NUMERICAL ANALYSIS AND COMPUTATION OF A MULTI-ORDER LAMINATED MICROSTRUCTURE

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Abstract. The mesh transformation method is applied in a finite element approximation to a multi-well problem. It is proved that, compared with standard finite element methods, significantly higher convergence rate for the finite element approximations of multi-level microstructures can be obtained by combining the mesh transformation method with the periodic relaxation technique. Numerical examples are given to show the method can be efficiently implemented in computing multi-level microstructures.

1. Introduction

We consider the problem of minimizing the integral functional

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

in a set of admissible deformations

$$\mathbb{U}(u_0;\ \Omega) := W_0^{1,\infty}(\Omega; R^2) = \{u \in W^{1,\infty}(\Omega; R^2) : u = 0,\ \text{on } \partial\Omega\}, \tag{1.2}$$

where $\Omega \subset R^2$ is a bounded open set with a Lipschitz continuous boundary $\partial\Omega$, and the integrand $f : R^{2\times 2} \to [0,\ \infty)$ is continuous with exactly four

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potential wells

$$W_1 = \begin{pmatrix} 1/2 & 0 \\ 0 & 2 \end{pmatrix}, \; W_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \; W_3 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \; W_4 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

i.e.

$$f(W_i) = 0, \quad i = 1, 2, 3, 4, \text{ and } f(W) > 0, \;\; \forall W \notin \{W_1, W_2, W_3, W_4\}, \tag{1.3}$$

and $f(A) \to \infty$, as $\|A\| \to \infty$.

It is well known that variational problems with non-quasi-convex integrands generally do not have solutions and the minimizing sequences produce finer and finer oscillations which lead to microstructures [1, 2]. The problem we consider here is a typical example which leads to a microstructure with four levels of laminates in laminates, or fourth-order laminated microstructure (see for example [3, 4]).

Numerical methods have been developed in the last twenty years to compute the simple laminated microstructure (see [25] for a survey on the conforming and nonconforming finite element approximations before 1996, see also [9, 10, 11, 12, 17, 19] among many others for more recent developments).

One of the main difficulties in the finite element approximations of microstructures is that the numerical solution is strongly mesh dependent and, unless the mesh is properly provided, it often produces false information on the microstructure in question [6, 7, 15, 16, 25], more precisely it typically produces one of the many spurious local minimizers of the discrete problem established on an unaligned mesh. To avoid strong mesh dependence of the finite element approximation, it is natural to involve the mesh distribution in a minimization procedure so that the mesh can align with the interfaces of the microstructure, which will then be capable of capturing the sharp interfaces and significantly reduce the approximation error [15, 19, 20, 21, 22, 23]. To guarantee the stability of the method, mesh quality control techniques can be applied [13, 14, 24, 26]. The size of the discrete problem is another crucial obstacle. Thanks to the periodic structure of the laminated microstructures (in fact it is in some sense a general property of microstructures, which is closely related to the definition of the quasi-convex envelope [8]), instead of solving the original problem, we may restrict ourselves to one period of the structure. This is the idea of the periodic relaxation method, which, along with some other advantages, significantly reduces the size of the problem [18]. For our problem, which leads to a fourth-order laminated microstructure, the mesh transformation method coupled with the periodic relaxation technique effectively reduces the size of the discrete problem to an equivalence of a second-order laminated microstructure, and increases the convergence rate to $O(h^{1/2})$ which is the convergence rate for a simple laminated microstructure by standard finite element methods [25].

In our method, we work on a computation domain $\Omega_C = (-1,\, 1)^2$. Let $\mathfrak{T}_h(\Omega_C)$ be a family of regular triangulations of Ω_C [5]. Denote the four sides of Ω_C by

$$S_i^{\pm}(\Omega_C) = \{x = (x_1, x_2) \in \partial\Omega_C : x_i = \pm 1\}, \quad i = 1, 2,$$

and the four vertices of Ω_C by

$$V(\Omega_C) = \{x = (x_1, x_2) \in \partial\Omega_C : x_1, x_2 = \pm 1\}.$$

For a given rotational matrix $R \in SO(2)$, define

$$\begin{aligned} P(\Omega_C; R) = \{&g \in (W^{1,\infty}(\Omega_C))^2 : g^{-1} \in (W^{1,\infty}(g(\Omega_C)))^2 \text{ and } \det \nabla g > 0, \\ &a.e. \text{ in } \Omega_C,\ g(x) = Rx, \forall x \in V(\Omega_C), (g - R)|_{S_i^+} = (g - R)|_{S_i^-}, i = 1, 2\}. \end{aligned}$$

The image $g(\Omega_C)$ of a map $g \in P(\Omega_C; R)$ is a periodic domain with its four vertices coinciding with those of $R(\Omega_C)$. Suppose $\Omega = g(\Omega_C)$, by a change of the integral variables and by setting $\bar{u}(x) = u(g(x))$, we have

$$F(\bar{u}, g; \Omega_C) := \int_{\Omega_C} f(\nabla \bar{u}(x)(\nabla g(x))^{-1})) \det \nabla g(x)\, dx = F(u; \Omega).$$

Thus the mesh transformation method combined with the periodic relaxation method leads to the following discrete problem

$$(MPR) \qquad \begin{cases} \text{find } (\bar{u},\, g) \in \tilde{\mathbb{U}}_h(0;\ \Omega_C) \times P_h(\Omega_C) \text{ such that} \\ F(\bar{u}, g;\ \Omega_C) = \inf_{(\bar{u}', g') \in \tilde{\mathbb{U}}_h(0;\ \Omega_C) \times P_h(\Omega_C)} F(\bar{u}', g';\ \Omega_C), \end{cases} \tag{1.4}$$

where

$$P_h(\Omega_C) = \{g \in P(\Omega_C; R) : \exists R \in SO(2),\ g|_K \text{ is affine } \forall K \in \mathfrak{T}_h(\Omega_C)\} \tag{1.5}$$

is the set of the admissible finite element mesh mappings and

$$\tilde{\mathbb{U}}_h(0;\Omega_C) = \mathbb{U}_h \cap \tilde{\mathbb{U}}(0;\Omega_C) \tag{1.6}$$

is the set of periodic finite element functions which vanish on the four vertices, *i.e.*

$$\begin{aligned}\tilde{\mathbb{U}}(0;\Omega_C) = \{\bar{u} \in W^{1,\infty}(\Omega_C;\ \mathbb{R}^2) : \bar{u}(x) = 0, \forall x \in V(\Omega_C),\\ \bar{u}|_{S_i^+(\Omega_C)} = \bar{u}|_{S_i^-(\Omega_C)}, i = 1, 2\},\end{aligned} \tag{1.7}$$

$$\mathbb{U}_h = \{\bar{u} \in (C(\overline{\Omega_C}))^m : \bar{u}|_K \text{ is affine } \forall K \in \mathfrak{T}_h(\Omega_C)\}. \tag{1.8}$$

The rest of the paper is organized as follows. In section 2, the fourth-order laminated microstructure is described. In section 3, we analyze the convergence rate of the method by constructing finite element approximations of the discrete problem. In section 4, we show some numerical examples. Finally, the conclusions are given in section 5.

2. The fourth-order laminated structure

We refer to [4] for an argument for the proof of the next lemma.

Lemma 2.1. *The infimum of $F(\cdot;\ \Omega)$ in $\mathbb{U}(0;\ \Omega)$ is not attainable, and the minimizing sequences leads to the homogeneous Young measure*

$$\nu_x \equiv \frac{2}{9}\delta_{W_1} + \frac{1}{3}\delta_{W_2} + \frac{1}{18}\delta_{W_3} + \frac{1}{6}\delta_{W_4}, \tag{2.1}$$

where δ_A is the Dirac measure centered at A.

The key observation is that for any two matrixes $A,\ B \in R^2$ with rank one connection, i.e. $\text{rank}(A - B) \leq 1$ or $A - B = \mathbf{a} \otimes \mathbf{n}$, and any given $\mu \in (0,\ 1)$, the sequence defined by

$$u_k(x) = B\,x + \left\{\int_0^{x\cdot\mathbf{n}} \chi_k(s)\,ds\right\}\mathbf{a}, \tag{2.2}$$

where $\chi_k(s) : R \to R$ is the characteristic function defined by

$$\chi_k(s) = \begin{cases} 0, & \text{if } 0 \leq kx - [kx] < \mu, \\ 1, & \text{if } \mu \leq kx - [kx] < 1, \end{cases} \tag{2.3}$$

with $[kx]$ being the integer part of kx, produces a simple laminated microstructure with interfaces normal to $\mathbf{n}$, which has piecewise constant deformation gradients

$$\nabla u_k = B + \chi_k(x \cdot \mathbf{n})\mathbf{a} \otimes \mathbf{n} = \begin{cases} B, & \text{if } 0 \leq kx - [kx] < \mu, \\ A, & \text{if } \mu \leq kx - [kx] < 1, \end{cases} \tag{2.4}$$

with volume fractions μ and $(1-\mu)$, and an average gradient

$$\overline{\nabla u_k} = \mu\, B + (1-\mu)A, \quad \forall k. \tag{2.5}$$

Furthermore, the sequence given by (2.2) leads to a homogeneous Young measure

$$\nu_x = \mu\, \delta_B + (1-\mu)\, \delta_A. \tag{2.6}$$

Now, let us illustrate how the Young measure (2.1) is realized by a fourth-order laminated microstructure.

First of all, notice that

$$0 = \frac{1}{3}\, A + \frac{2}{3}\, B, \tag{2.7}$$

where (see Figure 1)

$$A = \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} 1/2 & 0 \\ 0 & 0 \end{pmatrix}. \tag{2.8}$$

Since A and B is rank-one connected, more precisely, we have

$$B - A = \begin{pmatrix} 3/2 \\ 0 \end{pmatrix} \begin{pmatrix} 1, & 0 \end{pmatrix},$$

we see that 0 can be realized by a simple laminated microstructure having piecewise deformation gradients A and B with volume fractions $\lambda_1 = 2/3$ and $(1 - \lambda_1) = 1/3$ respectively, and with interfaces normal to $(1,\, 0)^T$.

Next, notice that

$$B = \frac{1}{2}\, C + \frac{1}{2}\, D, \tag{2.9}$$

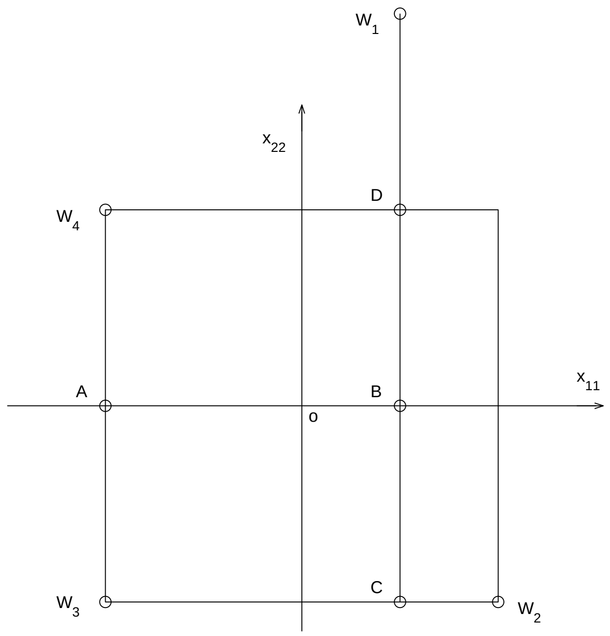

FIGURE 1. Potential wells on x_{11}-x_{22} plane.

where

$$C = \begin{pmatrix} 1/2 & 0 \\ 0 & -1 \end{pmatrix}, \qquad D = \begin{pmatrix} 1/2 & 0 \\ 0 & 1 \end{pmatrix}, \tag{2.10}$$

and that

$$A = \frac{1}{2} W_3 + \frac{1}{2} W_4. \tag{2.11}$$

Since

$$D - C = \begin{pmatrix} 0 \\ 2 \end{pmatrix} \begin{pmatrix} 0, & 1 \end{pmatrix}, \quad W_4 - W_3 = \begin{pmatrix} 0 \\ 2 \end{pmatrix} \begin{pmatrix} 0, & 1 \end{pmatrix},$$

we see that B (respectively A) can be realized by a simple laminated microstructure having piecewise deformation gradients C and D (respectively W_3 and W_4) with volume fractions $\lambda_2 = (1 - \lambda_2) = 1/2$ (respectively $\lambda_3 = (1 - \lambda_3) = 1/2$), and with interfaces normal to $(0, 1)^T$.

Thus, 0 can be realized by a second-order laminated microstructure, in which the simple laminates with average gradients A and B are embedded into the simple laminates with average gradient 0 to form the laminates in laminates microstructure. We denote such a fact by the following rank-one decomposition, which is a nested sum of rank-one connected pairs,

$$0 = \frac{2}{3}\left(\frac{1}{2}C + \frac{1}{2}D\right) + \frac{1}{3}\left(\frac{1}{2}W_3 + \frac{1}{2}W_4\right). \tag{2.12}$$

With similar arguments, it follows from

$$D = \frac{2}{3}W_1 + \frac{1}{3}C, \quad C = \frac{3}{4}W_2 + \frac{1}{4}W_3, \tag{2.13}$$

and the rank-one connections

$$W_1 - C = \begin{pmatrix} 0 \\ 3 \end{pmatrix} \begin{pmatrix} 0, & 1 \end{pmatrix}, \quad W_2 - W_3 = \begin{pmatrix} 2 \\ 0 \end{pmatrix} \begin{pmatrix} 1, & 0 \end{pmatrix}$$

that C can be realized by a simple laminated microstructure with piecewise deformation gradients W_2 and W_3 with volume fractions $\lambda_4 = 3/4$ and $(1 - \lambda_4) = 1/4$ respectively, and with interfaces normal to $(1, 0)^T$; and that D can be realized by a second-order laminated microstructure, which can be expressed in the following rank-one decomposition

$$D = \frac{2}{3}W_1 + \frac{1}{3}\left(\frac{3}{4}W_2 + \frac{1}{4}W_3\right). \tag{2.14}$$

Embed these laminated microstructure into the second laminated microstructure represented by (2.12), we obtain a fourth-order laminated microstructure (see Figure 2), which corresponds to the rank-one decomposition

$$\begin{aligned} 0 = \frac{2}{3}\left\{\frac{1}{2}\left[\frac{2}{3}W_1 + \frac{1}{3}\left(\frac{3}{4}W_2 + \frac{1}{4}W_3\right)\right] + \frac{1}{2}\left[\frac{3}{4}W_2 + \frac{1}{4}W_3\right]\right\} \\ + \frac{1}{3}\left\{\frac{1}{2}W_3 + \frac{1}{2}W_4\right\}. \end{aligned} \tag{2.15}$$

It follows easily from the above construction and the rank-one decomposition (2.12) that the fourth-order laminated microstructure is supported on $\{W_1, W_2, W_3, W_4\}$ and corresponds to the Young measure (2.1).

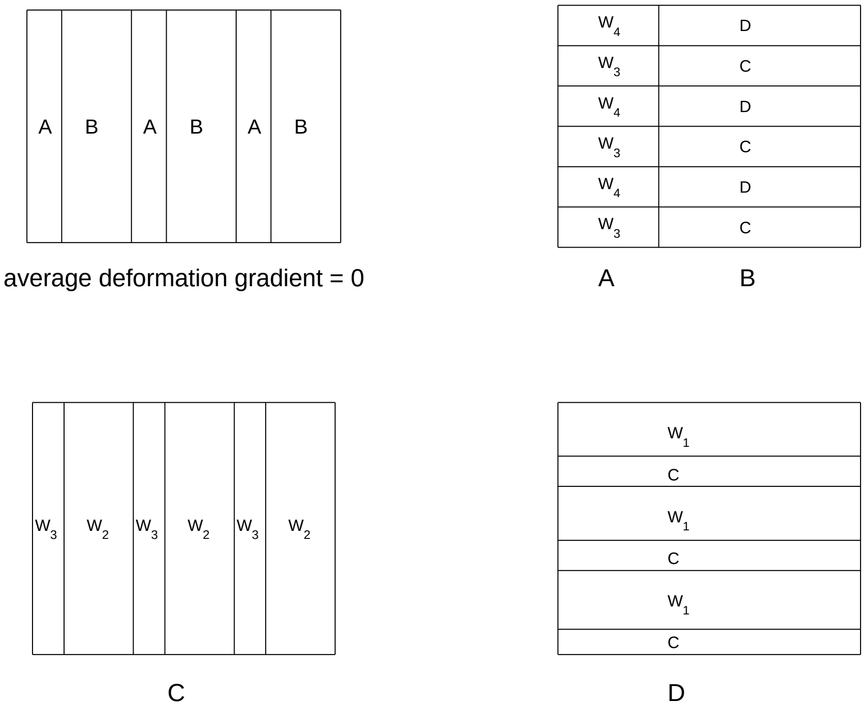

FIGURE 2. Decomposition of the fourth-order laminates in laminates.

3. Finite element approximation and its convergence rate

In this section, we will analyze the error of the finite element approximation by constructing a finite element approximation of the fourth-order laminated microstructure in the framework of (MPR) (see (1.4)).

We construct a periodic block of the fourth-order laminates in laminates as shown in Figure 3. Let h be the mesh size. By the nature of the mesh transformation method, the interfaces between the laminates' layers of W_3 and W_4, and of W_2 and W_3 can be exactly matched by the mesh lines, which guarantees that the integrand f is zero except on the interface layers as shown in Figure 3, and which also allow us to construct the laminates C, which consists of W_2 and W_3 laminates with volume fractions $\frac{3}{4}$ and $\frac{1}{4}$, in h scale. The width of the two interface layers between W_4 and the second-order laminates D is of order $O(h^\beta)$, where in D the twin width of W_1 and the laminates C is of order $O(h^\gamma)$. The width of the interface layers between W_1 and the laminates C is of order $O(h^\alpha)$. Hence, to evaluate $F(u_h;\ \Omega)$, we only need to calculate the integral on these interface layers.

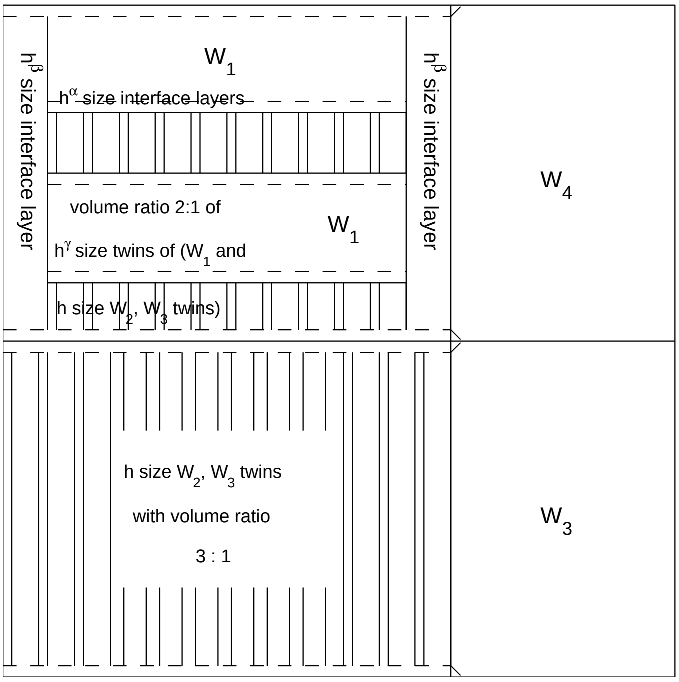

FIGURE 3. The structure of a periodic block of the fourth-order laminates in laminates.

Without loss of generality, we may assume

$$0 < \beta \le \gamma < \alpha \le 1, \tag{3.1}$$

so that ∇u_h is uniformly bounded, for example u_h is given by a linear interpolation on the interface layers. Thus, what remains to do is to calculate the measure of the interface layers Ω_L, which consists of two parts $\Omega_{L,\alpha}$ and $\Omega_{L,\beta}$. It is easily seen that

$$\text{meas}(\Omega_{L,\beta}) = c\, h^\beta, \tag{3.2}$$

and since there are $O(h^{-\gamma})$ interface layers of width h^α, we have

$$\text{meas}(\Omega_{L,\alpha}) = c\, h^{\alpha-\gamma}, \tag{3.3}$$

where by c we denote various constant independent of h. Thus, we have

$$F(u_h;\ \Omega) = F(u_h;\ \Omega_{L,\alpha}) + F(u_h;\ \Omega_{L,\beta}) \le c\,(h^\beta + h^{\alpha-\gamma}). \tag{3.4}$$

By (3.1), we have

$$\xi := \alpha + \beta - \gamma \le 1, \tag{3.5}$$

and to have the right hand side of inequality (3.4) minimized, we set

$$\alpha - \gamma = \beta. \tag{3.6}$$

The relations (3.5) and (3.6) lead to

$$\beta = \frac{\xi}{2} \leq \frac{1}{2}. \tag{3.7}$$

In particular, if we set

$$\alpha = 1, \quad \beta = \frac{1}{2}, \quad \gamma = \frac{1}{2}, \tag{3.8}$$

it follows from (3.5) and (3.7) that

$$\xi = 1, \quad \text{and} \quad \beta = \alpha - \gamma = \frac{1}{2}, \tag{3.9}$$

and thus the optimal convergence rate is obtained, that is

$$0 \leq F(u_h;\ \Omega) = F(u_h;\ \Omega_{L,\alpha}) + F(u_h;\ \Omega_{L,\beta}) \leq c\, h^{1/2}. \tag{3.10}$$

It is worth noticing that this is the convergence rate obtained by the standard finite element method for simple laminated microstructures [25].

Though the above analysis is made for the special case, the method can be easily generalized to other cases. For instance, if we replace the well W_2 by C, then the problem will lead to a third-order laminates in laminates, and with similar arguments we conclude that the convergence rate for the finite element approximation of such third-order laminated microstructures is $O(h)$.

4. Numerical results

Let the computation domain $\Omega_C = (-1,\ 1)^2$, and let $\mathfrak{T}_h(\Omega_C)$ be a family of $(N \times N)$ regular triangulations of Ω_C, where $h = h_N = 2\sqrt{2}/N$ with $N \geq 2$, introduced by the lines

$$\begin{cases} x = -1 + \frac{2}{N} i, & 0 \leq i \leq N; \\ y = -1 + \frac{2}{N} j, & 0 \leq j \leq N; \\ y = \pm(x + 2 - \frac{4}{N} k), & 0 < k < N. \end{cases}$$

Example 1. Replace the integrant $f(\nabla u)$ by $\hat{f}(\nabla u)$, which has potential wells $\{W_1, C, W_3, W_4\}$ instead of $\{W_1, W_2, W_3, W_4\}$, then the minimization problem

$$\inf_{u \in \mathbb{U}(0;\, \Omega)} \int_\Omega \hat{f}(\nabla u)\, dx \tag{4.1}$$

leads to a third-order laminates in laminates with a rank-one decomposition

$$0 = \frac{2}{3}\left\{\frac{1}{2}\left[\frac{2}{3}W_1 + \frac{1}{3}C\right] + \frac{1}{2}\left[\frac{3}{4}W_2 + \frac{1}{4}W_3\right]\right\} + \frac{1}{3}\left\{\frac{1}{2}W_3 + \frac{1}{2}W_4\right\}.$$

In our numerical experiments, we start with a four-well problem with energy wells C, W_3, W_4 and D (see Figure 1). With our scheme, a second order laminated structure is nicely produced on a 2×2 mesh with energy 0.16×10^{-14}. By comparison, with the standard finite element method, the corresponding minimizing energy obtained is 0.25, and the result is not much improved, and in fact can be even worse on finer meshes. Then, we work on the four-well problem with energy wells W_1, C, W_3 and W_4, taking a slight perturbation of the interpolation of the second order laminated structure on a refined mesh as the initial guess, to obtain the expected structure of laminates in laminates.

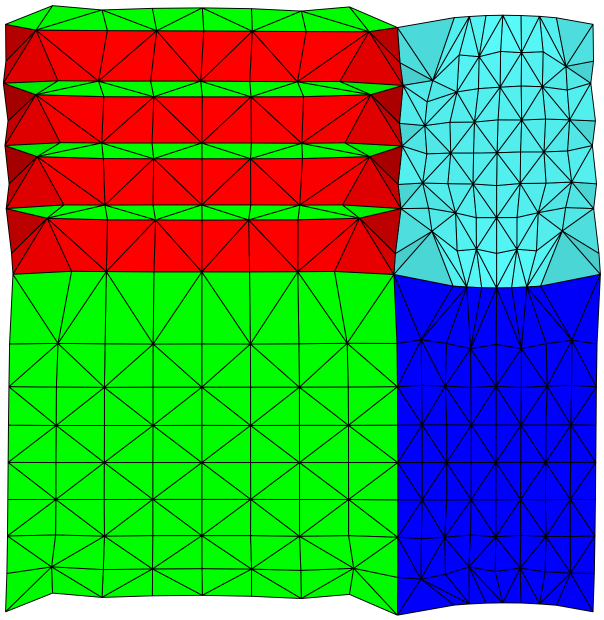

FIGURE 4. A third-order laminates in laminates on the 16×16 mesh.

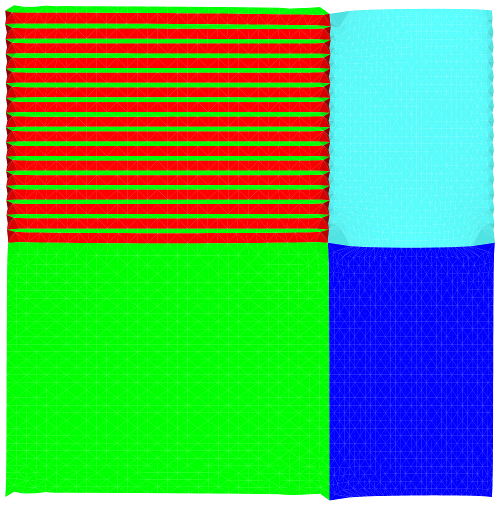

FIGURE 5. A third-order laminates in laminates on the 64×64 mesh.

Figure 4 and Figure 5 illustrate numerical results of the third-order laminates in laminates on the 16×16 and 64×64 mesh respectively. The convergence behavior of the method is shown in Figure 6. The convergence rate of the numerical result is approaching $O(h)$ as N increases, which agrees with our analysis and is significantly higher than the convergence rate $O(h^{1/4})$ of the standard finite element method.

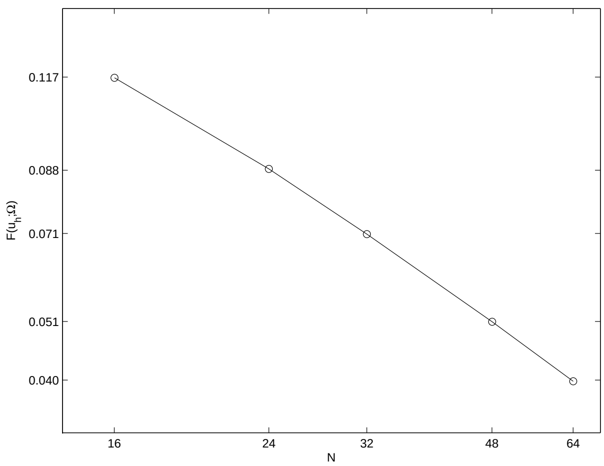

FIGURE 6. Convergence rate for the third-order laminates in laminates.

To have the mesh quality under control, we add some mesh quality control terms, such as

$$\tau \int_\Omega |\log(\det \nabla g)|\, dx$$

in the integral functional [24], which prevent the finite elements becoming too singular and thus help to improve the convergence behavior in searching for minimizers of the discrete problem.

Example 2. In this example, we consider computing the fourth-order laminated microstructure described in section 2 and section 3, which has potential wells $\{W_1, W_2, W_3, W_4\}$ and the rank-one decomposition

$$0 = \frac{2}{3}\left\{\frac{1}{2}\left[\frac{2}{3}W_1 + \frac{1}{3}\left(\frac{3}{4}W_2 + \frac{1}{4}W_3\right)\right] + \frac{1}{2}\left[\frac{3}{4}W_2 + \frac{1}{4}W_3\right]\right\} \\ + \frac{1}{3}\left\{\frac{1}{2}W_3 + \frac{1}{2}W_4\right\}.$$

Again, we start with a four-well problem with energy wells C, W_3, W_4 and D (see Figure 1) to obtain a second order laminated structure, and then, turn to work on the four-well problem with energy wells W_1, C, W_3 and W_4, taking a slight perturbation of the interpolation of the second order laminated structure on a refined mesh as the initial guess, to obtain a third order structure of laminates in laminates as shown in Figure 4, and finally, we work on the four-well problem with energy wells W_1, W_2, W_3 and W_4, taking a slight perturbation of the interpolation of the third order laminated structure on a refined mesh as the initial guess, to obtain the expected fourth order structure of laminates in laminates.

Figure 7 illustrates a numerical result of the fourth-order laminates in laminates on the 64×64 mesh. The convergence behavior of the method is shown in Figure 8. The convergence rate of the numerical result is approaching $O(h^{1/2})$ as N increases, which again agrees with our analysis and is significantly higher than the convergence rate $O(h^{1/5})$ of the standard finite element method.

5. Conclusions

Both the numerical analysis and numerical experiments show that the mesh transformation method is much more efficient than the standard finite

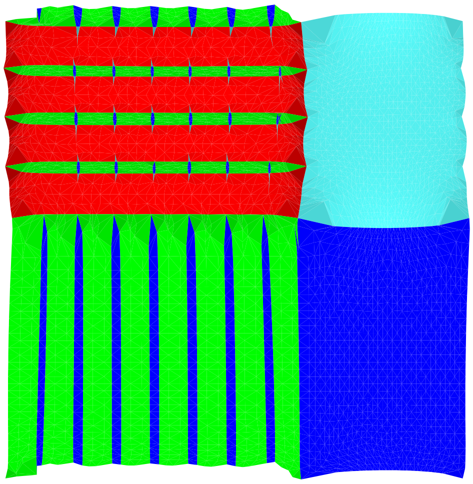

FIGURE 7. A fourth-order laminates in laminates on the 64×64 mesh.

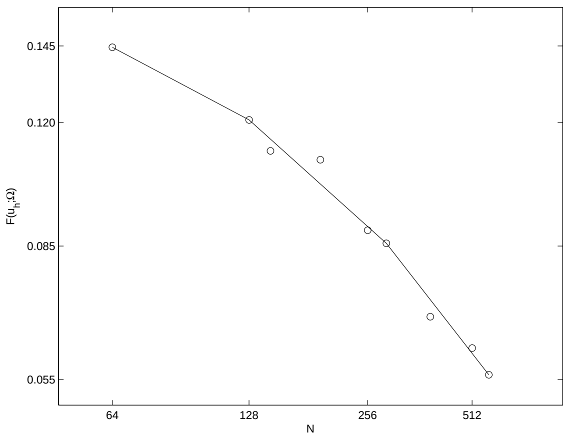

FIGURE 8. Convergence rate for the third-order laminates in laminates.

element method in computing the multi-order laminated microstructures. In fact, for the model problem considered in this paper, for a k-th order laminated microstructure $(k > 2)$, the convergence rate of the standard finite element method is $O(h^{1/(k+1)})$, while that of the mesh transformation method is $O(h^{1/(k-2)})$. More importantly, with the mesh transformation method, the spurious minimizers associated with the standard finite element discretization are effectively avoided, and the numerical solutions converge to the minimizers of the original problem.

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