A Coupled Numerical Method for Relaxed Minimizers and Inhomogeneous Microstructures

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Abstract

A numerical method is established to solve a coupled problem of minimizing a nonquasiconvex potential energy and its relaxed energy. Convergence of the method is proved. A numerical example shows that the method is successful and efficient in solving problems with nonlinear boundary data and inhomogeneous laminated microstructures.

1. Introduction

In many physical problems, such as those which involve phase transitions and hysteresis [**1**], one is often lead to consider the problem of minimizing a potential energy

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

with nonquasiconvex energy density $f : \Omega \times R^m \times R^{mn} \to R^1$ defined on a set of admissible functions

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

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**], which are characterized by the Young measure [**2**] and are closely related to the relaxed minimizers [**3**], namely the minimizers of the relaxed energy

$$QF(u;\ \Omega) \equiv \int_\Omega Qf(x,\ u(x),\ \nabla u(x))\, dx,$$

in $\mathbb{U}(u_0;\ \Omega)$, where $Qf(x,\ s,\ \xi)$ is the quasiconvex envelope of $f(x,\ s,\ \xi)$ [**4**]. In fact, under certain general hypotheses on f, we have [**3**]

$$\begin{aligned} QF(u;\Omega) = \Gamma^{-}\text{-}\lim F(u;\Omega) \equiv \min\{\liminf_{\alpha\to\infty} F(u_\alpha;\Omega) :\\ u_\alpha \in \mathbb{U}(u_0;\Omega), u_\alpha \rightharpoonup u \text{ in } W^{1,p}(\Omega;R^m)\}, \end{aligned} \tag{1.2}$$

where in (1.2) '$\rightharpoonup$' means 'converges weakly to' and $\Gamma^{-}\text{-}\lim F(u;\Omega)$ turns out to be the greatest 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 [**3**]). Since the explicit form of Qf is generally not available, (1.2) plays a very important role in the numerical computations of the relaxed minimizers and microstructures. Recently, a numerical method for the evaluation of $\Gamma^{-}\text{-}\lim F(u;\ \Omega)$ has been developed. The idea is that, for a continuous quasiconvex envelope $Qf(\cdot,\cdot,\cdot)$, $QF(u;\ \Omega)$ is a limit of the following finite sum as $h \to 0$

$$\sum_{K\in\mathfrak{T}_h(\Omega)} \int_K Qf(x_K, u(x_K), \nabla u(x_K))\, dx, \tag{1.3}$$

where $\mathfrak{T}_h(\Omega)$ is a triangulation of Ω with a mesh size h [**9**], and each integral $\int_K Qf(x_K, u(x_K), \nabla u(x_K))\, dx$ can be evaluated by finding a minimizing sequence for the problem [**3**]

$$\inf_{v\in\mathbb{U}(0;\ K)} \int_K f(x_K, u(x_K), \nabla u(x_K) + \nabla v(x))\, dx. \tag{1.4}$$

Thus the problem of evaluating $QF(u;\ \Omega)$ (see (1.2)) is reduced to a group of homogeneous subproblems (1.4) which are generally much easier to solve and can be solved in parallel. In the present paper, a coupled parallel numerical method is designed so that the numerical solutions of (1.4) are not only used to calculate $QF(u;\ \Omega)$ for a given u but also used to find a descent direction of it. Here in this paper, for simplicity, the rotational transformation method, which can be viewed as a special version of the mesh transformation method and the periodic relaxation method and can produce quite sharp numerical results for simple laminated microstructures [**6**], is applied to solve in parallel the homogeneous subproblems (1.4). In principle, any available numerical method, which can produce accurate numerical solutions to the homogeneous subproblems (1.4), can be used for our purpose. The method given in this paper has several advantages over the direct finite element approximation and the method given in [**5**], for example, (i) the relaxed minimizer and the Young measure are approximated simultaneously; (ii) the problem is solved by a coupled iteration of a group of subproblems which can be solved in parallel; (iii) every subproblem is homogeneous with linear boundary data and is defined on a standard domain; (iv) some high performance numerical methods for such subproblems are available and the investigations in this direction have great potential; (v) the total computing cost is much reduced, especially for locally laminated microstructures [**6, 7, 8**].

2. Numerical computation of $QF(u;\ \Omega)$

Let $D=(-1,\ 1)^n$. Define, for $u\in W^{1,p}(D;\ R^m)$ and $R\in SO(n)$,

$$\hat{F}_{i,K}(u,R;\,D)=\int_D f(x_{\scriptscriptstyle K},u_{h_i}(x_{\scriptscriptstyle K}),\nabla u_{h_i}(x_{\scriptscriptstyle K})+\nabla u(x)R^{-1})\,dx. \tag{2.1}$$

Let $\mathfrak{T}_{\hat{h}}(D)$ be regular triangulations of D and

$$\mathbb{U}_{\hat{h}}(D)(0;\ D)=\{u\in(C(\bar{D}))^m : u|_K\in(P_1(K))^m,\ \forall K\in\mathfrak{T}_{\hat{h}}(D), u=0 \text{ on } \partial D\}, \tag{2.2}$$

Numerical solutions to the problems (1.4) can then be obtained by applying periodic extension, rescaling, rotational transformations and truncations to the solutions of the following problems (see [**6**] for more details)

$$\begin{cases}\text{minimize } \hat{F}_{i,K}(u_{\hat{h}},R_{\hat{h}};\ D) \text{ for}\\ (u_{\hat{h}},R_{\hat{h}})\in\mathbb{U}_{\hat{h}}(0;\ D)\times SO(n).\end{cases} \tag{2.3}$$

Let $\lim_{i\to\infty}h_i=+0$, and let $\mathfrak{T}_{h_i}(\Omega)$ be regular triangulations of Ω with mesh size h_i [**9**] such that for all i, $\mathfrak{T}_{h_{i+1}}(\Omega)$ is a refinement of $\mathfrak{T}_{h_i}(\Omega)$. Let $\mathbb{U}_{h_i}(u_0;\ \Omega)$ be the set of the continuous piecewise affine functions defined on $\mathfrak{T}_i(\Omega)$ with boundary data u_0. Let $u_{h_i}\in\mathbb{U}_{h_i}(u_0;\ \Omega)$ and $u_{h_i}\to u$ in $W^{1,p}(\Omega;\ R^m)$. Define

$$\Upsilon^{i,j}_{\hat{h}}(\Omega)=\prod_{K\in\mathfrak{T}_{i+j}(\Omega)}(\mathbb{U}_{\hat{h}}(0;\ D)\times SO(n)). \tag{2.4}$$

We will call $\prod_{K\in\mathfrak{T}_{i+j}(\Omega)}(u^{i,K}_{\hat{h}},R^{i,K}_{\hat{h}})\in\Upsilon^{i,j}_{\hat{h}}(\Omega)$ the numerical microstructure corresponding to the function $u_{h_i}\in\mathbb{U}_{h_i}(u_0;\ \Omega)$ and denote it by $\upsilon^{i,j}_{\hat{h}}(u_{h_i})$ if, for all $K\in\mathfrak{T}_{i+j}(\Omega)$, $(u^{i,K}_{\hat{h}},R^{i,K}_{\hat{h}})$ are the solutions of (2.3). We have that

$$QF^{i,j}_{\hat{h}}(u_{h_i};\ \Omega)=2^{-n}\sum_{K\in\mathfrak{T}_{h_{i+j}}(\Omega)}\text{meas}(K)\int_D f(x_{\scriptscriptstyle K},u_{h_i}(x_{\scriptscriptstyle K}),\nabla u_{h_i}(x_{\scriptscriptstyle K})+\nabla u^{i,K}_{\hat{h}}(x)(R^{i,K}_{\hat{h}})^{-1})dx,$$

is a numerical approximation of $QF(u_{h_i};\ \Omega)$.

3. A coupled discrete problem and its numerical solution

The purpose of this section is to establish a numerical method to find a numerical solution to the problem of

$$\inf_{u\in\mathbb{U}_{h_i}(u_0;\ \Omega)} QF(u;\ \Omega) \tag{3.1}$$

and a corresponding numerical microstructure. The idea is to solve the discrete problem

$$(P)\begin{cases}\text{minimize } GF^{i,j}_{\hat{h}}(u,\upsilon;\ \Omega) \text{ for}\\ (u,\ \upsilon)\in\mathbb{U}_{h_i}(u_0;\ \Omega)\times\Upsilon^{i,j}_{\hat{h}}(\Omega),\end{cases} \tag{3.2}$$

by applying iteratively a coupled descent method to the following coupled discrete problems

$$(P1)\begin{cases}\text{minimize } GF^{i,j}_{\hat{h}}(u^\alpha,\upsilon^\alpha;\ \Omega) \text{ for}\\ \upsilon^\alpha\in\Upsilon^{i,j}_{\hat{h}}(\Omega),\end{cases} \tag{3.3}$$

and

$$(P2)\begin{cases}\text{minimize } GF^{i,j}_{\hat{h}}(u^\alpha+t_\alpha\delta u^\alpha,\upsilon^\alpha;\ \Omega)\\ \text{for} t_\alpha>0,\end{cases} \tag{3.4}$$

where, for $u\in\mathbb{U}_{h_i}(u_0;\ \Omega)$ and $\upsilon\in\Upsilon^{i,j}_{\hat{h}}(\Omega)$,

$$GF^{i,j}_{\hat{h}}(u,\upsilon;\ \Omega)=2^{-n}\sum_{K\in\mathfrak{T}_{h_{i+j}}(\Omega)}\text{meas}(K)\int_D f(x_{\scriptscriptstyle K},u(x_{\scriptscriptstyle K}),\nabla u(x_{\scriptscriptstyle K})+\nabla\upsilon^{i,K}_{\hat{h}}(x)(R^{i,K}_{\hat{h}})^{-1})\,dx,$$

and δu^α is a descent direction of $GF^{i,j}_{\hat{h}}(\cdot,\upsilon^\alpha;\Omega)$ at u_α. This can be summed up into the algorithm (A):

$$\begin{cases}\text{step 1: set } \alpha=0, \text{ give } u^0\in\mathbb{U}_{h_i}(u_0;\ \Omega);\\ \text{step 2: compute } \upsilon^\alpha \text{ by solving (P1)};\\ \text{step 3: if } \|\delta u^\alpha\|<\varepsilon,\ (u(\varepsilon),\upsilon(\varepsilon))=(u^\alpha,\upsilon^\alpha), \text{ stop};\\ \text{step 4: compute } t_\alpha \text{ by solving (P2)};\\ \text{step 5: define } u^{\alpha+1}=u^\alpha+t_\alpha\delta u^\alpha;\\ \text{step 6: set } \alpha=\alpha+1, \text{ go back to step 2,}\end{cases}$$

where $\varepsilon>0$ is a given tolerance.

4. Convergence of the method

The convergence of the method consists of two parts. The first part is that the sequences produced by the algorithm (A) converge to the solutions of the problem (P). The second part is that the solutions of the problem (P) converge to the relaxed minimizers and the corresponding microstructures.

THEOREM 4.1. *Let $u^0\in\mathbb{U}_{h_i}(u_0;\ \Omega)$ be arbitrarily given. Let $(u(\varepsilon_k),\ \upsilon(\varepsilon_k))\in\mathbb{U}_{h_i}(u_0;\ \Omega)\times\Upsilon^{i,j}_{\hat{h}}(\Omega)$ be obtained by algorithm (A) with the tolerance $\varepsilon_k\to 0^+$ as $k\to\infty$. Then, there exists a $(u_{h_i},\ \upsilon^{i,j}_{\hat{h}})\in\mathbb{U}_{h_i}(u_0;\ \Omega)\times$*

$\Upsilon^{i,j}_{\hat{h}}(\Omega)$ *and a subsequence of* $\{(u(\varepsilon_k),\ \upsilon(\varepsilon_k))\}$, *denoted again by* $\{(u(\varepsilon_k),\ \upsilon(\varepsilon_k))\}$, *such that*

$$(u(\varepsilon_k),\ \upsilon(\varepsilon_k)) \to (u_{h_i},\ \upsilon^{i,j}_{\hat{h}}), \quad as\ k \to \infty,$$
$$D(GF^{i,j}_{\hat{h}})(u_{h_i},\ \upsilon^{i,j}_{\hat{h}};\ \Omega) = 0,$$
$$GF^{i,j}_{\hat{h}}(u_{h_i},\ \upsilon^{i,j}_{\hat{h}};\ \Omega) = \inf_{\upsilon \in \Upsilon^{i,j}_{\hat{h}}(\Omega)} GF^{i,j}_{\hat{h}}(u_{h_i},\ \upsilon;\ \Omega),$$

and

$$D(QF^{i,j}_{\hat{h}})(u_{h_i};\ \Omega) = 0.$$

THEOREM 4.2. *There exists a nondecreasing function* $J(i)$ *and a nonincreasing function* $H(i,j)$ *such that for any sequence of solutions* $\{(u^{j,\hat{h}}_{h_i}, \upsilon^{i,j}_{\hat{h}})\}$ *of the problem (P) with* $i = 1,2,\ldots,\ j \geq J(i)$ *and* $0 < \hat{h} \leq H(i,j)$, *there is a subsequence of* $\{(u^{j,\hat{h}}_{h_i}, \upsilon^{i,j}_{\hat{h}})\}$, *denoted again by* $\{(u^{j,\hat{h}}_{h_i}, \upsilon^{i,j}_{\hat{h}})\}$, *and a function* $\hat{u} \in \mathbb{U}(u_0;\ \Omega)$ *satisfying*

$$\inf_{u \in \mathbb{U}(u_0;\ \Omega)} QF(u;\ \Omega) = \lim_{i\to\infty} GF^{i,j}_{\hat{h}}(u^{j,\hat{h}}_{h_i}, \upsilon^{i,j}_{\hat{h}};\ \Omega),$$
$$u^{j,\hat{h}}_{h_i} \rightharpoonup \hat{u} \quad in\ W^{1,p}(\Omega;\ R^m)\ as\ i \to \infty,$$
$$QF(\hat{u};\ \Omega) = \inf_{u \in \mathbb{U}(u_0;\ \Omega)} QF(u;\ \Omega).$$

5. A numerical example

Let $\Omega = (0,\ 1) \times (0,\ 1)$. Let $x = (x_1,\ x_2)^T \in \Omega$

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

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

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

$$F(u;\ \Omega) = \int_\Omega f(\nabla u(x)C(x))(\det(C(x)))^{-1}\, dx,$$
$$U(u_0;\ \Omega) = \{u \in W^{1,4}(\Omega;\ R^2) : u = u_0,\ \text{on}\ \partial\Omega\},$$

where

$$u_0^T(x) = \frac{1}{6}(-x_1 + \frac{\sqrt{1+8x_2}-1}{2}, x_1 - \frac{\sqrt{1+8x_2}-1}{2}).$$

It is easily verified that minimizing sequences of $\Gamma^{-}\text{-}\lim F(u_0;\ \Omega)$ lead to a Young measure

$$\mu(x) = \frac{2}{3}\delta_{BC^{-1}(x)} + \frac{1}{3}\delta_{-BC^{-1}(x)},$$

and

$$\Gamma^{-}\text{-}\lim F(u_0;\ \Omega) = QF(u_0;\ \Omega) = 0.$$

The following table shows the convergence of the algorithm (A) for the numerical relaxed minimizers and the numerical microstructures with $h_i = \frac{\sqrt{2}}{3}$, $j = 0$, $\hat{h} = \frac{\sqrt{2}}{9}$ and the initial data

$$u^0(x) = u_0(x) + x_1x_2(1-x_1)(1-x_2)\begin{pmatrix} -1 \\ 1 \end{pmatrix}.$$

where $QF = QF^{i,j}_{\hat{h}}(u^\alpha_{h_i};\ \Omega)$, $e_{0,2} = \|u^\alpha_{h_i} - u_{0h_i}\|_{0,2,\Omega}$ and $e_{1,2} = |u^\alpha_{h_i} - u_{0h_i}|_{1,2,\Omega}$ measure the error of the numerical relaxed minimizer, and where $d^\alpha(h_i, \hat{h})$ and $V^\alpha(h_i, \hat{h})$ measure the difference between the numerical microstructure and the Young measure on the deformation gradients (in $L^2(\Omega)$-norm) and the volume fraction (also in $L^2(\Omega)$-norm) respectively.

iterations	QF	$e_{0,2}$	$e_{1,2}$
$\alpha = 10$	2.9×10^{-2}	1.8×10^{-2}	6.2×10^{-2}
$\alpha = 20$	4.0×10^{-4}	1.9×10^{-4}	5.7×10^{-4}
$\alpha = 25$	4.0×10^{-4}	1.6×10^{-4}	5.8×10^{-4}
iterations	$\|\delta u^\alpha_{h_i}\|$	$d^\alpha(h_i, \hat{h})$	$V^\alpha(h_i, \hat{h})$
$\alpha = 10$	6.1×10^{-1}	9.9×10^{-2}	2.2×10^{-2}
$\alpha = 20$	4.4×10^{-3}	2.0×10^{-2}	4.0×10^{-3}
$\alpha = 25$	9.8×10^{-4}	2.2×10^{-2}	4.0×10^{-3}

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