AN ADAPTIVE FINITE ELEMENT METHOD FOR SOLVING A DOUBLE WELL PROBLEM DESCRIBING CRYSTALLINE MICROSTRUCTURE

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Abstract. The minimization of nonconvex functionals naturally arises in material sciences where deformation of certain alloys exhibit microstructures. As an example, minimizing sequences of the nonconvex Ericksen-James energy can be associated to deformations in martensitic materials that are observed in experiments, [1, 2]. — From the numerical point of view, classical conforming and nonconforming finite element discretizations have been observed to give minimizers with their quality being highly dependent on the underlying triangulation, see [7, 8, 21, 23, 24] for a survey. Recently, a new approach based on discontinuous finite elements has been proposed and analyzed in [12, 13]. The present paper is devoted to propose and analyze an adaptive method to resolve microstructures on arbitrary grids, giving a more accurate resolution of laminate microstructure.

Key words: Adaptive algorithm, finite element method, non-convex minimization, multi-well problem, microstructure, multiscale, nonlinear elasticity, shape-memory alloy, materials science.

AMS subject classifications: 65K10, 65M50, 65N30, 73C50, 73S10.

1 Introduction. In modern materials sciences, alloys are the subject of research that exhibit a memory shape effect: when cooled beyond a certain critical temperature, the crystal structure changes rapidly, and a new configuration of the atoms with less symmetry (martensitic phase) can be observed, exhibiting microstructure. When heating the alloy again, the original (austenite) phase is taken again and no microstructure exists any more. — The mathematical description of corresponding deformations existing in martensitic crystals has been given by Ball and James [1, 2], where they are characterized by minimizing sequences of a functional that is not convex (not even rank-one convex).

From the numerical point of view, standard finite element methods (of conforming or nonconforming type [Crouzeix or rotated (bi-, tri-)linear element]) turn out to be capable of simulating deformations giving microstructure, *provided* triangulations are employed that are aligned to the microstructure, see [10, 14, 21, 23, 24]. In order to free from these restrictions and to make a finite element model more flexible for instance for problems with acting forces and/or changing (in time) microstructures, a new ansatz based on *discontinuous elements* was recently proposed and analyzed in [12, 13]. The improved performance of this method is tested in computational experiments as well as supported through a rigorous convergence analysis, giving drastically improved orders of convergence, if compared to results for classical conforming and nonconforming ansatzes. We refer to Table 1 for a comparison of the distinct methods.

The goal of the present paper is to propose a new adaptive method to resolve laminated microstructure, with the main focus on the verification of improved convergence statements

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Finite element method	$\mathcal{E}_h(u_h)$	$\|u_h - F_\lambda x\|$	$\|(\nabla u_h - F_\lambda)\, w\|$	$\left\| \frac{\mu(\omega_\rho^\ell(u_h))}{\mu(\omega)} - \lambda^\ell \right\|$
classical conforming and nonconforming methods, see [23, 20]	$\mathcal{O}(h^{1/2})$	$\mathcal{O}(h^{1/8})$	$\mathcal{O}(h^{1/8})$	$\mathcal{O}(h^{1/16})$
discontinuous without interior L^2-term ($\alpha_3 = 0$), see [12]	$\mathcal{O}(h^2)$	$\mathcal{O}(h^{1/4})$	$\mathcal{O}(h^{1/4})$	$\mathcal{O}(h^{1/8})$
discontinuous with interior L^2-term ($\alpha_3 \neq 0$), see [12]	$\mathcal{O}(h^2)$	$\mathcal{O}(h^{1/2})$	$\mathcal{O}(h^{1/4})$	$\mathcal{O}(h^{1/4})$
discontinuous and adaptive without interior L^2-term ($\alpha_3 = 0$)	$\mathcal{O}(h^2)$	$\mathcal{O}(h^{3/10})$	$\mathcal{O}(h^{3/10})$	$\mathcal{O}(h^{3/20})$
discontinuous and adaptive with interior L^2-term ($\alpha_3 \neq 0$)	$\mathcal{O}(h^2)$	$\mathcal{O}(h^{3/5})$	$\mathcal{O}(h^{3/10})$	$\mathcal{O}(h^{3/10})$

Table 1: Summary of convergence results for the energy and other crucial quantities for different finite element methods. See the text for an explanation of the employed notation.

thereof. At first glance, adaptivity does not seem to make any sense in the context of microstructures under consideration, since there is no scaling in the solution where an adaptivity strategy can be based on. On the other hand — motivated by the numerical model of discontinuous ansatz functions — an adaptivity criterion can be based on the degree of discontinuity of a computed solution, i.e., the height of inter-element jumps. We will outline the strategy in section 3, and propose the new adaptive algorithm there. — The application of such an adaptivity strategy allows for convergence results that are superior to those of previous methods collected in Table 1, even for the method that is based on discontinuous ansatz functions. We refer to Theorem 3.1 in section 3 for further details on the performance of this algorithm.

The remainder of the article is as follows: section 2 provides the reader with the mathematical setup of the problem that is under consideration. The adaptive algorithm as well as the main result of convergence are presented in section 3. Its verification is subject of section 4.

2 The Ericksen-James energy functional. A common example of microstructures are simple laminates in which the deformation gradient oscillates on an infinitesimal scale in parallel layers between two states that are related to two symmetry-related variants of the martensitic phase. It follows from the frame-indifference principle that the minimum value of the elastic energy is attained on multiple, rotationally invariant wells. We study in this paper the approximation of deformations of martensitic crystals which can undergo an orthorhombic to monoclinic transformation, giving rise to a double well potential. We claim that the analysis can easily be extended to more complicated phase transitions like, e.g., the ”triple well case” describing cubic to tetragonal phase transitions in atomic lattice structure;

we refer to [21] for a corresponding study of the rotated (bi-, tri-)linear finite element. The Ericksen-James energy is given in the form

$$\mathcal{E}(v) = \int_\Omega \phi(\nabla v(x))\, d\Omega, \tag{1}$$

with the non-convex energy density $\phi(\cdot)$ and admissible deformations v to be defined below. For further details on the specific form of $\phi(\cdot)$, we refer to [24], e.g.. — Each well is of the form $\mathcal{U}_\ell = SO(3)U_\ell$, with $SO(3)$ being the group of proper rotations and the U_i, $i = 1, 2$ representing martensitic variants. In the double well case, we can assume (see [24]) that these wells are rank-one connected, i.e., there are $F_\ell \in \mathcal{U}_\ell$, $\ell = 1, 2$, such that the Hadamard condition is satisfied. This means that there are two non-vanishing vectors $a \in \mathrm{R}^3$ and $n \in \mathrm{R}^3$ such that

$$F_2 = F_1 + a \otimes n. \tag{2}$$

Without loss of generality, we assume $|n| = 1$.

We continue with the exposal of the general setting: $\Omega \subset \mathrm{R}^3$ is the reference domain of the crystal, which is assumed to be polygonal. Furthermore, the mapping $u : \Omega \to \mathrm{R}^3$ represents a continuous deformation of the crystal, with corresponding deformation gradients $\nabla u : \Omega \to \mathrm{R}^{3\times 3}$. — The energy density is assumed to satisfy

$$\begin{aligned} \phi(A) &\geq 0, & \forall\ \ A \in \mathrm{R}^{3\times 3}, \\ \phi(A) &= 0, & \iff \ \ A \in \mathcal{U}. \end{aligned} \tag{3}$$

We shall also assume that the energy density ϕ grows quadratically from the energy wells, that is,

$$\phi(F) \geq \kappa |||F - \pi(F)|||^2, \qquad \forall\ F \in \mathrm{R}^{3\times 3}, \tag{4}$$

with $\kappa > 0$ a constant and $\pi : \mathrm{R}^{3\times 3} \to \mathcal{U}$ a Borel measurable projection that is defined by

$$|||F - \pi(F)||| = \min_{G\in\mathcal{U}} |||F - G|||, \qquad \forall\ F \in \mathrm{R}^{3\times 3}, \tag{5}$$

where $|||\cdot|||$ denotes the Frobenius norm. Note that the projection $\pi(F)$ exists for any $F \in \mathrm{R}^{3\times 3}$ since $\mathcal{U}$ is compact, although it may not be unique.

As we already mentioned, we are interested in simple laminate microstructures. These can be enforced through the presciption of compatible boundary conditions,

$$u(x) = F_\lambda x, \qquad \forall\ x \in \partial\Omega, \tag{6}$$

where

$$F_\lambda = \lambda F_1 + (1 - \lambda) F_2, \tag{7}$$

and $\lambda \in (0,1)$ represents the mass fraction of the two variants. — The problem can be stated in the following way:

$$\inf\{\mathcal{E}(v) : \ v \in \mathcal{A}\}, \tag{8}$$

where

$$\mathcal{A} = \{v \in C(\Omega; \mathrm{R}^3) : \ v(x)|_{\partial\Omega} = F_\lambda x\}. \tag{9}$$

3 Proposal of the algorithm. We already mentioned the fact that classical conforming or nonconforming discretization ansatzes for the minimization of the energy function $\mathcal{E}(\cdot)$ (or its modification $\mathcal{E}_h(\cdot)$ in the nonconforming approach) give minimizers with its quality being highly mesh dependent. This is because of too strict continuity constraints of the finite element functions polluting the solution on meshes that are not aligned to the laminate microstructure.

In order to circumvent this problem and have a method that is essentially independent on the choice of the present triangulation, a finite element approach based on discontinuous ansatzes has been proposed in [12]. The inter-element continuity of the computed deformation is taken into account through a penalty term that is added to the bulk energy functional. Further, an analogous idea relaxes the boundary values in a way that small deviations from the prescribed boundary data are permitted, giving (only) small energy contributions. As a consequence, this reduces the pollution of the computed deformation through *averaged* boundary values. Then, the energy functional of the numerical model is as follows:

We are given a triangulation $\mathcal{T}_h$ of the domain Ω that can be parametrized by $h > 0$. Consider element-wise linear deformations $v_h \in \mathcal{A}_h \equiv \prod_{K\in\mathcal{T}_h} \mathcal{P}_1(K)$, having energy

$$\begin{aligned} \mathcal{E}_h^\beta(v_h) = & \sum_{K\in\mathcal{T}_h} \int_K \phi(\nabla v_h(x)) \, d\Omega \\ & + \alpha_{11}\Big(\sum_{K\in\mathcal{T}_h} h^{1-\beta} \int_{\partial K} \big|[v_h](x)\big| \, d\sigma\Big)^2 + \alpha_{12}\Big(\sum_{K\in\mathcal{T}_h} h^{1-\beta} \int_{\partial K} \big|[v_h](x)\big|^2 \, d\sigma\Big) \\ & + \alpha_2 \sum_{K\in\mathcal{T}_h} h^{2\beta} \int_{\partial K\cap\partial\Omega} |v_h(x) - F_\lambda x|^2 \, d\sigma + \alpha_3 \sum_{K\in\mathcal{T}_h} h^{2\beta} \int_K |v_h(x) - F_\lambda x|^2 \, d\Omega, \end{aligned} \tag{10}$$

and do the following minimization, for a given parameter $\beta \in [0,1]$,

$$\min_{v_h\in\mathcal{A}_h} \mathcal{E}_h^\beta(v_h). \tag{11}$$

In this algorithm, the parameter β plays a roll to distinguish between the discretization size ($\beta = 0$) and the thickness of the laminates $\mathcal{O}(h^{1-\beta})$, i.e., the structure of the solution. As it turns out from the analysis in [12], the algorithm gives most accurate computations of the microstructure for the choice $\beta = 1/2$.

Based on the idea of distinguishing between the scaling of the *variants* of the martensitic phase, i.e., the laminates, and *transitions between variants*, which has proved to be fruitful

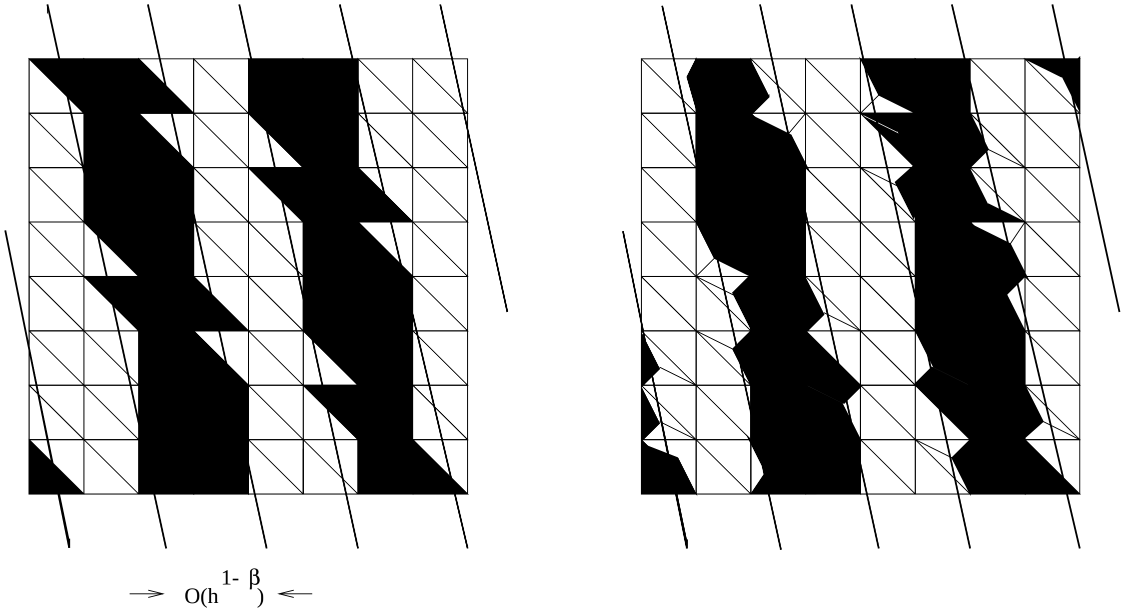

Figure 1: Sketch of the adaptive refinement strategy in two dimensions: white corresponds to slope $+1$, black to slope -1. The figures show a possible first adaptive refinement of a given basic triangulation.

in the formulation of the previous algorithm, we will now extend this idea to the context of adaptivity. The idea is now to *expand* the area "supporting" variants by reducing the domains of variant transitions at the same time.

The adaptive algorithm proposed here consists of two parts: A refinement criterion of the present underlying triangulation, and the formulation of an energy functional that changes for each new triangulation, parametrized by $i \geq 0$, using different values $\beta_i \geq 1$. From this point of view, the presented algorithm distinguishes between features on *three* different length scales: the basic discretization length h, the thickness of the laminates $\mathcal{O}(h^{1-\beta})$ and the transition thickness between two variants, $\mathcal{O}(h^{\beta_i})$, with the latter being subject to the adaptive algorithm. Therefore, the objective is to reduce the area where transition of martensitic variants occurs. Figure 1 shows the principal properties of the adaptive algorithm: the scope of it is to increase the flexibility in the minimization process and to avoid severe restrictions to the solution in this process that are caused by the underlying triangulation of the domain Ω. — Let us start with the proposal of the *adaptive energy functional:*

Let the tuple $\{\mathcal{T}_h^i, \beta^i\}_{i=0}^{i_F}$ be given, and consider a modified energy for deformations $v_h^i \in$

$\mathcal{A}_h^i \equiv \prod_{K_i \in \mathcal{T}_h^i} \mathcal{P}_1(K_i)$,

$$\begin{aligned} \mathcal{E}_{h,\beta}^{\beta_i}(v_h^i) &= \sum_{K \in \mathcal{T}_h^i} \int_K \phi(\nabla v_h^i(x))\, d\Omega \\ &+ \alpha_{11}\Big(\sum_{K \in \mathcal{T}_h^i} h^{2-\beta_i-\beta} \int_{\partial K} \big|[v_h^i](x)\big|\, d\sigma \Big)^2 + \alpha_{12}\Big(\sum_{K \in \mathcal{T}_h^i} h^{3-2\beta_i-\beta} \int_{\partial K} \big|[v_h^i](x)\big|^2\, d\sigma \Big) \\ &+ \alpha_2 \sum_{K \in \mathcal{T}_h^i} h^{2\beta} \int_{\partial K \cap \partial\Omega} |v_h^i(x) - F_\lambda x|^2\, d\sigma + \alpha_3 \sum_{K \in \mathcal{T}_h^i} h^{2\beta} \int_K |v_h^i(x) - F_\lambda x|^2\, d\Omega, \end{aligned} \tag{12}$$

for $0 \le i \le i_F$, and a choice $i_F = \mathcal{O}(\log_2(h^{-\beta/2}))$.

Remark 3.1 *1. The value for i_F is a consequence of an easy dimensionality argument and follows from the fact that we have $\mathcal{O}(h^{-3})$ degrees of freedom (i.e., elements) in three dimensions. Since we have $\mathcal{O}(h^{\beta-1})$ layers marking transitions of laminates, we are provided with $\mathcal{O}(h^{-2-\beta})$ degrees of freedom maximum per each transition layer. From this consideration, the smallest triangles coming from a refinement process are of order $\mathcal{O}(h^{1+\beta/2})$.*

2. If we carry out a corresponding investigation for a 2D-version of the model (1), (8), $\Omega \subset \mathrm{R}^2$, and for deformations $v \in \mathcal{B}$,

$$\mathcal{B} = \big\{ v \in C(\Omega; \mathrm{R}^2) : v(x)\big|_{\partial\Omega} = F_\lambda x \big\},$$

the value of i_F has to be changed to $\mathcal{O}(\log_2(h^{-\beta}))$, and, correspondingly, $\beta_{i_F} = 1 + \beta$ in this case.

The adaptive algorithm can then be stated in the following way, for $0 \le i \le i_F$, and with the initial triangulation $\mathcal{T}_h^0 \equiv \mathcal{T}_h$ from above:

1. Given $v_h^i \in \mathcal{A}_h^i$, apply the refinement strategy

$$\mathcal{S}_i \equiv \mathcal{S}_i(v_h^i) : \mathcal{T}_h^i \to \mathcal{T}_h^{i+1}, \tag{13}$$

   according to the following criterion: Refine by bisection adjacent elements $K \in \mathcal{T}_h^i$, that share an edge $\mathcal{F} \in \partial K$, where the jump of v_h^i across $\mathcal{F}$ satisfies the following bound, for a given number $\alpha = \mathcal{O}(1)$,

$$\max_{x \in \mathcal{F}} \big|[v_h^i](x)\big| \ge \alpha h^{\beta_i}. \tag{14}$$

2. Set $i := i + 1$ and go back to 1. in case $i < i_F$. For $i = i_F$, go to the next step.

3. For $i = i_F$, compute a minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ of

$$\min_{v_h^{i_F} \in \mathcal{A}_h^{i_F}} \mathcal{E}_{h,\beta}^{\beta_{i_F}}(v_h^{i_F}), \qquad \text{with} \qquad \beta_{i_F} = 1 + \frac{\beta}{2}. \tag{15}$$

Remark 3.2 *Note that the second and third term with the leading factors α_{11} and α_{12} in (12) have a weight in h with an exponent that couples the laminate thickness with the thickness of the transition area.*

In order to assure a monotonous behavior of the algorithm and thus an optimal performance of the method, the refinement process $\mathcal{S}_i$ has to be properly chosen in the sense of the following definition.

Definition 1 *Given a quasiuniform triangulation $\mathcal{T}_h^0 := \mathcal{T}$, we call a refinement strategy $\mathcal{S} := \{\mathcal{S}_i\}_{i=0}^{i_F-1}$, with $\mathcal{S}_i : \mathcal{T}_h^i \to \mathcal{T}_h^{i+1}$ admissible if there exists a sequence $\{\mathcal{T}_h^i, v_h^i\}_{i=0}^{i_F}$, and a constant $\tilde{C} = \tilde{C}(\alpha_{11}, \alpha_{12})$ that is independent on the number i, with deformations $v_h^i \in \mathcal{A}_h^i$ satisfying*

$$\mathcal{E}_{h,\beta}^{\beta_i}(v_h^i) \leq \tilde{C}h^2, \qquad \text{for} \quad 0 \leq i \leq i_F. \tag{16}$$

The description of the simply laminated microstructure can now be fixed in the following way: The orientation of it is determined by its normal vector $n \in \mathrm{R}^3$. In the following, we make also use of vectors $w \in \mathrm{R}^3$ along the laminates, that satisfy $w \cdot n = 0$. Furthermore, we study the accuracy of representing the volume fractions $\lambda^1 := \lambda$ and $\lambda^2 := (1 - \lambda)$. We refer to Subsection 4.4 for further details. — We are now in a position to present the main result of this work.

Theorem 3.1 *Suppose $u \in \mathcal{A}$ to be an infimizer of problem (8), (9). Consider the algorithm (14), (15), with a sequence of triangulations and values $1 \leq \beta_i \leq 1 + \frac{\beta}{2}$ given by*

$$\beta_i = 1 + \log_h(2^{-i}).$$

Then, there exists an admissible refinement strategy $\mathcal{S}$ of a given initial quasiuniform triangulation $\mathcal{T}_h^0 = \mathcal{T}_h$, such that a minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ of problem (15) satisfies the following approximation properties, for the optimal parameter choice $\beta = 2/5$,

1. *(case: $\alpha_3 = 0$) for positive $\alpha_{11}, \alpha_{12}, \alpha_2 = \mathcal{O}(1)$,*
   - *(a)* $\mathcal{E}_{h,2/5}^{\beta_{i_F}}(u_h^{i_F}) \leq Ch^2$,
   - *(b)* $\|u_h^{i_F} - F_\lambda x\|_{L^2(\Omega)} \leq Ch^{3/10}$,
   - *(c)* $\|\{\nabla u_h^{i_F} - F_\lambda\}w\|_{L^2(\Omega)} \leq Ch^{3/10}$,
   - *(d)* $\left|\frac{\mu(\omega_\rho^\ell(u_h^{i_F}))}{\mu(\omega)} - \lambda^\ell\right| \leq Ch^{3/20}, \qquad \text{for } \ell \in \{1, 2\}$,
2. *(case: $\alpha_3 \neq 0$) for positive $\alpha_{11}, \alpha_{12}, \alpha_2, \alpha_3 = \mathcal{O}(1)$,*
   - *(a)* $\mathcal{E}_{h,2/5}^{\beta_{i_F}}(u_h^{i_F}) \leq Ch^2$,
   - *(b)* $\|u_h^{i_F} - F_\lambda x\|_{L^2(\Omega)} \leq Ch^{3/5}$,
   - *(c)* $\|\{\nabla u_h^{i_F} - F_\lambda\}w\|_{L^2(\Omega)} \leq Ch^{3/10}$,

(d) $\left|\frac{\mu(\omega_\rho^\ell(u_h^{i_F}))}{\mu(\omega)} - \lambda^\ell\right| \leq C h^{3/10}, \qquad \text{for } \ell \in \{1,2\},$

for all subsets $\omega \subset \Omega$ *and* $h < \rho < 1$. *The applied generic constant* C *is only dependent on the parameters of the continuous problem (8) and the values* $\alpha_{11}, \alpha_{12}, \alpha_2, \alpha_3$ *but independent on the mesh size* h *and* i_F.

Remark 3.3 *1. Note that the thickness of layers of the approximate simply laminated microstructure is now of magnitude* $\mathcal{O}(h^{3/5})$ *— in contrast to the previous model (10) where we computed minimizing deformations exhibiting laminated microstructure of thickness* $\mathcal{O}(h^{1/2})$. *In particular, this method allows for a better approximation of the prescribed boundary data.*

2. *We emphasize the interplay between the adaptive construction of an admissibly refined triangulation* $\mathcal{T}_h^{i_F}$ *of the domain and the iterative adjustment of the energy functional with respect to the* $\{\beta_i\}_{i=0}^{i_F}$ *to end up with the final form* $\mathcal{E}_{h,\beta}^{\beta_{i_F}}(\cdot)$: *to some extent, the initial triangulation is made compatible to the laminate microstructure through the refinement strategy, whereas the modification of the energy functional "increases" the continuity requirements on a computed minimizer in each iteration step* $0 \leq i \leq i_F$, *only allowing for decreasing jumps across element interfaces.*

3. *In actual computations, the admissible character of refined triangulations has to be checked in each iteration step; for instance, we can employ minimizing deformations* $u_h^i \in \mathcal{A}_h^i$ *of the energies*

$$\mathcal{E}_{h,\beta}^{\beta_i}(v_h^i), \qquad \forall\, v_h^i \in \mathcal{A}_h^i \tag{17}$$

as indicators of a refinement strategy $\left\{\mathcal{S}_i(u_h^i)\right\}_{i=0}^{i_F-1}$, *but the admissible character of this refinement strategy has to be verified.*

4. *The statements in Theorem 3.1 are given for the three-dimensional Ericksen-James energy. According to Remark 3.1, the situation slightly changes, if we are concerned with the modified Ericksen-James energy in two space dimensions. In this case, the thickness of laminates is of order* $\mathcal{O}(h^{2/3})$ *for the optimal parameter* $\beta = 1/3$, *and the following results hold,*

   (a) *(case:* $\alpha_3 = 0$*) for positive* $\alpha_{11}, \alpha_{12}, \alpha_2 = \mathcal{O}(1)$,

      i. $\mathcal{E}_{h,1/3}^{\beta_{i_F}}(u_h^{i_F}) \leq C h^2$,

      ii. $\|u_h^{i_F} - F_\lambda x\|_{L^2(\Omega)} \leq C h^{1/3}$,

      iii. $\|\{\nabla u_h^{i_F} - F_\lambda\} w\|_{L^2(\Omega)} \leq C h^{1/3}$,

      iv. $\left|\frac{\mu(\omega_\rho^\ell(u_h^{i_F}))}{\mu(\omega)} - \lambda^\ell\right| \leq C h^{1/6}, \qquad \text{for } \ell \in \{1,2\},$

   (b) *(case:* $\alpha_3 \neq 0$*) for positive* $\alpha_{11}, \alpha_{12}, \alpha_2, \alpha_3 = \mathcal{O}(1)$,

      i. $\mathcal{E}_{h,1/3}^{\beta_{i_F}}(u_h^{i_F}) \leq C h^2$, *ii.* $\|u_h^{i_F} - F_\lambda x\|_{L^2(\Omega)} \le Ch^{2/3}$,

iii. $\|\{\nabla u_h^{i_F} - F_\lambda\} w\|_{L^2(\Omega)} \le Ch^{1/3}$,

iv. $\left|\frac{\mu(\omega_\rho^\ell(u_h^{i_F}))}{\mu(\omega)} - \lambda^\ell\right| \le Ch^{1/3}, \qquad \text{for } \ell \in \{1,2\}.$

The verification of these statements follows from the analysis of the three-dimensional model below and Remark 3.1.

The verification of Theorem 3.1 is subject of section 4. For its proof, we need to test a couple of auxiliary results. The general line of analyzing problems of this class has first been developed in [23, 24, 21], and we also follow it in our proofs. Also, we benefit very much from the analysis of the algorithm (10) performed in [12] and refer to there in order to shorten the proofs.

4 Analysis for the discontinuous element without interior L^2-term. The following investigations refer to the case α_3 in the energy functional (12). Then, given a number $0 \le i \le i_F$, there are three terms in the energy functional that compete with each other: the first is the bulk energy term that already comes from the continuous version $\mathcal{E}(\cdot)$. The two remaining terms release strict continuity constraints across elements to be satisfied in the continuous problem by penalizing (high) jumps: The last term in $\mathcal{E}_{h,\beta}^{\beta_i}(\cdot)$ allows slight fluctuations of the boundary data to improve the flexibility of the finite element method to model laminate microstructure on nonaligned grids.

4.1 Discontinuous Finite elements. Given a triangulation $\mathcal{T}_h^i$, the Lagrange interpolation operator

$$\mathcal{I}_h^i : C(\bigcup_{K\in\mathcal{T}_h^i} K) \to \prod_{K\in\mathcal{T}_h^i} \mathrm{Aff}_i(K),$$

with $\mathrm{Aff}_i(K)$ the set of affine-linear functions on the triangle $K \in \mathcal{T}_h^i$ is defined in a standard way as a point interpolate. From this, inverse inequalities are valid since they hold on each triangle, compare [9].

Lemma 4.1 *Let k and l be two integers such that $0 \le k \le l \le 2$. We have the following inverse inequalities for any $K \in \mathcal{T}_h^i$, and any $v_h^i \in \mathrm{Aff}_i(K)$,*

1. $|v_h^i|_{l,K} \le Ch^{k-l}|v_h^i|_{k,K}, \qquad \forall\ K \in \mathcal{T}_h^i$,
2. $|v_h^i|_{l,\infty,K} \le Ch^{k-l-3/2}|v_h^i|_{k,K}, \qquad \forall\ K \in \mathcal{T}_h^i$.

4.2 Properties of Minimizers of the Functional $\mathcal{E}_h^\beta(\cdot)$. The next lemma shows that it is always possible to find deformations $u_h^i \in \prod_{K\in\mathcal{T}_h^i} \mathrm{Aff}_i(K)$ on an admissible refinement of $\mathcal{T}_h \equiv \mathcal{T}_h^0$ that satisfy $\mathcal{E}_{h,\beta}^{\beta_i}(u_h^i) \le Ch^2$, for $\beta \in [0,1]$, and $0 \le i \le i_F$.

Lemma 4.2 *Given a quasiuniform triangulation $\mathcal{T}_h^0 \equiv \mathcal{T}_h$. Then, there exists an admissible refinement strategy $\mathcal{S}$ and a minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ satisfying the bound*

$$\mathcal{E}_{h,\beta}^{\beta_{i_F}}(u_h^{i_F}) \le Ch^2.$$

Proof. This result will be shown by an extended argument that constitutes the proof for the case $i = 0$, as it is given in [12]. It will be presented in the following to show the existence of an admissible refinement giving triangulations $\{\mathcal{T}_h^i\}_{i=0}^{i_F}$ such that the above energy inequality is valid.

We define a deformation $C(\Omega) \ni w : \Omega \to \mathrm{R}^3$, given by

$$w(x) = F_0 x + \Big[\int_0^{x\cdot n} \xi(\frac{s}{\gamma h^{1-\beta}})\ ds\Big] a, \tag{18}$$

where $\xi(\tilde{s}) : \mathrm{R} \to \mathrm{R}$ is a characteristic function with period 1,

$$\xi(\tilde{s}) = \begin{cases} 0 & \text{for all } 0 \le s \le \lambda, \\ 1 & \text{for all } \lambda < s < 1, \end{cases} \tag{19}$$

and $\gamma = \mathcal{O}(1)$ an arbitrary choice. $\gamma = \mathcal{O}(1)$ an arbitrary choice. It is evident, that the following inequality holds true,

$$|w(x) - F_\lambda x| \le C h^{1-\beta}, \qquad \forall\ x \in \Omega. \tag{20}$$

We now have

$$\nabla w(x) = F_0 + \xi(\frac{x\cdot n}{\gamma h^{1-\beta}}) a \otimes n. \tag{21}$$

We are given a triangulation $\mathcal{T}_h^0 = \{K_l^0\}_{l\in L^0}$ such that in general $w \ne \mathcal{I}_{\mathcal{T}_h^0}(w)$. Because of w being piecewise affine there exists a *refinement* $\tilde{\mathcal{T}}_h^0 = \{\tilde{K}_{lj}^0\}_{l\in L^0, j\in J_l^0}$ of $\mathcal{T}_h^0$, with

$$\mathcal{T}_h^0 \ni K_l^0 = \bigcup_{j\in J_l^0} \tilde{K}_{lj}^0, \qquad \tilde{K}_{lj}^0 \in \tilde{\mathcal{T}}_h^0,$$

s.t. holds: $w = \mathcal{I}_{\tilde{\mathcal{T}}_h^0}(w)$.

In our notation, $\mathrm{card}J_l^0 = 1$ stands for no refinement, whereas $\mathrm{card}J_l^0 > 1$ denotes a refinement of $K_l^0 \in \mathcal{T}_h^0$. — Now, using the triangulation $\mathcal{T}_h^0 = \{K_l\}_{l\in L^0}$, we will now construct a deformation $v_h^0 \in \mathcal{A}_h^0$ from w presented in (18),

$$v_h^0(x) = \begin{cases} w(x), & \text{for all } K_l^0 \in \mathcal{T}_h^0, \text{ s.t. } \mathrm{card}J_l^0 = 1, \\ \mathrm{Ext}_{K_l^0}(w)(x), & \text{for all } K_l^0 \in \mathcal{T}_h^0, \text{ s.t. } \mathrm{card}J_l^0 > 1. \end{cases} \tag{22}$$

where, for each set I, we can define an extension operator

$$\mathrm{Ext}_{K_l^0} : \prod_{\{\tilde{K}_{lj}^0\}_{j\in J_l} := K_l^0 \in \mathcal{T}_h^0} \mathrm{Aff}(\tilde{K}_{lj}^0) \to \mathrm{Aff}(K_l^0),$$

with $\mathrm{Ext}_{K_l^0}(w)(x)$ further defined to be a linear extension of $w\big|_{\tilde{K}_{lj_0}^0}$ onto $\{\tilde{K}_{lj}^0\}_{j\in J_l^0} := K_l^0 \in \mathcal{T}_h^0$, satisfying

$$\nabla \mathrm{Ext}_{K_l^0}(w)(x) := \nabla v_h^0(x)\big|_{\tilde{K}_{lj_0}^0}, \qquad \text{with } \mu(\tilde{K}_{lj_0}^0) \ge \mu(\tilde{K}_{lj}^0), \ \ \forall\ j \in J_l^0.$$

This gives a deformation candidate $v_h^0 = \mathcal{I}_{\mathcal{T}_h^0}(v_h^0)$. It is now easy to compute the energy $\mathcal{E}_{h,\beta}^{\beta_0}(v_h^0)$, thus verifying the statement of the Lemma for the choice $i = 0$.

We will now prove the existence of an admissible refinement strategy $\mathcal{S}$, with a sequence $\{\mathcal{T}_h^i, v_h^i\}_{i=0}^{i_F}$, for $v_h^i \in \mathcal{A}_h^i$. For this purpose, we can make use of the previously introduced technical apparatus, selecting refined triangulations $\tilde{\mathcal{T}}_h^i = \{\tilde{K}_{lj}^i\}_{l\in L^i, j\in J^i}$ of the triangulation $\mathcal{T}_h^i = \{K_l^i\}_{l\in L^i}$, with

$$\mathcal{T}_h^i \ni K_l^i = \bigcup_{j\in J_l^i} \tilde{K}_{lj}^i, \qquad \tilde{K}_{lj}^i \in \tilde{\mathcal{T}}_h^i,$$

for all $0 \le i \le i_F$.
According to the definition, the deformation $v_h^{i-1} \in \mathcal{A}_h^{i-1}$ exhibits jumps close to the subsets of the domain Ω where a change of variants arises. Therefore, these elements are subject to refinement according to $\mathcal{S}_i$ (via bisection). We can then define the following deformation $v_h^i \in \mathcal{A}_h^i$, for $i \ge 1$,

$$v_h^i(x) = \begin{cases} v_h^{i-1}(x), & \text{for all } K_l^i \in \mathcal{T}_h^i, \text{ s.t. } \mathrm{card} J_l^i = 1, \\ \mathrm{Ext}_{K_l^i}(w)(x), & \text{for all } K_l^i \in \mathcal{T}_h^i, \text{ s.t. } \mathrm{card} J_l^i > 1, \end{cases} \tag{23}$$

with the extension operator $\mathrm{Ext}_{K_l^i}$ defined before. — This provides us with candidates $v_h^i \in \mathcal{A}_h^i$, for $0 \le i \le i_F$, and it can be immediately seen that there holds $\mathcal{E}_{h,\beta}^{\beta_i}(v_h^i) \le \tilde{C}h^2$, $0 \le i \le i_F$. We presented an admissible refinement strategy $\mathcal{S}$, consisting of sequence of tuples $\{v_h^i, \mathcal{T}_h^i\}_{i=0}^{i_F}$, with $v_h^i \in \mathcal{A}_h^i$.

The existence of a minimizer now follows from standard arguments, see e.g. [12], Lemma 2.2. The upper energy bound for a minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ on the final mesh $\mathcal{T}_h^{i_F}$ is immediate. $\square$

We can now benefit from this result. Note that the continuity constraints given in the penalized energy functional $\mathcal{E}_{h,\beta}^{\beta_i}$ on a computed minimizing deformation on the triangulation $\mathcal{T}_h^i$ are enforced for increasing numbers i. This is the consequence of the following Theorem that plays a crucial role in the subsequent convergence analysis. Moreover, it shows that the adaptive energy functional (12) performs best in the sense of convergence for the choice $\beta = 2/5$. — In the subsequent proof, we see the interplay of the different features arising in the algorithm, scaled by β and β_i.

Theorem 4.1 *Suppose $\mathcal{T}_h^{i_F}$ to be constructed through an admissible refinement process. Then, a minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ of the energy functional $\mathcal{E}_{h,\beta}^{\beta_{i_F}}(\cdot)$ given in (12) satisfies the following estimate,*

$$\Big|\Big|\Big| \sum_{K\in\mathcal{T}_h^{i_F}} \int_K \{\nabla u_h^{i_F}(x) - F_\lambda\}\, d\Omega \Big|\Big|\Big| \le C\Big\{h^{3\beta/2} + h^{1-\beta}\Big\}, \qquad \text{for } \beta \in [0,1].$$

Proof. Set $\mathcal{A}_{i_F} \ni z_h^{i_F}(x) = u_h^{i_F}(x) - F_\lambda x$. Then, we have

(24)
$$\begin{aligned}\sum_{K\in\mathcal{T}_h^{i_F}} \int_K \nabla z_h^{i_F}(x)\, d\Omega &= \sum_{K\in\mathcal{T}_h^{i_F}} \int_{\partial K} z_h^{i_F}(x) \otimes \nu\, d\sigma \\ &= \sum_{\mathcal{F}\subset\partial K, K\in\mathcal{T}_h^{i_F}, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} z_h^{i_F}(x)\otimes\nu\, d\sigma + \sum_{\mathcal{F}\subset\partial K, K\in\mathcal{T}_h^{i_F}, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} z_h^{i_F}(x)\otimes\nu\, d\sigma := I + II.\end{aligned}$$

Owing to the fact that two neighboring elements share one face, with their related normal vectors changing their sign, we can continue with the first term as follows,

(25)
$$\begin{aligned}|||I||| &\le \Big|\Big|\Big| \sum_{\mathcal{F}\subset\partial K, K\in\mathcal{T}_h^{i_F}, \mathcal{F}\not\subset\partial\Omega} \Big|\int_{\mathcal{F}} (z_h^{i_F,+} - z_h^{i_F,-})(x)\otimes\nu\big|_{K^+}\, d\sigma\Big|\Big|\Big| \\ &\le \sum_{\mathcal{F}\subset\partial K, K\in\mathcal{T}_h^{i_F}, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} \big|[u_h]^{i_F}(x)\big|\, d\sigma \le C h^{3\beta/2}.\end{aligned}$$

The last bound is a consequence of Lemma 4.2 and the evaluation $\beta_{i_F} = 1 + \frac{\beta}{2}$ in the energy (12). Another application of Lemma 4.2 further leads to an upper bound for the term II,

(26)
$$\begin{aligned}|||II||| &\le \sum_{\mathcal{F}\subset\partial K, K\in\mathcal{T}_h^{i_F}, \mathcal{F}\subset\partial\Omega} \int_{\mathcal{F}} |z_h^{i_F}(x)|\, d\sigma \le C \sum_{\mathcal{F}\subset\partial K, K\in\mathcal{T}_h^{i_F}, \mathcal{F}\subset\partial\Omega} h\Big(\int_{\mathcal{F}} |z_h^{i_F}(x)|^2\, d\sigma\Big)^{1/2} \\ &\le C\Big(\sum_{\mathcal{F}\subset\partial K, K\in\mathcal{T}_h^{i_F}, \mathcal{F}\subset\partial\Omega} \int_{\mathcal{F}} |z_h^{i_F}(x)|^2\, d\sigma\Big)^{1/2} \le C h^{1-\beta}.\end{aligned}$$

This furnishes the proof of the theorem. □

Remark 4.1 *1. A corresponding analysis has been given for problem (10) in [12], where the following error bound was proven,*

$$\Big|\Big|\Big| \sum_{K\in\mathcal{T}_h^{i_F}} \int_K \{\nabla u_h^{i_F}(x) - F_\lambda\}\, d\Omega \Big|\Big|\Big| \le C\Big\{h^\beta + h^{1-\beta}\Big\}, \qquad \text{for } \beta\in[0,1].$$

2. For the two-dimensional Ericksen-James model (see Remark 3.1 and Remark 3.3), the following crucial bound is valid,

$$\Big|\Big|\Big| \sum_{K\in\mathcal{T}_h^{i_F}} \int_K \{\nabla u_h^{i_F}(x) - F_\lambda\}\, d\Omega \Big|\Big|\Big| \le C\Big\{h^{2\beta} + h^{1-\beta}\Big\}, \qquad \text{for } \beta\in[0,1].$$

This indicates $\beta = 1/3$ to be the optimal value.

The following theorem quantifies the deviation of the computed minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ from the minimizer $u \in \mathcal{A}$ in $L^2(\Omega)$.

Theorem 4.2 *A minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ of $\mathcal{E}_{h,\beta}^{\beta_{i_F}}(\cdot)$ given in (12) satisfies the estimate*

$$\Big(\sum_{K \in \mathcal{T}_h^{i_F}} \int_K |u_h^{i_F} - F_\lambda x|^2 \; d\Omega \Big)^{1/2} \le C \Big\{ \Big(\sum_{K \in \mathcal{T}_h^{i_F}} \int_K \big| \{ \nabla u_h^{i_F} - F_\lambda \} w \big|^2 \; d\Omega \Big)^{1/2} + h^{1-\beta} + h^{3\beta/4} \Big\}.$$

Proof. We will again use the abbreviative notation $z_h^{i_F}(x) = u_h^{i_F}(x) - F_\lambda x$, $x \in \Omega$. Using integration by parts, we find:

$$\begin{aligned} \int_\Omega |z_h^{i_F}(x)|^2 \; d\Omega = & \sum_{K \in \mathcal{T}_h^{i_F}} \int_{\partial K} |z_h^{i_F}(x)|^2 (w \cdot x)(w \cdot \nu) \; d\sigma \\ & - \sum_{K \in \mathcal{T}_h^{i_F}} \int_K (\nabla |z_h^{i_F}(x)|^2 \cdot w)(w \cdot x) \; d\Omega := I_1 + I_2, \end{aligned} \tag{27}$$

with an arbitrary vector $w \in \mathrm{R}^3$, $|w| = 1$. — The second term can be controlled as follows,

$$\begin{aligned} |I_2| &= \Big| \sum_{K \in \mathcal{T}_h^{i_F}} \int_K (\nabla |z_h^{i_F}(x)|^2 \cdot w)(w \cdot x) \; d\Omega \Big| \\ &\le C \max_{x \in \overline{\Omega}} |w \cdot x| \Big(\sum_{K \in \mathcal{T}_h^{i_F}} \int_K |\nabla z_h^{i_F}(x) w|^2 \; d\Omega \Big)^{1/2} \Big(\int_\Omega |z_h^{i_F}(x)|^2 \; d\Omega \Big)^{1/2} \\ &\le \frac{1}{4} \int_\Omega |z_h^{i_F}(x)|^2 \; d\Omega + C \sum_{K \in \mathcal{T}_h^{i_F}} \int_K |\nabla z_h^{i_F}(x) w|^2 \; d\Omega. \end{aligned} \tag{28}$$

In order to handle the term I_1, we distinguish between the edges in the interior of the domain and those on the boundary $\partial\Omega$,

$$\begin{aligned} I_1 = & \sum_{\mathcal{F} \subset \partial K, K \in \mathcal{T}_h^{i_F}, \mathcal{F} \subset \partial\Omega} \int_{\mathcal{F}} |z_h^{i_F}(x)|^2 (w \cdot x)(w \cdot \nu) \; d\sigma \\ & + \sum_{\mathcal{F} \subset \partial K, K \in \mathcal{T}_h^{i_F}, \mathcal{F} \not\subset \partial\Omega} \int_{\mathcal{F}} |z_h^{i_F}(x)|^2 (w \cdot x)(w \cdot \nu) \; d\sigma := I_{11} + I_{12}. \end{aligned} \tag{29}$$

Because of the existence of a minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ having energy $\mathcal{E}_{h,\beta}^{\beta_{i_F}}(u_h^{i_F}) \le Ch^2$, we immediately obtain

$$|I_{11}| \le C \sum_{\mathcal{F} \subset \partial K, \partial K \subset \partial\Omega} \int_{\mathcal{F}} |z_h^{i_F}(x)|^2 \; d\sigma \le Ch^{2(1-\beta)}. \tag{30}$$

In order to bound I_{12}, we shall distinguish along each face between ν^+ and ν^-, depending on the direction of the outer normal of adjacent triangles K^+, $K^- \in \mathcal{T}_h^{i_F}$, for $\overline{K^+} \cap \overline{K^-} \neq \emptyset$,

$$
\begin{aligned}
I_{12} &= \sum_{\mathcal{F}\subset\partial K, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} \left\{ |z_h^{i_F,+}(x)|^2 (w\cdot x)(w\cdot\nu^+) + |z_h^{i_F,-}(x)|^2 (w\cdot x)(w\cdot\nu^-) \right\} d\sigma \\
&= \sum_{\mathcal{F}\subset\partial K, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} \left\{ |z_h^{i_F,+}(x)|^2 - |z_h^{i_F,-}(x)|^2 \right\} (w\cdot x)(w\cdot\nu^+)\, d\sigma \\
&= \sum_{\mathcal{F}\subset\partial K, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} \left(\left\{ z_h^{i_F,+} - z_h^{i_F,-} \right\}(x) \cdot \left\{ z_h^{i_F,+} + z_h^{i_F,-} \right\}(x) \right) (w\cdot x)(w\cdot\nu^+)\, d\sigma \\
&= \sum_{\mathcal{F}\subset\partial K, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} \left([u_h^{i_F}](x) \cdot \left\{ z_h^{i_F,+} + z_h^{i_F,-} \right\}(x) \right) (w\cdot x)(w\cdot\nu^+)\, d\sigma \\
&\leq C \sum_{\mathcal{F}\subset\partial K, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} \left| [u_h^{i_F}](x) \right| \left\{ |z_h^{i_F,+}(x)| + |z_h^{i_F,-}(x)| \right\} d\sigma \\
&\leq C \sum_{\mathcal{F}\subset\partial K, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} \Big(\int_F \left| [u_h^{i_F}](x) \right|^2 d\sigma \Big)^{1/2} \Big(\int_{\mathcal{F}} \left\{ |z_h^{i_F,+}(x)| + |z_h^{i_F,-}(x)| \right\}^2 d\sigma \Big)^{1/2}.
\end{aligned} \tag{31}
$$

Because of Lemma 4.1, we can continue,

$$
\begin{aligned}
&\leq C \sum_{\mathcal{F}\subset\partial K, \mathcal{F}\not\subset\partial\Omega} \Big(\int_{\mathcal{F}} \left| [u_h^{i_F}](x) \right|^2 d\sigma \Big)^{1/2} h_K^{-1/2} \Big(\int_K |z_h^{i_F}(x)|^2\, d\Omega \Big)^{1/2} \\
&\leq C \sum_{\mathcal{F}\subset\partial K, \mathcal{F}\not\subset\partial\Omega} \int_{\mathcal{F}} \frac{1}{h_K} \left| [u_h^{i_F}](x) \right|^2 d\sigma + \frac{1}{4} \int_\Omega |z_h^{i_F}(x)|^2\, d\Omega.
\end{aligned} \tag{32}
$$

Because of the result

$$
\sum_{K\in\mathcal{T}_h^{i_F}} \int_{\partial K} \left| [u_h^{i_F}](x) \right|^2 d\sigma \leq C h^{1+2\beta}, \tag{33}
$$

which is an immediate consequence of Lemma 4.2, we can now insert (28) through (33) in (27) and the proof is finished. □

The following theorem gives a bound for errors on interior edges in terms of the error on elements. For this purpose, we will introduce subdomains $\omega_h \subset \overline{\Omega}$ being "pseudo-parallelepipeds". By this, we mean a perturbed parallelepiped, with faces being piecewise affine linear curves to be considered as $\mathcal{O}(h)$ perturbations of plains that constitute the parallelepiped $\omega \supset \omega_h$.

Theorem 4.3 *Assume $\{\mathcal{T}_h^i\}_{i=1}^{i_F}$ to be a sequence of admissibly refined triangulations. Then, there exists a constant $C = C(\omega) > 0$ such that for any pseudo-parallelepiped $\omega_h = \{K_s\}_{s\in L} \subset$*

$\overline{\Omega}$ *which is a union of elements* $K_s \in \mathcal{T}_h^{i_F} = \{K_s\}_{s\in I}$, *with* $I \supset L$, *the following is valid,*

$$\begin{aligned}\Big(\sum_{\mathcal{F}\subset\partial K, \mathcal{F}\cap\partial\omega_h\neq\emptyset, K\in\mathcal{T}_h^{i_F}, K\subset\omega_h} \int_{\mathcal{F}} |u_h^{i_F,\bullet}(x) - F_\lambda x|^2 \, d\sigma\Big)^{1/2} \\ \leq \frac{C}{\Lambda(\omega)}\Big(\int_{\omega_h} |u_h^{i_F}(x) - F_\lambda x|^2 \, d\Omega\Big)^{1/2} + Ch^{3\beta/4} \\ + C\Big(\int_{\omega_h} |u_h^{i_F}(x) - F_\lambda x|^2 \, d\Omega\Big)^{1/4}\Big(\sum_{K\subset\omega_h}\int_K \big|\big|\big|\nabla u_h^{i_F}(x) - F_\lambda\big|\big|\big|^2\Big)^{1/4},\end{aligned}$$

where $\Lambda(\omega)$ *is the length of the shortest edge of the corresponding parallelepiped* ω *and where* $u_h^{i_F,\bullet}\Big|_{\partial K\cap\partial\omega_h\neq\emptyset}$ *is the trace of* $u_h^{i_F}\Big|_{K\subset\omega_h}$ *on* $\partial K \cap \partial\omega_h$.

Remark 4.2 *We omit the proof of this theorem, and refer to Theorem 2.3 and its proof in [12]. Note that the improved second term on the right hand side is a consequence of the application of inequality (33).*

4.3 Approximation of limiting macroscopic deformations.

The results presented in this section are improved versions of theorems presented in [12] that hold for the adaptive energy (12). The improved orders on the right hand side of the estimates are based on the results derived in the previous section. — Since the proofs of the subsequent statements can immediately be copied from corresponding ones in [12] by taking benefit from the Theorems 4.1, 4.2 and 4.3, we will omit them here and just report on the results.

Lemma 4.3 *Suppose* $\{\mathcal{T}_h^i\}_{i=0}^{i_F}$ *to be a sequence of admissibly refined triangulations. Then there holds,*

$$\sum_{K\in\mathcal{T}_h^{i_F}} \int_K \big|\big|\big|\nabla v_h^{i_F}(x) - \pi(\nabla v_h^{i_F}(x))\big|\big|\big|^2 \, d\Omega \leq C\,\mathcal{E}_{h,\beta}^{\beta_{i_F}}(v_h^{i_F}), \qquad \forall\ v_h^{i_F} \in \mathcal{A}_h^{i_F}.$$

The next two statements quantify the accuracy of the computed minimizer in the direction of the laminates.

Lemma 4.4 *Suppose* $\{\mathcal{T}_h^i\}_{i=0}^{i_F}$ *to be a sequence of admissibly refined triangulations. Then, for any* $w \in \mathrm{R}^3$ *satisfying* $w \cdot n = 0$, *there exists a constant* $C > 0$ *such that the following bound holds for a minimizer* $u_h^{i_F} \in \mathcal{A}_h^{i_F}$,

$$\Big(\sum_{K\in\mathcal{T}_h^{i_F}} \int_K \big|\{\pi(\nabla u_h^{i_F}(x)) - F_\lambda\}w\big|^2 \, d\Omega\Big)^{1/2} \leq C\Big\{\big(\mathcal{E}_{h,\beta}^{\beta_{i_F}}(u_h^{i_F})\big)^{1/4} + h^{3\beta/4} + h^{(1-\beta)/2}\Big\}$$

with $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ *being a minimizer of problem (11).*

Theorem 4.4 *Suppose $\{\mathcal{T}_h^i\}_{i=0}^{i_F}$ to be a sequence of admissibly refined triangulations. For any $w \in \mathrm{R}^3$ satisfying $w \cdot n = 0$, there exists a constant $C > 0$ such that*

$$\Big(\sum_{K\in\mathcal{T}_h^{i_F}} \int_K \big|\{\nabla u_h^{i_F}(x) - F_\lambda\} w\big|^2 \, d\Omega\Big)^{1/2} \le C\Big\{\big(\mathcal{E}_{h,\beta}^{\beta_{i_F}}(u_h^{i_F})\big)^{1/4} + h^{3\beta/4} + h^{(1-\beta)/2}\Big\}.$$

The next theorem states averaged local approximation of the wells by the deformation gradients.

Theorem 4.5 *Suppose $\{\mathcal{T}_h^i\}_{i=0}^{i_F}$ to be a sequence of admissibly refined triangulations. For any parallelepiped $\omega \subset \overline{\Omega}$, there exists a constant $C = C(\omega) > 0$, such that the following bound holds for a minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$,*

$$\Big|\Big|\Big| \sum_{K\in\mathcal{T}_h^{i_F}, K\cap\omega_h\neq\emptyset} \int_K \{\nabla u_h^{i_F}(x) - F_\lambda\} \, d\Omega \Big|\Big|\Big|$$
$$\le C\Big\{h + h^{1/2}\big(\mathcal{E}_{h,\beta}^{\beta_{i_F}}(u_h^{i_F})\big)^{1/2} + h^\beta + \big(\mathcal{E}_{h,\beta}^{\beta_{i_F}}(u_h^{i_F})\big)^{1/8} + h^{(1-\beta)/4} + h^{3\beta/8}\Big\}.$$

4.4 Approximation of simply laminated microstructure. Again, the verification of the results presented here make use of the sharp inequalities presented in the last section, and the proofs of corresponding statements given in [12] can be immediately applied. From this reason, we again omit the presentation of the corresponding proofs, and refer the interested reader to [12]. — For the formulation of the results, let us introduce some additional notation:
For any subset $\omega \subset \Omega$, $\rho > 0$ and $v_h^i \in \mathcal{A}_h^i$, with $0 \le i \le i_F$, we introduce the sets

$$\omega^\ell(v_h^i) = \bigcup_{K\in\mathcal{T}_h} \big\{x \in \omega \cap K : \Pi(\nabla v_h^i(x)) = F_\ell, \text{ and } \|\nabla v_h^i(x) - F_\ell\| < \rho\big\},$$

for $\ell \in \{1, 2\}$. – In here, we made use of the operator $\Pi : \mathrm{R}^{3\times3} \to \{U_1, U_2\}$ that is related to the operator π in the following way,

$$\pi(F) = \Theta(F)\Pi(F), \qquad \text{with} \qquad \Theta : \mathrm{R}^{3\times3} \to SO(3), \quad \forall\, F \in \mathrm{R}^{3\times3}.$$

Then we have the following result:

Theorem 4.6 *Suppose $\{\mathcal{T}_h^i\}_{i=0}^{i_F}$ to be a sequence of admissibly refined triangulations. There exists a constant $C > 0$ such that a minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ satisfies the following bound,*

$$\Big(\sum_{K\in\mathcal{T}_h^{i_F}} \int_K \big|\big|\big|\nabla u_h^{i_F}(x) - \Pi(\nabla u_h^{i_F}(x))\big|\big|\big|^2 \, d\Omega\Big)^{1/2} \le C\Big\{\big(\mathcal{E}_{h,\beta}^{\beta_{i_F}}(u_h^{i_F})\big)^{1/4} + h^{3\beta/4} + h^{(1-\beta)/2}\Big\}.$$

Finally, the following theorem quantifies the ability of the adaptive method (14), (15) to approximize the laminate microstructure.

Theorem 4.7 *Suppose $\{\mathcal{T}_h^i\}_{i=0}^{i_F}$ to be a sequence of admissibly refined triangulations. For any rectangular parallelepiped $\omega \subset \Omega$, and any $\rho > 0$, there exists a constant $C = C(\omega, \rho) > 0$, such that a minimizer $u_h^{i_F} \in \mathcal{A}_h^{i_F}$ enjoys the following bound, for $\ell \in \{1, 2\}$,*

$$\Big| \frac{\mu(\omega_\rho^\ell(u_h^{i_F}))}{\mu(\omega)} - \lambda^\ell \Big| \leq C \Big\{ \big(\mathcal{E}_{h,\beta}^{\beta_{i_F}}(u_h^{i_F}) \big)^{1/8} + h^{3\beta/8} + h^{(1-\beta)/4} \Big\}.$$

This investigation furnishes item 1) in Theorem 3.1. — Now, in order to verify the second part of it, dealing with the case α_3, we refer again to [12] where a corresponding case is investigated.

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