

# A MESH TRANSFORMATION METHOD FOR COMPUTING MICROSTRUCTURES

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ABSTRACT. A numerical method is established to solve the problem of minimizing a nonquasiconvex potential energy. Convergence of the method is proved both in the case on its own and in the case when it is combined with a weak boundary condition. Numerical examples are given to show that the method, especially when applied together with a continuation method and some other numerical techniques, is not only successful and efficient in solving problems with laminated microstructures but also capable of computing more complicated microstructures.

## 1. INTRODUCTION

Microstructure is a phenomenon found in many physical problems, such as those which involve phase transitions and hysteresis [1, 2]. A related mathematical problem is to minimize a potential energy

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

with nonquasiconvex energy density  $f : \Omega \times R^m \times R^{mn} \rightarrow R^1$  on 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 a Lipschitz continuous boundary  $\partial\Omega$  and  $1 < p < \infty$ .

It is well known that such a variational problem fails, in general, to have a solution, and the minimizing sequences of the potential energy can develop finer and finer oscillations and lead to microstructures [1, 3, 4], which are characterized by the Young measures [5]. To compute the microstructures, or rather the highly

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oscillating minimizing sequences of  $F(\cdot, \Omega)$  in  $\mathbb{U}(u_0; \Omega)$ , is challenging and is of great interests both in theory and in applications. Great progress has been made in recent years, and many numerical methods have been established (see [6]-[24] among many others, see [15] for more references).

It is known that, by applying an iterative method with a piecewise affine finite element approximation, the numerical computation of microstructures for a problem involving an inhomogeneous energy density and nonlinear boundary conditions can be transformed into the numerical computations of microstructures for a group of related homogeneous problems, *i.e.* the problems with energy densities of the form  $f(\nabla u)$  and with linear boundary conditions. Hence, It is of essential importance to establish efficient numerical methods for computing microstructures for homogeneous problems, which is the focus of this paper.

For problems involving microstructures, numerical analyses and experiments revealed that the numerical results often depend strongly on the mesh and shape functions, and can sometimes lead to pseudo-microstructures [4, 10, 15]. A rotational transformation method established by Li [21] somehow reduces the mesh dependence of the numerical results, and it turns out to be successful in computing laminated microstructures. In the present paper, the idea of the rotational transformation method is further extended into a mesh transformation method where the rotational transformation of the mesh is replaced by a piecewise linear transformation. Basically the mesh transformation method gives more freedom in searching for a minimizer of the corresponding discrete problem and allows the mesh to be aligned with the interfaces between phases or phase variants, for example the mesh can be transformed to fit arbitrary volume fractions of a simple laminate (see section 3), and thus not only reduces further the mesh dependence but also reduces the possibility of being trapped into a local minimizer. Furthermore, compared with the rotational transformation method, the mesh transformation method provides more flexibility for the computation of microstructures which are not simple laminates (see section 3 and see [24] for more involved applications).

In section 2, the mesh transformation method is established and analyzed, convergence of the method is proved. We also consider to replace the "hard" boundary condition  $u|_{\partial D} = Ax$  by adding a boundary integral term  $\beta \int_{\partial D} |u - Ax| dx$  to the potential energy. The mesh transformation method combined with this technique shows better performance in the numerical experiments and is also proved to be convergent. The mesh transformation method combines with more subtle boundary technique for periodic boundary conditions can be found

in [23]. In section 3, the implementation of the mesh transformation method and the applications of some other techniques, such as the incremental crystallization method [21] and the continuation method, are discussed, and the numerical results for two model problems are given.

## 2. THE METHOD AND ITS ANALYSIS

Let  $\Omega \subset R^n$  be a bounded open set with a Lipschitz continuous boundary. Let  $f : R^{mn} \rightarrow R^1$  be a continuous function which satisfies the following hypotheses for a constant  $p > 1$ :

$$\begin{aligned} \text{(h1): } & \max\{0, a_1 + b_1|\xi|^p\} \leq f(\xi) \leq a_2 + b_2|\xi|^p, \\ \text{(h2): } & |f(\xi) - f(\eta)| \leq C(1 + |\xi|^{p-1} + |\eta|^{p-1})|\xi - \eta|, \end{aligned}$$

where  $a_1 \in R^1$ ,  $a_2 > 0$ ,  $b_2 \geq b_1 > 0$  and  $C > 0$  are constants. Consider the problem of minimizing the functional

$$F(u; \Omega) = \int_{\Omega} f(\nabla u(x)) dx \quad (2.1)$$

on a set of admissible functions with a linear boundary condition

$$\mathbb{U}(A; \Omega) = \{u \in W^{1,p}(\Omega; R^m) : u(x) = Ax, \text{ on } \partial\Omega\}, \quad (2.2)$$

where  $A \in R^{mn}$  is a given matrix, which may be assumed to be 0 if  $f(\cdot)$  is replaced by  $f(A + \cdot)$  ( *c.f.* [8]), however to help the readers to see clearly how the matrix  $A$  is involved in the computation we simply leave it as it is.

Without loss of generality, assume

$$\Omega \subset B(0; 1), \quad (2.3)$$

where  $B(0; 1) = \{x \in R^n : \|x\|_2 < 1\}$  is the open unit ball of  $R^n$ . Define

$$D = (-1, 1)^n. \quad (2.4)$$

We have obviously

$$\Omega \subset B(0; 1) \subset B(0; \sqrt{n}) = \bigcap_{R \in SO(n)} R(D), \quad (2.5)$$

where  $SO(n)$  is the set of all  $n \times n$  rotational transformation matrices  $R$  with the determinant  $\det R = 1$ . The hypercube  $D$  will serve as the working domain for our numerical computation.

For a given  $R \in SO(n)$ , define

$$T(D; R) = \{ \text{bijections } L : D \rightarrow R(D) \mid L \in W^{1,\infty}(D), L^{-1} \in W^{1,\infty}(R(D)) \\ \text{and } \det \nabla L > 0, a.e. \text{ in } D \},$$

and

$$T(D) = \{L \in T(D; R) : \text{for some } R \in SO(n)\}.$$

**Lemma 2.1.** *For any  $L \in T(D)$ , we have*

$$\inf_{u \in \mathbb{U}(A; L(D))} F(u; L(D)) = \inf_{u \in \mathbb{U}(A; \Omega)} \frac{1}{\text{meas}(\Omega)} F(u; \Omega), \quad (2.6)$$

where  $\text{meas}(\cdot)$  is the Lebesgue measure in  $R^n$ .

*Proof.* It is well known (cf. [25, 26]) that

$$Qf(A) = \inf_{u \in \mathbb{U}(A; \Omega')} \frac{1}{\text{meas}(\Omega')} F(u; \Omega')$$

for all bounded open set  $\Omega' \subset R^n$ , where  $Qf(\cdot)$  is the quasiconvex envelope of  $f(\cdot)$  [25, 27]. Thus the lemma follows, since  $\text{meas}(D) = \text{meas}(L(D)) = 1$  for all  $L \in T(D)$ .  $\square$

**Lemma 2.2.** *For any  $L \in T(D)$  and  $\bar{u} \in \mathbb{U}(A; L(D))$ , let  $u(x) : D \rightarrow R^m$  be defined by*

$$u(x) = \bar{u}(L(x)) - A L(x). \quad (2.7)$$

*Then  $u \in \mathbb{U}(0; D)$  and*

$$\int_D f(A + \nabla u(x)(\nabla L(x))^{-1}) \det \nabla L(x) dx = F(\bar{u}; L(D)). \quad (2.8)$$

*Proof.* The relation  $u \in \mathbb{U}(0; D)$  follows directly from (2.7) and (2.2). By a change of variables, we have (2.8).  $\square$

As a direct corollary of lemmas 2.1 and 2.2, we have

**Corollary 2.1.** *Let  $L \in T(D)$ . Define*

$$F(u, L; D) = \int_D f(A + \nabla u(x)(\nabla L(x))^{-1}) \det \nabla L(x) dx. \quad (2.9)$$

*Then*

$$\inf_{u \in \mathbb{U}(0; D)} F(u, L; D) = \inf_{u \in \mathbb{U}(A; \Omega)} \frac{1}{\text{meas}(\Omega)} F(u; \Omega). \quad (2.10)$$

Let  $\mathfrak{T}_h$  be regular triangulations of  $D$  with mesh sizes  $h$  [28]. Let

$$T_h(D) = \{L \in T(D) : L|_K \text{ is affine for all } K \in \mathfrak{T}_h\}, \quad (2.11)$$

$$\mathbb{U}_h = \{u \in (C(\overline{D}))^m : u|_K \text{ is affine } \forall K \in \mathfrak{T}_h\} \quad (2.12)$$

and

$$\mathbb{U}_h(A; D) = \{u \in \mathbb{U}_h : u|_{\partial D} = Ax\}. \quad (2.13)$$

In the mesh transformation method, we solve the following discrete problem :

$$(DP) \quad \begin{cases} \text{find } (u, L) \in \mathbb{U}_h(0; D) \times T_h(D) \text{ such that} \\ F(u, L; D) = \inf_{(u', L') \in \mathbb{U}_h(0; D) \times T_h(D)} F(u', L'; D). \end{cases} \quad (2.14)$$

**Theorem 2.1.** *Let  $\lim_{i \rightarrow \infty} h_i = 0$  and  $\lim_{i \rightarrow \infty} \varepsilon_i = 0$ . Let the functions  $(u_{h_i}, L_{h_i}) \in \mathbb{U}_{h_i}(0; D) \times T_{h_i}(D)$  be a sequence of approximate solutions to (DP) (see remark 2.1) with*

$$F(\bar{u}_{h_i}, L_{h_i}(D)) \leq \inf_{(u, L) \in \mathbb{U}_{h_i}(0; D) \times T_{h_i}(D)} F(u, L; D) + \varepsilon_i.$$

Then

$$\lim_{i \rightarrow \infty} F(\bar{u}_{h_i}, L_{h_i}(D)) = \lim_{i \rightarrow \infty} F(u_{h_i}, L_{h_i}; D) = \inf_{u \in \mathbb{U}(A; D)} F(u, D), \quad (2.15)$$

where  $\bar{u}_{h_i}(x) = u_{h_i}(L_{h_i}^{-1}(x)) + AL_{h_i}^{-1}(x)$  (see (2.7)).

*Proof.* It follows from lemma 2.1 that

$$\inf_{u \in \mathbb{U}(A; D)} F(u; D) = \inf_{u \in \mathbb{U}(0; D)} F(u, L_{h_i}; D) \leq F(u_{h_i}, L_{h_i}; D). \quad (2.16)$$

On the other hand, for the identity  $I : D \rightarrow D$ , we have

$$F(u_{h_i}, L_{h_i}; D) \leq \inf_{u \in \mathbb{U}_{h_i}(0; D)} F(u, I; D) + \varepsilon_i. \quad (2.17)$$

By the standard finite element approximation theory [28], we have

$$\lim_{h_i \rightarrow 0} \inf_{u \in \mathbb{U}_{h_i}(0; D)} F(u, I; D) = \inf_{u \in \mathbb{U}(0; D)} F(u, I; D). \quad (2.18)$$

Combining (2.18) with (2.16), (2.17), (2.8) and (2.10), we obtain (2.15).  $\square$

**Corollary 2.2.** *As a consequence of lemma 2.1, lemma 2.2 and theorem 2.1, we have*

$$\begin{aligned} Qf(A) &= \frac{1}{\text{meas}(\Omega)} \inf_{u \in \mathbb{U}(A; \Omega)} F(u; \Omega) \\ &= \lim_{h \rightarrow 0} \inf_{(u, L) \in \mathbb{U}_h(0; D) \times T_h(D)} F(u, L; D), \end{aligned}$$

where  $Qf(\cdot)$  is the quasiconvex envelope of  $f(\cdot)$  [25, 26, 27].

Let  $(u_h, L_h) \in \mathbb{U}_h(0; D) \times T_h(D)$  be a sequence of solutions to (DP) with  $h \rightarrow 0$ , then they can be used to construct a minimizing sequence of  $F(\cdot, \Omega)$  in  $\mathbb{U}(A; \Omega)$  in the following standard way (see for example [26]). Assume  $h \ll 1$ , let  $R_h \in SO(n)$  be such that  $L_h \in T(D; R_h)$ . Define

$$\Omega(h) = \{x : x \in h(2R_h z + L_h(D)) \subset \Omega \text{ for some } z \in \mathbb{Z}^n\},$$

where  $\mathbb{Z}$  is the set of all integers. Let  $\varphi_h : \Omega \rightarrow R^1$  be a truncation function defined by

$$\varphi_h(x) = \begin{cases} 1, & \text{if } x \in \Omega_h, \\ 0, & \text{otherwise.} \end{cases}$$

Define  $\hat{u}_h : \Omega \rightarrow R^m$  by

$$\hat{u}_h(x) = \varphi_h(x) h u_h(L_h^{-1}(h^{-1}x)) + Ax, \quad (2.19)$$

where  $L_h^{-1}$  is defined on the whole space of  $R^n$  by a periodic extension

$$L_h^{-1}(x') = L_h^{-1}(x), \forall x' \in R^n, x \in L_h(\bar{D}) \text{ and } \frac{1}{2}(x' - x) \in R_h(\mathbb{Z}^n). \quad (2.20)$$

**Theorem 2.2.** *Let  $(u_h, L_h) \in \mathbb{U}_h(0; D) \times T_h(D)$  be a sequence of approximate solutions to (DP) (see theorem 2.1) with  $h \rightarrow 0$ . Let  $\hat{u}_h$  be defined by (2.19). Then*

$$\hat{u}_h \in \mathbb{U}(A; \Omega), \quad \hat{u}_h \rightarrow Ax \text{ in } L^p(\Omega; R^m) \quad (2.21)$$

and

$$\lim_{h \rightarrow 0} F(\hat{u}_h; \Omega) = \inf_{u \in \mathbb{U}(A; \Omega)} F(u; \Omega). \quad (2.22)$$

*Proof.* The relation (2.21) follows directly from the definition of  $\hat{u}_h$ . Let  $R_h \in SO(n)$  be such that  $L_h \in T(D; R_h)$ , and let  $\mathbb{Z}_h = \{z \in \mathbb{Z}^n : h(2R_h z + L_h(D)) \subset \Omega\}$ . Then, a straight forward calculation yields

$$\begin{aligned} F(\hat{u}; \Omega) &= F(Ax; \Omega \setminus \Omega(h)) + F(\hat{u}_h; \Omega(h)) \\ &= F(Ax; \Omega \setminus \Omega(h)) + \sum_{z \in \mathbb{Z}_h} F(\hat{u}_h; hL_h(D)) \\ &= F(Ax; \Omega \setminus \Omega(h)) + \sum_{z \in \mathbb{Z}_h} h^n F(u_h, L_h; D). \end{aligned} \quad (2.23)$$

Since  $\lim_{h \rightarrow 0} \text{meas}(\Omega \setminus \Omega(h)) = 0$  and

$$\sum_{z \in \mathbb{Z}_h} h^n = \text{meas}(\Omega(h)),$$

(2.22) follows from (2.23) and corollary 2.2. □

As a consequence of theorem 2.2, by solving the discrete problems (DP) (see (2.14)), we obtain a minimizing sequence  $\{\hat{u}_h\}$  (see (2.19)) of  $F(\cdot; \Omega)$  in  $\mathbb{U}(A; \Omega)$ . However, in numerical computations, the strict satisfaction of the boundary condition  $u|_{\partial D} = 0$  causes energy accumulation in the area near the boundary and can even sometimes cause difficulties in the formation of oscillations, or in other words numerical microstructures. To reduce such a boundary effect, we consider, instead of the problem (DP), the following discrete problem :

$$(DPI) \quad \begin{cases} \text{find } (u, L) \in \mathbb{U}_h(D) \times T_h(D) \text{ such that} \\ F_{\alpha,r}(u, L; D) = \inf_{(u', L') \in \mathbb{U}_h(D) \times T_h(D)} F_{\alpha,r}(u', L'; D), \end{cases} \quad (2.24)$$

where  $\alpha > 0$  and  $0 < r < p$  are parameters to be given in the computation and

$$F_{\alpha,r}(u, L; D) = F(u, L; D) + \alpha h^{-r} \int_{\partial L(D)} |u(L^{-1}(x))|^p dx. \quad (2.25)$$

It is obvious that for all  $\alpha > 0$  and  $0 < r < p$

$$\inf_{(u', L') \in \mathbb{U}_h(D) \times T_h(D)} F_{\alpha,r}(u', L'; D) \leq \inf_{(u', L') \in \mathbb{U}_h(0; D) \times T_h(D)} F(u', L'; D). \quad (2.26)$$

**Lemma 2.3.** *Let  $(\tilde{u}_{h_i}, L_{h_i}) \in \mathbb{U}_{h_i}(D) \times T_{h_i}(D)$  be a sequence of solutions (see remark 2.1) to (DPI) with  $\lim_{i \rightarrow \infty} h_i = 0$ . Then,*

$$\lim_{i \rightarrow \infty} F(\tilde{u}_{h_i}, L_{h_i}; D) = \lim_{i \rightarrow \infty} F_{\alpha,r}(\tilde{u}_{h_i}, L_{h_i}; D) = \inf_{u \in \mathbb{U}(A; D)} F(u; D), \quad (2.27)$$

and the sequence  $\{|\nabla \tilde{u}_{h_i} (\nabla L_{h_i})^{-1}|^p \det \nabla L_{h_i}\}_{i=1}^{\infty}$  are equi-uniformly integral continuous [29] in the sense that for any given  $\varepsilon > 0$ , there exists  $\delta(\varepsilon) > 0$  such that for all  $i$  and any measurable set  $E \subset D$

$$\int_E |\nabla \tilde{u}_{h_i}(x) (\nabla L_{h_i}(x))^{-1}|^p \det \nabla L_{h_i}(x) dx < \varepsilon, \text{ if } \text{meas}(L_{h_i}(E)) < \delta.$$

*Proof.* Let  $R_{h_i} \in SO(n)$  be such that  $L_{h_i} \in T(D; R_{h_i})$ . Since  $SO(n)$  is a compact set in  $R^{2 \times 2}$ , without loss of generality, we may assume that for some  $R \in SO(n)$

$$R_{h_i} \rightarrow R \text{ in } R^{2 \times 2}. \quad (2.28)$$

Denote  $P_{h_i} = R R_{h_i}^{-1}$  and define  $\bar{u}_{h_i} : R(D) \rightarrow R^m$  by

$$\bar{u}_{h_i}(x) = A x + \tilde{u}_{h_i}(L_{h_i}^{-1}(P_{h_i}^{-1}x)). \quad (2.29)$$

Then, by a change of variables of integration and noticing that  $\det P_{h_i} = 1$ , we have

$$F(\bar{u}_{h_i}; R(D)) = \int_D f(A + \nabla \tilde{u}_{h_i}(x) (\nabla L_{h_i}(x))^{-1} P_{h_i}^{-1}) \det \nabla L_{h_i}(x) dx. \quad (2.30)$$

It follows from (2.30) and (h1) that

$$\begin{aligned} |F(\bar{u}_{h_i}; R(D))| &\leq C \int_D (1 + |\nabla \tilde{u}_{h_i}(x) (\nabla L_{h_i}(x))^{-1}|^p) \det \nabla L_{h_i}(x) dx \\ &\leq C (1 + F(\tilde{u}_{h_i}, L_{h_i}; D)). \end{aligned} \quad (2.31)$$

By (h1), (h2), (2.26), (2.31) and corollary 2.2, we have

$$\begin{aligned} &|F(\bar{u}_{h_i}; R(D)) - F(\tilde{u}_{h_i}, L_{h_i}; D)| \\ &\leq C \int_D (1 + |A + \nabla \tilde{u}_{h_i}(x) (\nabla L_{h_i}(x))^{-1} P_{h_i}^{-1}|^p \\ &\quad + |A + \nabla \tilde{u}_{h_i}(x) (\nabla L_{h_i}(x))^{-1}|^p) |P_{h_i} - I| \det \nabla L_{h_i}(x) dx \\ &\leq C |P_{h_i} - I| (1 + F(\bar{u}_{h_i}; R(D)) + F(\tilde{u}_{h_i}, L_{h_i}; D)) \leq C |P_{h_i} - I|. \end{aligned} \quad (2.32)$$

(2.26), (2.28), (2.32) and corollary 2.1-2.2 imply

$$\limsup_{i \rightarrow \infty} F(\bar{u}_{h_i}; R(D)) \leq \inf_{u \in \mathbb{U}(A; R(D))} F(u; R(D)). \quad (2.33)$$

It follows from (2.33) and (h1) that  $\{\bar{u}_{h_i}\}_{i=1}^{\infty}$  are bounded in  $W^{1,p}(R(D); R^m)$ . Thus, without loss of generality, we may assume [25] that

$$\bar{u}_{h_i} \rightharpoonup u_{\infty}, \quad \text{in } W^{1,p}(R(D); R^m), \quad (2.34)$$

Where ' $\rightharpoonup$ ' means 'converges weakly to'. Since, by (2.25), (2.26) and (2.29),

$$\int_{\partial D} |\bar{u}_{h_i} - A x|^p dx = \int_{\partial L_{h_i}(D)} |\tilde{u}_{h_i}(L_{h_i}^{-1}(x))|^p dx \leq C h_i^r, \quad (2.35)$$

(2.34) and the Sobolev imbedding theorem [30] imply that  $u_{\infty} \in \mathbb{U}(A; R(D))$ . Let

$$QF(u; R(D)) = \int_{R(D)} Qf(\nabla u(x)) dx, \quad \text{for } u \in W^{1,p}(R(D); R^m).$$

Then, by (2.34), we have [26, 31]

$$QF(u_{\infty}; R(D)) \leq \liminf_{i \rightarrow \infty} QF(\bar{u}_{h_i}; R(D)) \leq \liminf_{i \rightarrow \infty} F(\bar{u}_{h_i}; R(D)). \quad (2.36)$$

By (2.33), (2.36) and

$$\inf_{u \in \mathbb{U}(A; R(D))} QF(u; R(D)) = \inf_{u \in \mathbb{U}(A; R(D))} F(u; R(D)) \quad (2.37)$$



(cf. [26, 31]), we have

$$\inf_{u \in \mathbb{U}(A; R(D))} QF(u; R(D)) = QF(u_\infty; R(D)) = \lim_{i \rightarrow \infty} QF(\bar{u}_{h_i}; R(D)). \quad (2.38)$$

Now, (2.27) follows from (2.26), (2.28), (2.32), (2.33), (2.37) and (2.38). It is a result given by Kinderlehrer and Pedregal [32, 33] that (2.34), (2.38) and (h1) imply that  $\{|\nabla \bar{u}_{h_i}|^p\}_{i=1}^\infty$  are equi-uniformly integral continuous, and thus the lemma holds as a consequence.  $\square$

**Lemma 2.4.** (*Poincaré-Friedrichs inequality*) For  $d < 1$  and  $R \in SO(n)$ , let  $D(d, R) = \{x \in R(D) : \text{dist}(x, \partial R(D)) < d\}$ . Let  $u \in W^{1,p}(R(D); R^m)$ . Then, we have

$$\|u\|_{0,p,D(d,R)}^p \leq 2^{p-1} (\|u\|_{0,p,\partial R(D)}^p + \frac{1}{p} d^p |u|_{1,p,D(d,R)}^p). \quad (2.39)$$

*Proof.* Without loss of generality, we assume that  $R = I$ . Let  $x' \in [-1, 1]^{n-1}$ . For  $x_n \in (-1, -1 + d)$  and  $u \in C^1(\bar{D}; R^m)$ , we have

$$\begin{aligned} |u(x', x_n)|^p &= |u(x', -1) + \int_{-1}^{x_n} \frac{\partial u(x', x_n)}{\partial x_n} dx_n|^p \\ &\leq 2^{p-1} (|u(x', -1)|^p + |\int_{-1}^{x_n} \frac{\partial u(x', x_n)}{\partial x_n} dx_n|^p) \\ &\leq 2^{p-1} (|u(x', -1)|^p + (x_n + 1)^{p-1} \int_{-1}^{x_n} |\frac{\partial u(x', x_n)}{\partial x_n}|^p dx_n). \end{aligned}$$

Integrating over  $D^-(d, n) = \{x \in D(d) : x_n \in (-1, -1 + d)\}$ , we obtain

$$\|u\|_{0,p,D^-(d,n)}^p \leq 2^p (\|u\|_{0,p,\partial D_n^-}^p + \frac{1}{p} d^p |u|_{1,p,D^-(d,n)}^p),$$

where  $\partial D_n^- = \{x \in \partial D : x_n = -1\}$ . Applying the above argument on the other parts of  $\partial D$ , summing up the obtained results and considering that  $C^1(\bar{D}; R^m)$  is dense in  $W^{1,p}(D; R^m)$  [30], we have the conclusion.  $\square$

**Theorem 2.3.** Let  $(\tilde{u}_{h_i}, L_{h_i}) \in \mathbb{U}_{h_i} \times T_{h_i}(D)$  be a sequence of solutions (see remark 2.1) to (DPI) with  $\lim_{i \rightarrow \infty} h_i = 0$ . Let  $u_{h_i} : D \rightarrow R^m$  be defined by

$$u_{h_i}(x) = \psi_{h_i}(L_{h_i}(x)) \tilde{u}_{h_i}(x), \quad (2.40)$$

where  $\psi_{h_i} \in C^\infty(L_{h_i}(\bar{D}))$  are truncation functions satisfying

$$\psi_{h_i}(x) = \begin{cases} 0, & \text{if } x \in \partial L_{h_i}(D), \\ 1, & \text{if } \text{dist}(x, \partial L_{h_i}(D)) \geq h_i^s, \end{cases} \quad (2.41)$$

$$|\nabla \psi_{h_i}(x)| \leq C h_i^{-s}, \quad \forall x \in L_{h_i}(\bar{D}), \quad (2.42)$$

and where  $C > 1$  and  $0 < s < r/p$  are constants. Then  $u_{h_i} \in \mathbb{U}(0; D)$  and

$$\lim_{i \rightarrow \infty} F(u_{h_i}, L_{h_i}; D) = \inf_{u \in \mathbb{U}(A; D)} F(u; D). \quad (2.43)$$

*Proof.* It is obvious that  $u_{h_i} \in \mathbb{U}(0; D)$ . Let

$$L_{h_i}^s(D) = \{x \in L_{h_i}(D) : \text{dist}(x, \partial L_{h_i}(D)) \geq h_i^s\}$$

and denote  $L_{h_i}^{-1}(L_{h_i}(D) \setminus L_{h_i}^s(D)) = D \setminus L_{h_i}^{-1}(L_{h_i}^s(D))$  by  $D_{h_i}^s$ . Since  $u_{h_i} = \tilde{u}_{h_i}$  on  $D \setminus D_{h_i}^s$ , it follows from (h2) and the Hölder's inequality [30] that

$$\begin{aligned} & |F(u_{h_i}, L_{h_i}; D) - F(\tilde{u}_{h_i}, L_{h_i}; D)| = |F(u_{h_i}, L_{h_i}; D_{h_i}^s) - F(\tilde{u}_{h_i}, L_{h_i}; D_{h_i}^s)| \\ & \leq C [(\text{meas}(L_{h_i}(D_{h_i}^s)))^{\frac{p-1}{p}} + (\int_{D_{h_i}^s} |A + \nabla u_{h_i}(\nabla L_{h_i})^{-1}|^p \det \nabla L_{h_i} dx)^{\frac{p-1}{p}} \\ & \quad + (\int_{D_{h_i}^s} |A + \nabla \tilde{u}_{h_i}(\nabla L_{h_i})^{-1}|^p \det \nabla L_{h_i} dx)^{\frac{p-1}{p}}] \\ & \quad \cdot (\int_{D_{h_i}^s} |(\nabla u_{h_i} - \nabla \tilde{u}_{h_i})(\nabla L_{h_i})^{-1}|^p \det \nabla L_{h_i} dx)^{\frac{1}{p}} \\ & = C (I_1^{\frac{p-1}{p}} + I_2^{\frac{p-1}{p}} + I_3^{\frac{1}{p}}) I_4^{\frac{1}{p}}. \end{aligned} \quad (2.44)$$

It follows from (2.41), (2.42) and the Hölder's inequality that

$$\begin{aligned} I_4 & \leq C (\int_{D_{h_i}^s} |\nabla \tilde{u}_{h_i}(\nabla L_{h_i})^{-1}|^p \det \nabla L_{h_i} dx + h_i^{-ps} \int_{L_{h_i}(D_{h_i}^s)} |\tilde{u}_{h_i}(L_{h_i}^{-1}(x))|^p dx) \\ & \leq C (I_{21} + h_i^{-ps} I_{22}), \end{aligned} \quad (2.45)$$

$$I_2 \leq C (I_1 + I_{21} + h_i^{-ps} I_{22}), \quad (2.46)$$

Since

$$\text{meas}(L_{h_i}(D_{h_i}^s)) \leq C h_i^s, \quad (2.47)$$

it follows from lemma 2.3 that

$$\lim_{i \rightarrow \infty} I_1 = \lim_{i \rightarrow \infty} I_{21} = \lim_{i \rightarrow \infty} I_3 = 0. \quad (2.48)$$

By lemma 2.4,

$$I_{22} \leq C (\int_{\partial L_{h_i}(D)} |\tilde{u}_{h_i}(L_{h_i}^{-1}(x))|^p dx + h_i^{ps} \int_{D_{h_i}^s} |\nabla \tilde{u}_{h_i}(\nabla L_{h_i})^{-1}|^p \det \nabla L_{h_i} dx).$$

By (2.25), (2.26) (2.47) and lemma 2.3, this gives

$$\lim_{i \rightarrow \infty} h_i^{-ps} I_{22} \leq \lim_{i \rightarrow \infty} C (h_i^{r-ps} + \int_{D_{h_i}^s} |\nabla \tilde{u}_{h_i} (\nabla L_{h_i})^{-1}|^p \det \nabla L_{h_i} dx) = 0. \quad (2.49)$$

Thus, (2.43) follows as a consequence of (2.44)-(2.49) and lemm 2.3.  $\square$

**Theorem 2.4.** *Let  $(\tilde{u}_h, L_h) \in \mathbb{U}_h(D) \times T_h(D)$  be a sequence of solutions (see remark 2.1) to (DPI) with  $h \rightarrow 0$ . Let  $u_h : R^n \rightarrow R^m$  be defined by (2.40). Let  $\hat{u}_h : \Omega \rightarrow R^m$  be defined by (2.19). Then*

$$\hat{u}_h \in \mathbb{U}(A; \Omega), \text{ and } \hat{u}_h \rightarrow Ax \text{ in } L^p(\Omega; R^m) \quad (2.50)$$

and

$$\lim_{h \rightarrow 0} F(\hat{u}_h; \Omega) = \inf_{u \in \mathbb{U}(A; \Omega)} F(u; \Omega). \quad (2.51)$$

*Proof.* With the same arguments as in the proof of theorem 2.2, and by theorem 2.3, we have the result.  $\square$

*Remark 2.1.* The minima of (DP) and (DPI) may not be attainable. However, this is not of practical concern, since the results of this section remain valid as long as the numerical solutions to (DP) and (DPI) satisfy

$$\lim_{h \rightarrow 0} (F(u_h, L_h; \Omega) - \inf_{(u', L') \in \mathbb{U}_h(0; D) \times T_h(D)} F(u', L'; D)) = 0 \quad (2.52)$$

and

$$\lim_{h \rightarrow 0} (F_{\alpha, r}(\tilde{u}_h, L_h; \Omega) - \inf_{(u', L') \in \mathbb{U}_h(D) \times T_h(D)} F_{\alpha, r}(u', L'; D)) = 0 \quad (2.53)$$

respectively.

### 3. NUMERICAL EXAMPLES

In applying the mesh transformation method established in section 2, We need to solve (DP) or (DPI) numerically. Since the numerical solutions are expected to converge weakly in  $W^{1,p}(\Omega; R^m)$  to the affine function  $Ax$  [26, 21], to enhance the formation of such oscillations, we add a penalty term

$$\beta h^{-q} \int_D |u_h(x)|^p \det \nabla L_h(x) dx \quad (3.1)$$

to the potential energy (see also [21]) where  $\beta > 0$  and  $0 < q < p$  are parameters. An optimization method, for example gradient iterative methods [6, 10] and Methods using simulated annealing and Monte Carlo techniques [11, 12], can

then be applied to solve the obtained discrete problems. In the following numerical examples, the conjugate gradient method is used. To increase the accuracy of the numerical approximation, after an initial convergent criterion is satisfied, the parameters  $\alpha$  in (2.24) and  $\beta$  in (3.1) can be reduced gradually as long as the integrals  $\int_{\partial L_h(D)} |u_h(x)|^p dx$  and  $\int_D |u_h(x)|^p \det \nabla L_h(x) dx$  do not increase too much (for example less than 3 times) [21] which is usually the case when a "good" oscillation pattern is formed. The incremental crystallization method [21] can also be applied in the optimization procedure, roughly speaking the optimization is restricted to a subsequently increasing subsets  $D_1 \subset D_2 \subset \dots \subset D_k = D$  of  $D$  and the algorithm goes on to the next domain only after certain convergent criterion is satisfied. Another technique used in the following examples is the continuation method. The idea is that problems with topologically similar microstructures may be linked by a parameter and by tracing the varying microstructure we may very well obtain a microstructure which is otherwise very difficult, if not impossible, to approximate numerically.

In the following examples,  $n = m = 2$ ,  $D = (-1, 1)^2$  and a family of regular triangulations  $\mathfrak{T}_h(D)$  for  $h_N = 2\sqrt{2}/N$  with  $N \geq 2$  is introduced by the lines

$$\begin{cases} x = -1 + \frac{2}{N}i, & 0 \leq i \leq N; \\ y = -1 + \frac{2}{N}j, & 0 \leq j \leq N; \\ y = x - \frac{2}{N}k, & -N + 1 \leq k \leq N - 1. \end{cases} \quad (3.2)$$

For numerical solutions  $(u_h, L_h) \in \mathbb{U}_h \times T_h(D)$ , we denote

$$\bar{F}_h = F(u_h, L_h; D), \quad (3.3)$$

which should converge to  $Qf(A)$  (see (2.15), (2.27) and corollary 2.2), and denote

$$I_h(D) = \left( \int_{L_h(D)} |u_h(L_h^{-1}(x))|^2 dx \right)^{1/2}, \quad (3.4)$$

$$I_h(\partial D) = \left( \int_{\partial L_h(D)} |u_h(L_h^{-1}(x))|^2 dx \right)^{1/2}, \quad (3.5)$$

which are expected to be of the order of  $h$  when the mesh scale oscillations are obtained.

**Example 1.** Let  $\mathbf{a} = (-\frac{5}{8}, \frac{5}{6})^T$  and  $\mathbf{n} = (-\frac{4}{5}, \frac{3}{5})^T$ . Let

$$B = \mathbf{a} \otimes \mathbf{n} = \begin{pmatrix} \frac{1}{2} & -\frac{3}{8} \\ -\frac{2}{3} & \frac{1}{2} \end{pmatrix}. \quad (3.6)$$

Let  $f : R^{2 \times 2} \rightarrow R$  be defined by

$$f(\xi) = \langle \xi - B, \xi - B \rangle \cdot \langle \xi + B, \xi + B \rangle, \quad (3.7)$$

where  $\langle a, b \rangle = \text{tr}(\xi^T \eta)$  is the inner product of  $R^{2 \times 2}$ . The linear boundary conditions  $A(\lambda)x$  with

$$A(\lambda) = \lambda B + (1 - \lambda)(-B) = (2\lambda - 1)B, \quad 0 < \lambda < 1, \quad (3.8)$$

are considered.

It is obvious that  $B$  and  $-B$ , which are in rank one connection (see (3.6)), are the two potential wells of  $F(u; \Omega)$ , and it is easily seen [5, 26] that

$$QF(A(\lambda)) = 0, \quad (3.9)$$

and the Young measure of a minimizing sequence of  $F(\cdot; \Omega)$  in  $\mathbb{U}(A(\lambda); \Omega)$  is homogeneous and is given by

$$\mu^\lambda(\xi) = \lambda \delta_B(\xi) + (1 - \lambda) \delta_{-B}(\xi), \quad (3.10)$$

where  $\delta_E$  is the Dirac measure centered at  $E$ . Thus, the numerical solutions  $(u_h^\lambda, L_h^\lambda) \in \mathbb{U}_h(D) \times T_h(D)$  to (DPI) (or (DP)) are expected to satisfy [5, 26] (see also section 2)

$$A(\lambda) + \nabla u_h^\lambda (\nabla L_h^\lambda)^{-1} \rightharpoonup \mu^\lambda, \quad \text{in the sense of measure}, \quad (3.11)$$

$$F(u_h^\lambda, L_h^\lambda; D) \rightarrow 0. \quad (3.12)$$

To reflect such a weak convergence of the numerical solutions, we use the following notations:

$$e_\infty(u_h^\lambda, L_h^\lambda; K) = \min\{|A(\lambda) + \nabla u_h^\lambda (\nabla L_h^\lambda)^{-1} \pm B|\}, \quad \forall K \in \mathfrak{T}_h(D),$$

$$E_{2,h}^\lambda = \left( \sum_{K \subset C(k)} (e_\infty(u_h^\lambda, L_h^\lambda; K))^2 \text{meas}(L_h^\lambda(K)) \right)^{1/2},$$

$$L_h^\pm(D, \lambda) = \{x \in D : |A(\lambda) + \nabla u_h^\lambda(x) (\nabla L_h^\lambda(x))^{-1} \mp B| = e_\infty(u_h^\lambda, L_h^\lambda; K)\},$$

$$e_{\lambda,h} = \max\left\{ \left| \frac{\text{meas}(L_h^+(D, \lambda))}{\lambda} - 1 \right|, \left| \frac{\text{meas}(L_h^-(D, \lambda))}{1 - \lambda} - 1 \right| \right\}.$$

Numerical results with various  $\lambda$  and  $h = \sqrt{2}/8$  ( $N = 16$ ) obtained by solving (DPI) with the penalty term (3.1), using the conjugate gradient method combined with the incremental crystallization and continuation techniques, are shown in table 1. The numerical results for a fixed  $\lambda = 0.6$  and  $N = 8, 16, 32$  are shown in table 2. In the computation, we set  $\alpha h^{-r} = 2.5$ ,  $\beta h^{-q} = 0.12$  and  $\lambda_0 = 0.5$  initially, and when the norm of the gradient of the energy drops to  $10^{-5}$  we set  $\lambda$  to its final value and allow  $\alpha h^{-r}$  and  $\beta h^{-q}$  to decrease gradually to the order of

$10^{-8}$  and  $10^{-4}$  respectively as long as the increase of the corresponding integrals  $I_h(D)$  and  $I_h(\partial D)$  do not exceed 3 times of their original values.

| $\lambda$ | $\bar{F}_h$            | $E_{2,h}^\lambda$     | $e_{\lambda,h}$       | $I_h(D)$              | $I_h(\partial D)$     |
|-----------|------------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| 0.5       | $1.30 \times 10^{-11}$ | $4.90 \times 10^{-6}$ | $1.60 \times 10^{-6}$ | $3.75 \times 10^{-2}$ | $1.28 \times 10^{-3}$ |
| 0.6       | $7.47 \times 10^{-11}$ | $1.17 \times 10^{-5}$ | $1.02 \times 10^{-4}$ | $3.61 \times 10^{-2}$ | $3.99 \times 10^{-3}$ |
| 0.7       | $1.17 \times 10^{-11}$ | $4.65 \times 10^{-6}$ | $267 \times 10^{-3}$  | $3.18 \times 10^{-2}$ | $8.66 \times 10^{-3}$ |
| 0.8       | $4.39 \times 10^{-9}$  | $8.46 \times 10^{-5}$ | $7.43 \times 10^{-3}$ | $2.46 \times 10^{-2}$ | $1.39 \times 10^{-2}$ |
| 0.9       | $3.94 \times 10^{-7}$  | $5.43 \times 10^{-4}$ | $1.79 \times 10^{-3}$ | $1.81 \times 10^{-2}$ | $3.47 \times 10^{-2}$ |

TABLE 1. Numerical results for  $N = 16$  with DPI+p+c.

| N  | $\bar{F}_h$            | $E_{2,h}^\lambda$     | $e_{\lambda,h}$       | $I_h(D)$              | $I_h(\partial D)$     |
|----|------------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| 8  | $1.21 \times 10^{-12}$ | $1.49 \times 10^{-6}$ | $2.58 \times 10^{-3}$ | $7.22 \times 10^{-2}$ | $1.17 \times 10^{-3}$ |
| 16 | $7.47 \times 10^{-11}$ | $1.17 \times 10^{-5}$ | $1.02 \times 10^{-4}$ | $3.61 \times 10^{-2}$ | $3.99 \times 10^{-3}$ |
| 32 | $1.52 \times 10^{-12}$ | $1.68 \times 10^{-6}$ | $3.70 \times 10^{-5}$ | $1.80 \times 10^{-2}$ | $1.80 \times 10^{-3}$ |

TABLE 2. Numerical results for  $\lambda = 0.6$  with DPI+p+c.

| Method  | $\bar{F}_h$            | $E_{2,h}^\lambda$     | $e_{\lambda,h}$       | $I_h(D)$              | $I_h(\partial D)$     |
|---------|------------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| DPI+p+c | $1.30 \times 10^{-11}$ | $4.90 \times 10^{-6}$ | $1.60 \times 10^{-6}$ | $3.75 \times 10^{-2}$ | $1.28 \times 10^{-3}$ |
| DPI+p-c | $6.42 \times 10^{-4}$  | $3.46 \times 10^{-2}$ | $8.86 \times 10^{-3}$ | $6.50 \times 10^{-2}$ | $1.79 \times 10^{-1}$ |
| DPI-p+c | $2.92 \times 10^{-12}$ | $2.32 \times 10^{-6}$ | $9.00 \times 10^{-4}$ | $3.62 \times 10^{-2}$ | $4.62 \times 10^{-3}$ |
| DPI-p-c | $3.87 \times 10^{-4}$  | $2.67 \times 10^{-2}$ | $6.07 \times 10^{-3}$ | $6.84 \times 10^{-2}$ | $1.76 \times 10^{-1}$ |
| DP+p+c  | $8.18 \times 10^{-2}$  | $4.84 \times 10^{-1}$ | $1.05 \times 10^{-2}$ | $4.98 \times 10^{-2}$ | null                  |
| DP-p+c  | $1.26 \times 10^{-1}$  | $7.06 \times 10^{-1}$ | $4.86 \times 10^{-2}$ | $5.25 \times 10^{-2}$ | null                  |
| DP+p-c  | $8.18 \times 10^{-2}$  | $4.83 \times 10^{-1}$ | $1.05 \times 10^{-2}$ | $5.01 \times 10^{-2}$ | null                  |
| DP-p-c  | $1.06 \times 10^{-1}$  | $5.66 \times 10^{-1}$ | $1.06 \times 10^{-2}$ | $6.85 \times 10^{-2}$ | null                  |

TABLE 3. Numerical results for  $\lambda = 0.6$  with various methods.

In table 3, we compare the numerical results obtained by solving (DPI) (or (DP)) with (or without) the penalty term (3.1) (referred to as  $\pm p$  respectively), using (or not using) the continuation technique (referred to as  $\pm c$  respectively), for  $\lambda = 0.6$  and  $N = 16$ .

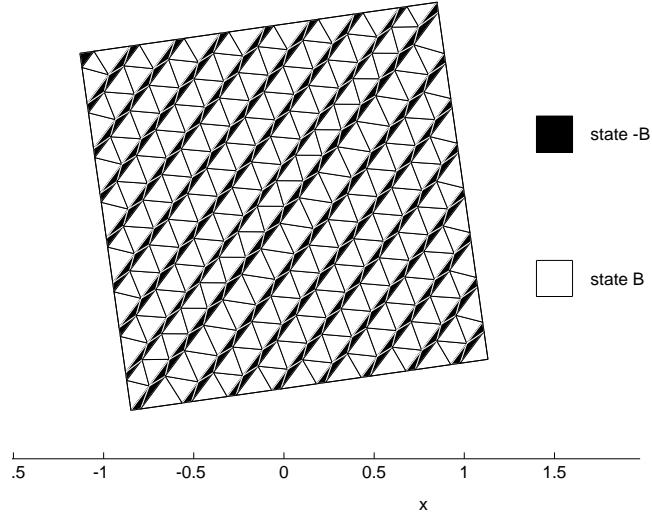


FIGURE 1. Numerical microstructure for  $\lambda = 0.8$  by DPI+p+c.

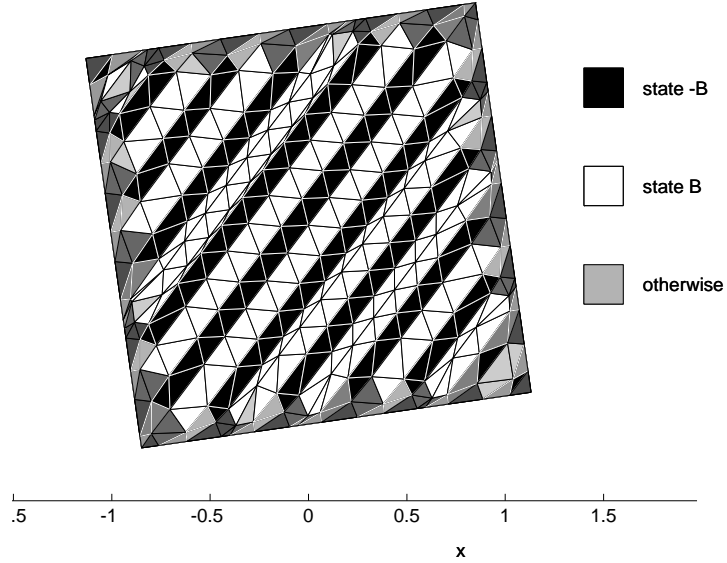


FIGURE 2. Numerical microstructure for  $\lambda = 0.6$  by DP-p-c.

A numerical microstructure for  $\lambda = 0.8$  and  $N = 16$  obtained by (DPI+p+c) is shown in figure 1 and a numerical microstructure for  $\lambda = 0.6$  and  $N = 16$  obtained by (DP-p-c) is shown in figure 2. In both cases we can see clearly the advantage of the mesh transformation method. From numerical results shown in the tables and the figures, it is obvious that (DPI) works generally better than

(DP), and the continuation technique also shows its power, especially in the case of (DPI) where the boundary effect is reduced to a minimum, and finally the penalty term (3.1) reduces the error  $e_{\lambda,h}$  which means a better approximation to the Young measure  $\mu^\lambda$ .

**Example 2.** Consider an optimal design problem [26, 34, 35] where the integrand is given by

$$f(\xi) = \begin{cases} 1 + |\xi|^2, & \text{if } \xi \neq 0, \\ 0, & \text{if } \xi = 0. \end{cases} \quad (3.13)$$

It is known [26, 34, 35] that in the case  $n = m = 2$

$$Qf(\xi) = \begin{cases} 1 + |\xi|^2, & \text{if } \rho(\xi) \geq 1, \\ 2\rho(\xi) - 2|\det \xi|, & \text{if } \rho(\xi) \leq 1, \end{cases} \quad (3.14)$$

where

$$\rho(\xi) = (|\xi|^2 + 2|\det \xi|)^{1/2}. \quad (3.15)$$

Let

$$B = \begin{pmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}. \quad (3.16)$$

We consider the affine boundary conditions associate with matrices

$$A(\lambda) = \lambda B = \begin{pmatrix} \lambda & -\frac{\lambda}{2} \\ -\frac{\lambda}{2} & \frac{\lambda}{2} \end{pmatrix}. \quad (3.17)$$

By (3.14),

$$Qf(A(\lambda)) = \begin{cases} 1 + \frac{7}{4}\lambda^2, & \text{if } |\lambda| \geq \frac{2}{3}, \\ \frac{1}{2}|\lambda|(6 - |\lambda|), & \text{if } |\lambda| \leq \frac{2}{3}. \end{cases} \quad (3.18)$$

Since there is a removable discontinuity point at the very heart, the unique potential well of the integrand,  $f$  given by (3.13) is not a nice function for numerical approximations. So, we consider of an application of the continuation method, which is essential to the numerical approximations. Instead of dealing with  $f$ , we introduce a sequence of integrands  $f_k : R^{2 \times 2} \rightarrow R$ ,  $k = 1, 2, \dots$ ,

$$f_k(\xi) = \begin{cases} 1 + |\xi|^2, & \text{if } |\xi| \geq \frac{1}{k}, \\ (1 + k^2)|\xi|^2, & \text{if } |\xi| \leq \frac{1}{k}. \end{cases} \quad (3.19)$$



It is easily seen that

$$Qf - 2\sqrt{2}\frac{1}{k^2} \leq f_k \leq f_{k+1} \leq f, \quad \forall k. \quad (3.20)$$

Hence, for all open set  $\Omega \in R^2$  and  $A \in R^{2 \times 2}$ , we have [26]

$$\lim_{k \rightarrow \infty} \inf_{u \in \mathbb{U}(A; \Omega)} F_k(u; \Omega) = \inf_{u \in \mathbb{U}(A; \Omega)} F(u; \Omega), \quad (3.21)$$

where  $F_k(u; \Omega) = \int_{\Omega} f_k(\nabla u(x)) dx$ .

Let  $u_k \in \mathbb{U}(A; \Omega)$  satisfy

$$F_k(u_k; \Omega) \leq \inf_{u \in \mathbb{U}(A; \Omega)} F_k(u; \Omega) + \varepsilon_k, \quad (3.22)$$

with  $\lim_{k \rightarrow \infty} \varepsilon_k = 0$ . Then, it follows from (3.20)–(3.22) that

$$\limsup_{k \rightarrow \infty} F_i(u_k; \Omega) \leq \inf_{u \in \mathbb{U}(A; \Omega)} F(u; \Omega). \quad (3.23)$$

Since, by (3.23) and (h1),  $\{u_k\}_{k=1}^{\infty}$  are uniformly bounded in  $W^{1,p}(\Omega; R^2)$  and since a affine boundary condition is considered, without loss of generality, we may assume that there exists a homogeneous Young measure  $\mu$  on  $R^{2 \times 2}$ , which is a probability measure [5], such that

$$\lim_{k \rightarrow \infty} F_i(u_k; \Omega) = \int_{\Omega} \langle f_i(\cdot), \mu \rangle dx = \text{meas}(\Omega) \langle f_i(\cdot), \mu \rangle, \quad \forall i. \quad (3.24)$$

On the other hand, for a probability measure  $\mu$  on  $R^{2 \times 2}$ , it follows from

$$0 \leq \langle f(\cdot) - f_i(\cdot), \mu \rangle \leq \mu(\{\xi \in R^{2 \times 2} : 0 < |\xi| < i^{-1}\}), \quad (3.25)$$

and

$$\lim_{i \rightarrow \infty} \mu(\{\xi : 0 < |\xi| < i^{-1}\}) = \mu\left(\bigcap_{i=1}^{\infty} \{\xi : 0 < |\xi| < i^{-1}\}\right) = \mu(\emptyset) = 0. \quad (3.26)$$

Combining (3.23)–(3.26), we obtain

$$\int_{\Omega} \langle f(\cdot), \mu \rangle dx = \inf_{u \in \mathbb{U}(A; \Omega)} F(u; \Omega). \quad (3.27)$$

The above analysis indicates that while a sequence  $\{u_k\}_{k=1}^{\infty}$ , which satisfies (3.22) and has a homogeneous Young measure representation  $\mu$ , is generally not a minimizing sequence of  $F(\cdot; \Omega)$  in  $\mathbb{U}(A; \Omega)$ , a modification can be made to  $\{u_k\}_{k=1}^{\infty}$  to produce such a minimizing sequence which has the Young measure representation  $\mu$ .

In our numerical experiments the method (DPI+p), *i.e.* (DPI) with the penalty term (3.1), is applied. To solve the discrete problem for large  $k$ , the continuation method is again applied. We either take  $\lambda$  as a parameter or consider the parameterized integrands

$$f_{k,l}(\xi) = \begin{cases} 1 + |\xi|^2, & \text{if } |\xi| \geq \frac{l}{k}, \\ (1 + l^{-2}k^2)|\xi|^2, & \text{if } |\xi| \leq \frac{l}{k}. \end{cases} \quad (3.28)$$

The parameters  $\lambda$  or  $l$  in (3.28) will be varied incrementally from their initial values, say  $\lambda_0 = 0.025$  and  $l_0 = \frac{k}{1+\|A(\lambda)\|}$ , to the final value of  $\lambda$  and 1 respectively, and in each step a convergent criterion, say the norm of the energy gradient less than  $10^{-4}$ , is to be satisfied. Both of the processes, encourage the deformation gradients to fall into the energy well, which is very small for large  $k$ , and thus greatly improve the performance of the algorithm. It should be brought into attention here however that the value  $k$  is limited by the mesh size  $h$ , in other words, to solve the problem with large  $k$  the mesh size  $h$  must be sufficiently small. In showing the numerical results, we denote the relative error of  $\bar{F}_h$  by  $E_r(\bar{F}_h)$  and define

$$C(k) = \{\xi \in R^{2 \times 2} : |\xi| \leq \frac{1}{k}\},$$

$$e_\infty(u_h^\lambda, L_h^\lambda; K) = \|A(\lambda) + \nabla u_h^\lambda (\nabla L_h^\lambda)^{-1}\|_K, \quad \text{for } K \subset C(k),$$

$$E_{\infty,h}^\lambda(C(k)) = \max_{K \subset C(k)} e_\infty(u_h^\lambda, L_h^\lambda; K),$$

$$E_{2,h}^\lambda(C(k)) = \left( \sum_{K \subset C(k)} (e_\infty(u_h^\lambda, L_h^\lambda; K))^2 \text{meas}(L_h^\lambda(K)) \right)^{1/2}.$$

In table 4, numerical results for  $k = 30$ ,  $N = 16$  and various  $\lambda$  are shown. Table 5 shows the numerical results for  $\lambda = 0.3$ ,  $k = 30$  and  $N = 8, 16, 32, 64$ , and it is clearly shown that  $I_h(D)$  and  $I_h(\partial D)$  decrease as  $N$  increases (or equivalently as  $h$  decreases), this means the weakly convergence of the finite element solutions. Table 6 shows the numerical results for  $N = 16$ ,  $\lambda = 0.3$  and  $k = 15, 30, 60$ . In table 6, we see that  $E_r(\bar{F}_h)$  decreases as  $k$  increases, this indicates the finite element solutions satisfy (3.21), we see also the gradients in the wells  $C(k)$  (see  $E_{\infty,h}^\lambda(C(k))$  and  $E_{2,h}^\lambda(C(k))$ ) converge sharply to 0 as  $k$  increases, this implies the convergence of the Young measure.

Numerical microstructures for  $\lambda = 0.3$  obtained by the algorithm with different initial data and the combinations of the rotation transformation method, the incremental crystallization method and the continuation method are shown in

| $\lambda$ | $E_r(\bar{F}_h)$      | $E_{\infty,h}^\lambda(C(k))$ | $E_{2,h}^\lambda(C(k))$ | $I_h(D)$              | $I_h(\partial D)$     |
|-----------|-----------------------|------------------------------|-------------------------|-----------------------|-----------------------|
| 0.05      | $7.62 \times 10^{-2}$ | $9.93 \times 10^{-3}$        | $6.10 \times 10^{-5}$   | $1.79 \times 10^{-2}$ | $4.21 \times 10^{-2}$ |
| 0.15      | $3.08 \times 10^{-3}$ | $3.04 \times 10^{-2}$        | $1.02 \times 10^{-4}$   | $3.10 \times 10^{-2}$ | $7.15 \times 10^{-2}$ |
| 0.25      | $5.93 \times 10^{-2}$ | $2.65 \times 10^{-2}$        | $1.09 \times 10^{-4}$   | $3.72 \times 10^{-2}$ | $7.00 \times 10^{-2}$ |
| 0.35      | $6.01 \times 10^{-2}$ | $2.67 \times 10^{-2}$        | $1.66 \times 10^{-4}$   | $4.48 \times 10^{-2}$ | $7.36 \times 10^{-2}$ |
| 0.45      | $2.51 \times 10^{-2}$ | $2.62 \times 10^{-2}$        | $1.44 \times 10^{-4}$   | $4.57 \times 10^{-2}$ | $1.16 \times 10^{-1}$ |
| 0.55      | $1.11 \times 10^{-2}$ | $3.32 \times 10^{-2}$        | $1.40 \times 10^{-4}$   | $4.31 \times 10^{-2}$ | $1.22 \times 10^{-1}$ |

TABLE 4. Numerical results for  $N = 16$  and  $k = 30$ .

| N  | $E_r(\bar{F}_h)$      | $E_{\infty,h}^\lambda(C(k))$ | $E_{2,h}^\lambda(C(k))$ | $I_h(D)$              | $I_h(\partial D)$     |
|----|-----------------------|------------------------------|-------------------------|-----------------------|-----------------------|
| 8  | $2.92 \times 10^{-2}$ | $1.89 \times 10^{-2}$        | $2.77 \times 10^{-5}$   | $6.33 \times 10^{-2}$ | $9.75 \times 10^{-2}$ |
| 16 | $4.13 \times 10^{-2}$ | $2.17 \times 10^{-2}$        | $7.93 \times 10^{-5}$   | $3.85 \times 10^{-2}$ | $6.42 \times 10^{-2}$ |
| 32 | $4.58 \times 10^{-2}$ | $2.53 \times 10^{-2}$        | $6.17 \times 10^{-5}$   | $2.42 \times 10^{-2}$ | $4.51 \times 10^{-2}$ |
| 64 | $6.37 \times 10^{-2}$ | $2.72 \times 10^{-2}$        | $1.44 \times 10^{-4}$   | $1.39 \times 10^{-2}$ | $3.23 \times 10^{-2}$ |

TABLE 5. Numerical results for  $\lambda = 0.3$  and  $k = 30$ .

| k  | $E_r(\bar{F}_h)$      | $E_{\infty,h}^\lambda(C(k))$ | $E_{2,h}^\lambda(C(k))$ | $I_h(D)$              | $I_h(\partial D)$     |
|----|-----------------------|------------------------------|-------------------------|-----------------------|-----------------------|
| 15 | $8.37 \times 10^{-2}$ | $5.67 \times 10^{-2}$        | $1.09 \times 10^{-3}$   | $3.31 \times 10^{-2}$ | $4.87 \times 10^{-2}$ |
| 30 | $6.78 \times 10^{-2}$ | $2.73 \times 10^{-2}$        | $1.78 \times 10^{-4}$   | $4.33 \times 10^{-2}$ | $7.23 \times 10^{-2}$ |
| 60 | $2.76 \times 10^{-2}$ | $8.75 \times 10^{-3}$        | $8.49 \times 10^{-6}$   | $4.69 \times 10^{-2}$ | $8.33 \times 10^{-2}$ |

TABLE 6. Numerical results for  $\lambda = 0.3$  and  $N = 16$ .

figure 3 – figure 8. It can be clearly seen, as is expected since the Young measure is wildly nonunique in this case [34, 35], that these numerical microstructures are not simple laminates and are quite different from each other.

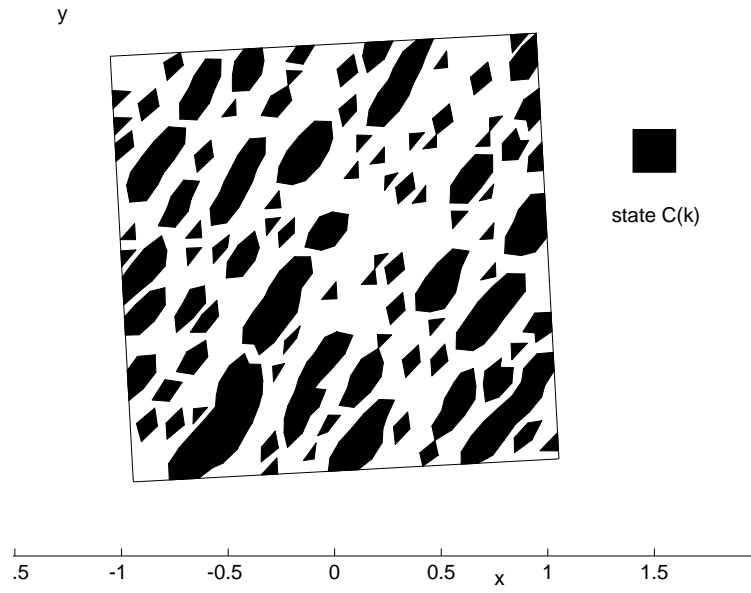


FIGURE 3. A numerical microstructure for  $\lambda = 0.3$ ,  $k = 30$ .

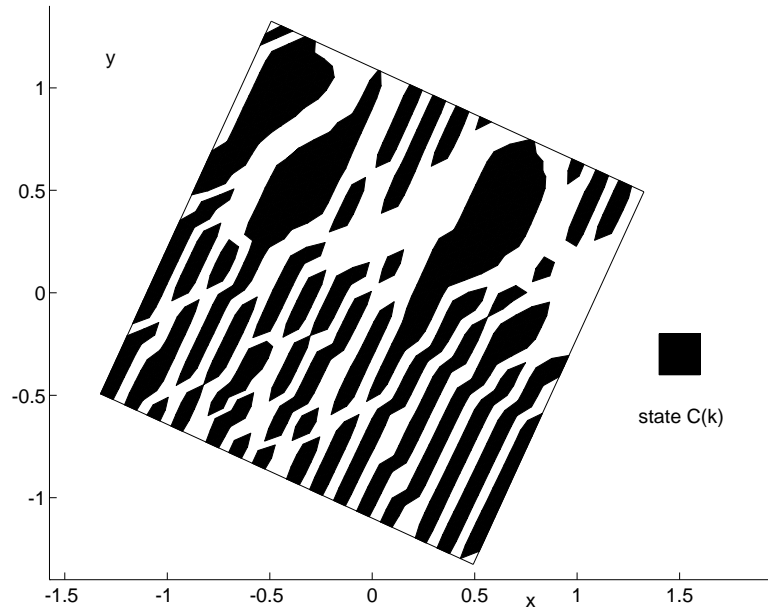


FIGURE 4. A numerical microstructure for  $\lambda = 0.3$ ,  $k = 30$ .

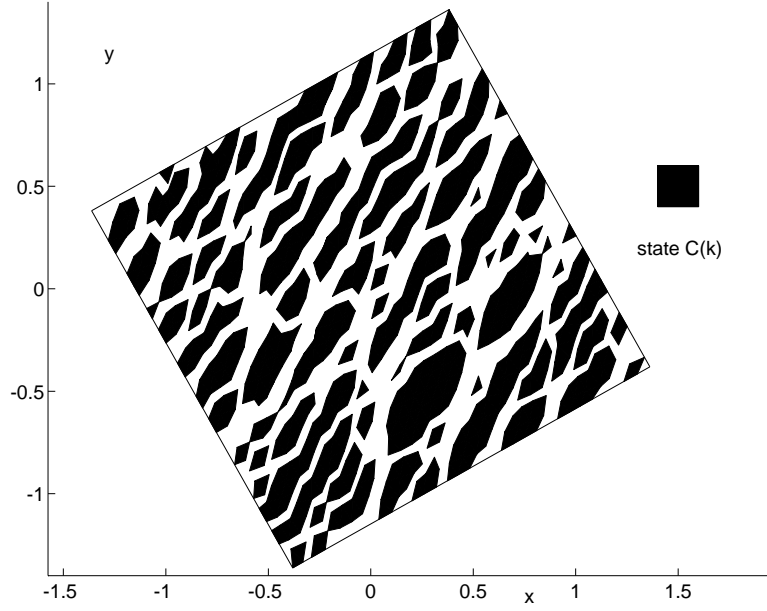


FIGURE 5. A numerical microstructure for  $\lambda = 0.3$ ,  $k = 30$ .

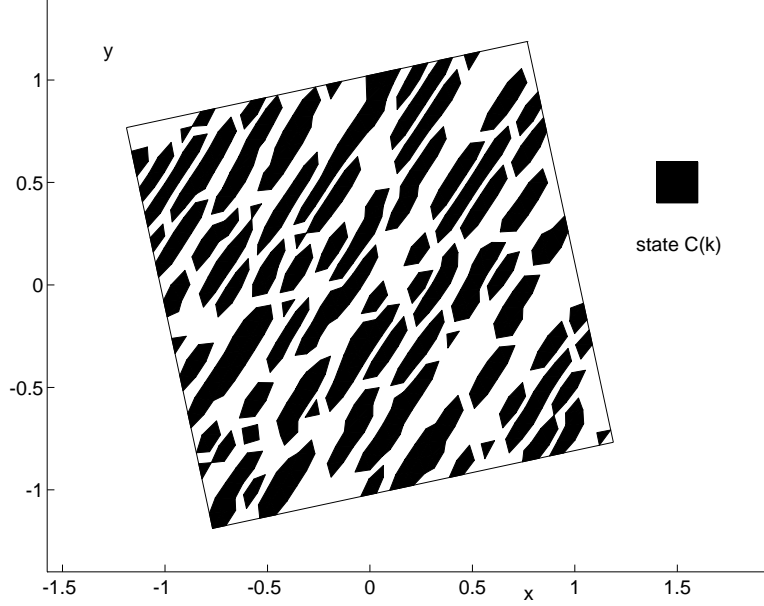


FIGURE 6. A numerical microstructure for  $\lambda = 0.3$ ,  $k = 30$ .

While the numerical microstructures shown in figure 3 – figure 7 are obtained by  $N = 32$  and  $k = 30$ , the numerical microstructure in figure 8 is obtained by  $N = 64$  and  $k = 60$ . We see that the mesh size oscillations are obtained.

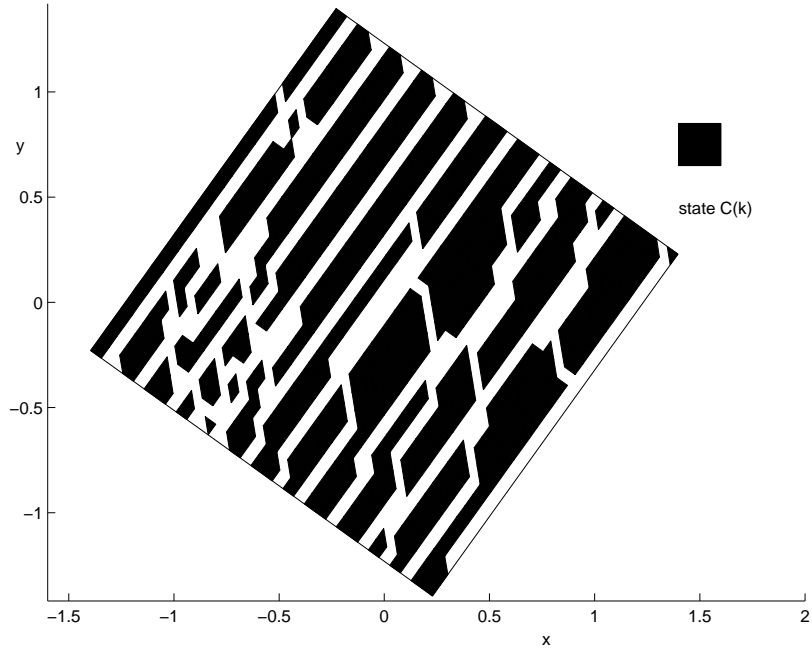


FIGURE 7. A numerical microstructure for  $\lambda = 0.3$ ,  $k = 30$ .

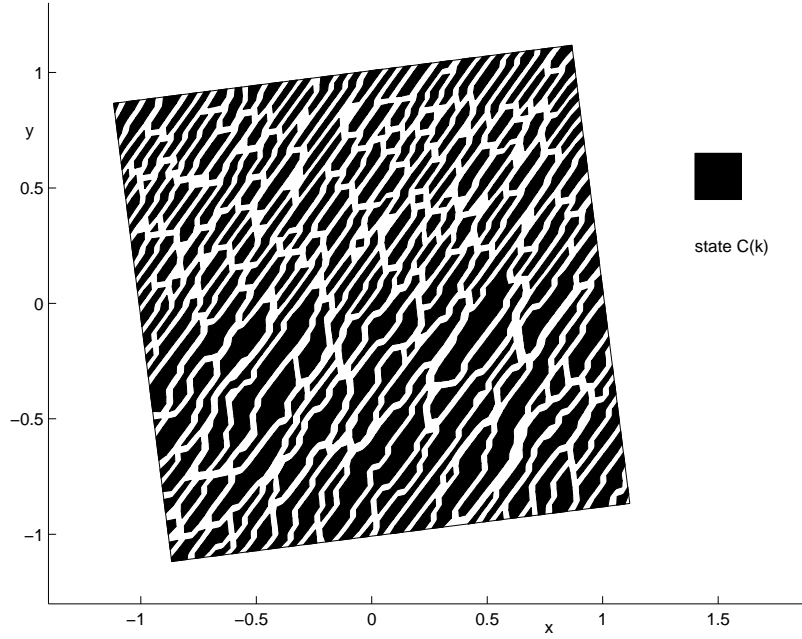


FIGURE 8. A numerical microstructure for  $\lambda = 0.3$ ,  $k = 60$ .

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