A PERIODIC RELAXATION METHOD FOR COMPUTING MICROSTRUCTURES

ZHIPING LI

SCHOOL OF MATHEMATICAL SCIENCES, PEKING UNIVERSITY, BEIJING 100871, P.R.CHINA

ABSTRACT. A new numerical method, periodic relaxation method, for computing microstructure is established. Convergence of the method is proved. It is shown that higher order error bounds can be obtained with the method, and in particular, numerical solutions with computer accuracy can be expected to obtain for simple laminated microstructures. Numerical examples are given.

1. INTRODUCTION

It is well known, by a theory established by Ball and James [1, 2], that microstructure, which is a typical phenomenon in material sciences, can be well characterized by increasingly fine oscillating minimizing sequences of a nonquasiconvex potential energy. In corresponding mathematics context, put it in a simplest setting, it is a problem of minimizing an integral functional

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

with a nonquasiconvex energy density $f : R^{mn} \to R^1$ in a set of admissible functions

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

where $\Omega \subset R^n$ is a bounded open set with a Lipschitz continuous boundary $\partial\Omega$, A is a $m \times n$ real matrix and $1 < p < \infty$, and microstructures can be viewed

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as the Young measure limit of gradients of a minimizing sequence of $F(\cdot;\ \Omega)$ in $\mathbb{U}(A;\ \Omega)$ [1, 2].

To compute the microstructures, or rather the highly oscillating minimizing sequences of $F(\cdot,\ \Omega)$ in $\mathbb{U}(A;\ \Omega)$ and the Young measure, is of great interests and importance both in the mathematical theory and in applications, and it is also challenging (see [3]-[9] among many others).

Numerical analysis show that, in general, a microstructure can not be approximated with high accuracy by standard finite element function spaces. For example, for a simple laminated microstructure the optimal error bound for the energy is only $\mathrm{O}(h^{1/2})$ [5, 6, 9]. The low accuracy is mainly caused by the transition layers between the phases and by the boundary layer, which generally exist to gurantee a finite element approximation to be continuous and to satisfy the boundary condition. It is known that the error estimates can be improved if the finite element meshes are aligned with the microstructure [5, 6], and such a requirement can be achieved by the rotational transformation method [10]. In fact, the transition layers can completely be removed for simple laminated microstructures by the mesh transformation method [11], and thus the optimal error bound for the energy can be improved to $\mathrm{O}(h)$ (see [5, 6] for the arguments). Further improvement on the error bound can be obtained by applying some boundary layer removing techniques such as replacing the boundary condition $u = A\,x$ on $\partial\Omega$ by adding to $F(\cdot;\ \Omega)$ penalty terms [10, 11]

$$\alpha h^{-s} \int_{\Omega} |u(x) - A\,x|^p \, dx \tag{1.3}$$

and

$$\beta h^{-r} \int_{\partial\Omega} |u(x) - A\,x|^p \, dx. \tag{1.4}$$

These techniques greatly increase the accuracy of the numerical results. However, as a by-product, they can cause "floating" effect on numerical solutions u_h, *i.e.*

$$\frac{1}{\mathrm{meas}(\Omega)} \int_{\Omega} \nabla u_h(x) \, dx \neq A, \tag{1.5}$$

and this implies a possibility of "over-relaxation" which means an energy lower than the infimum being obtained by the numerical solutions (see section 3).

In the present paper, a more efficient boundary layer removing technique, periodic relaxation method, which is "floating" free and can completely prevent the formation of a boundary layer in numerical solutions, is established. The method generally produces sharper numerical results. In particular, an application of the periodic relaxation method (PR) together with the mesh transformation method (MT) to a problem with a simple laminated microstructure can produce "floating" free numerical results with neither a boundary layer nor transition layers, which implies the computer accuracy for the numerical approximations to simple laminated microstructures. We remark that, even though from the theoretical point of view they are only a matter of an "equivalent" transformation of the problem, in numerical computations the (PR and MT) methods reduce significantly the possibility of being trapped into a local minimizer and thus do produce much better numerical results (see section 3, see also [10, 11]). We also point out here that for a numerical method based directly on conforming finite elements the transition layers are generally inevitable (consider the case of second order laminates as an example), on the other hand, a direct application of nonconforming finite element methods can cause "over-relaxation" [8]. These observations suggest that further investigations are necessary to create high accuracy numerical methods for computing microstructures which are more complicated than simple laminated microstructures (see [13] for an approach for the case of conforming finite element methods).

The rest of the paper is planned as follows. In section 2, the periodic relaxation method, which is built in the framework of the mesh transformation method, is introduced and the convergence of the method is proved. Numerical examples are given in section 3.

2. Periodic relaxation method and its analysis

Let $\Omega \subset R^n$ be a bounded open set with a Lipschitz continuous boundary. Let $f : R^{mn} \to R^1$ be a continuous function and satisfy the following hypotheses:

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

(h2): $|f(\xi) - f(\eta)| \le C(1 + |\xi|^{p-1} + |\eta|^{p-1})(|\xi - \eta|)$,

where $a_1 \in R^1$, $a_2 > 0$, $b_2 \ge b_1 > 0$ and $C > 0$ are constants.

As in the rotational transformation method [10] and the mesh transformation method [11], $D = (-1,\ 1)^n$ will be taken as the computing domain for our numerical computation.

For a given $R \in SO(n)$, which is the set of all $n \times n$ orthogonal matrices with determinant equal to 1, define

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

and define

$$T(D) = \{L \in T(D;\ R) : \text{for some } R \in SO(n)\}. \tag{2.1}$$

Let $\mathfrak{T}_h$ be regular triangulations of D with mesh sizes h [14]. Let

$$T_h(D) = \{L \in T(D) : L|_K \text{ is affine } \forall K \in \mathfrak{T}_h\}, \tag{2.2}$$

$$\mathbb{U}_h = \{u \in (C(\overline{D}))^m : u|_K \text{ is affine } \forall K \in \mathfrak{T}_h\}, \tag{2.3}$$

$$\mathbb{U}_h(A; D) = \{u \in \mathbb{U}_h : u|_{\partial D} = A\,x\}, \tag{2.4}$$

and

$$F(u, L;\ D) = \int_D f(A + \nabla u(x)(\nabla L(x))^{-1})) \det \nabla L(x)\, dx. \tag{2.5}$$

Then the mesh transformation method yields the following discrete problem :

$$(MT) \quad \begin{cases} \text{find } (u,\ L) \in \mathbb{U}_h(0;\ D) \times T_h(D) \text{ such that} \\ F(u, L;\ D) = \inf_{(u',L') \in \mathbb{U}_h(0;\ D) \times T_h(D)} F(u', L';\ D). \end{cases} \tag{2.6}$$

In the periodic relaxation method, (2.6) is modified as follows. Let

$$S_i^{\pm}(D) = \{x = (x_1, \ldots, x_n) \in \partial D : x_i = \pm 1\},$$

which are the $(n-1)$ faces of D, and let

$$V(D) = \{x = (x_1, \ldots, x_n) \in \partial D : x_i = \pm 1, \forall i\},$$

which is the set of all vertices of $\bar{D}$. In the following, a function $\phi : \bar{D} \to R^n$ is said to be periodic and denoted by $\phi|_{S_i^+} = \phi|_{S_i^-}, \forall i$, if $\phi(x) = \phi(y)$ for all $x \in S_i^+$ and $y \in S_i^-$ satisfying $-1 \le x_j = y_j \le 1,\ \ \forall j \ne i$.

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

$$P(D;\ R) = \{L \in (W^{1,\infty}(D))^n : L^{-1} \in (W^{1,\infty}(L(D)))^n \text{ and } \det \nabla L > 0,$$
$$a.e. \text{ in } D,\ L(x) = R(x), \forall x \in V(D), (L-R)|_{S_i^+} = (L-R)|_{S_i^-}, \forall i\},$$

and define

$$P(D) = \{L \in P(D;\ R) : \text{for some } R \in SO(n)\}. \tag{2.7}$$

$$P_h(D) = \{L \in P(D) : L|_K \text{ is affine } \forall K \in \mathfrak{T}_h\}, \tag{2.8}$$

$$\tilde{\mathbb{U}}(A; D) = \{u \in W^{1,\infty}(D;\ R^m) : u(x) = A\,x, \forall x \in V(D),$$
$$(u(x) - A\,x)|_{S_i^+(D)} = (u(x) - A\,x)|_{S_i^-(D)}, \forall i\}, \tag{2.9}$$

$$\tilde{\mathbb{U}}_h(A; D) = \mathbb{U}_h \cap \tilde{\mathbb{U}}(A; D). \tag{2.10}$$

The following discrete problem is considered in the periodic relaxation method:

$$(PR) \quad \begin{cases} \text{find } (u,\ L) \in \tilde{\mathbb{U}}_h(0;\ D) \times P_h(D) \text{ such that} \\ F(u, L;\ D) = \inf_{(u', L') \in \tilde{\mathbb{U}}_h(0;\ D) \times P_h(D)} F(u', L';\ D). \end{cases} \tag{2.11}$$

Remark 2.1. The functions in $P(D)$ and $\tilde{\mathbb{U}}(0;\ D)$ are so defined that they may be viewed as periodic with period 2 with respect to each variable x_i, $i = 1, 2, \ldots, n$.

Lemma 2.1. *For any $L \in P(D)$, denote*

$$\tilde{\mathbb{U}}(A; L, D) = \{\bar{u} \in W^{1,\infty}(L(D);\ R^m) :$$
$$\bar{u}(x) = u(L^{-1}(x)) + A\,x,\ u \in \tilde{\mathbb{U}}(0; D)\}.$$

We have

$$\inf_{u \in \tilde{\mathbb{U}}(A; L, D)} \frac{1}{\text{meas}(D)} F(u;\ L(D)) \le \inf_{u \in \mathbb{U}(A; \Omega)} \frac{1}{\text{meas}(\Omega)} F(u;\ \Omega), \tag{2.12}$$

where $\text{meas}(\cdot)$ *is the Lebesgue measure in* R^n*, and for all* $\bar{u} \in \tilde{\mathbb{U}}(A; L, D)$

$$\frac{1}{\text{meas}(D)} \int_{L(D)} \nabla \bar{u}(x)\, dx = A. \tag{2.13}$$

Proof. It is well known [12, 15] 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 $f(\cdot)$ [12, 15], *i.e.* the greatest quasiconvex function less than or equal to f. Noticing also that the hypotheses (h1) and (h2) imply the continuity of $F(\cdot; L(D))$ in the strong topology of $W^{1,p}(L(D);\ R^m)$, and for any $L \in P(D)$, $\mathbb{U}(A; L(D)) \cap W^{1,\infty}(L(D);\ R^m)$, which is a subset of $\tilde{\mathbb{U}}(A; L, D)$, is dense in $\mathbb{U}(A; L(D))$, and $\text{meas}(D) = \text{meas}(L(D))$, we have (2.12). (2.13) follows from the periodicity of $\bar{u}(x) - A\,x$, which is a consequence of the periodicity of $\tilde{\mathbb{U}}(0; L, D)$ and $L(D)$. □

Lemma 2.2. *For any $L \in P(D)$ and $u \in \tilde{\mathbb{U}}(0; D)$, let $\bar{u} : L(D) \to R^m$ be defined by*

$$\bar{u}(L(x)) = u(x) + A\,L(x), \quad \forall x \in D. \tag{2.14}$$

Then, $\bar{u} \in \tilde{\mathbb{U}}(A; L, D)$ and

$$F(\bar{u};\ L(D)) = F(u, L;\ D). \tag{2.15}$$

Proof. $\bar{u} \in \tilde{\mathbb{U}}(A; L, D)$ follows directly from (2.9) and (2.14). By a change of integral variables and by (2.5), we have (2.15). □

Lemma 2.3. *For any $L \in P(D)$, we have*

$$\inf_{u \in \tilde{\mathbb{U}}(0;D)} \frac{1}{\text{meas}(D)} F(u, L;\ D) \le \inf_{u \in \mathbb{U}(A;\Omega)} \frac{1}{\text{meas}(\Omega)} F(u;\ \Omega). \tag{2.16}$$

Proof. Since the image of $\tilde{\mathbb{U}}(0; D)$ under the mapping (2.14) is exactly $\tilde{\mathbb{U}}(A; L, D)$, (2.16) follows as a consequence of (2.12) and (2.15). □

Remark 2.2. It is in view of remark 2.1 and (2.16) that we name (2.11) the periodic relaxation method.

Theorem 2.1. *For any $L \in P(D)$, we have*

$$\inf_{u \in \tilde{\mathbb{U}}(0;D)} \frac{1}{\text{meas}(D)} F(u, L;\ D) = \inf_{u \in \mathbb{U}(A;\Omega)} \frac{1}{\text{meas}(\Omega)} F(u;\ \Omega). \tag{2.17}$$

Proof. Let $L \in P(D;\ R)$ with $R \in SO(n)$ and $u \in \tilde{\mathbb{U}}(0; D)$ be given. Let $\lambda \ll 1$, denote $L_{\lambda,z}(D) = \lambda(2R\,z + L(D))$, define

$$\Omega(\lambda) = \{x : x \in L_{\lambda,z}(D) \subset \Omega \text{ for some } z \in \mathbb{Z}^n \text{ and } \operatorname{dist}(L_{\lambda,z}(D),\ \partial\Omega) \geq \lambda\}, \tag{2.18}$$

where $\mathbb{Z}$ is the set of all integers. Let $\varphi_\lambda : \bar{\Omega} \to [0,\ 1]$ be a smooth truncation function satisfying

$$\varphi_\lambda(x) = \begin{cases} 1, & \text{if } x \in \Omega(\lambda), \\ 0, & \text{if } x \in \partial\Omega; \end{cases} \tag{2.19}$$

$$|\nabla\varphi_\lambda(x)| \leq C\lambda^{-1},\ \forall x \in R^n, \tag{2.20}$$

where, in (2.20) and in what follows C is a constant independent of λ. Define $\hat{u}_\lambda : \Omega \to R^m$ by

$$\hat{u}_\lambda(x) = \lambda\,\varphi_\lambda(x)u(L^{-1}(\lambda^{-1}x)) + Ax, \tag{2.21}$$

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

$$L^{-1}(x') = L^{-1}(x), \forall x' \in R^n,\ x \in L(\bar{D}) \text{ and } \frac{1}{2}(x' - x) \in R(\mathbb{Z}^n). \tag{2.22}$$

Then, $\hat{u}_\lambda \in \mathbb{U}(A;\ \Omega) \cap W^{1,\infty}(\Omega;\ R^m)$ and

$$\nabla\hat{u}_\lambda(x) = A + \nabla u(L^{-1}(\lambda^{-1}x))(\nabla L(L^{-1}(\lambda^{-1}x)))^{-1},\ \forall x \in \Omega(\lambda), \tag{2.23}$$

$$|\nabla\hat{u}_\lambda(x)| \leq C,\ \ \forall x \in \Omega. \tag{2.24}$$

A straightforward calculation using the periodic properties of $\hat{u}_\lambda$ and $L(D)$ and the facts that $\operatorname{meas}(D) = \operatorname{meas}(L(D))$ and $\operatorname{meas}(\Omega \setminus \Omega(\lambda)) = O(\lambda)$ yield

$$\left|\frac{1}{\operatorname{meas}(\Omega)}F(\hat{u}_\lambda;\ \Omega) - \frac{1}{\operatorname{meas}(D)}F(u, L;\ D)\right| \leq C\lambda. \tag{2.25}$$

(2.25) implies that

$$\inf_{u\in\mathbb{U}(A;\Omega)} \frac{1}{\operatorname{meas}(\Omega)}F(u;\ \Omega) \leq \inf_{u\in\tilde{\mathbb{U}}(0;D)} \frac{1}{\operatorname{meas}(D)}F(u, L;\ D) \tag{2.26}$$

Thus, by (2.16) and (2.26), the theorem is proved. □

Remark 2.3. The periodic extension of L^{-1} given by (2.22) is not uniquely defined for $x \in L(\partial D)$. However, $\hat{u}_\lambda$ is well defined.

Next, we consider the convergence of the solutions of the discrete problems (2.11)

Theorem 2.2. *For the discrete problem* (2.11)*, we have*

$$\lim_{h\to 0}\inf_{(u,\,L)\in\tilde{\mathbb{U}}_h(0;D)\times P_h(D)}\frac{1}{\mathrm{meas}(D)}F(u,L;\;D)=\inf_{u\in\mathbb{U}(A;\Omega)}\frac{1}{\mathrm{meas}(\Omega)}F(u;\;\Omega). \tag{2.27}$$

Furthermore, let $(u_h,\;L_h)\in\tilde{\mathbb{U}}_h(0;D)\times P_h(D)$ *be a sequence satisfying*

$$F(u_h,\;L_h;\;D)<\inf_{(u,\,L)\in\tilde{\mathbb{U}}_h(0;D)\times P_h(D)}\frac{1}{\mathrm{meas}(D)}F(u,L;\;D)+\mathrm{meas}(D)\,\varepsilon_h \tag{2.28}$$

with $\varepsilon_h>0$ *and* $\lim_{h\to 0}\varepsilon_h=0$. *Then, there exists* $0<\lambda(h)\ll 1$ *satisfying* $\lim_{h\to 0}\lambda(h)=0$ *such that* $\hat{u}_h\in\mathbb{U}(A;\;\Omega)$ *defined by*

$$\hat{u}_h(x)=\lambda(h)\,\varphi_{\lambda(h)}(x)u_h(L_h^{-1}(\lambda^{-1}(h)x))+Ax, \tag{2.29}$$

where $\varphi_\lambda:\bar{\Omega}\to[0,\;1]$ *is a smooth function satisfying* (2.19) *and* (2.20)*, is a minimizing sequence of* $F(\cdot\,;\;\Omega)$ *in* $\mathbb{U}(A;\;\Omega)$*, and*

$$\frac{1}{\mathrm{meas}(\Omega)}F(\hat{u}_h;\;\Omega)<\inf_{(u,\,L)\in\tilde{\mathbb{U}}_h(0;D)\times P_h(D)}\frac{1}{\mathrm{meas}(D)}F(u,L;\;D)+2\,\varepsilon_h. \tag{2.30}$$

Proof. Denote id the identity map on R^n. We have

$$\tilde{\mathbb{U}}(0;D)\times P(D)\supset\tilde{\mathbb{U}}_h(0;D)\times P_h(D)\supset\mathbb{U}_h(0\,;\;D)\times SO(n)\supset\mathbb{U}(0\,;\;D)_h\times\{id\}. \tag{2.31}$$

Since for all $u\in\mathbb{U}_h(A\,;\;D)$ we have

$$F(u_A,id;\;D)=F(u;\;D),$$

where $u_A(x)=u(x)-A\,x\in\mathbb{U}_h(0\,;\;D)$, and [5]

$$\lim_{h\to 0}\inf_{u\in\mathbb{U}_h(A\,;\,D)}\frac{1}{\mathrm{meas}(D)}F(u;\;D)=\inf_{u\in\mathbb{U}(A\,;\,D)}\frac{1}{\mathrm{meas}(D)}F(u;\;D),$$

(2.27) follows from (2.31) and theorem 2.1. The existence of $\lambda(h)$ leading to (2.30) follows directly from (2.25) and (2.28). ☐

As a consequence of (2.31), we have

Corollary 2.1. *Periodic relaxation method (PR) generally produces sharper numerical results than the standard finite element method and the rotational transformation method* [10]. *More precisely, we have*

$$\inf_{u\in\mathbb{U}(A;D)} F(u;\ D) \le \inf_{(u,\ L)\in\tilde{\mathbb{U}}_h(0;D)\times P_h(D)} F(u,L;\ D)$$
$$\le \inf_{(u,\ L)\in\mathbb{U}_h(0;D)\times SO(n)} F(u,L;\ D) \le \inf_{u\in\mathbb{U}_h(A;D)} F(u;\ D), \quad (2.32)$$

where the equalities hold only in special cases.

Corollary 2.2. *Assume that the problem of minimizing $F(\cdot;\ \Omega)$ in $\mathbb{U}(A;\ \Omega)$ admits a Young measure μ_x which is independent of x and is supported on a finite set $\{Y_1, Y_2, \ldots, Y_k\}$. Assume that there exists $(u_h,\ L_h) \in \tilde{\mathbb{U}}_h(0; D) \times P_h(D)$ such that*

$$\mu_x = \sum_{\alpha=1}^{k}[\frac{1}{\mathrm{meas}(D)}\int_D \delta_{(A+\nabla u_h(y)-Y_\alpha)}\ \det\nabla L_h(y)\,dy]\,\delta_{Y_\alpha}, \quad (2.33)$$

where δ_Y is the Dirac measure centered at $Y \in R^{mn}$. Then, the problem can be solved to an arbitrary precision (up to the computer accuracy) by the periodic relaxation method (2.11).

Proof. It follows from (2.33) that [12]

$$\inf_{u\in\mathbb{U}(A;\Omega)} \frac{1}{\mathrm{meas}(\Omega)} F(u;\ \Omega) = \frac{1}{\mathrm{meas}(D)} F(u_h, L_h;\ D). \quad (2.34)$$

In addition, by theorem 2.2, a minimizing sequence $\bar{u}_{h,i} \in \mathbb{U}(A\,;\ \Omega)$ can be constructed by (2.29) by choosing a sequence $0 < \lambda_i(h) \ll 1$ satisfying $\lim_{i\to\infty}\lambda_i(h) = 0$. □

Remark 2.4. It is easily verified that simple laminated microstructures satisfy the assumptions of corollary 2.2, thus they can be approximated by (PR) up to the computer accuracy.

Remark 2.5. It is worth noticing that $P_h(D)$ is not a closed set because of the restriction $\det\nabla L > 0$. This implies that the problem (2.11) may not have a solution. The restriction $\det \nabla L > 0$ may also cause locking in the computation, which deteriorates the performance of the algorithm. To overcome these difficulties, the restriction $\det \nabla L > 0$ can be realized by a penalty method, or simply replaced by $\det \nabla L \geq \varepsilon_h > 0$ in the computation.

Remark 2.6. While the periodic relaxation method is an extension of the rotational transformation method, it is not an extension of the mesh transformation method since $T_h(D)$ is not a subset of $P_h(D)$. In fact, $\dim(T_h(D)) > \dim(P_h(D))$ if $n \geq 3$.

Remark 2.7. As for the boundary layer removing effect, the periodic relaxation method not only avoids the formation of a boundary layer but also causes no "floating", *i.e.* the relation $\int_D \nabla u_h(x)(\nabla L_h(x))^{-1} \det \nabla L_h(x)\, dx = 0$ is kept for the numerical solutions, and thus the Young measure approximation μ_h obtained by (PR) satisfies (see (2.13))

$$\int_{R^{mn}} Y \, d\mu_h(Y) = A.$$

This is one of the advantages of (PR) over the penalty type techniques used in [10, 11] (see section 3 for numerical results).

3. Numerical Examples

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

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

For numerical solutions $(u_h^\lambda,\ L_h^\lambda) \in \bar{\mathbb{U}}_h(0;\ D) \times P_h(D)$, we denote

$$\bar{F}_h^\lambda = \frac{1}{\operatorname{meas}(D)} F(u_h^\lambda, L_h^\lambda;\ D),$$

which should converge to $Qf(A)$ (see (2.17), (2.27)).

Example 1. Consider the Ericksen-James two dimensional energy model for elastic crystals [16, 17, 18] with $f(A) = \phi(A^T A)$ and

$$\phi(C) = \kappa_1(\operatorname{tr} C - 2)^2 + \kappa_2 C_{12}^2 + \kappa_3((\frac{C_{11} - C_{22}}{2})^2 - \varepsilon^2)^2, \tag{3.1}$$

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 [16, 17, 18] that this energy has two symmetry related rotationally invariant elastic energy wells $SO(2)U_0$ and $SO(2)U_1$, where

$$U_0 = \begin{pmatrix} \sqrt{1-\varepsilon} & 0 \\ 0 & \sqrt{1+\varepsilon} \end{pmatrix}, \quad U_1 = \begin{pmatrix} \sqrt{1+\varepsilon} & 0 \\ 0 & \sqrt{1-\varepsilon} \end{pmatrix}, \tag{3.2}$$

and for a rotation

$$R = \begin{pmatrix} \eta_1\eta_2 & \pm\varepsilon \\ \mp\varepsilon & \eta_1\eta_2 \end{pmatrix}, \tag{3.3}$$

U_0 and RU_1 are in rank-one connection, more precisely

$$RU_1 = U_0 + \mathbf{a} \otimes \mathbf{n}, \tag{3.4}$$

where $\mathbf{a} = \sqrt{2}\varepsilon(\eta_1, \ \mp\eta_2)$ and $\mathbf{n} = \frac{1}{\sqrt{2}}(1, \ \pm 1)$.

In our numerical experiments, we take $\kappa_1 = 10$, $\kappa_2 = 3$, $\kappa_3 = 1$, $\varepsilon = 0.1$ and $\mathbf{n} = \frac{1}{\sqrt{2}}(1, \ -1)$, and we consider affine boundary conditions $u(x) = A_\lambda x$ on $\partial\Omega$ with

$$A_\lambda = (1-\lambda)U_0 + \lambda RU_1, \quad 0 < \lambda < 1. \tag{3.5}$$

By [2], the Young measure derived from any minimizing sequence satisfying such a boundary condition is unique and is given by

$$\mu_x^\lambda(\xi) \equiv \mu^\lambda(\xi) = (1-\lambda)\delta_{A_0}(\xi) + \lambda\delta_{A_1}(\xi), \tag{3.6}$$

where δ_E is the Dirac measure centered at E. Thus the numerical solutions are expected to have a banded structure alternating between the two variants A_0 and A_1 with the average ratio $1-\lambda$ to λ. Noticing that

$$Qf(A(\lambda)) = 0,$$

and

$$f(A_\lambda) = 4(\kappa_1 + 4\kappa_2 + \kappa_3)\varepsilon^4\lambda^2(1-\lambda)^2,$$

we regard as a basic requirement that a meaningful numerical solution should have its average energy density much less than ε^4. In other words, we expect to have $\bar{F}_h^\lambda \ll 10^{-4}$.

To present our numerical results, we introduce the following notations:

$$e_\infty(u_h^\lambda, L_h^\lambda;\ K) = \min_{x\in K}\{|A_\lambda + \nabla u_h^\lambda(x)(\nabla L_h^\lambda(x))^{-1} - A_i|,\ i = 0, 1\},$$

$$E_{\infty,h}^\lambda = \max_{K\in\mathfrak{T}_h(D)} e_\infty(u_h^\lambda, L_h^\lambda;\ K),$$

$$E_{2,h}^\lambda = (\sum_{K\in\mathfrak{T}_h(D)} (e_\infty(u_h^\lambda, L_h^\lambda;\ K))^2 \ \mathrm{meas}(L_h^\lambda(K)))^{1/2},$$

$$L_h^i(D,\lambda) = \{x\in D : |A_\lambda + \nabla u_h^\lambda(x)(\nabla L_h^\lambda(x))^{-1} - A_i| = e_\infty(u_h^\lambda, L_h^\lambda;\ K) \quad \text{if } x \in K\}, \quad i = 0, 1,$$

$$e_{\lambda,h} = \max\{|\frac{\mathrm{meas}(L_h^0(D,\lambda))}{(1-\lambda)\ \mathrm{meas}(D)} - 1|,\ |\frac{\mathrm{meas}(L_h^1(D,\lambda))}{\lambda\ \mathrm{meas}(D)} - 1|\},$$

where $E_{\infty,h}^\lambda$ and $E_{2,h}^\lambda$ measure the error between the numerical wells and the analytical ones in L^∞ and L^2 norms respectively, $e_{\lambda,h}$ is the maximum relative error of the average band width ratio.

The conjugate gradient method is used in searching for the minimizers of (PR). The numerical results obtained by the period relaxation method (PR) are given in table 1. We can see in table 1 that very sharp numerical results can be obtained by coarse meshes, which is one of the advantages of the periodic relaxation method. In figure 1 and figure 2, two typical numerical solutions, which represent the same microstructure for $\lambda = 0.4$ are shown.

Example 2. Let the energy density $f : R^{2\times 2} \to R$ be given by

$$f(A) = \langle A - B,\ A - B\rangle \cdot \langle A + B,\ A + B\rangle, \quad \forall A \in R^{2\times 2}, \tag{3.7}$$

λ	N	$\bar{F}_h^\lambda$	$e_{\lambda,h}$	$E_{\infty,h}^\lambda$	$E_{2,h}^\lambda$
0.50	4	3.919×10^{-27}	1.437×10^{-13}	3.939×10^{-13}	1.240×10^{-12}
0.45	4	1.588×10^{-23}	1.802×10^{-10}	2.508×10^{-11}	7.747×10^{-11}
0.40	4	2.000×10^{-9}	2.171×10^{-9}	3.350×10^{-10}	8.769×10^{-10}
0.35	4	1.720×10^{-12}	4.560×10^{-5}	1.016×10^{-5}	2.565×10^{-5}
0.30	4	1.211×10^{-11}	2.511×10^{-4}	2.199×10^{-5}	6.405×10^{-5}
0.25	4	8.904×10^{-21}	7.642×10^{-9}	6.496×10^{-10}	1.718×10^{-10}
0.20	5	4.375×10^{-17}	6.549×10^{-7}	5.800×10^{-8}	1.360×10^{-7}
0.19	5	6.635×10^{-12}	2.638×10^{-4}	2.273×10^{-5}	5.307×10^{-5}

TABLE 1. Numerical results obtained by PR for example 1.

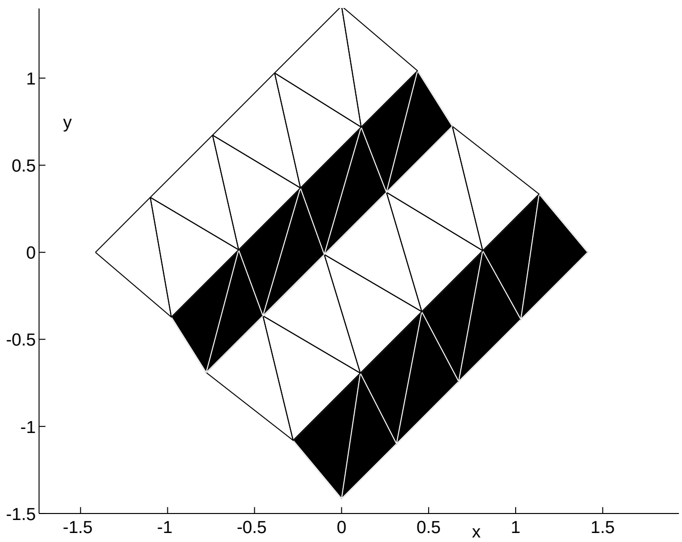

FIGURE 1. A periodic brick of banded microstructure for $\lambda = 0.4$ obtained by PR ($\theta = \frac{\pi}{4}$), where the white and black elements are in the wells A_0 and A_1 respectively.

where $\langle A,\ C\rangle = \sum_{i,j=1}^{2} a_{ij}c_{ij}$ denotes the inner product in $R^{2\times 2}$. Let $B \in R^{2\times 2}$ be given by

$$\begin{pmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{3.8}$$

Consider affine boundary conditions $u(x) = A_\lambda x$ on $\partial\Omega$ with

$$A_\lambda = \lambda A + (1-\lambda)(-A) = (2\lambda - 1)A, \tag{3.9}$$

where A is the unique solution of the system

$$\alpha A + \operatorname{adj} A = \beta B, \tag{3.10}$$

and where in (3.10)

$$\alpha = \frac{7+\sqrt{45}}{2}, \quad \beta = (\frac{\sqrt{45}(7+\sqrt{45})}{2})^{1/2}. \tag{3.11}$$

By [8], A and $-A$ are in rank-one connection and

$$f(A) = f(-A) = \inf\{f(B) : \det B = 0\} = Qf(0) = \frac{1}{4}. \tag{3.12}$$

Since quasiconvexity implies rank-one convexity [12], (3.12) gives

$$Qf(A_\lambda) = \frac{1}{4}, \quad \forall \lambda \in [0,\ 1]. \tag{3.13}$$

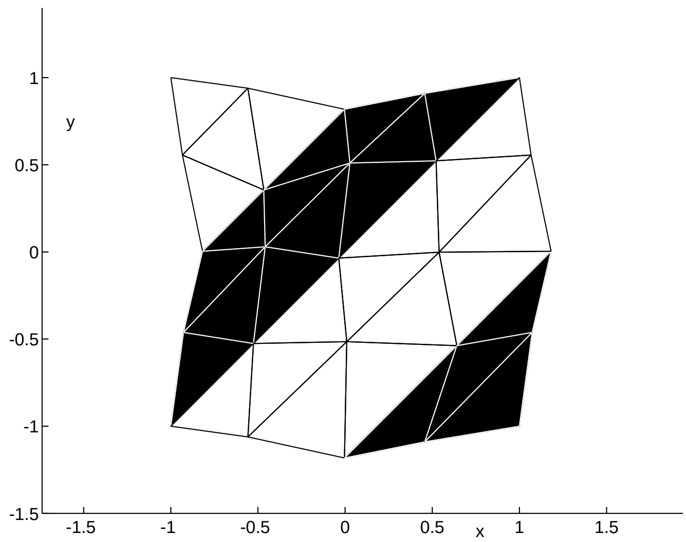

FIGURE 2. A periodic brick of banded microstructure for $\lambda = 0.4$ obtained by PR ($\theta = 0$), where the white and black elements are in the wells A_0 and A_1 respectively.

Thus we have

$$\inf_{u \in \mathbb{U}(A_\lambda;\Omega)} \frac{1}{\text{meas}(\Omega)} F(u;\ \Omega) = \frac{1}{4}, \quad \forall \lambda \in [0,\ 1], \tag{3.14}$$

and the Young measure derived from any minimizing sequence satisfying the boundary condition $u(x) = A_\lambda x$ on $\partial\Omega$ is given by [8]

$$\mu_x^\lambda(\xi) \equiv \mu^\lambda(\xi) = \lambda\delta_A(\xi) + (1-\lambda)\delta_{-A}(\xi). \tag{3.15}$$

Numerical results obtained by the periodic relaxation method (PR) and by the mesh transformation method with penalty terms (1.3) and (1.4) (MTP2) [11] are shown in table 2 and table 3 respectively, where

$$E_r(\bar{F}_h^\lambda) = \frac{4}{\text{meas}(D)} F(u_h^\lambda, L_h^\lambda;\ D) - 1$$

measures the relative error of the energy density, and the other notations are the same as those used in example 1. It is clearly seen in the tables that PR produced sharp numerical results for all λ and MTP2 produced numerical results with obvious "floating" which becomes more severe as λ is further away from 0.5.

λ	N	$E_r(\bar{F}_h^\lambda)$	$e_{\lambda,h}$	$E_{\infty,h}^\lambda$	$E_{2,h}^\lambda$
0.5	4	$< 10^{-16}$	4.738×10^{-10}	7.996×10^{-9}	1.339×10^{-8}
0.6	4	6.767×10^{-9}	1.238×10^{-7}	2.729×10^{-5}	6.305×10^{-5}
0.7	4	4.873×10^{-7}	1.170×10^{-6}	3.464×10^{-4}	5.373×10^{-4}
0.8	4	6.659×10^{-6}	2.465×10^{-5}	2.268×10^{-3}	1.982×10^{-3}

Table 2. Numerical results obtained by PR for example 2.

λ	N	$E_R(\bar{F}_h^\lambda)$	$e_{\lambda,h}$	$E_{\infty,h}^\lambda$	$E_{2,h}^\lambda$
0.5	10	7.219×10^{-6}	2.598×10^{-4}	1.816×10^{-3}	1.174×10^{-3}
0.6	10	-3.481×10^{-2}	3.287×10^{-5}	6.084×10^{-2}	8.685×10^{-2}
0.7	10	-1.428×10^{-1}	3.076×10^{-3}	1.143×10^{-1}	1.714×10^{-1}
0.8	10	-3.325×10^{-1}	1.528×10^{-2}	1.675×10^{-1}	2.542×10^{-1}

Table 3. Numerical results obtained by MTP2 for example 2.

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E-mail address: `zpli@math.pku.edu.cn`