLEMS

Let f satisfy (H1). Let u_{h_i} and $\mathfrak{T}_{h_{i+j}}(\Omega)$ be given. Consider the problems of minimizing the integral functional

$$F_{i,K}(u; \Omega) = \int_{\Omega} f_{i,K}(\nabla u(x)) dx \quad (3.1)$$

in the set of admissible functions

$$\mathbb{U}(u_0; K) = \{u \in W^{1,p}(K; R^m) : u = u_0, \text{ on } \partial K\}, \quad (3.2)$$

for all $K \in \mathfrak{T}_{h_{i+j}}(\Omega)$. It will be much more convenient if the problems can be solved numerically on a common reference configuration.

Let $\hat{K} \subset B(0; 1)$ be a given n -simplex with $0 \in \hat{K}$, where

$$B(x_0; r) = \{x \in R^n : \|x - x_0\| < r\}.$$

Lemma 3.1. *For each $K \in \mathfrak{T}_{h_{i+j}}(\Omega)$, there exists a $n \times n$ matrix B_K with $\det B_K > 0$ and a point $x_K \in K$ such that the linear mapping*

$$x = G_K(\hat{x}) \equiv h_K B_K \hat{x} + x_K \quad (3.3)$$

maps $\hat{K}$ on to K , that is

$$K = G_K(\hat{K}), \quad (3.4)$$

where $h_K = \text{diam}(K)$ is the diameter of K . Furthermore, there exists a constant C which is independent of i, j and K such that

$$\|B_K\| \leq C, \quad \|B_K^{-1}\| \leq C, \quad \forall K \in \mathfrak{T}_{h_{i+j}}(\Omega), \quad \forall i, j. \quad (3.5)$$

Proof. Since every $K \in \mathfrak{T}_{h_{i+j}}(\Omega)$ is a n -simplex, the first part of the lemma is obvious. (3.5) follows from the fact that $\mathfrak{T}_{h_{i+j}}(\Omega)$ are regular triangulations of Ω [10]. $\square$

Let $B_K, K \in \mathfrak{T}_{h_{i+j}}(\Omega)$, be given by lemma 3.1. Then a natural 1-1 correspondence between $U(0; K)$ and $U(0; \hat{K})$ can be established by

$$\hat{u}(\hat{x}) = h_K^{-1} u(h_K B_K \hat{x} + x_K), \quad \forall u \in U(0; K). \quad (3.6)$$

Theorem 3.1. For all $K \in \mathfrak{T}_{h_{i+j}}(\Omega)$, we have

$$\inf_{v \in U(0; K)} \int_K f_{i,K}(\nabla v(x)) dx = \frac{\text{meas}(K)}{\text{meas}(\hat{K})} \inf_{\hat{v} \in U(0; \hat{K})} \int_{\hat{K}} f_{i,K}(\nabla \hat{v}(\hat{x}) B_K^{-1}) d\hat{x}. \quad (3.7)$$

Proof. Let $u \in U(0; K)$ and $\hat{u} \in U(0; \hat{K})$ be related by (3.6). Then, it follows from (3.3) and (3.4) that

$$\int_K f_{i,K}(\nabla u(x)) dx = \int_{\hat{K}} f_{i,K}(\nabla \hat{u}(\hat{x}) B_K^{-1}) h_K^n \det B_K d\hat{x}.$$

Since

$$h_K^n \det B_K = \frac{\text{meas } K}{\text{meas}(\hat{K})},$$

we have

$$\int_K f_{i,K}(\nabla u(x)) dx = \frac{\text{meas}(K)}{\text{meas}(\hat{K})} \int_{\hat{K}} f_{i,K}(\nabla \hat{u}(\hat{x}) B_K^{-1}) d\hat{x}. \quad (3.8)$$

This implies (3.7), since (3.6) is a 1-1 correspondence. $\square$

Theorem 3.2. Let $\{\hat{u}_\alpha\}_{\alpha=1}^\infty$ be a minimizing sequence of

$$\hat{F}_{i,K}(\hat{u}; \hat{K}) = \int_{\hat{K}} f_{i,K}(\nabla \hat{u}(\hat{x}) B_K^{-1}) d\hat{x} \quad (3.9)$$

in $U(0; \hat{K})$. Then

$$u_\alpha(x) = h_K \hat{u}_\alpha(h_K^{-1} B_K^{-1}(x - x_K)), \quad \alpha = 1, 2, \dots \quad (3.10)$$

is a minimizing sequence of $F_{i,K}(\cdot; K)$ in $U(0; K)$.

Proof. Since (3.10) implies that u_α and $\hat{u}_\alpha$ are related by (3.6), it follows from (3.8) that

$$F_{i,K}(u_\alpha; K) = \frac{\text{meas}(K)}{\text{meas}(\hat{K})} \hat{F}_{i,K}(\hat{u}_\alpha; \hat{K}), \quad \forall \alpha.$$

Thus, by theorem 3.1, we have

$$\lim_{\alpha \rightarrow \infty} F_{i,K}(u_\alpha; K) = \frac{\text{meas}(K)}{\text{meas}(\hat{K})} \inf_{\hat{u} \in U(0; \hat{K})} \hat{F}_{i,K}(\hat{u}; \hat{K}) = \inf_{u \in U(0; K)} F_{i,K}(u; K).$$

This completes the proof. $\square$

Instead of solving the subproblems (2.15) directly, theorem 3.1 and theorem 3.2 allow us to obtain numerical solutions to (2.15) by solving the problems

$$\inf_{\hat{u} \in U(0; \hat{K})} \int_{\hat{K}} f_{i,K}(\nabla \hat{u}(\hat{x}) B_K^{-1}) d\hat{x} \quad (3.11)$$

for all $K \in \mathfrak{T}_{h_{i+j}}(\Omega)$.

Remark 3.1. Since for all $K \in \mathfrak{T}_{h_{i+j}}(\Omega)$ the problems (3.11) are defined on a same standard domain $\hat{K}$, the programming is much simplified.

Remark 3.2. The problems (3.11) are independent of each other and thus can be solved parallelly by any available numerical methods, for example, the rotational transformation method [24], the periodic relaxation method [25] and the mesh transformation method [27] can be applied to compute simple laminated microstructures, and methods to compute finite order laminated microstructures can be found in [26, 28].

For simplicity, we consider to solve the problem of minimizing the functional $\hat{F}_{i,K}(\cdot; \hat{K})$ in $U(0; \hat{K})$ (see (3.11)) by the rotational transformation method [24]. Similar results can be obtained by applying other methods. Let $D = (-1, 1)^n$. Let $\hat{\mathfrak{T}}_{\hat{h}}(D)$ be regular triangulations [10] of D , and let

$$U_{\hat{h}}(0; D) = \{u \in (C(\bar{D}))^m : u|_{D_e} \in (P_1(D_e))^m, \forall D_e \in \hat{\mathfrak{T}}_{\hat{h}}(D); \\ u = 0, \text{ on } \partial D\}, \quad (3.12)$$

$$SO^+(n) = \{R \in R^{n \times n} : R = R^T, R^T R = I, \det R = 1\}.$$

Define

$$\hat{F}_{i,K}(u, R; D) = \int_D f_{i,K}(\nabla u(\hat{x}) R^{-1} B_K^{-1}) d\hat{x}. \quad (3.13)$$

The rotational transformation problem leads to the following finite problem

$$\begin{cases} \text{Find } (u_{\hat{h}}, R_{\hat{h}}) \in U_{\hat{h}}(0; D) \times SO^+(n) \text{ such that} \\ \hat{F}_{i,K}(u_{\hat{h}}, R_{\hat{h}}; D) = \inf_{(u', R') \in U_{\hat{h}}(0; D) \times SO^+(n)} \hat{F}_{i,K}(u', R'; D), \end{cases} \quad (3.14)$$

which can be solved by the gradient method combined with the incremental crystallization method [24]. Briefly speaking, (3.14) is first solved on a small subset D_0 of D to produce a crystal core, and then it is solved iteratively on an incrementally increasing subset D_β , $\beta = 1, 2, \dots, M$ of D with $D_M = D$.

Lemma 3.2. Let $(u_{\hat{h}}^{i,K}, R_{\hat{h}}^{i,K}) \in U_{\hat{h}}(0; D) \times SO^+(n)$ be a solution to (3.14). Then, the function $\bar{u}_{\hat{h}}^{i,K} : R_{\hat{h}}^{i,K}(D) \rightarrow \mathbb{R}^m$ defined by

$$\bar{u}_{\hat{h}}^{i,K}(\hat{x}) = u_{\hat{h}}^{i,K}((R_{\hat{h}}^{i,K})^{-1}\hat{x}) \quad (3.15)$$

is a minimizer of $\hat{F}_{i,K}(\cdot; R_{\hat{h}}^{i,K}(D))$ in $U_{\hat{h}}(0; R_{\hat{h}}^{i,K}(D))$. As a consequence, we have

$$\inf_{u \in U_{\hat{h}}(0; R_{\hat{h}}^{i,K}(D))} \hat{F}_{i,K}(u; R_{\hat{h}}^{i,K}(D)) = \inf_{(u', R') \in U_{\hat{h}}(0; D) \times SO^+(n)} \hat{F}_{i,K}(u', R'; D).$$

Proof. A straightforward calculation by using the 1-1 correspondence between $U_{\hat{h}}(0; D)$ and $U_{\hat{h}}(0; R_{\hat{h}}^{i,K}(D))$ shows the result. $\square$

Lemma 3.3. ([24]) For all i, K , we have

$$\begin{aligned} & \frac{1}{\text{meas}(\hat{K})} \inf_{u \in U(0; \hat{K})} \hat{F}_{i,K}(u; \hat{K}) = Qf_{i,K}(0) \\ & = \frac{1}{\text{meas}(D)} \lim_{\hat{h} \rightarrow 0} \inf_{(u', R') \in U_{\hat{h}}(0; D) \times SO^+(n)} \hat{F}_{i,K}(u', R'; D). \end{aligned} \quad (3.16)$$

Proof. Let $(u_{\hat{h}}^{i,K}, R_{\hat{h}}^{i,K}) \in U_{\hat{h}}(0; D) \times SO^+(n)$ be a solution to (3.14) and let $\bar{u}_{\hat{h}}^{i,K}$ be defined by (3.15), then

$$\begin{aligned} \inf_{u \in U(0; R_{\hat{h}}^{i,K}(D))} \hat{F}_{i,K}(u; R_{\hat{h}}^{i,K}(D)) & \leq \hat{F}_{i,K}(\bar{u}_{\hat{h}}^{i,K}; R_{\hat{h}}^{i,K}(D)) \\ & = \hat{F}_{i,K}(u_{\hat{h}}^{i,K}, R_{\hat{h}}^{i,K}; D) \leq \inf_{u \in U_{\hat{h}}(0; D)} \hat{F}_{i,K}(u; D). \end{aligned}$$

Since (see [13, 24])

$$\begin{aligned} \inf_{u \in U(0; R_{\hat{h}}^{i,K}(D))} \hat{F}_{i,K}(u; R_{\hat{h}}^{i,K}(D)) & = \text{meas}(D)Qf_{i,K}(0), \\ \lim_{\hat{h} \rightarrow 0} \inf_{u \in U_{\hat{h}}(0; D)} \hat{F}_{i,K}(u; D) & = \inf_{u \in U(0; D)} \hat{F}_{i,K}(u; D) = \text{meas}(D)Qf_{i,K}(0), \end{aligned}$$

and

$$\inf_{u \in U(0; \hat{K})} \hat{F}_{i,K}(u; \hat{K}) = \text{meas}(\hat{K})Qf_{i,K}(0),$$

(3.16) is proved. $\square$

Let $(u_{\hat{h}}^{i,K}, R_{\hat{h}}^{i,K}) \in U_{\hat{h}}(0; D) \times SO^+(n)$ be a sequence of solutions to (3.14) with $\hat{h} \rightarrow 0$, then $\bar{u}_{\hat{h}}^{i,K}$ defined by (3.15) can be used to construct a minimizing sequence of $\hat{F}_{i,K}(\cdot; \hat{K})$ in $U(0; \hat{K})$.

A standard way of doing so (see [13]) is to first extend $\bar{u}_{\hat{h}}^{i,K}$ periodically from $R_{\hat{h}}^{i,K}(D)$ to the whole of R^n and then define

$$\hat{u}_{\hat{h}}^{i,K}(\hat{x}) = \begin{cases} \hat{h} \bar{u}_{\hat{h}}^{i,K}(\hat{h}^{-1} \hat{x}), & \text{if } \hat{x} \in \hat{K}_{\hat{h}}, \\ 0, & \text{otherwise,} \end{cases} \quad (3.17)$$

where

$$\hat{K}_{\hat{h}} = \{x : x \in \hat{h}(2R_{\hat{h}}^{i,K}(z) + R_{\hat{h}}^{i,K}(D)) \subset \hat{K} \text{ for some } z \in \mathbf{Z}^n\}$$

and where $\mathbf{Z}$ is the set of all integers.

Theorem 3.3. *Let $(u_{\hat{h}}^{i,K}, R_{\hat{h}}^{i,K}) \in U_{\hat{h}}(0; D) \times SO^+(n)$ be a sequence of solutions to (3.14) with $\hat{h} \rightarrow 0$ such that*

$$|u_{\hat{h}}^{i,K}|_{1,p,D} \leq C, \quad \forall \hat{h}, \quad (3.18)$$

where C is a constant independent of $\hat{h}$. Then, the sequence $\{\hat{u}_{\hat{h}}^{i,K}\} \subset U(0; \hat{K})$ defined by (3.17) is such that

$$\hat{u}_{\hat{h}}^{i,K} \rightharpoonup 0, \quad \text{in } W^{1,p}(\hat{K}; R^m), \quad \text{as } \hat{h} \rightarrow 0, \quad (3.19)$$

$$\lim_{\hat{h} \rightarrow 0} \hat{F}_{i,K}(\hat{u}_{\hat{h}}^{i,K}; \hat{K}) = \inf_{u \in U(0; \hat{K})} \hat{F}_{i,K}(u; \hat{K}). \quad (3.20)$$

Proof. (3.19) is obvious. By lemma 3.2 and lemma 3.3, to show (3.20), we only need to verify that

$$\lim_{\hat{h} \rightarrow 0} [\hat{F}_{i,K}(\hat{u}_{\hat{h}}^{i,K}; \hat{K}) - \frac{\text{meas}(\hat{K})}{\text{meas}(D)} \hat{F}_{i,K}(\bar{u}_{\hat{h}}^{i,K}; R_{\hat{h}}^{i,K}(D))] = 0.$$

This can be obtained easily by a straightforward calculation using (3.17) and the fact that $f_{i,K}(0)$ is bounded and $\lim_{\hat{h} \rightarrow 0} \text{meas}(\hat{K} \setminus \hat{K}_{\hat{h}}) = 0$. $\square$

Another method to construct a minimizing sequence of $\hat{F}_{i,K}(\cdot; \hat{K})$ in $U(0; \hat{K})$ out of $\{(u_h^{i,K}, R_h^{i,K})\}$ is given by Li [24]. Assume that

$$u_h^{i,K} \rightharpoonup 0, \quad \text{in } W^{1,p}(D; R^m), \quad \text{as } \hat{h} \rightarrow 0. \quad (3.21)$$

By the Kondracov compactness theorem [6], this implies

$$u_h^{i,K} \rightarrow 0, \quad \text{in } L^p(D; R^m), \quad \text{as } \hat{h} \rightarrow 0. \quad (3.22)$$

Define

$$\delta_h^{i,K} = \min\{1, \max(\hat{h}, \int_D |u_h^{i,K}(\hat{x})|^p d\hat{x})\}, \quad (3.23)$$

$$\hat{K}(\lambda) = \{x \in \hat{K} : \text{dist}(x, \partial \hat{K}) < \lambda\}. \quad (3.24)$$

Let $\varphi_h^{i,K} : R^n \rightarrow [0, 1]$ be such that $\varphi_h^{i,K} \in C^\infty(R^n)$,

$$\varphi_h^{i,K}(x) = \begin{cases} 1, & \text{if } x \in \hat{K} \setminus \hat{K}(2(\delta_h^{i,K})^{1/\hat{p}}); \\ 0, & \text{if } x \in R^n \setminus (\hat{K} \setminus \hat{K}(\hat{h})), \end{cases} \quad (3.25)$$

and

$$|\nabla \varphi_h^{i,K}(x)| \leq (\delta_h^{i,K})^{-1/\hat{p}}, \quad \forall x \in R^n, \quad (3.26)$$

where $\hat{p} > p$ is an arbitrarily given constant. Define

$$\check{u}_h^{i,K}(\hat{x}) = \varphi_h^{i,K}(\hat{x}) \bar{u}_h^{i,K}(\hat{x}), \quad (3.27)$$

with $\bar{u}_h^{i,K}$ defined by (3.15). We have the following result [24].

Theorem 3.4. *Let $(u_h^{i,K}, R_h^{i,K}) \in U_{\hat{h}}(0; D) \times SO^+(n)$ be a sequence of solutions to (3.14) satisfying (3.21) and the condition (see [15, 18, 19])*

$$\textbf{(C): } \{|\nabla u_h^{i,K}|^p\} \text{ are precompact in } L^1(D; R^m).$$

Then, the sequence $\{\check{u}_h^{i,K}\} \subset U(0; \hat{K})$ defined by (3.27) satisfies

$$\check{u}_h^{i,K} \rightharpoonup 0, \quad \text{in } W^{1,p}(\hat{K}; R^m), \quad \text{as } \hat{h} \rightarrow 0, \quad (3.28)$$

$$\lim_{\hat{h} \rightarrow 0} \hat{F}_{i,K}(\check{u}_h^{i,K}; \hat{K}) = \inf_{u \in U(0; \hat{K})} \hat{F}_{i,K}(u; \hat{K}). \quad (3.29)$$

Remark 3.3. In practice, $\bar{u}_h^{i,K}|_{\hat{K}}$ can be directly used as a numerical solution to (3.11) as long as (3.21) and the condition (C) are satisfied, and this can usually provide sharper numerical results (see [24]).

Remark 3.4. Under the hypotheses (h1)-(h3), a minimizing sequence satisfying (3.21) is known to exist [13], furthermore Kinderlehrer and Pedregal [18, 19] proved that such a sequence satisfies the condition (C). To guarantee the finite element solutions $\{u_h^{i,K}\}$ satisfy (3.21), a penalty term $\mu \hat{h}^{-q} \int_D |u_h^{i,K}|^p dx$ with $\mu > 0$ and $q \in (0, p)$ can be added to $\hat{F}_{i,K}(\cdot, \cdot; D)$ (see [24] for details).

4. NUMERICAL SOLUTIONS TO Γ -lim $F(u; \Omega)$

Using the numerical solutions to the subproblems (3.14) obtained in Sec. 3, we can now evaluate Γ -lim $F(u; \Omega)$.

Theorem 4.1. *Let f satisfy (H1)-(H3). Let $(u_h^{i,K}, R_h^{i,K}) \in U_h(0; D) \times SO^+(n)$ be a sequence of solutions to (3.14) with $\hat{h} \rightarrow 0$. Then*

$$\Gamma\text{-lim } F(u; \Omega) = 2^{-n} \lim_{i \rightarrow \infty} \lim_{j \rightarrow \infty} \lim_{\hat{h} \rightarrow 0} \sum_{K \in \mathfrak{T}_{h_{i+j}}(\Omega)} \text{meas } K \hat{F}_{i,K}(u_h^{i,j}, R_h^{i,j}; D). \quad (4.1)$$

Proof. By theorem 3.1 and lemma 3.2,

$$\inf_{v \in U(0; K)} \int_K f_{i,K}(\nabla v(x)) dx = \frac{\text{meas}(K)}{\text{meas}(\hat{K})} \frac{\text{meas}(\hat{K})}{\text{meas}(D)} \lim_{\hat{h} \rightarrow 0} \hat{F}_{i,K}(u_h^{i,K}, R_h^{i,K}; D).$$

This and theorem 2.1 give (4.1), since $\text{meas}(D) = 2^n$. $\square$

Furthermore, we can construct a minimizing sequence of Γ -lim $F(u; \Omega)$ by the numerical solutions of the subproblems.

Theorem 4.2. *Let f satisfy (h1)-(h3). Let $(u_h^{i,K}, R_h^{i,K}) \in U_h(0; D) \times SO^+(n)$ be solutions to (3.14). Let $\hat{u}_h^{i,K}$ be defined by (3.17). Let the functions $u_h^{i,K} \in U(u_0; \Omega)$ be defined by*

$$u_h^{i,j}(x) = u_{h_i}(x) + h_K \hat{u}_h^{i,K}(h_K^{-1} B_K^{-1}(x - x_K)), \quad \text{if } x \in K, \forall K \in \mathfrak{T}_{h_{i+j}}(\Omega). \quad (4.2)$$

Then, we have

$$\Gamma^- \text{-} \lim F(u; \Omega) = \lim_{i \rightarrow \infty} \lim_{j \rightarrow \infty} \lim_{\hat{h} \rightarrow 0} F(u_{\hat{h}}^{i,j}; \Omega). \quad (4.3)$$

Furthermore, there exist a nondecreasing function $J(i)$ and a nonincreasing function $H(i, j)$ such that the sequence $\{u^i\}$ defined by

$$u^i(x) = u_{\hat{h}}^{i,j}(x), \quad \forall x \in \Omega, \forall i \text{ and } j \geq J(i), \quad 0 < \hat{h} \leq A(i, j),$$

is a minimizing sequence of $\Gamma^- \text{-} \lim F(u; \Omega)$, that is

$$u^i \rightharpoonup u \quad \text{in } W^{1,p}(\Omega; \mathbb{R}^m), \quad (4.4)$$

$$\Gamma^- \text{-} \lim F(u; \Omega) = \lim_{i \rightarrow \infty} F(u^i; \Omega). \quad (4.5)$$

Proof. The minimizing property of $(u_{\hat{h}}^{i,K}, R_{\hat{h}}^{i,K})$ ensure that (3.18) holds. Thus, theorem 3.3 and theorem 3.2 give that, for all i and K ,

$$\tilde{u}_{\hat{h}}^{i,K}(x) = h_K \hat{u}_{\hat{h}}^{i,K}(h_K^{-1} B_K^{-1}(x - x_K))$$

are minimizing sequences of (2.15) satisfying (2.16). Hence the conclusions of the theorem follows from theorem 2.2. $\square$

Theorem 4.3. *Let f satisfy (h1)-(h3). Let $(u_{\hat{h}}^{i,K}, R_{\hat{h}}^{i,K}) \in U_{\hat{h}}(0; D) \times SO^+(n)$ be solutions to (3.14) satisfying (3.21) and the condition (C). Let $\tilde{u}_{\hat{h}}^{i,K}$ be defined by (3.27). Let the functions $u_{\hat{h}}^{i,K} \in U(u_0; \Omega)$ be defined by*

$$u_{\hat{h}}^{i,j}(x) = u_{h_i}(x) + h_K \tilde{u}_{\hat{h}}^{i,K}(h_K^{-1} B_K^{-1}(x - x_K)), \quad \text{if } x \in K, \quad \forall K \in \mathfrak{T}_{h_{i+j}}(\Omega). \quad (4.6)$$

Then, the conclusions of theorem 4.2 hold.

Proof. The theorem follows from theorem 3.4, theorem 3.2 and theorem 2.2. $\square$

5. NUMERICAL EXAMPLES

Example 1. Let $\Omega = (0, 1) \times (0, 1)$. Let $B, C(x) \in \mathbb{R}^{2 \times 2}$ be given by

$$B = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix}, \quad C(x) = \begin{pmatrix} 1 & 0 \\ 0 & \frac{\sqrt{1+8x_2}}{2} \end{pmatrix}, \quad (5.1)$$

where $x = (x_1, x_2)^T \in \Omega$. Let $f : R^{2 \times 2} \rightarrow R^1$ be defined by

$$f(A) = \langle A - B, A - B \rangle \langle A + B, A + B \rangle, \quad (5.2)$$

and where $\langle D, E \rangle = \text{tr}(DE^T)$. Let

$$F(u; \Omega) = \int_{\Omega} f(\nabla u(x)C(x))(\det(C(x)))^{-1} dx, \quad (5.3)$$

$$U(0; \Omega) = \{u \in W^{1,4}(\Omega; R^2) : u = 0, \text{ on } \partial\Omega\}. \quad (5.4)$$

The Aim is to calculate the value of Γ -lim $F(0; \Omega)$ and to find a minimizing sequence for it.

The problem can be solved analytically. Let $\hat{\Omega} = \Omega$ and let $\Phi : \Omega \rightarrow \hat{\Omega}$ be given by

$$\begin{cases} \hat{x}_1 = x_1, \\ \hat{x}_2 = \frac{\sqrt{1+8x_2}-1}{2}. \end{cases} \quad (5.5)$$

Let $\hat{u}$ be defined by $\hat{u}(\hat{x}) = u(\Phi^{-1}(\hat{x}))$. Let

$$\hat{F}(\hat{u}; \hat{\Omega}) = \int_{\hat{\Omega}} f(\nabla \hat{u}(\hat{x})) d\hat{x}. \quad (5.6)$$

Then, it is easily verified that $\hat{F}(\hat{u}; \hat{\Omega}) = F(u; \Omega)$ and that

$$\Gamma\text{-lim } F(0; \Omega) = \Gamma\text{-lim } \hat{F}(0; \hat{\Omega}) = \int_{\hat{\Omega}} Qf(0) d\hat{x} = Qf(0). \quad (5.7)$$

Noticing that

$$B - (-B) = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} \sqrt{2} \\ -\sqrt{2} \end{pmatrix} \begin{pmatrix} -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix} = \vec{a} \otimes \vec{n}, \quad (5.8)$$

that is the two potential wells B and $-B$ are in rank one connection, and that

$$\frac{1}{2}B + \frac{1}{2}(-B) = 0, \quad (5.9)$$

we see that [13]

$$Qf(0) = \frac{1}{2}f(B) + \frac{1}{2}f(-B) = 0, \quad (5.10)$$

and a minimizing sequence for $\Gamma\text{-}\lim \hat{F}(0; \hat{\Omega})$ can be given by a laminated microstructure which is essentially defined by [30]

$$\hat{u}_k(\hat{x}) = B\hat{x} + \left[\int_0^{\hat{x} \cdot \vec{n}} \chi_k(s) ds \right] \vec{a}, \quad (5.11)$$

where $\vec{a} \otimes \vec{n} = 2B$ is given by (5.8) and

$$\chi_k(s) = \begin{cases} 0, & \text{if } \sqrt{2}ks \in (2l, 2l+1), \forall l \in \mathbb{Z}, \\ 1, & \text{if } \sqrt{2}ks \in (2l-1, 2l), \forall l \in \mathbb{Z} \end{cases} \quad (5.12)$$

Thus, we have, by (5.7) and (5.10)

$$\Gamma\text{-}\lim F(0; \Omega) = 0, \quad (5.13)$$

and a minimizing sequence for $\Gamma\text{-}\lim F(0; \Omega)$ essentially defined by

$$u_k(x) = \hat{u}_k(\Phi(x)), k = 1, 2, 3, \dots \quad (5.14)$$

The sequence defined by (5.14) give a curved laminated microstructure which has a inhomogeneous Young measure representation [5, 13]

$$\mu(x) = \frac{1}{2} \delta_{BC^{-1}(x)} + \frac{1}{2} \delta_{-BC^{-1}(x)}, \quad (5.15)$$

Where δ_A is the Dirac measure in $R^{2 \times 2}$ centered at A . Since the interfaces across which the gradients of $\hat{u}_k(\hat{x})$ are discontinuous are given by parallel lines

$$\hat{x}_2 = \hat{x}_1 - \frac{l}{k}, \quad \hat{x}_1 \in (0, 1), \quad l = 0, \pm 1, \pm 2, \dots, \pm(k-1),$$

the interfaces across which the gradients of $u_k(x)$ are discontinuous are given by a family of parabolas

$$x_2 = \frac{1}{2} \left(x_1 - \frac{l}{k} \right) \left(x_1 - \frac{l}{k} + 1 \right), \quad x_1 \in (0, 1), \quad l = 0, \pm 1, \dots, \pm(k-1). \quad (5.16)$$

The numerical results obtained by the method developed in the previous sections with various values of h_i and $\hat{h}$ are shown in table 1, and a numerical curved microstructure which is recovered from the numerical result with $h_i = 0.05$ is shown in Figure 1, where black and white curved stripes represent laminates with deformation gradients close to $BC^{-1}(x)$ and $-BC^{-1}(x)$ respectively.

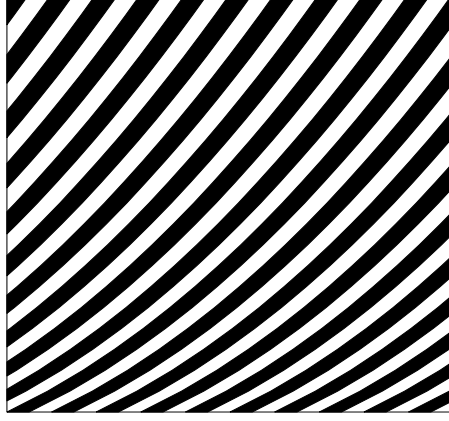


FIGURE 1. A numerical curved microstructure.

	$h_i = 0.2$ $\hat{h} = 0.16667$	$h_i = 0.1$ $\hat{h} = 0.1111$	$h_i = 0.05$ $\hat{h} = 0.0333$
$\Gamma\text{-}\lim F(0; \Omega)$	0.2115×10^{-6}	0.5401×10^{-7}	0.2213×10^{-7}
$d_\infty(h_i, \hat{h})$	0.5120×10^{-3}	0.2950×10^{-3}	0.1946×10^{-3}
$e(h_i, \hat{h})$	$\leq 0.5268 \times 10^{-8}$	$\leq 0.5268 \times 10^{-8}$	$\leq 0.5268 \times 10^{-8}$

TABLE 1. Numerical results for the example.

$d_\infty(h_i, \hat{h})$ and $e(h_i, \hat{h})$ in table 1, which measure the difference between the numerical solutions $u_{h_i, \hat{h}}(x)$ and the Young measure $\mu(x)$, are defined as follows

$$d_p(h_i, \hat{h}) = \sup_{x \in X_{h_i}} \{ \|\nabla u_{h_i, \hat{h}}(x) - BC^{-1}(x)\|_p, \|\nabla u_{h_i, \hat{h}}(x) + BC^{-1}(x)\|_p \},$$

$$e_k(h_i, \hat{h}) = \text{meas}\{x \in \Omega : \|\nabla u_{h_i, \hat{h}}(x) + (-1)^k BC^{-1}(x)\|_\infty \leq d_\infty(h_i, \hat{h}) + 4h_i\},$$

$$e(h_i, \hat{h}) = \max_{k=1,2} \{ |e_k(h_i, \hat{h}) - \frac{1}{2} \text{meas}(\Omega)| \},$$

where

$$X_{h_i} = \{x = (x_1, x_2) \in \Omega : x_2 = (l + \frac{1}{2}h_i), l = 0, 1, \dots, [h_i^{-1}] - 1.\}.$$

Example 2. Consider a two dimensional model for elastic crystals with the Ericksen-James energy density [12, 17]

$$f(A) = \Phi(A^T A), \tag{5.17}$$

with

$$\Phi(C) = \kappa_1(\text{tr } C - 2)^2 + \kappa_2 C_{12}^2 + \kappa_3 \left(\left(\frac{C_{11} - C_{22}}{2} \right)^2 - \varepsilon^2 \right)^2, \quad (5.18)$$

where $C = \nabla u^T \nabla u$ is the right Cauchy-Green strain tensor, $\kappa_i > 0$, $i = 1, 2, 3$ are constant elastic moduli, and $\varepsilon > 0$ is the transformation strain. It is well known that the energy density has two rank-one connected potential wells $SO(2)U_0$ and $SO(2)U_1$, where

$$U_0 = \begin{pmatrix} \sqrt{1-\varepsilon} & 0 \\ 0 & \sqrt{1+\varepsilon} \end{pmatrix}, \quad U_1 = \begin{pmatrix} \sqrt{1+\varepsilon} & 0 \\ 0 & \sqrt{1-\varepsilon} \end{pmatrix}, \quad (5.19)$$

and, by forming properly arranged laminated microstructures with the two energy wells, the material can have a plenty of stress-free large deformations. Numerical examples of such kind can be found in [28].

Figure 2 shows such a stress-free large deformation, obtained by our numerical method, of an originally straight bar being bent into a part of a ring, where the arrows illustrate the normal directions of the interfaces of the first-order laminates on the elements and the gray scale indicates the volume fractions of $SO(2)U_0$ and $SO(2)U_1$ in the laminates, more precisely, the greater the volume fraction of $SO(2)U_0$ is in the laminate on an element the darker the element is painted.

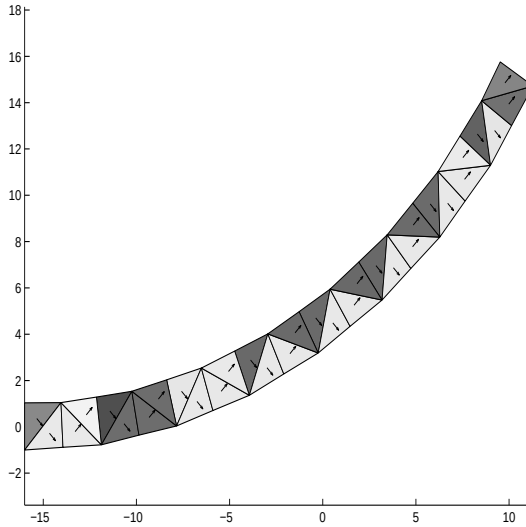


FIGURE 2. Numerical non-homogeneous laminated microstructure of a stress-free large deformation of a straight bar.

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