NONCONFORMING FINITE ELEMENT APPROXIMATION
OF CRYSTALLINE MICROSTRUCTURE

By

Bo Li

and

Mitchell Luskin

IMA Preprint Series # 1420
July 1996
NONCONFORMING FINITE ELEMENT APPROXIMATION OF
CRYSTALLINE MICROSTRUCTURE

BO LI AND MITCHELL LUSKIN

ABSTRACT. We consider a class of nonconforming finite element approximations
of a simply laminated microstructure which minimizes the nonconvex variational
problem for the deformation of martensitic crystals which can undergo either an or-
thorhombic to monoclinic (double well) or a cubic to tetragonal (triple well) trans-
formation. We first establish a series of error bounds in terms of elastic energies for
the $L^2$ approximation of derivatives of the deformation in the direction tangential to
parallel layers of the laminate, for the $L^2$ approximation of the deformation, for the
weak approximation of the deformation gradient, for the approximation of volume
fractions of deformation gradients, and for the approximation of nonlinear integ-
als of the deformation gradient. We then use these bounds to give corresponding
convergence rates for quasi-optimal finite element approximations.

1. INTRODUCTION

The nonconvex elastic energy used to model martensitic crystals is generally mini-
mized only by a microstructure [3, 4, 9, 19, 23, 26, 32]. A common example of such
a microstructure is a simple laminate in which the deformation gradient oscillates
on a fine or infinitesimal scale in parallel layers between two stress-free homogeneous
states.

Finite element approximations of energy-minimizing laminates necessarily have a
finite thickness. Although conforming finite element methods can be proven to give
convergent approximations to the microstructure [28, 29, 31, 32], they cannot gen-
erally give a laminate which oscillates on the scale of the mesh size for arbitrarily
oriented meshes [12, 32].

Date: June 7, 1996.
1991 Mathematics Subject Classification. 49M15, 65C20, 65N30, 73C50, 73K20.
Key words and phrases. finite element, nonconforming, microstructure, martensitic transforma-
tion, error estimate.

This work was supported in part by the NSF through grant DMS 95-05077, by the AFOSR
through grant AF/F49620-96-1-0057, by the Institute for Mathematics and its Applications, and by
a grant from the Minnesota Supercomputer Institute.
Nonconforming finite element approximations are not required to be globally continuous [10, 38], so it is reasonable to think that they would be able to give a more accurate approximation to fine-scale microstructure [32]. The class of nonconforming finite element methods analyzed in this paper were successfully used to compute crystalline microstructure in [25]. These elements were first proposed, tested, and analyzed in [39] for the Stokes problem. A short discussion on one of these elements in the setting of the mixed finite element method can be found in [2]. This class of elements was analyzed for general second-order elliptic problems in [24]. In this paper, we prove the convergence of these nonconforming methods to an energy-minimizing microstructure for the nonconvex elastic energies which model martensitic crystals which can undergo either an orthorhombic to monoclinic transformation (double well) or a cubic to tetragonal (triple well) transformation. The results in this paper also hold for a general rotationally invariant, double well energy density.

In the recently developed geometrically nonlinear theory of martensitic crystals, the elastic energy density attains its minimum value (below the transformation temperature) on a set

$$\text{SO}(3) U_1 \cup \cdots \cup \text{SO}(3) U_N,$$

where \text{SO}(3) is the group of proper rotations defined by

$$\text{SO}(3) = \{ Q \in \mathbb{R}^{3 \times 3} : Q^T = Q^{-1} \text{ and } \det Q = 1 \},$$

and where the symmetry-related matrices, \( U_1, \cdots, U_N \), for \( N > 1 \), represent the martensitic variants. The martensitic variants \( U_1, \cdots, U_N \) are linear transformations which transform the lattice of the austenitic phase into the lattice of the martensitic phase. In the above, \( \mathbb{R}^{3 \times 3} \) is the set of all \( 3 \times 3 \) real matrices.

A martensitic crystal which can undergo an orthorhombic to monoclinic transformation has two symmetry-related martensitic variants, that is, \( N = 2 \), and hence the elastic energy density has two wells [4, 32]. A more commonly observed martensitic transformation is the cubic to tetragonal transformation [3, 4, 32]. In this case, there are three associated symmetry-related martensitic variants, so \( N = 3 \), and the elastic energy density has therefore three wells.

For certain boundary conditions, the elastic energy of the martensitic crystal cannot be minimized by a deformation and can be lowered as much as possible only by a sequence of deformations whose gradients oscillate so that the limiting volume fraction is nonzero for more than one gradient [4, 32]. Based on the hypothesis that the crystal structure is determined by the principle of energy minimization, the geometrically nonlinear theory describes the crystalline microstructure as the limiting configuration of energy-minimizing sequences of deformations [3, 4, 9, 19, 23, 26, 32].
Both of our nonconforming finite elements are defined on rectangular parallelepipeds. The first one has its degrees of freedom given by the values at the centers of the faces of the rectangular parallelepipeds. The second one has its degrees of freedom given by the averages over the six faces of the rectangular parallelepipeds. To prove the convergence of this class of nonconforming finite element methods for the nonconvex energies which model crystalline microstructure, we prove some important properties of the nonconforming finite element deformations. They include a discrete version of a slight variation of the divergence theorem, a Poincaré type inequality which is more general than that in [24], and a discrete version of the usual trace theorem in Sobolev spaces [1]. These properties will be used as key technical tools in establishing various kinds of error bounds in terms of the elastic energy.

Our analysis utilizes the theory of numerical analysis for the microstructure in nonconvex variational problems that was developed in [13, 16], and extended in [6, 7, 8, 21, 34]. This theory was also used to analyze the finite element approximation of microstructure in micromagnetics [33]. The approximation of relaxed variational problems has been analyzed in [5, 20, 35, 36, 37, 40, 41]. A nonconforming finite element approximation for a nonconvex variational problem with not only an elastic energy but also a non-physical penalty term was analyzed in [21].

An analysis of the finite element approximation for a physical, rotationally invariant energy was first given in [31] for the orthorhombic to monoclinic transformation. This analysis has been extended to the cubic to orthorhombic transformation [28], to more general boundary conditions [27, 29], and to the method of reduced integration [11]. The estimates in these papers and in this paper show that all of the local minima of the energy (restricted to the finite element space) which satisfy a quasi-optimality condition give accurate approximations to the energy-minimizing microstructure for the deformation, the volume fractions of the deformation gradients, and the nonlinear integrals of the deformation gradient.

In this paper, we further generalize the results in [28, 31] to the approximation by the two nonconforming finite elements. Our results show that the approximation errors due to the nonconformity of the employed nonconforming finite elements are negligible compared with the errors of the approximation of microstructure which are already present in the conforming approximation. Therefore, the asymptotic rate of convergence that we obtain for the nonconforming methods is equal to the rate found for the conforming methods.

We refer to [32] for an introduction to the modeling and computation of crystalline microstructure and for a more extensive survey of results and references.

We organize the rest of the paper as follows. In §2, we describe the underlying continuum model for crystals which can undergo either an orthorhombic to monoclinic or a cubic to tetragonal martensitic transformation. In §3, we review the definition
and basic properties of the class of nonconforming finite element spaces that we analyze. Further properties of nonconforming finite element deformations are given in §4. These properties are then used to establish a series of error bounds in terms of the elastic energy for the nonconforming finite element approximations in §5 – §7. Finally, in §8, we first prove the existence of finite element energy minimizers and then derive the corresponding error estimates for quasi-optimal nonconforming finite element approximations.

2. Multi-well Energy Minimization Problems

We first briefly review some basic definitions and properties of martensitic crystals which can undergo either an orthorhombic to monoclinic or a cubic to tetragonal phase transformation. For more details, we refer to [3, 4, 32].

The energy wells for an orthorhombic to monoclinic transformation are determined by the martensitic variants

\[ U_1 = (I + \eta e_2 \otimes e_1)D, \quad U_2 = (I - \eta e_2 \otimes e_1)D, \]

where \( I \) is the identity transformation from \( \mathbb{R}^3 \) to \( \mathbb{R}^3 \), \( \eta > 0 \) is a material parameter, \( \{e_1, e_2, e_3\} \) is an orthonormal basis for \( \mathbb{R}^3 \), and \( D \) is a diagonal, positive definite, linear transformation given by

\[ D = d_1 e_1 \otimes e_1 + d_2 e_2 \otimes e_2 + d_3 e_3 \otimes e_3 \]

for some \( d_1, d_2, d_3 > 0 \). We recall that the tensor \( a \otimes n \) for \( a, n \in \mathbb{R}^3 \) defines the linear transformation \( (a \otimes n)v = (n \cdot v)a \) for \( v \in \mathbb{R}^3 \).

The energy wells for a cubic to tetragonal transformation are determined by the martensitic variants

\[ U_1 = \eta_1 I + (\eta_2 - \eta_1)e_1 \otimes e_1, \quad U_2 = \eta_1 I + (\eta_2 - \eta_1)e_2 \otimes e_2, \quad U_3 = \eta_1 I + (\eta_2 - \eta_1)e_3 \otimes e_3, \]

where \( \eta_1 > 0 \) and \( \eta_2 > 0 \) are material parameters such that \( \eta_1 \neq \eta_2 \), and \( \{e_1, e_2, e_3\} \) is again an orthonormal basis for \( \mathbb{R}^3 \).

For convenience, we define the set of indices \( K \) to be \( K = \{1, 2\} \) for the orthorhombic to monoclinic transformation and \( K = \{1, 2, 3\} \) for the cubic to tetragonal transformation. We also denote

\[ U_i = \text{SO}(3)U_i, \quad i \in K, \quad \text{and} \quad \mathcal{U} = \bigcup \{U_i : i \in K\}. \]

The following lemma, proved in [3, 4, 32], serves as a key crystallographical basis for our analysis.
Lemma 2.1. (1) For each $i \in K$ there is no rank-one connection between $\mathcal{U}_i$ and itself, that is, there do not exist $F_0, F_1 \in \mathcal{U}_i$ with $F_0 \neq F_1$ such that

$$F_1 = F_0 + a \otimes n$$

for some $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$.

(2) For any $i, j \in K, i \neq j$, there are exactly two rank-one connections between $\mathcal{U}_i$ and $\mathcal{U}_j$, that is, for any $F_0 \in \mathcal{U}_i$ there are exactly two distinct $F_1 \in \mathcal{U}_j$ such that

$$F_1 = F_0 + a \otimes n$$

for some $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$. In this case, we have also for any $\lambda \in (0, 1)$ that

$$(1 - \lambda)F_0 + \lambda F_1 \notin \mathcal{U}.$$  

Moreover, we have for the orthorhombic to monoclinic transformation that

$$n \in \{\pm e_1, \pm e_2\},$$

and for the cubic to tetragonal transformation that

$$n \in \left\{\pm \frac{1}{\sqrt{2}}(e_i + e_j), \pm \frac{1}{\sqrt{2}}(e_i - e_j)\right\}.$$  

We now consider a crystal that can undergo either an orthorhombic to monoclinic or a cubic to tetragonal transformation. We denote by $\Omega$ the reference configuration of the crystal which is taken to be the homogeneous austenitic phase at the transformation temperature. We assume that $\Omega \subset \mathbb{R}^3$ is a bounded domain with a Lipschitz continuous boundary. We denote deformations by $y : \Omega \rightarrow \mathbb{R}^3$ and corresponding deformation gradients by $\nabla y : \Omega \rightarrow \mathbb{R}^{3 \times 3}$. We denote the elastic energy density at a fixed temperature below the transformation temperature by the continuous function $\phi : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$. The elastic energy of a deformation $y$ is then given by

$$\mathcal{E}(y) = \int_{\Omega} \phi(\nabla y(x)) \, dx.$$  

To model the underlying martensitic transformations, we assume that the energy density $\phi$ is minimized on the energy wells $\mathcal{U}_i = \text{SO}(3)\mathcal{U}_i$, $i \in K$, so we assume (after adding a constant to the energy density) that

$$\phi(F) \geq 0, \quad \forall F \in \mathbb{R}^{3 \times 3},$$

$$\phi(F) = 0 \quad \text{if and only if} \quad F \in \mathcal{U} = \bigcup \{\mathcal{U}_i : i \in K\}.$$  

We shall also assume that the energy density $\phi$ grows quadratically away from the energy wells, that is,

$$\phi(F) \geq \kappa \|F - \pi(F)\|^2, \quad \forall F \in \mathbb{R}^{3 \times 3},$$  

(2.2)
where \( \kappa > 0 \) is a constant and \( \pi : \mathbb{R}^{3 \times 3} \rightarrow \mathcal{U} \) is a Borel measurable projection defined by

\[
\| F - \pi(F) \| = \min_{G \in \mathcal{U}} \| F - G \|, \quad \forall F \in \mathbb{R}^{3 \times 3}.
\]

In the above and in the following we use the matrix norm defined by

\[
\| F \|^2 = \text{trace} \left( F^T F \right) = \sum_{i,j=1}^{3} F_{ij}^2, \quad \forall F = (F_{ij}) \in \mathbb{R}^{3 \times 3}.
\]

The projection \( \pi(F) \) exists for any \( F \in \mathbb{R}^{3 \times 3} \) since \( \mathcal{U} \) is compact, although the projection may not be unique. It is unique, however, if \( \| F - \pi(F) \| \) is small enough \([32]\).

Let \( F_0, F_1 \in \mathcal{U} \) be rank-one connected so as to satisfy

\[
F_1 = F_0 + a \otimes n
\]

for some \( a, n \in \mathbb{R}^3, |n| = 1 \). By Lemma 2.1, we may assume without loss of generality that \( F_0 \in \mathcal{U}_1 \) and \( F_1 \in \mathcal{U}_2 \) and also that

\[
n = e_1
\]

for the orthorhombic to monoclinic transformation and

\[
n = \frac{1}{\sqrt{2}} (e_1 + e_2)
\]

for the cubic to tetragonal transformation. Let \( \lambda \) be a constant such that \( 0 < \lambda < 1 \) and let

\[
F_\lambda = (1 - \lambda) F_0 + \lambda F_1.
\]

We define the set of admissible deformations which are compatible with the simple laminate to be

\[
W^{1,\infty}_\lambda(\Omega; \mathbb{R}^3) \equiv \{ y \in W^{1,\infty}(\Omega; \mathbb{R}^3) : y(x) = F_\lambda x, \forall x \in \partial \Omega \}.
\]

Our multi-well energy minimization problem is to minimize the elastic energy (2.1) among all deformations \( y \in W^{1,\infty}_\lambda(\Omega; \mathbb{R}^3) \). Ball and James have shown that there exist no energy minimizers for this minimization problem and that any energy minimizing sequence will converge to a unique microstructure which is composed of the gradient \( F_0 \) with volume fraction \( 1 - \lambda \) and the gradient \( F_1 \) with volume fraction \( \lambda \) \([4]\).

We note that the proofs given in this paper for the orthorhombic to monoclinic transformation hold without modification for the more general problem with a rotationally invariant, double well energy (that is, \( N=2 \), in (1.1)) if there exists a rotation
$Q \in \text{SO}(3)$ and vectors $a, n \in \mathbb{R}^3$, $|n| = 1$, such that

$$QU_2 = U_1 + a \otimes n.$$ 

3. Nonconforming Finite Elements

We will denote a generic point in $\mathbb{R}^3$ by $(x_1, x_2, x_3)$. Our first finite element is defined by the triple $(Q, P_Q, \Sigma_Q^p)$; where $Q = [\alpha_1 - l_1, \alpha_1 + l_1] \times [\alpha_2 - l_2, \alpha_2 + l_2] \times [\alpha_3 - l_3, \alpha_3 + l_3]$ is a rectangular parallelepiped with its center at $(\alpha_1, \alpha_2, \alpha_3)$ and the lengths of its edges are $2l_1, 2l_2, 2l_3$, where $l_1, l_2, l_3 > 0$;

$$P_Q = \text{span} \left\{ 1, x_1, x_2, x_3, \left( \frac{x_1}{l_1} \right)^2 - \left( \frac{x_2}{l_2} \right)^2, \left( \frac{x_3}{l_3} \right)^2 \right\};$$

and

$$\Sigma_Q^p = \{ q(c_{\mathcal{F}_i}) : i = 1, \ldots, 6 \},$$

where $c_{\mathcal{F}_i}, i = 1, \ldots, 6$, are the centers of the faces $\mathcal{F}_i, i = 1, \ldots, 6$, of the rectangular parallelepiped $Q$. Our second element is defined to be the triple $(Q, P_Q, \Sigma_Q^a)$. The polynomial space $P_Q$ is the same as defined in (3.1) and the set of degrees of freedom is defined by

$$\Sigma_Q^a = \left\{ \frac{1}{|\mathcal{F}_i|} \int_{\mathcal{F}_i} q \, dS : i = 1, \ldots, 6 \right\},$$

where $\mathcal{F}_i, i = 1, \ldots, 6$, are the faces of $Q$, and $|\mathcal{F}_i|$ is the area of the face $\mathcal{F}_i$ for $i = 1, \ldots, 6$.

In the sequel, we will restrict ourselves to considering rectangular domains with faces parallel to coordinate planes. The results presented in this paper can be immediately extended to domains which are the union of rectangular parallelepipeds. However, we will assume for simplicity of exposition that $\Omega = (0, L_1) \times (0, L_2) \times (0, L_3)$ for some $L_k > 0$, $k = 1, 2, 3$. To construct a rectangular partition $\tau_h$ of $\Omega$, we define the one-dimensional partitions of $[0, L_k]$, for $k = 1, 2, 3$, by

$$0 = x^0_k < x^1_k < \cdots < x^{m_k}_k = L_k,$$

where the $m_k$ are positive integers. We then define the rectangular parallelepipeds

$$\mathcal{R}_{i_1,i_2,i_3} = [x^{i_1-1}_1, x^{i_1}_1] \times [x^{i_2-1}_2, x^{i_2}_2] \times [x^{i_3-1}_3, x^{i_3}_3]$$

for $1 \leq i_1 \leq m_1$, $1 \leq i_2 \leq m_2$, $1 \leq i_3 \leq m_3$, and the rectangular partition

$$\tau_h = \{ \mathcal{R}_{i_1,i_2,i_3} : 1 \leq i_1 \leq m_1, 1 \leq i_2 \leq m_2, 1 \leq i_3 \leq m_3 \}.$$ 

The mesh size parameter $h$ is defined by $h = \max\{h_k : 1 \leq k \leq 3\}$, where $h_k \equiv \max\{x^i_k - x^{i-1}_k : 1 \leq i \leq m_k\}$ is the maximal discretization size in the $k$th coordinate.
direction for \( k = 1, 2, 3 \). We will always assume that the rectangular partitions \( \tau_h \) are quasi-uniform, that is, there exists a constant \( \sigma > 0 \), independent of \( h \), such that
\[
\min\{x^i_k - x^{i-1}_k : i = 1, \ldots, m_k, k = 1, 2, 3\} \geq \sigma h.
\]

For the first finite element, we define the set of nodal points \( N_h \) to be the set of all centers \( c_F \) of faces \( F \) of elements in \( \tau_h \). The finite element spaces over the partition \( \tau_h \) are then defined respectively to be
\[
V^p_h \equiv \{v_h \in L^2(\Omega) : v_h|_\mathcal{R} \in P_\mathcal{R}, \ \forall \mathcal{R} \in \tau_h; \ \text{adjoining } v_h \ \text{have the same}
\]
values at shared nodal points, that is, \( v_h \) is continuous on \( N_h \},
\]
\[
V^a_h \equiv \{v_h \in L^2(\Omega) : v_h|_\mathcal{R} \in P_\mathcal{R}, \ \forall \mathcal{R} \in \tau_h;
\]
\[
\int_F v_h|_{\mathcal{R}'} \ dS = \int_F v_h|_{\mathcal{R}''} \ dS, \ \forall \text{faces } \mathcal{F} = \mathcal{R}' \cap \mathcal{R}'' \neq \emptyset, \ \mathcal{R}', \mathcal{R}'' \in \tau_h \}.
\]

We denote by \( \mathcal{A}^p_h \) the set of admissible finite element deformations \( y_h : \Omega \to \mathbb{R}^3 \) such that each component of \( y_h \) belongs to \( V^p_h \) and such that \( y_h(c_F) = F_\lambda c_F \) if \( c_F \) is the center of an element face \( F \) lying in \( \partial \Omega \). Similarly, we denote \( \mathcal{A}^a_h \) to be the set of admissible finite element deformations \( y_h : \Omega \to \mathbb{R}^3 \) such that each component of \( y_h \) belongs to \( V^a_h \) and such that
\[
\int_F y_h(x) \ dS = \int_F F_\lambda x \ dS
\]
for any element face \( F \subset \partial \Omega \). Note that the deformation \( y_h(x) = F_\lambda x, \ x \in \Omega \), belongs to both \( \mathcal{A}^p_h \) and \( \mathcal{A}^a_h \). We denote for convenience \( V_h = V^p_h \cup V^a_h \) and \( \mathcal{A}_h = \mathcal{A}^p_h \cup \mathcal{A}^a_h \).

It is obvious that both of the spaces \( V^p_h \) and \( V^a_h \) are finite-dimensional affine subspaces of \( L^2(\Omega) \). They are also affine finite element spaces [10]. For \( v_h \in V^p_h \) or \( v_h \in V^a_h \), we have in general that \( v_h \notin C(\bar{\Omega}) \) since \( v_h \) is continuous only at some points of the faces of adjacent elements. Thus, \( V^p_h, V^a_h \not\subset C(\bar{\Omega}) \), and hence, neither \( \mathcal{A}^p_h \) nor \( \mathcal{A}^a_h \) is contained in \( W^{1,\infty}_\lambda(\Omega; \mathbb{R}^3) \) which is a subset of \( C(\bar{\Omega}; \mathbb{R}^3) \) by the embedding theorem [1]. Therefore, in view of minimizing the elastic energy over \( W^{1,\infty}_\lambda(\Omega; \mathbb{R}^3) \subset W^{1,\infty}(\Omega; \mathbb{R}^3) \), the above finite elements are nonconforming.

We now denote the Lagrange interpolation operator \( I_h^p : C(\bar{\Omega}) \to V_h \) to be either \( I_h^p : C(\bar{\Omega}) \to V^p_h \) or \( I_h^a : C(\bar{\Omega}) \to V^a_h \), which are defined respectively by \( I_h^p v \in V^p_h \) and \( I_h^a v \in V^a_h \), and
\[
I^p_h v(c_F) = v(c_F), \quad \forall c_F \in N_h,
\]
\[
\int_F I^a_h v \ dS = \int_F v \ dS, \quad \forall \text{faces } F \subset \partial \mathcal{R}, \forall \mathcal{R} \in \tau_h,
\]
for any $v \in C(\bar{\Omega})$. We will also use the same notation $I_h$, $I_h^p$ and $I_h^a$ to denote the restrictions of these operators to an element of the partition $\tau_h$.

For any element $\mathcal{R} \in \tau_h$ and a face $\mathcal{F} \subset \partial \mathcal{R}$, we define the functional $T^p_{\mathcal{F}} : C(\mathcal{F}) \to \mathbb{R}$ by $T^p_{\mathcal{F}}(w) = w(c_{\mathcal{F}})$ for $w \in C(\mathcal{F})$, where $c_{\mathcal{F}}$ is the center of the face $\mathcal{F}$, when considering the $V_h^p$-approximation, and the functional $T^a_{\mathcal{F}} : L^2(\mathcal{F}) \to \mathbb{R}$ by $T^a_{\mathcal{F}}(w) = (\frac{1}{|\mathcal{F}|}) \int_{\mathcal{F}} w \, dS$ for $w \in L^2(\mathcal{F})$, when considering the $V_h^a$-approximation. Similar functionals of suitable deformations can be defined component-wise. Without confusion, the same notation $T^p_{\mathcal{F}}$ or $T^a_{\mathcal{F}}$ will be used for functionals defined on both scalar functions and vectorial deformations.

We will use the letter $C$ to denote a generic positive constant which is independent of the mesh size $h$. For convenience, we also define for any integer $k \geq 0$ and $p \in [1, \infty]$ the space

$$W_h^{k,p}(\Omega) \equiv \{ v \in L^p(\Omega) : v|_{\mathcal{R}} \in W^{k,p}(\mathcal{R}), \forall \mathcal{R} \in \tau_h \},$$

and we equip $W_h^{k,p}(\Omega)$ with the following semi-norm and norm:

$$| \cdot |_{k,p,h} \equiv \begin{cases} \left( \sum_{\mathcal{R} \in \tau_h} | \cdot |_{k,p,\mathcal{R}}^p \right)^{\frac{1}{p}}, & \text{if } 1 \leq p < \infty, \\ \max_{\mathcal{R} \in \tau_h} | \cdot |_{k,\infty,\mathcal{R}}, & \text{if } p = \infty; \end{cases}$$

$$\| \cdot \|_{k,p,h} \equiv \begin{cases} \left( \sum_{\mathcal{R} \in \tau_h} \| \cdot \|_{k,p,\mathcal{R}}^p \right)^{\frac{1}{p}}, & \text{if } 1 \leq p < \infty, \\ \max_{\mathcal{R} \in \tau_h} \| \cdot \|_{k,\infty,\mathcal{R}}, & \text{if } p = \infty; \end{cases}$$

where, for $\mathcal{R} \in \tau_h$, $| \cdot |_{k,p,\mathcal{R}}$ and $\| \cdot \|_{k,p,\mathcal{R}}$ are the usual semi-norm and norm on the Sobolev space $W^{k,p}(\mathcal{R})$ [1]. If $p = 2$ we write $H_h^k(\Omega)$ for $W_h^{k,p}(\Omega)$ and omit $p$ in all of the above semi-norm and norm expressions. We define the spaces $W_h^{k,p}(\Omega; \mathbb{R}^3)$ and $H_h^k(\Omega; \mathbb{R}^3)$ in a similar way and use the same notation $| \cdot |_{k,p,h}$, $\| \cdot \|_{k,p,h}$, $| \cdot |_{k,h}$, and $\| \cdot \|_{k,h}$ for the associated semi-norms and norms.

We now collect some useful properties of the finite element spaces $V_h^p$ and $V_h^a$ in the following lemmas.

**Lemma 3.1.** For any $v_h \in V_h = V_h^p \cup V_h^a$ restricted to any $\mathcal{R} \in \tau_h$, we have

$$\frac{\partial v_h}{\partial x_k} \in \text{span} \{1, x_k\}, \quad k = 1, 2, 3. \quad (3.3)$$

It follows that

$$v_h(\hat{x}_1, \hat{x}_2, \hat{x}_3) - v_h(\hat{x}_1, x_2, x_3) = v_h(x_1, \hat{x}_2, \hat{x}_3) - v_h(x_1, x_2, x_3), \quad (3.4)$$

$$v_h(\hat{x}_1, \hat{x}_2, \hat{x}_3) - v_h(x_1, \hat{x}_2, x_3) = v_h(\hat{x}_1, x_2, \hat{x}_3) - v_h(x_1, x_2, x_3), \quad (3.5)$$

$$v_h(\hat{x}_1, \hat{x}_2, \hat{x}_3) - v_h(x_1, x_2, \hat{x}_3) = v_h(\hat{x}_1, \hat{x}_2, x_3) - v_h(x_1, x_2, x_3). \quad (3.6)$$

for any $(\hat{x}_1, \hat{x}_2, \hat{x}_3) \in \mathcal{R}$ and $(x_1, x_2, x_3) \in \mathcal{R}$. 
Proof. The equation (3.3) follows directly from the definition of the finite element polynomial space \( P_Q \) (3.1). The result (3.4) follows from (3.3) since \( \partial v_h / \partial x_1 \) is independent of \( x_2 \) and \( x_3 \), so
\[
v_h(\hat{x}_1, \hat{x}_2, \hat{x}_3) - v_h(x_1, x_2, x_3) = \int_{x_1}^{\hat{x}_1} \frac{\partial v_h}{\partial x_1}(\xi, \hat{x}_2, \hat{x}_3) \, d\xi
\]
\[
= \int_{x_1}^{\hat{x}_1} \frac{\partial v_h}{\partial x_1}(\xi, x_2, x_3) \, d\xi
\]
\[
= v_h(\hat{x}_1, x_2, x_3) - v_h(x_1, x_2, x_3).
\]

The results (3.5) and (3.6) follow similarly. 

\[\Box\]

Lemma 3.2. Let \( k \) and \( l \) be two integers such that \( 0 \leq k \leq l \leq 2 \). We have the following inverse inequalities for any \( \mathcal{R} \in \tau_h \) and any \( v_h \in V_h = V_h^p \cup V_h^a \)
\[
(3.7) \quad |v_h|_{l, \mathcal{R}} \leq C h^{k-l} |v_h|_{k, \mathcal{R}},
\]
\[
(3.8) \quad |v_h|_{l, h} \leq C h^{k-l} |v_h|_{k, h},
\]
\[
(3.9) \quad |v_h|_{l, \infty, \mathcal{R}} \leq C h^{k-l-\frac{3}{2}} |v_h|_{k, \mathcal{R}},
\]
\[
(3.10) \quad |v_h|_{l, \infty, h} \leq C h^{k-l-\frac{3}{2}} |v_h|_{k, h}.
\]

Proof. Since both \( V_h^p \) and \( V_h^a \) are affine finite element spaces, the results of this lemma can be proven by a standard argument via affine mappings [10].

\[\Box\]

Lemma 3.3. We have for any \( \mathcal{R} \in \tau_h \) and any face \( \mathcal{F} \subset \partial \mathcal{R} \) that
\[
(3.11) \quad \int_{\mathcal{F}} |v - T^a_{\mathcal{F}}(v)|^2 \, dS \leq C h |v|_{1, \mathcal{R}}^2, \quad \forall v \in H^1(\mathcal{R}).
\]

We also have that
\[
(3.12) \quad \int_{\mathcal{F}} |v_h - T^p_{\mathcal{F}}(v_h)|^2 \, dS \leq C h |v_h|_{1, \mathcal{R}}^2, \quad \forall v_h \in V_h^p.
\]

Proof. We will prove (3.11) and (3.12) on the reference domain \( \hat{\mathcal{R}} = (0, 1) \times (0, 1) \times (0, 1) \) with face \( \hat{\mathcal{F}} = \{0\} \times (0, 1) \times (0, 1) \). We can then obtain the results (3.11) and (3.12) on the element \( \mathcal{R} \in \tau_h \) and the face \( \mathcal{F} \subset \partial \mathcal{R} \) by an affine scaling.

For \( v \in C^\infty(\hat{\mathcal{R}}) \) we have that
\[
v(0, x_2, x_3) - \int_0^1 \int_0^1 v(0, \hat{x}_2, \hat{x}_3) \, d\hat{x}_2 \, d\hat{x}_3
\]
\[
= v(x_1, x_2, x_3) - \int_0^1 \int_0^1 v(x_1, \hat{x}_2, \hat{x}_3) \, d\hat{x}_2 \, d\hat{x}_3
\]
\begin{align}
(3.13) & \quad - \int_0^{x_1} \frac{\partial v}{\partial x_1}(\hat{x}_1, x_2, x_3) \, d\hat{x}_1 + \int_0^1 \int_0^1 \int_0^{x_1} \frac{\partial v}{\partial x_1}(\hat{x}_1, \hat{x}_2, \hat{x}_3) \, d\hat{x}_1 \, d\hat{x}_2 \, d\hat{x}_3 \\
&= \int_0^1 \int_0^1 \left[ v(x_1, x_2, x_3) - v(x_1, \hat{x}_2, \hat{x}_3) \right] \, d\hat{x}_2 \, d\hat{x}_3 \\
&\quad - \int_0^{x_1} \frac{\partial v}{\partial x_1}(\hat{x}_1, x_2, x_3) \, d\hat{x}_1 + \int_0^1 \int_0^1 \int_0^{x_1} \frac{\partial v}{\partial x_1}(\hat{x}_1, \hat{x}_2, \hat{x}_3) \, d\hat{x}_1 \, d\hat{x}_2 \, d\hat{x}_3.
\end{align}

Now,
\begin{align}
(3.14) & \quad v(x_1, x_2, x_3) - v(x_1, \hat{x}_2, \hat{x}_3) \\
&= [v(x_1, x_2, x_3) - v(x_1, \hat{x}_2, x_3)] + [v(x_1, \hat{x}_2, x_3) - v(x_1, \hat{x}_2, \hat{x}_3)] \\
&= \int_{\hat{x}_2}^{x_2} \frac{\partial v}{\partial x_2}(x_1, \hat{x}_2, x_3) \, d\hat{x}_2 + \int_{\hat{x}_3}^{x_3} \frac{\partial v}{\partial x_3}(x_1, \hat{x}_2, \hat{x}_3) \, d\hat{x}_3.
\end{align}

We obtain from substituting (3.14) into (3.13) that
\begin{align}
(3.15) & \quad v(0, x_2, x_3) - \int_0^1 \int_0^1 v(0, \hat{x}_2, \hat{x}_3) \, d\hat{x}_2 \, d\hat{x}_3 \\
&= \int_0^1 \int_0^1 \int_{\hat{x}_2}^{x_2} \frac{\partial v}{\partial x_2}(x_1, \hat{x}_2, x_3) \, d\hat{x}_2 \, d\hat{x}_3 \\
&\quad + \int_0^1 \int_0^1 \int_{\hat{x}_3}^{x_3} \frac{\partial v}{\partial x_3}(x_1, \hat{x}_2, \hat{x}_3) \, d\hat{x}_3 \, d\hat{x}_2 \, d\hat{x}_3 \\
&\quad - \int_0^{x_1} \frac{\partial v}{\partial x_1}(\hat{x}_1, x_2, x_3) \, d\hat{x}_1 + \int_0^1 \int_0^1 \int_0^{x_1} \frac{\partial v}{\partial x_1}(\hat{x}_1, \hat{x}_2, \hat{x}_3) \, d\hat{x}_1 \, d\hat{x}_2 \, d\hat{x}_3.
\end{align}

We can then obtain by squaring both sides of (3.15), integrating with respect to \((x_1, x_2, x_3)\) over the domain \((0,1) \times (0,1) \times (0,1)\), and using the Cauchy-Schwarz inequality that
\begin{align}
(3.16) & \quad \left| \int_0^1 \int_0^1 v(0, x_2, x_3) - \int_0^1 \int_0^1 v(0, \hat{x}_2, \hat{x}_3) \, d\hat{x}_2 \, d\hat{x}_3 \right|^2 \, dx_2 \, dx_3 \\
&= \int_0^1 \int_0^1 \int_0^1 \left| v(0, x_2, x_3) - \int_0^1 \int_0^1 v(0, \hat{x}_2, \hat{x}_3) \, d\hat{x}_2 \, d\hat{x}_3 \right|^2 \, dx_1 \, dx_2 \, dx_3 \\
&\leq 8 \left| \frac{\partial v}{\partial x_1} \right|_{0, \hat{\mathcal{R}}}^2 + 4 \left| \frac{\partial v}{\partial x_2} \right|_{0, \hat{\mathcal{R}}}^2 + 4 \left| \frac{\partial v}{\partial x_3} \right|_{0, \hat{\mathcal{R}}}^2.
\end{align}

The inequality (3.11) for \(\hat{\mathcal{R}}\) and \(\hat{\mathcal{F}}\) now follows from the density of \(C^\infty(\hat{\mathcal{R}})\) in \(H^1(\hat{\mathcal{R}})\) and the continuous embedding \(H^1(\hat{\mathcal{R}}) \hookrightarrow L^2(\hat{\mathcal{F}})\) \([1]\).
We note that we cannot prove the inequality (3.12) for all \( v \in H^1(\mathcal{R}) \) because 
\( T^F_v(v) = v(c_F) \) is not a well-defined operator on \( H^1(\mathcal{R}) \) since \( H^1(\tilde{\mathcal{R}}) \) is not continuously embedded in \( C(\tilde{\mathcal{R}}) \) [1]. To prove the inequality (3.12) with \( \mathcal{R} \) and \( \mathcal{F} \) replaced by \( \tilde{\mathcal{R}} \) and \( \tilde{\mathcal{F}} \), respectively, for \( v_h \in P_{\tilde{\mathcal{R}}} \), the finite element polynomial space (3.1), we derive as above the identity

\[
v_h(0, x_2, x_3) - v_h(0, 1/2, 1/2) = \int_{1/2}^{x_2} \frac{\partial v_h}{\partial x_2}(x_1, \tilde{x}_2, x_3) \, d\tilde{x}_2 + \int_{1/2}^{x_3} \frac{\partial v_h}{\partial x_3}(x_1, 1/2, \tilde{x}_3) \, d\tilde{x}_3 \\
- \int_0^{x_1} \frac{\partial v_h}{\partial x_1}(\tilde{x}_1, x_2, x_3) \, d\tilde{x}_1 + \int_0^{x_1} \frac{\partial v_h}{\partial x_1}(\tilde{x}_1, 1/2, 1/2) \, d\tilde{x}_1.
\]

(3.17)

Since by Lemma 3.1, \( \partial v_h/\partial x_k \in \text{span} \{1, x_k\} \), for \( k = 1, 2, 3 \), we have from (3.17) that

\[
v_h(0, x_2, x_3) - v_h(0, 1/2, 1/2) = \int_{1/2}^{x_2} \frac{\partial v_h}{\partial x_2}(x_1, \tilde{x}_2, x_3) \, d\tilde{x}_2 + \int_{1/2}^{x_3} \frac{\partial v_h}{\partial x_3}(x_1, x_2, \tilde{x}_3) \, d\tilde{x}_3 \\
- \int_0^{x_1} \frac{\partial v_h}{\partial x_1}(\tilde{x}_1, x_2, x_3) \, d\tilde{x}_1 + \int_0^{x_1} \frac{\partial v_h}{\partial x_1}(\tilde{x}_1, 1/2, 1/2) \, d\tilde{x}_1.
\]

(3.18)

We can then obtain by squaring both sides of (3.18), integrating with respect to \( (x_1, x_2, x_3) \) over the domain \((0,1) \times (0,1) \times (0,1)\), and using the Cauchy-Schwarz inequality that

\[
\int_0^1 \int_0^1 |v_h(0, x_2, x_3) - v_h(0, 1/2, 1/2)|^2 \, dx_2 \, dx_3 \leq 8 \left( \frac{\left| \frac{\partial v_h}{\partial x_1} \right|^2}{0, \tilde{\mathcal{R}}} + 4 \left| \frac{\partial v_h}{\partial x_2} \right|^2 0, \tilde{\mathcal{R}} + 4 \left| \frac{\partial v_h}{\partial x_3} \right|^2 0, \tilde{\mathcal{R}} \right).
\]

(3.19)

\[\square\]

Lemma 3.4. We have

\[
\|\nabla I_h v\|_{0, \infty, h} \leq C\|\nabla v\|_{0, \infty, \Omega}, \quad \forall v \in W^{1, \infty}(\Omega).
\]

(3.20)

Proof. The proof easily follows from the quasi-uniformity of the partition \( \tau_h \) [10].

\[\square\]
4. Properties of Nonconforming Finite Element Deformations

In this section, we will give some further properties of the considered nonconforming finite element deformations. We first prove a discrete version of a slight variation of the divergence theorem.

**Theorem 4.1.** We have for any \( y_h \in A_h = A^p_h \cup A^q_h \) that

\[
\sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \nabla y_h(x) \, dx = \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} F_\lambda \, dx.
\]

**Proof.** Applying the divergence theorem to each integral on \( \mathcal{R} \in \tau_h \) in the summation and noticing the cancellation of contributions from adjacent elements to their common faces, we see by the definition of \( A^p_h \) that (4.1) holds if \( y_h \in A^q_h \).

For \( y_h \in A^p_h \), we set \( z_h(x) = y_h(x) - F_\lambda x, \, x \in \Omega \). We also denote by \( c_\mathcal{F} \) the center of a face \( \mathcal{F} \) of an element in \( \tau_h \). Thus, by the definition of \( A^p_h \), we have \( z_h(c_\mathcal{F}) = 0 \) if \( \mathcal{F} \subset \partial \Omega \). Moreover, we have

\[
\sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \nabla z_h(x) \, dx = \sum_{\mathcal{R} \in \tau_h} \int_{\partial \mathcal{R}} z_h(x) \otimes \nu \, dS
\]

\[
= \sum_{\mathcal{R} \in \tau_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} [z_h(x) - z_h(c_\mathcal{F})] \otimes \nu|_\mathcal{F} \, dS,
\]

where \( \nu \) is the unit exterior normal to the underlying boundary.

Fix \( \mathcal{R} = [\alpha_1 - l_1, \alpha_1 + l_1] \times [\alpha_2 - l_2, \alpha_2 + l_2] \times [\alpha_3 - l_3, \alpha_3 + l_3] \in \tau_h \). Set \( \mathcal{F}_\pm = [\alpha_1 - l_1, \alpha_1 + l_1] \times [\alpha_2 - l_2, \alpha_2 + l_2] \times \{\alpha_3 \pm l_3\} \). It follows from (3.6) that

\[
z_h(x_1, x_2, \alpha_3 + l_3) - z_h(\alpha_1, \alpha_2, \alpha_3 + l_3) = z_h(x_1, x_2, \alpha_3 - l_3) - z_h(\alpha_1, \alpha_2, \alpha_3 - l_3).
\]

Noting that \( \nu|_{\mathcal{F}_+} = -\nu|_{\mathcal{F}_-} = e_3 \), we then have

\[
\int_{\mathcal{F}_+} [z_h(x) - z_h(c_\mathcal{F}_+)] \otimes \nu|_{\mathcal{F}_+} \, dS + \int_{\mathcal{F}_-} [z_h(x) - z_h(c_\mathcal{F}_-)] \otimes \nu|_{\mathcal{F}_-} \, dS
\]

\[
= \left[ \int_{\alpha_1 - l_1}^{\alpha_1 + l_1} \int_{\alpha_2 - l_2}^{\alpha_2 + l_2} \{[z_h(x_1, x_2, \alpha_3 + l_3) - z_h(\alpha_1, \alpha_2, \alpha_3 + l_3)]
\]

\[
- [z_h(x_1, x_2, \alpha_3 - l_3) - z_h(\alpha_1, \alpha_2, \alpha_3 - l_3)] \right] \, dx_1 \, dx_2 \otimes e_3
\]

\[
= 0.
\]

The same argument applies to any other pair of faces \( \mathcal{F}_\pm \subset \partial \mathcal{R} \). Therefore,

\[
\sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} [z_h(x) - z_h(c_\mathcal{F})] \otimes \nu|_{\mathcal{F}} \, dS = 0.
\]
The arbitrariness of $\mathcal{R} \in \tau_h$ then implies that the sum in (4.2) is zero. This proves (4.1) for $y_h \in \mathcal{A}_h^a$ as well. \hfill \Box

We now prove a Poincaré type inequality for all of the finite element deformations in $\mathcal{A}_h$. This result is more general than that proven in [24].

**Theorem 4.2.** There exists a constant $C > 0$ such that for all $w \in \mathbb{R}^3$ with $|w| = 1$ and all $y_h \in \mathcal{A}_h$,

\[
\int_{\Omega} |y_h(x) - F_\lambda x|^2 \, dx \\
\leq C \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \{ |[\nabla y_h(x) - F_\lambda] \, w|^2 + h \| \nabla y_h(x) - F_\lambda \|^2 \} \, dx.
\]

**Proof.** Fix an arbitrary $w \in \mathbb{R}^3$ with $|w| = 1$. For $y_h \in \mathcal{A}_h$, set again $z_h(x) = y_h(x) - F_\lambda x$, $x \in \Omega$. By integration by parts we obtain [44]

\[
\int_{\Omega} |z_h(x)|^2 \, dx = \sum_{\mathcal{R} \in \tau_h} \int_{\partial \mathcal{R}} |z_h(x)|^2 (w \cdot x) (w \cdot \nu) \, dS \\
- \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} (\nabla |z_h(x)|^2 \cdot w) (w \cdot x) \, dx \\
\equiv I_1 + I_2.
\]  

We estimate the second term $I_2$ by the Cauchy-Schwarz inequality to get

\[
|I_2| \leq \left| \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \left( \nabla |z_h(x)|^2 \cdot w \right) (w \cdot x) \, dx \right| \\
\leq 2 \max_{x \in \Omega} |w \cdot x| \left( \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} |\nabla z_h(x)w|^2 \, dx \right)^{\frac{1}{2}} \left( \int_{\Omega} |z_h(x)|^2 \, dx \right)^{\frac{1}{2}} \\
\leq \frac{1}{2} \int_{\Omega} |z_h(x)|^2 \, dx + C \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} |\nabla z_h(x)w|^2 \, dx.
\]

To estimate $I_1$, we first consider the $\mathcal{A}_h$-approximation. So, we fix $y_h \in \mathcal{A}_h^a$. Observing that $T_\mathcal{F}^a(y_h) = 0$ for any element face $\mathcal{F} \subset \partial \Omega$, we obtain by the definition of $\mathcal{A}_h^a$ that

\[
I_1 = \sum_{\mathcal{R} \in \tau_h} \int_{\partial \mathcal{R}} |z_h(x)|^2 (w \cdot x) (w \cdot \nu) \, dS
\]
\[\begin{align*}
&= \sum_{R \in \tau_h} \sum_{\mathcal{F} \subset \partial R} \int_{\mathcal{F}} \left| z_h(x) - T^a_{\mathcal{F}}(z_h) \right|^2 (\nu \cdot x)(\nu \cdot \nu|_{\mathcal{F}}) \, dS \\
&= \sum_{R \in \tau_h} \sum_{\mathcal{F} \subset \partial R} \int_{\mathcal{F}} \left| z_h(x) - T^a_{\mathcal{F}}(z_h) \right|^2 (\nu \cdot x)(\nu \cdot \nu|_{\mathcal{F}}) \, dS \\
&\quad + \sum_{R \in \tau_h} \sum_{\mathcal{F} \subset \partial R} \int_{\mathcal{F}} \left| T^a_{\mathcal{F}}(z_h) \right|^2 (\nu \cdot x)(\nu \cdot \nu|_{\mathcal{F}}) \, dS \\
&\quad + \sum_{R \in \tau_h} \sum_{\mathcal{F} \subset \partial R} \int_{\mathcal{F}} 2T^a_{\mathcal{F}}(z_h) \cdot [z_h(x) - T^a_{\mathcal{F}}(z_h)] (\nu \cdot x)(\nu \cdot \nu|_{\mathcal{F}}) \, dS \\
&= \sum_{R \in \tau_h} \sum_{\mathcal{F} \subset \partial R} \int_{\mathcal{F}} \left| z_h(x) - T^a_{\mathcal{F}}(z_h) \right|^2 (\nu \cdot x)(\nu \cdot \nu|_{\mathcal{F}}) \, dS \\
&\quad + 2 \sum_{R \in \tau_h} \sum_{\mathcal{F} \subset \partial R} \int_{\mathcal{F}} T^a_{\mathcal{F}}(z_h) \cdot [z_h(x) - T^a_{\mathcal{F}}(z_h)] (\nu \cdot x)(\nu \cdot \nu|_{\mathcal{F}}) \, dS \\
&\equiv J^a_1 + 2J^a_2,
\end{align*}\]

where we combined adjacent elements and canceled their contributions to the common face to obtain that one summed term is equal to zero. It follows directly from (3.11) that

\[|J^a_1| \leq \left| \sum_{R \in \tau_h} \sum_{\mathcal{F} \subset \partial R} \int_{\mathcal{F}} \left| z_h(x) - T^a_{\mathcal{F}}(z_h) \right|^2 (\nu \cdot x)(\nu \cdot \nu|_{\mathcal{F}}) \, dS \right| \leq C h \| \nabla z_h \|_{0, \mathcal{R}}.\]

Setting \( g_\nu(x) = (\nu \cdot x)(\nu \cdot \nu) \), we have

\[J^a_2 \equiv \sum_{R \in \tau_h} \sum_{\mathcal{F} \subset \partial R} \int_{\mathcal{F}} T^a_{\mathcal{F}}(z_h) \cdot [z_h(x) - T^a_{\mathcal{F}}(z_h)] g_\nu(x) \, dS \]

\[= \sum_{R \in \tau_h} \sum_{\mathcal{F} \subset \partial R} \int_{\mathcal{F}} T^a_{\mathcal{F}}(z_h) \cdot [z_h(x) - T^a_{\mathcal{F}}(z_h)] [g_\nu(x) - T^a_{\mathcal{F}}(g_\nu)] \, dS.\]

For a fixed face \( \mathcal{F} \subset \partial R \) of some element \( R \in \tau_h \), we have by the inverse estimate (3.9) that

\[|T^a_{\mathcal{F}}(z_h)| \leq \| z_h \|_{0, \infty, \mathcal{R}} \leq C h^{-\frac{3}{2}} \| z_h \|_{0, \mathcal{R}}.\]

We also have by (3.11) that

\[\int_{\mathcal{F}} \left| z_h(x) - T^a_{\mathcal{F}}(z_h) \right|^2 \, dS \leq C h \| \nabla z_h \|_{0, \mathcal{R}}^2.\]
and

\[ \int_{\mathcal{F}} |g_\nu(x) - T_\mathcal{F}^\nu(g_\nu)|^2 \, dS \leq Ch \|
abla g_\nu\|_{0,\mathcal{R}}^2 \leq Ch^4. \]

Consequently,

\[
|J_2^p| \leq \sum_{\mathcal{R} \in \tau_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} |T_\mathcal{F}^p(z_h)| \left( \int_{\mathcal{F}} |z_h(x) - T_\mathcal{F}^p(z_h)|^2 \, dS \right)^{1/2} \left( \int_{\mathcal{F}} |g_\nu(x) - T_\mathcal{F}^\nu(g_\nu)|^2 \, dS \right)^{1/2} \leq Ch \sum_{\mathcal{R} \in \tau_h} \|z_h\|_{0,\mathcal{R}} \|\nabla z_h\|_{0,\mathcal{R}} \leq Ch \|z_h\|_{0,\Omega} \|\nabla z_h\|_{0,\Omega} \leq \frac{1}{8} \|z_h\|_{0,\Omega}^2 + Ch^2 \|\nabla z_h\|_{0,\Omega}^2.
\]

(4.11)

Now we consider the \( \mathcal{A}_h^p \)-approximation. Fix \( y_h \in \mathcal{A}_h^p \). We have as above that \( T_\mathcal{F}^p(z_h) = 0 \) for any element face \( \mathcal{F} \subset \partial \Omega \), so (cf. (4.8))

\[
I_1 \equiv \sum_{\mathcal{R} \in \tau_h} \int_{\partial \mathcal{R}} |z_h(x) - T_\mathcal{F}^p(z_h)|^2 (w \cdot x)(w \cdot \nu) \, dS
\]

(4.12)

\[ + 2 \sum_{\mathcal{R} \in \tau_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} T_\mathcal{F}^p(z_h) \cdot [z_h(x) - T_\mathcal{F}^p(z_h)] (w \cdot x)(w \cdot \nu) \, dS \equiv J_1^p + 2J_2^p. \]

It similarly follows from (3.12) that

\[
|J_1^p| \equiv \left| \sum_{\mathcal{R} \in \tau_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} |z_h(x) - T_\mathcal{F}^p(z_h)|^2 (w \cdot x)(w \cdot \nu) \, dS \right| \leq Ch \|\nabla z_h\|_{0,\Omega}^2.
\]

(4.13)

Let us fix again \( \mathcal{R} = [\alpha_1 - l_1, \alpha_1 + l_1] \times [\alpha_2 - l_2, \alpha_2 + l_2] \times [\alpha_3 - l_3, \alpha_3 + l_3] \in \tau_h \) and a pair of its faces \( \mathcal{F}_\pm = [\alpha_1 - l_1, \alpha_1 + l_1] \times [\alpha_2 - l_2, \alpha_2 + l_2] \times \{\alpha_3 \pm l_3\} \). We have that \( g_\nu(x) = \pm g(x) \) on \( \mathcal{F}_\pm \), where \( g(x) = (w \cdot e_3)(w \cdot x) \). We also have by (3.6) that

\[ z_h(x_1, x_2, \alpha_3 + l_3) - z_h(\alpha_1, \alpha_2, \alpha_3 + l_3) = z_h(x_1, x_2, \alpha_3 - l_3) - z_h(\alpha_1, \alpha_2, \alpha_3 - l_3). \]

It then follows from the above identity, the inverse inequality (3.9), and (3.12) that

\[ \left| \int_{\mathcal{F}_+} z_h(c_{\mathcal{F}_+}) \cdot [z_h(x) - z_h(c_{\mathcal{F}_+})] g(x) \, dS \right| \]
\begin{align*}
- \int_{\mathcal{F}_-} z_h(c_{\mathcal{F}_-}) \cdot [z_h(x) - z_h(c_{\mathcal{F}_-})] g(x) \, dS \\
= & \left| \int_{\alpha_1 - l_1}^{\alpha_1 + l_1} \int_{\alpha_2 - l_2}^{\alpha_2 + l_2} [z_h(x_1, x_2, \alpha_3 + l_3) - z_h(\alpha_1, \alpha_2, \alpha_3 + l_3)] \\
& \cdot [g(x_1, x_2, \alpha_3 + l_3) z_h(\alpha_1, \alpha_2, \alpha_3 + l_3) \\
& - g(x_1, x_2, \alpha_3 - l_3) z_h(\alpha_1, \alpha_2, \alpha_3 - l_3)] \, dx_1 \, dx_2 \right| \\
\leq & \int_{\alpha_3 - l_3}^{\alpha_3 + l_3} \frac{\partial}{\partial x_3} (g(x) z_h(\alpha_1, \alpha_2, x_3)) \, dx_3 \right| \, dx_1 \, dx_2 \\
\leq & C h \| z_h \|_{1, \infty, \mathcal{R}} \int_{\mathcal{F}_+} \left| z_h(x) - z_h(c_{\mathcal{F}_+}) \right| \, dS \\
\leq & C h^2 \| z_h \|_{1, \infty, \mathcal{R}} \left( \int_{\mathcal{F}_+} \left| z_h(x) - z_h(c_{\mathcal{F}_+}) \right|^2 \, dS \right)^{\frac{1}{2}} \\
\leq & C h \left( \| z_h \|_{0, \mathcal{R}} \| \nabla z_h \|_{0, \mathcal{R}} + \| \nabla z_h \|_{0, \mathcal{R}}^2 \right).
\end{align*}

This argument also applies to other pairs of faces of \( \mathcal{R} \in \tau_h \). Hence, we can also conclude in this case that

\begin{equation}
| J_{\mathcal{F}}^P | \leq C h \| z_h \|_{0, \Omega} \| \nabla z_h \|_{0, h} + C h \| \nabla z_h \|_{0, h}^2
\end{equation}

The assertion of the theorem now follows from (4.6) – (4.15). \( \square \)

A local trace inequality was used in [21] to derive estimates for a nonconforming finite element approximation of a variational problem. But even an improved version of such a local result (cf. Lemma 3.4 in [24]) cannot be applied here to our situation. We thus give a global version of a discrete trace theorem for our finite element deformations.

**Theorem 4.3.** There exists a constant \( C > 0 \) such that for any rectangular parallelepiped \( \omega \subset \Omega \) which is a union of elements \( \mathcal{R} \) of a rectangular mesh \( \tau_h \),

\[
\sum_{\mathcal{R} \cap \partial \omega \neq \emptyset} \sum_{\mathcal{F} \in \partial \mathcal{R} \cap \partial \omega} h^2 | y_h(c_{\mathcal{F}}) - F_{\lambda} c_{\mathcal{F}} |^2 \leq \frac{C}{\Lambda(\omega)} \int_{\omega} | y_h(x) - F_{\lambda} x |^2 \, dx
\]
\begin{align}
(4.16) \quad &+ C \left( \int_\omega |y_h(x) - F_\lambda x|^2 \, dx \right)^{\frac{1}{2}} \left( \sum_{R \subset \omega} \int_R \| \nabla y_h(x) - F_\lambda \|^2 \, dx \right)^{\frac{1}{2}} \\
&\text{for all } y_h \in A_h^p, \text{ and} \\
&\sum_{R \subset \omega} \sum_{\mathcal{F} \subset \partial R \cap \partial \omega} \int_{\mathcal{F}} |y_h(x) - F_\lambda x|^2 \, dS \\
(4.17) \quad &\leq \frac{C}{\Lambda(\omega)} \int_\omega |y_h(x) - F_\lambda x|^2 \, dx + C h \sum_{R \subset \omega} \int_R \| \nabla y_h(x) - F_\lambda \|^2 \, dx \\
&+ C \left( \int_\omega |y_h(x) - F_\lambda x|^2 \, dx \right)^{\frac{1}{2}} \left( \sum_{R \subset \omega} \int_R \| \nabla y_h(x) - F_\lambda \|^2 \, dx \right)^{\frac{1}{2}} \\
&\text{for all } y_h \in A_h^p, \text{ where } \Lambda(\omega) \text{ is the length of the shortest edge of } \omega.
\end{align}

Proof. Assume that \( \omega = [\omega_1^-, \omega_1^+] \times [\omega_2^-, \omega_2^+] \times [\omega_3^-, \omega_3^+] \). Fix \( y_h \in A_h \) and set \( z_h(x) = y_h(x) - F_\lambda x, x \in \Omega \). Also, fix an arbitrary element face \( \mathcal{F}_0 \subset \partial \omega \) of an element \( R \subset \omega \). Assume without loss of generality that the corresponding unit exterior normal at \( \mathcal{F}_0 \) with respect to \( \partial \omega \) is \( \nu = \nu|_{\mathcal{F}_0} = -e_1 \). Denote by

\( \mathcal{S}_0 = \{ x + y : x \in \mathcal{F}_0 \text{ and } y = se_1 \text{ where } s \in [0, \omega_1^+ - \omega_1^-] \} \subset \omega \)

the cylinder composed of elements of \( \tau_h \) with generating line parallel to \( e_1 \), one base \( \mathcal{F}_0 \subset \omega \), and the other base also on \( \partial \omega \). We denote the corresponding height (the length of the generating line segment) of the cylinder \( \mathcal{S}_0 \) by \( \Lambda_1 = \omega_1^+ - \omega_1^- \). Notice that \( \Lambda_1 \) is in fact the length of one edge of the rectangular parallelepiped \( \omega \). Suppose further that the element faces which are in the cylinder \( \mathcal{S}_0 \) and are parallel to \( \mathcal{F}_0 \) are given by \( \mathcal{F}_i, \, i = 0, \cdots, k \), and that these faces lie respectively in the planes \( x_1 = \alpha_{1}^{(i)} \), for some \( \alpha_1^{-} = \alpha_{1}^{(0)} < \cdots < \alpha_{1}^{(k)} = \omega_1^+ \).

Case 1: \( y_h \in A_h^p \). Denoting by \( c_{\mathcal{F}_i} \) the center of the face \( \mathcal{F}_i \) for \( i = 0, \cdots, k \), we have by the fact \( \Lambda_1 = \alpha_{1}^{(k)} - \alpha_{1}^{(0)} \) that

\begin{align}
(4.18) \quad &\sum_{i=0}^{k-1} \left[ \left( \alpha_{1}^{(k)} - \alpha_{1}^{(i+1)} \right) |z_h(c_{\mathcal{F}_{i+1}})|^2 - \left( \alpha_{1}^{(k)} - \alpha_{1}^{(i)} \right) |z_h(c_{\mathcal{F}_i})|^2 \right] \\
&= -\Lambda_1 |z_h(c_{\mathcal{F}_0})|^2.
\end{align}

If \( 0 \leq i \leq k - 1 \), then

\[ \left| \left( \alpha_{1}^{(k)} - \alpha_{1}^{(i+1)} \right) |z_h(c_{\mathcal{F}_{i+1}})|^2 - \left( \alpha_{1}^{(k)} - \alpha_{1}^{(i)} \right) |z_h(c_{\mathcal{F}_i})|^2 \right| \]
\[ = \left| (\alpha^{(k)}_1 - \alpha^{(i)}_1) \left[ |z_h(c_{F_{i+1}})|^2 - |z_h(c_{F_i})|^2 \right] + (\alpha^{(i)}_1 - \alpha^{(i+1)}_1) |z_h(c_{F_{i+1}})|^2 \right| \]
\[ \leq \Lambda_1 \left[ |z_h(c_{F_{i+1}}) - z_h(c_{F_i})| \cdot |z_h(c_{F_{i+1}}) + z_h(c_{F_i})| + h |z_h(c_{F_{i+1}})|^2 \right]. \]

This, together with (4.18) and the inverse inequality (3.9), leads to
\[ h^2 |z_h(c_{F_0})|^2 \leq h^3 \sum_{\mathcal{R} \in \mathcal{S}_0} \left[ ||\nabla z_h||_{0,\infty,\mathcal{R}} ||z_h||_{0,\infty,\mathcal{R}} + \frac{1}{\Lambda_1} ||z_h||_{0,\infty,\mathcal{R}}^2 \right] \]
\[ \leq C \sum_{\mathcal{R} \in \mathcal{S}_0} \left[ ||\nabla z_h||_{0,\mathcal{R}} ||z_h||_{0,\mathcal{R}} + \frac{1}{\Lambda(\omega)} ||z_h||_{0,\mathcal{R}}^2 \right]. \] (4.19)

Case 2: \( y_h \in \mathcal{A}_h^a \). Noting that \( \alpha^{(k)}_1 - \alpha^{(0)}_1 = \Lambda_1 \), we have
\[ \sum_{\mathcal{R} \in \mathcal{S}_0} \int_{\mathcal{R}} \frac{\partial}{\partial x_1} \left[ (\alpha^{(k)}_1 - x_1) |z_h(x)|^2 \right] dx \]
\[ = \sum_{\mathcal{R} \in \mathcal{S}_0} \int_{\partial \mathcal{R}} (\alpha^{(k)}_1 - x_1) |z_h(x)|^2 (\nu \cdot e_1) dS \]
\[ = -\Lambda_1 \int_{\mathcal{F}_0} |z_h(x)|^2 dS + \sum_{i=1}^{k-1} \left( \alpha^{(k)}_1 - \alpha^{(i)}_1 \right) \int_{\mathcal{F}_i} \left[ |z_h^+(x)|^2 - |z_h^-(x)|^2 \right] dS, \]
where for a fixed face \( \mathcal{F}_i \), \( 1 \leq i \leq k - 1 \), we denote by \( z_h^\pm \) the restriction of \( z_h \) to \( \mathcal{F}_i \) for \( z_h \) defined on the adjacent element sharing the common face \( \mathcal{F}_i \) such that the corresponding unit exterior normal of the element boundary \( \nu \) satisfies \( \nu|_{\mathcal{F}_i} = \pm e_1 \). Consequently, we have that
\[ \int_{\mathcal{F}_0} |z_h(x)|^2 dS \]
\[ \leq \sum_{\mathcal{R} \in \mathcal{S}_0} \int_{\mathcal{R}} \left[ \frac{1}{\Lambda_1} |z_h(x)|^2 + 2|z_h(x)||\nabla z_h(x)|| \right] dx \]
\[ + \sum_{i=1}^{k-1} \left| \int_{\mathcal{F}_i} \left[ |z_h^+(x)|^2 - |z_h^-(x)|^2 \right] dS \right| \]
\[ = \sum_{\mathcal{R} \in \mathcal{S}_0} \left( \frac{1}{\Lambda_1} ||z_h||_{0,\mathcal{R}}^2 + 2 ||z_h||_{0,\mathcal{R}} ||\nabla z_h||_{0,\mathcal{R}} \right) \]
\[ + \sum_{i=1}^{k-1} \left| \int_{\mathcal{F}_i} \left[ |z_h^+(x)| - T_{\mathcal{F}_i}^a(z_h) + T_{\mathcal{F}_i}^a(z_h) \right]^2 \right|^2 \] (4.20)
- \left| z^-_h(x) - T^a_{\mathcal{F}_i}(z_h) + T^a_{\mathcal{F}_i}(z_h) \right|^2 dS \right| \\
= \sum_{\mathcal{R} \subseteq \mathcal{S}_0} \left( \frac{1}{\Lambda_1} \| z_h \|_{0, \mathcal{R}}^2 + 2 \| z_h \|_{0, \mathcal{R}} \| \nabla z_h \|_{0, \mathcal{R}}^2 \right) \\
+ \sum_{i=1}^{k-1} \left| \int_{\mathcal{F}_i} \left[ \left| z^+_h(x) - T^a_{\mathcal{F}_i}(z_h) \right|^2 - \left| z^-_h(x) - T^a_{\mathcal{F}_i}(z_h) \right|^2 \right] dS \right| \\
\leq C \sum_{\mathcal{R} \subseteq \mathcal{S}_0} \left[ \frac{1}{\Lambda(\omega)} \| z_h \|_{0, \mathcal{R}}^2 + \| z_h \|_{0, \mathcal{R}} \| \nabla z_h \|_{0, \mathcal{R}} + h \| \nabla z_h \|_{0, \mathcal{R}}^2 \right],

where in the last step we used (3.12).

Since every such cylinder \( \mathcal{S}_0 \subset \omega \) will only be used twice corresponding to its two bases on \( \partial \omega \), we therefore obtain (4.16) and (4.17) from (4.19) and (4.20), respectively, by summing over all boundary faces \( \mathcal{F}_0 \subset \partial \omega \) of elements \( \mathcal{R} \subset \omega \) such that \( \partial \mathcal{R} \cap \partial \omega \neq \emptyset \). \( \square \)

**Remark 4.1.** We can generalize the above theorem to cover more general closed subdomains \( \omega \subset \hat{\Omega} \) which are still unions of rectangular elements of \( \tau_h \). For such an \( \omega \) we denote by \( \Lambda(\omega) \) the smallest height of all cylinders \( \mathcal{S}_0 \subset \omega \) composed of elements of \( \tau_h \) which have generating lines parallel to the coordinate axes and for which both bases lie in the boundary \( \partial \omega \). Both of the inequalities (4.16) and (4.17) remain valid.

5. **Approximation of Limiting Macroscopic Deformations**

We define

\[ \mathcal{E}_h(y_h) = \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \phi(\nabla y_h(x)) \, dx, \quad \forall y_h \in \mathcal{A}_h. \]

The following result which will be frequently used is a direct consequence of the quadratic growth rate of the energy density around the energy wells (2.2).

**Lemma 5.1.** We have

\[ \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \| \nabla y_h(x) - \pi(\nabla y_h(x)) \|^2 dx \leq \kappa^{-1} \mathcal{E}_h(y_h), \quad \forall y_h \in \mathcal{A}_h. \]

In the following lemma, we recall that we have assumed that

\[ F_1 = F_0 + a \otimes n, \]

\[ (5.1) \]
and that we have assumed without loss of generality in the cubic to tetragonal case by Lemma 2.1 that

\begin{equation}
(5.2) \quad n = \frac{1}{\sqrt{2}}(e_1 + e_2).
\end{equation}

**Lemma 5.2.** For any \( w \in \mathbb{R}^3 \) satisfying \( w \cdot n = 0 \), there exists a constant \( C > 0 \) such that

\begin{equation}
(5.3) \quad \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \left| \left[ \pi(\nabla y_h(x)) - F_\lambda \right] w \right|^2 dx \leq C \mathcal{E}_h(y_h)^{\frac{1}{2}}, \quad \forall y_h \in \mathcal{A}_h.
\end{equation}

**Proof.** We first consider the orthorhombic to monoclinic transformation. In this case we have

\( \pi(F) \in \text{SO}(3)F_0 \cup \text{SO}(3)F_1, \quad \forall F \in \mathbb{R}^{3 \times 3}. \)

Consequently, we have by the rank-one connection (5.1) and by the identity

\( F_\lambda = (1 - \lambda)F_0 + \lambda F_1 = F_0 + \lambda a \otimes n \)

that

\begin{equation}
(5.4) \quad |\pi(F)w| = |F_0w| = |F_1w| = |F_\lambda w|, \quad \forall F \in \mathbb{R}^{3 \times 3},
\end{equation}

for any \( w \in \mathbb{R}^3 \) such that \( w \cdot n = 0 \). It then follows from Theorem 4.1, the Cauchy-Schwarz inequality, and the identity (5.4) that for any \( y_h \in \mathcal{A}_h \),

\begin{align*}
\sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \left| \left[ \pi(\nabla y_h(x)) - F_\lambda \right] w \right|^2 dx &= 2F_\lambda w \cdot \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \left[ F_\lambda - \pi(\nabla y_h(x)) \right] w \, dx \\
&\leq C \left[ \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \left\| \nabla y_h(x) - \pi(\nabla y_h(x)) \right\|^2 \, dx \right]^\frac{1}{2} \\
&\leq C \mathcal{E}_h(y_h)^{\frac{1}{2}},
\end{align*}

which implies (5.3) for the orthorhombic to monoclinic transformation.

Now we consider the cubic to tetragonal transformation. Set

\( w_1 = e_1 - e_2 + e_3 \quad \text{and} \quad w_2 = e_1 - e_2 - e_3. \)

It is easy to check that

\( w_1 \cdot n = w_2 \cdot n = 0, \)
and

\[ |U_i w_j| = \sqrt{2\eta_i^2 + \eta_2^2}, \quad i = 1, 2, 3, \quad j = 1, 2. \]

Consequently, we can obtain (5.4) and hence (5.5) again for \( w = w_1 \) and \( w = w_2 \), respectively. Thus, (5.3) is also proved for the cubic to tetragonal transformation since \( \{w_1, w_2\} \) is an orthonormal basis for the two-dimensional subspace \( \{w \in \mathbb{R}^3 : w \cdot n = 0\} \).

The following theorem is a direct consequence of the above two lemmas. It gives error bounds for the approximation of directional derivatives of deformations to the limiting macroscopic deformation gradient \( F_\lambda \) in the direction tangential to the parallel layers of the laminate. It will play a key role in establishing all of the other error bounds.

**Theorem 5.1.** For any \( w \in \mathbb{R}^3 \) satisfying \( w \cdot n = 0 \), there exists a constant \( C > 0 \) such that

\[ \sum_{\mathcal{R} \in \mathcal{R}_h} \int_{\mathcal{R}} |[\nabla y_h(x) - F_\lambda w]|^2 \, dx \leq C \left[ \mathcal{E}_h(y_h)^{\frac{1}{2}} + \mathcal{E}_h(y_h) \right], \quad \forall y_h \in \mathcal{A}_h. \]

We now give error bounds for the strong \( L^2 \) approximation of deformations to the limiting macroscopic homogeneous deformation \( F_\lambda x, x \in \Omega \).

**Theorem 5.2.** There is a constant \( C > 0 \) such that

\[ \int_{\Omega} |y_h(x) - F_\lambda x|^2 \, dx \leq C \left[ \mathcal{E}_h(y_h)^{\frac{1}{2}} + \mathcal{E}_h(y_h) + h \right], \quad \forall y_h \in \mathcal{A}_h. \]

**Proof.** For any \( y_h \in \mathcal{A}_h \), we have by Lemma 5.1 that

\[
\sum_{\mathcal{R} \in \mathcal{R}_h} \int_{\mathcal{R}} ||\nabla y_h(x) - F_\lambda||^2 \, dx \\
\leq 2 \int_{\mathcal{R}} ||\nabla y_h(x) - \pi(\nabla y_h(x))||^2 \, dx + 2 \int_{\mathcal{R}} ||\pi(\nabla y_h(x)) - F_\lambda||^2 \, dx \\
\leq C \mathcal{E}_h(y_h) + C,
\]

which together with Theorem 4.2 implies the desired inequality. \qed

We now establish error bounds for the weak approximation of deformation gradients to the limiting macroscopic deformation gradient \( F_\lambda \).

**Theorem 5.3.** For any rectangular parallelepiped \( \omega \subset \Omega \) whose boundary \( \partial \omega \) is composed of faces parallel to the coordinate planes, there exists a constant \( C = C(\omega) > 0 \)
such that for all $y_h \in A_h$

\begin{equation}
\left\| \sum_{R \in \tau_h} \int_{\omega \cap R} [\nabla y_h(x) - F_\lambda] \, dx \right\| \leq C \left[ \mathcal{E}_h(y_h)^{\frac{1}{2}} + \mathcal{E}_h(y_h)^{\frac{1}{2}} + h^{\frac{1}{2}} \right].
\end{equation}

Proof. Denoting

$$\omega_h = \bigcup \{ R \in \tau_h : R \subset \omega \},$$

we have for any $y_h \in A_h$ that

\begin{align*}
\sum_{R \in \tau_h} \int_{\omega \cap R} [\nabla y_h(x) - F_\lambda] \, dx &= \sum_{R \in \tau_h, R \subset \omega_h} \int_R [\nabla y_h(x) - F_\lambda] \, dx + \sum_{R \in \tau_h} \int_{(\omega - \omega_h) \cap R} [\nabla y_h(x) - F_\lambda] \, dx \\
&\equiv K_1 + K_2.
\end{align*}

Since

$$\text{meas} (\omega - \omega_h) \leq Ch,$$

we can estimate $K_2$ by virtue of the triangle inequality, the Cauchy-Schwarz inequality, and Lemma 5.1 to get

\begin{align*}
\| K_2 \| &\equiv \left\| \sum_{R \in \tau_h} \int_{(\omega - \omega_h) \cap R} [\nabla y_h(x) - F_\lambda] \, dx \right\| \\
&\leq \left\| \sum_{R \in \tau_h} \int_{(\omega - \omega_h) \cap R} [\nabla y_h(x) - \pi(\nabla y_h(x))] \, dx \right\| \\
&\quad + \left\| \sum_{R \in \tau_h} \int_{(\omega - \omega_h) \cap R} [\pi(\nabla y_h(x)) - F_\lambda] \, dx \right\| \\
&\leq Ch^{\frac{1}{2}} \left[ \sum_{R \in \tau_h} \int_R \| \nabla y_h(x) - \pi(\nabla y_h(x)) \|^2 \, dx \right]^{\frac{1}{2}} + Ch \\
&\leq Ch^{\frac{1}{2}} \mathcal{E}_h(y_h)^{\frac{1}{2}} + Ch.
\end{align*}

To estimate $K_1$ we first assume that $y_h \in A_h^a$. It then follows from the divergence theorem and the definition of the $A_h^a$-approximation that

$$K_1 \equiv \sum_{R \in \tau_h, R \subset \omega_h} \int_R [\nabla y_h(x) - F_\lambda] \, dx$$
\[
\|K_1\| \leq \sum_{\mathcal{R} \in \mathcal{T}_h, \mathcal{R} \cap \Omega_h \neq \emptyset} \sum_{\mathcal{F} \in \partial \mathcal{R} \cap \partial \Omega_h} \int_{\mathcal{F}} |y_h(x) - F_\lambda x| \, dS \leq (\text{meas } \partial \omega_h)^{1/2} \left[ \sum_{\mathcal{R} \cap \Omega_h \neq \emptyset} \sum_{\mathcal{F} \in \partial \mathcal{R} \cap \partial \omega_h} \int_{\mathcal{F}} |y_h(x) - F_\lambda x|^2 \, dS \right]^{1/2} \leq C (\text{meas } \partial \omega)^{1/2} \left\{ \frac{1}{\Lambda(\omega_h)} \int_{\omega_h} |y_h(x) - F_\lambda x|^2 \, dx + h \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \|
abla y_h(x) - F_\lambda\|^2 \, dx \right. \\
\left. + \left( \int_{\omega_h} |y_h(x) - F_\lambda x|^2 \, dx \right)^{1/2} \left( \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \|
abla y_h(x) - F_\lambda\|^2 \, dx \right)^{1/2}\right\}^{1/2}, \\
\leq C \left\{ \frac{1}{\Lambda(\omega_h)} \int_{\Omega} |y_h(x) - F_\lambda x|^2 \, dx + h \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \|
abla y_h(x) - F_\lambda\|^2 \, dx \right. \\
\left. + \left( \int_{\Omega} |y_h(x) - F_\lambda x|^2 \, dx \right)^{1/2} \left( \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \|
abla y_h(x) - F_\lambda\|^2 \, dx \right)^{1/2}\right\}^{1/2},
\]

since \(\Lambda(\omega) \leq CA(\omega_h)\). This, together with (5.6) and Theorem (5.2), implies that

\[(5.10) \quad \|K_1\| \leq C \left[ \mathcal{E}_h(y_h)^{1/4} + \mathcal{E}_h(y_h)^{1/4} + h^{1/4} \right].
\]

Now let us assume that \(y_h \in \mathcal{A}^p_h\). By the same argument as in the proof of Theorem 4.1, cf. (4.3) and (4.4), we have

\[
K_1 \equiv \sum_{\mathcal{R} \in \mathcal{T}_h, \mathcal{R} \cap \Omega_h} \int_{\mathcal{R}} [\nabla y_h(x) - F_\lambda] \, dx = \sum_{\mathcal{R} \in \mathcal{T}_h, \mathcal{R} \cap \Omega_h} \int_{\partial \mathcal{R}} [y_h(x) - F_\lambda x] \otimes \nu \, dS.
\]
\[
\begin{align*}
= & \sum_{\mathcal{R} \in \mathcal{E}_h, \mathcal{R} \subset \omega_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} \{[y_h(x) - F_\lambda x] - [y_h(c_\mathcal{F}) - F_\lambda c_\mathcal{F}]\} \otimes \nu \, dS \\
& + \sum_{\mathcal{R} \in \mathcal{E}_h, \mathcal{R} \subset \omega_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} [y_h(c_\mathcal{F}) - F_\lambda c_\mathcal{F}] \otimes \nu \, dS \\
= & \sum_{\mathcal{R} \in \mathcal{E}_h, \mathcal{R} \subset \omega_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} [y_h(c_\mathcal{F}) - F_\lambda c_\mathcal{F}] \otimes \nu \, dS \\
= & \sum_{\mathcal{R} \subset \omega_h, \partial \mathcal{R} \cap \partial \omega_h \neq \emptyset} \sum_{\mathcal{F} \subset \partial \mathcal{R} \cap \partial \omega_h} \int_{\mathcal{F}} [y_h(c_\mathcal{F}) - F_\lambda c_\mathcal{F}] \otimes \nu \, dS.
\end{align*}
\]

Using a similar argument to that for \( y_h \in \mathcal{A}^p_h \), we can obtain (5.10) again for \( y_h \in \mathcal{A}^p_h \) by (4.16), (5.6), and Theorem 5.2.

Finally, (5.7) follows from (5.8), (5.9), and (5.10).

\[\Box\]

6. Approximation of Martensitic Variants

Let us now define the projection operator \( \pi_{12} : \mathbb{R}^{3 \times 3} \to \mathcal{U}_1 \cup \mathcal{U}_2 \) by
\[
\|F - \pi_{12}(F)\| = \min_{G \in \mathcal{U}_1 \cup \mathcal{U}_2} \|F - G\|, \quad \forall F \in \mathbb{R}^{3 \times 3}.
\]

For the orthorhombic to monoclinic transformation, we note that \( \pi_{12} = \pi \). The next lemma gives an estimate for \( \pi_{12} - \pi \) for the cubic to tetragonal transformation by showing that the measure of the set of points in which the gradient of energy minimizing sequences of deformations is near \( \mathcal{U}_3 \) converges to zero. Thus, the next lemma reduces the three-well problem for the cubic to tetragonal transformation to a two-well problem.

**Lemma 6.1.** For the cubic to tetragonal transformation, there exists a constant \( C > 0 \) such that
\[
\sum_{\mathcal{R} \in \mathcal{E}_h} \int_{\mathcal{R}} \|\pi(\nabla y_h(x)) - \pi_{12}(\nabla y_h(x))\|^2 \, dx \leq C\varepsilon_h(y_h)\frac{1}{2}, \quad \forall y \in \mathcal{A}_h.
\]

**Proof.** We have by a simple calculation that
\[
\inf_{F \in \mathcal{U}_3} |[F - F_\lambda]e_3| \geq |\eta_2 - \eta_1|.
\]

Denoting
\[
\Omega_3 = \bigcup_{\mathcal{R} \in \mathcal{E}_h} \{x \in \mathcal{R} : \pi(\nabla y_h(x)) \in \mathcal{U}_3\}
\]
for \( y_h \in \mathcal{A}_h \), we have by Lemma 5.2 that
\[
\text{meas } \Omega_3 = \sum_{\mathcal{R} \in \mathcal{T}_h} \text{meas } \{ x \in \mathcal{R} : \pi(\nabla y_h(x)) \in \mathcal{U}_3 \} \\
\leq |\eta_2 - \eta_1|^{-2} \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} |[\pi(\nabla y_h(x)) - F_\lambda]e_3|^2 \, dx \\
\leq C\mathcal{E}_h(y_h)^{\frac{1}{2}},
\]
since \( e_3 \cdot n = 0 \) (recall that \( n = 2^{-1/2}(e_1 + e_2) \)). The result (6.1) then follows from the inequality
\[
\sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \|\pi(\nabla y(x)) - \pi_{12}(\nabla y_h(x))\|^2 \, dx \\
= \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R} \cap \Omega_3} \|\pi(\nabla y(x)) - \pi_{12}(\nabla y_h(x))\|^2 \, dx \\
\leq 4(2\eta_1^2 + \eta_2^2) \text{meas } \Omega_3 \\
\leq C\mathcal{E}_h(y_h)^{\frac{1}{2}},
\]
since \( \|\pi(F)\| = \|\pi_{12}(F)\| = \sqrt{2\eta_1^2 + \eta_2^2} \) for all \( F \in \mathbb{R}^{3 \times 3} \).

We next define the operators \( \Theta : \mathbb{R}^{3 \times 3} \to \text{SO}(3) \) and \( \Pi : \mathbb{R}^{3 \times 3} \to \{F_0, F_1\} \) by the relation
\[
\pi_{12}(F) = \Theta(F)\Pi(F), \quad \forall F \in \mathbb{R}^{3 \times 3}.
\]
The following theorem gives an error bound for the convergence of deformation gradients to the set of variants \( \{F_0, F_1\} \).

**Theorem 6.1.** There exists a constant \( C > 0 \) such that
\[
\sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \|\nabla y_h(x) - \Pi(\nabla y_h(x))\|^2 \, dx \leq C \left[ \mathcal{E}_h(y_h)^{\frac{1}{2}} + \mathcal{E}_h(y_h) \right], \quad \forall y_h \in \mathcal{A}_h.
\]

**Proof.** For any \( w \in \mathbb{R}^3 \) such that \( w \cdot n = 0 \), we have
\[
\Pi(F)w = F_0w = F_1w = F_\lambda w, \quad \forall F \in \mathbb{R}^{3 \times 3}.
\]
Thus, it follows from (6.3) that
\[
[\Theta(F) - I]F_0w = [\Theta(F) - I]F_1w = [\pi_{12}(F) - F_\lambda]w \\
= [\pi_{12}(F) - \pi(F)]w + [\pi(F) - F_\lambda]w, \quad \forall F \in \mathbb{R}^{3 \times 3}.
\]
We can then apply the triangle inequality to the above identity with \( F = \nabla y_h(x), \ x \in \mathcal{R}, \) for any \( y_h \in \mathcal{A}_h \) and any element \( \mathcal{R} \in \tau_h, \) and estimate the corresponding two terms by Lemma 6.1 and Lemma 5.2 to obtain for \( w \cdot n = 0 \) that

\[
\sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \left[ |\Theta\left(\nabla y_h(x)\right) - I\right] F_0 w|^2 dx \\
\leq 2 \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \left[ |\pi_{12}(\nabla y_h(x)) - \pi(\nabla y_h(x))| w|^2 dx \\
+ 2 \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \left| \pi(\nabla y_h(x)) - F_{\lambda} \right| w|^2 dx \\
\leq C \mathcal{E}_h(y_h)^{\frac{1}{2}}.
\]

(6.4)

Choose \( w_1 \in \mathbb{R}^3 \) and \( w_2 \in \mathbb{R}^3 \) so that \( w_1 \cdot n = w_2 \cdot n = 0 \) and \( w_1, w_2 \) are linearly independent. Set \( m = F_0 w_1 \times F_0 w_2. \) Since

\[
Qm = QF_0 w_1 \times QF_0 w_2, \quad \forall Q \in \text{SO}(3),
\]

we have for all \( F \in \mathbb{R}^{3 \times 3} \) that

\[
\left[ \Theta(F) - I \right] m = \{ \Theta(F) F_0 w_1 \times \Theta(F) F_0 w_2 \} - \{ F_0 w_1 \times F_0 w_2 \} \\
= \{ \left[ \Theta(F) - I \right] F_0 w_1 \times \Theta(F) F_0 w_2 \} - \{ F_0 w_1 \times \left[ I - \Theta(F) \right] F_0 w_2 \}.
\]

This together with (6.4) implies that

\[
\sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \left[ |\Theta\left(\nabla y_h(x)\right) - I\right] m|^2 dx \leq C \mathcal{E}_h(y_h)^{\frac{1}{2}}.
\]

(6.5)

Now \( \{ F_0 w_1, F_0 w_2, m \} \) is a basis for \( \mathbb{R}^3, \) so we can conclude from (6.4) and (6.5) that for all \( y_h \in \mathcal{A}_h \)

\[
\sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} ||\Theta\left(\nabla y_h(x)\right) - I||^2 dx \leq C \left[ \mathcal{E}_h(y_h)^{\frac{1}{2}} + \mathcal{E}_h(y_h) \right].
\]

(6.6)

We complete the proof by applying the triangle inequality to the identity

\[
F - \Pi(F) = [F - \pi(F)] + [\pi(F) - \pi_{12}(F)] + [\pi_{12}(F) - \Pi(F)] \\
= [F - \pi(F)] + [\pi(F) - \pi_{12}(F)] + [\Theta(F) - I] \Pi(F), \quad \forall F \in \mathbb{R}^{3 \times 3},
\]

with \( F = \nabla y_h(x) \) for any \( y_h \in \mathcal{A}_h, \ x \in \mathcal{R}, \) and \( \mathcal{R} \in \tau_h, \) and by estimating the three terms by Lemma 5.1, Lemma 6.1, and (6.6).
7. Approximation of Simply Laminated Microstructure

For any subset $\omega \subset \Omega$, $\rho > 0$, and $y_h \in \mathcal{A}_h$, we define the sets
\[
\omega^0_{\rho}(y_h) = \bigcup_{R \in \mathcal{R}} \{ x \in \omega \cap R : \Pi(\nabla y_h(x)) = F_0 \text{ and } \|\nabla y_h(x) - F_0\| < \rho \}, \]
\[
\omega^1_{\rho}(y_h) = \bigcup_{R \in \mathcal{R}} \{ x \in \omega \cap R : \Pi(\nabla y_h(x)) = F_1 \text{ and } \|\nabla y_h(x) - F_1\| < \rho \}.
\]

The following theorem states that for any rectangular parallelepiped $\omega \subset \bar{\Omega}$ and for any energy minimizing sequence $\{y_h\}$ the volume fraction that the piecewise defined gradient $\nabla y_h$ is near $F_0$ converges to $1 - \lambda$ and the volume fraction that $\nabla y_h$ is near $F_1$ converges to $\lambda$.

\textbf{Theorem 7.1.} For any rectangular parallelepiped $\omega \subset \Omega$ whose faces are parallel to the coordinate planes, and any $\rho > 0$, there exists a constant $C = C(\omega, \rho) > 0$ such that for all $y_h \in \mathcal{A}_h$,

\[
\left| \frac{\text{meas} \omega^0_{\rho}(y_h)}{\text{meas} \omega} - (1 - \lambda) \right| + \left| \frac{\text{meas} \omega^1_{\rho}(y_h)}{\text{meas} \omega} - \lambda \right| 
\leq C \left[ \mathcal{E}_h(y_h)^{\frac{1}{2}} + \mathcal{E}_h(y_h)^{\frac{1}{3}} + h^\frac{1}{2} \right].
\]

(7.1)

\textbf{Proof.} Fix $y_h \in \mathcal{A}_h$. It follows from the definition of $\omega^0_{\rho} \equiv \omega^0_{\rho}(y_h)$ and $\omega^1_{\rho} \equiv \omega^1_{\rho}(y_h)$ that

\[
\left[ \text{meas} \omega^0_{\rho} - (1 - \lambda) \text{meas} \omega \right] F_0 + \left[ \text{meas} \omega^1_{\rho} - \lambda \text{meas} \omega \right] F_1
\]
\[
= \sum_{R \in \mathcal{R}} \int_{\omega \cap R} \left[ \Pi(\nabla y_h(x)) - F_\lambda \right] dx 
\]
\[
- \sum_{R \in \mathcal{R}} \int_{(\omega - \{\omega^0_{\rho} \cup \omega^1_{\rho}\}) \cap R} \Pi(\nabla y_h(x)) dx.
\]

(7.2)

We have by Theorem 6.1 and Theorem 5.3 that

\[
\left\| \sum_{R \in \mathcal{R}} \int_{\omega \cap R} \left[ \Pi(\nabla y_h(x)) - F_\lambda \right] dx \right\|
\]
\[
\leq \left\| \sum_{R \in \mathcal{R}} \int_{\omega \cap R} \left[ \Pi(\nabla y_h(x)) - \nabla y_h(x) \right] dx \right\| + \left\| \sum_{R \in \mathcal{R}} \int_{\omega \cap R} \left[ \nabla y_h(x) - F_\lambda \right] dx \right\|
\]
\[
(7.3)
\]
\[
\leq \left( \text{meas} \omega \right)^{\frac{1}{2}} \left[ \sum_{R \in \mathcal{R}} \int_{\mathcal{R}} \| \Pi(\nabla y_h(x)) - \nabla y_h(x) \|^2 dx \right]^{\frac{1}{2}}
\]
\[ + \left\| \sum_{R \in \tau_h} \int_{\omega \cap R} [\nabla y_h(x) - F_\lambda] \, dx \right\| \]
\[ \leq C \left[ \mathcal{E}_h(y_h)^{\frac{1}{3}} + \mathcal{E}_h(y_h)^{\frac{1}{3}} + h^{\frac{1}{3}} \right]. \]

Since \( \|\Pi(F)\| = \sqrt{2\eta_1^2 + \eta_2^2} \) for all \( F \in \mathbb{R}^{3 \times 3} \), we can conclude by the definition of \( \omega_0^0 \) and \( \omega_0^1 \) and by Theorem 6.1 that

\[ \left\| \sum_{R \in \tau_h} \int_{(\omega - (\omega_0^0 \cup \omega_0^1)) \cap R} \Pi(\nabla y_h(x)) \, dx \right\| \]
\[ \leq C \text{meas}(\omega - \{\omega_0^0 \cup \omega_0^1\}) \]
\[ \leq \frac{C}{\rho} \sum_{R \in \tau_h} \int_{(\omega - (\omega_0^0 \cup \omega_0^1)) \cap R} \|\Pi(\nabla y_h(x)) - \nabla y_h(x)\| \, dx \]
\[ \leq \frac{C(\text{meas} \omega)^{\frac{1}{2}}}{\rho} \left[ \sum_{R \in \tau_h} \int_{R} \|\Pi(\nabla y_h(x)) - \nabla y_h(x)\|^2 \, dx \right]^{\frac{1}{2}} \]
\[ \leq C \left[ \mathcal{E}_h(y_h)^{\frac{1}{4}} + \mathcal{E}_h(y_h)^{\frac{1}{2}} \right]. \]

Therefore, we have by (7.3) and (7.4) that
\[ \left\| \left[ \text{meas} \omega_0^0 - (1 - \lambda)\text{meas} \omega \right] F_0 + \left[ \text{meas} \omega_0^1 - \lambda \text{meas} \omega \right] F_1 \right\| \]
\[ \leq C \left[ \mathcal{E}_h(y_h)^{\frac{1}{4}} + \mathcal{E}_h(y_h)^{\frac{1}{2}} + h^{\frac{1}{4}} \right], \]

which implies (7.1) because \( F_0 \) and \( F_1 \) are linearly independent. \( \Box \)

We now denote by \( V \) the Sobolev space of all measurable functions \( f(x, F) : \Omega \times \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R} \) such that
\[ \|f\|_{V}^2 = \int_{\Omega} \left[ \text{ess} \sup_{F \in \mathbb{R}^{3 \times 3}} \|\nabla_{F} f(x, F)\| \right]^2 \, dx + \|G_f\|_{1, \Omega}^2 < \infty, \]
where
\[ G_f(x) = f(x, F_1) - f(x, F_0), \quad x \in \Omega. \]

The following theorem gives error bounds for the approximation of nonlinear integrals of deformation gradients which represent macroscopic thermodynamic densities.

**Theorem 7.2.** There exists a constant \( C > 0 \) such that
\[ \left\| \sum_{R \in \tau_h} \int_{R} \left\{ f((x, \nabla y_h(x)) - [(1 - \lambda)f(x, F_0) + \lambda f(x, F_1))] \right\} \, dx \right\| \]}
\[ \leq C \| \mathcal{E}_{\mathcal{H}}(y_h) + \mathcal{E}_{\mathcal{H}}(y_h) + h^\frac{1}{2} \|_V, \quad \forall f \in V, \forall y_h \in \mathcal{A}_h. \]

**Proof.** We have
\[
\sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \{ f((x, \nabla y_h(x)) - (1 - \lambda)f(x, F_0) + \lambda f(x, F_1)) \} \, dx
\]
\[
= \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} [f(x, \nabla y_h(x)) - f(x, \Pi(\nabla y_h(x)))] \, dx
\]
\[
+ \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \{ f(x, \Pi(\nabla y_h(x))) - [(1 - \lambda)f(x, F_0) + \lambda f(x, F_1)] \} \, dx
\]
\[
= M_1 + M_2.
\]

The first term \(M_1\) can be easily estimated by the Cauchy-Schwarz inequality and Theorem 6.1 to give
\[
|M_1| \leq \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \left[ \text{ess sup}_{F \in \mathbb{R}^{3 \times 3}} \| \nabla f(x, F) \| \right] \| \nabla y_h(x) - \Pi(\nabla y_h(x)) \| \, dx
\]
\[
\leq \left\{ \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \left[ \text{ess sup}_{F \in \mathbb{R}^{3 \times 3}} \| \nabla f(x, F) \|^2 \right] \right\}^{\frac{1}{2}}
\]
\[
\cdot \left\{ \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \| \nabla y_h(x) - \Pi(\nabla y_h(x)) \|^2 \, dx \right\}^{\frac{1}{2}}
\]
\[
\leq C \| f \|_V \left[ \mathcal{E}_{\mathcal{H}}(y_h)^{\frac{1}{2}} + \mathcal{E}_{\mathcal{H}}(y_h)^{\frac{1}{2}} \right].
\]

To estimate the second term \(M_2\), we use the identity
\[
f(x, \Pi(F)) - [(1 - \lambda)f(x, F_0) + \lambda f(x, F_1)]
\]
\[
= \frac{1}{|a|^2} \{ a \cdot [\Pi(F) - F_a] \} G_f(x), \quad \forall F \in \mathbb{R}^{3 \times 3},
\]
to show that
\[
M_2 = \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \{ f(x, \Pi(\nabla y_h(x))) - [(1 - \lambda)f(x, F_0) + \lambda f(x, F_1)] \} \, dx
\]
\[
= \sum_{\mathcal{R} \in \mathcal{T}_h} \int_{\mathcal{R}} \frac{1}{|a|^2} \{ a \cdot [\Pi(\nabla y_h(x)) - \nabla y_h(x)] \} \, G_f(x) \, dx
\]
NONCONFORMING APPROXIMATION OF MICROSTRUCTURE

\[ + \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \frac{1}{|a|^2} \left\{ a \cdot [\nabla y_h(x) - F_{\lambda}] n \right\} G_f(x) \, dx \]

(7.7)

\[ = \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \frac{1}{|a|^2} \left\{ a \cdot [\Pi(\nabla y_h(x)) - \nabla y_h(x)] n \right\} G_f(x) \, dx \]

\[ + \sum_{\mathcal{R} \in \tau_h} \int_{\partial \mathcal{R}} \frac{1}{|a|^2} \left\{ a \cdot [y_h(x) - F_{\lambda} x] \right\} (n \cdot \nu) G_f(x) \, dS \]

\[ - \sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} \frac{1}{|a|^2} \left\{ a \cdot [y_h(x) - F_{\lambda} x] \right\} [\nabla G_f(x) \cdot n] \, dx \]

\[ \equiv P_1 + P_2 + P_3. \]

We can estimate \( P_1 \) and \( P_3 \) by the Cauchy-Schwarz inequality, Theorem 6.1, and Theorem 5.2 by

(7.8) \[ |P_1| \leq C \left( \int_{\Omega} |G_f(x)|^2 \, dx \right)^{\frac{1}{2}} \left[ \mathcal{E}_h(y_h)^{\frac{1}{2}} + \mathcal{E}_h(y_h)^{\frac{1}{2}} \right], \]

(7.9) \[ |P_3| \leq C \left( \int_{\Omega} |\nabla G_f(x)n|^2 \, dx \right)^{\frac{1}{2}} \left[ \mathcal{E}_h(y_h)^{\frac{1}{2}} + \mathcal{E}_h(y_h)^{\frac{1}{2}} + h^{\frac{1}{2}} \right]. \]

To estimate \( P_2 \), we denote again \( z_h(x) = y_h(x) - F_{\lambda} x, x \in \Omega \). We rewrite \( P_2 \) as

\[ P_2 \equiv \sum_{\mathcal{R} \in \tau_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} \frac{1}{|a|^2} \left\{ a \cdot z_h(x) \right\} G_f(x) (n \cdot \nu) \, dS \]

\[ = \sum_{\mathcal{R} \in \tau_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} \frac{1}{|a|^2} \left\{ a \cdot [z_h(x) - T_\mu^a(z_h)] \right\} [G_f(x) - T_\mu^a (G_f)] (n \cdot \nu) \, dS \]

for \( y_h \in \mathcal{A}_h^a \) by the definition of \( \mathcal{A}_h^a \) and

\[ P_2 \equiv \sum_{\mathcal{R} \in \tau_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} \frac{1}{|a|^2} \left\{ a \cdot z_h(x) \right\} G_f(x) (n \cdot \nu) \, dS \]

\[ = \sum_{\mathcal{R} \in \tau_h} \sum_{\mathcal{F} \subset \partial \mathcal{R}} \int_{\mathcal{F}} \frac{1}{|a|^2} \left\{ a \cdot [z_h(x) - z_h (c_\mathcal{F})] \right\} G_f(x) (n \cdot \nu) \, dS \]

for \( y_h \in \mathcal{A}_h^p \) by the definition of \( \mathcal{A}_h^p \). By the same argument as for estimating \( J_2^a \) and \( J_2^p \) in the proof of Theorem 4.2 (cf. (4.10), (4.11), (4.14), and (4.15)) and by Lemma
3.3 and (5.6), we have

\[ |P_2| \leq Ch \left( \sum_{R \in \tau_h} \int_R \| \nabla y_h(x) - F_{\lambda} \|^2 \, dx \right)^{\frac{1}{2}} \left( \int_{\Omega} \| \nabla G_f(x) \|^2 \, dx \right)^{\frac{1}{2}} \]

(7.10) \[ \leq Ch \left[ \mathcal{E}_h(y_h)^{\frac{1}{2}} + 1 \right] \| \nabla G_f \|_{0,\Omega}. \]

Finally, the assertion of the theorem follows from (7.5)–(7.10). \qed

8. Error Estimates for Quasi-optimal Deformations

We first establish the existence of finite element energy minimizers as well as the error bound for the corresponding minimum energy.

**Theorem 8.1.** There exist a constant \( C > 0 \) and \( y_h \in A_h \) such that

\[ \mathcal{E}_h(y_h) = \min_{u_h \in A_h} \mathcal{E}_h(u_h) \leq Ch^{\frac{1}{2}}. \]

**Proof.** Fix a mesh \( \tau_h \). We have by the inverse inequality (3.8), Lemma 5.1, and Theorem 5.2 that

\[ \| u_h \|_{1,\infty,h} \leq Ch^{-\frac{3}{2}} \| u_h \|_{1,h} \]

(8.1) \[ \leq Ch^{-\frac{3}{2}} \left[ \mathcal{E}_h(u_h)^{\frac{1}{2}} + \mathcal{E}_h(u_h)^{\frac{1}{2}} + 1 \right], \quad \forall u_h \in A_h. \]

Moreover, the continuity of the energy density \( \phi \) implies the continuity of the energy functional \( \mathcal{E}_h \) on the finite-dimensional affine space \( A_h \). Therefore, the bound (8.1) implies the existence of a finite element energy minimizer by compactness.

To finish the proof, we need to construct a finite element deformation \( y_h \in A_h \) such that

\[ \mathcal{E}_h(y_h) \leq Ch^{\frac{1}{2}}. \]

This can be demonstrated by an argument similar to that in [8, 31, 32] since the space of our finite element polynomials (3.1) contains all linear polynomials and since the interpolation operator \( I_h : C(\bar{\Omega}) \to V_h \) satisfies the inequality (3.20). \qed

The number of local minima of the energy functional \( \mathcal{E}_h \) on \( A_h \) grows arbitrarily large as the mesh size \( h \to 0 \) [32]. Many of these local minima are approximations on different length scales to the same optimal microstructure [32]. Thus, it is reasonable to give error estimates for finite element approximations \( y_h \in A_h \) satisfying the quasi-optimality condition

(8.2) \[ \mathcal{E}_h(y_h) \leq \gamma \inf_{u_h \in A_h} \mathcal{E}(u_h) \]
for some constant $\gamma > 1$ independent of $h$. Our estimates show that all of the local minima of $E_h$ on $A_h$ which satisfy the quasi-optimality condition give accurate approximations to the energy-minimizing microstructure for the deformation, the volume fractions of the deformation gradients, and the nonlinear integrals of the deformation gradient.

It follows directly from the above theorem and all of the error bounds established in §5, §6, and §7 that we can obtain the following error estimates for all quasi-optimal finite element deformations $y_h \in A_h$ and for any family of rectangular meshes $\tau_h$ satisfying the quasi-uniformity condition (3.2).

**Corollary 8.1.** For any $w \in \mathbb{R}^3$ satisfying $w \cdot n = 0$, there exists a constant $C > 0$ such that

$$
\sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} |[\nabla y_h(x) - F_x]w|^2 \, dx \leq C h^{\frac{1}{4}}
$$

for any $y_h \in A_h$ which satisfies the quasi-optimality condition (8.2).

**Corollary 8.2.** There exists a constant $C > 0$ such that

$$
\sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} |y_h(x) - F_x|^2 \, dx \leq C h^{\frac{1}{4}}
$$

for any $y_h \in A_h$ which satisfies the quasi-optimality condition (8.2).

**Corollary 8.3.** If $\omega \subset \bar{\Omega}$ is a rectangular parallelepiped whose faces are parallel to the coordinate planes, then there exists a constant $C = C(\omega) > 0$ such that

$$
\left\|\sum_{\mathcal{R} \in \tau_h} \int_{\omega \cap \mathcal{R}} [\nabla y_h(x) - F_x] \, dx \right\| \leq C h^{\frac{1}{16}}
$$

for any $y_h \in A_h$ which satisfies the quasi-optimality condition (8.2).

**Corollary 8.4.** There exists a constant $C > 0$ such that

$$
\sum_{\mathcal{R} \in \tau_h} \int_{\mathcal{R}} |\nabla y_h(x) - \Pi(\nabla y_h(x))|^2 \, dx \leq C h^{\frac{1}{4}}
$$

for any $y_h \in A_h$ which satisfies the quasi-optimality condition (8.2).

**Corollary 8.5.** If $\omega \subset \bar{\Omega}$ is a rectangular parallelepiped whose faces are parallel to the coordinate planes and $\rho > 0$, then there exists a constant $C = C(\omega, \rho) > 0$ such that

$$
\left| \frac{\text{meas}_{\omega}^0(y_h)}{\text{meas} \omega} - (1 - \lambda) \right| + \left| \frac{\text{meas}_{\omega}^1(y_h)}{\text{meas} \omega} - \lambda \right| \leq C h^{\frac{1}{16}}
$$
for any $y_h \in A_h$ which satisfies the quasi-optimality condition (8.2).

**Corollary 8.6.** There exists a constant $C > 0$ such that

$$
\left| \sum_{R \in \mathcal{R}} \int_R \{f(x, \nabla y_h(x)) - [(1 - \lambda)f(x, F_0) + \lambda f(x, F_1)]\} \, dx \right| \leq C \|f\|_{V h^{1/2}}
$$

for any $f \in V$ and any $y_h \in A_h$ which satisfies the quasi-optimality condition (8.2).

**References**


Nonconforming Approximation of Microstructure


School of Mathematics, University of Minnesota, 206 Church Street, S.E., Minneapolis, MN 55455, U.S.A.

E-mail address: bli@math.umn.edu, luskin@math.umn.edu
<table>
<thead>
<tr>
<th>#</th>
<th>Author/s</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>1325</td>
<td>M. Luskin</td>
<td>Approximation of a laminated microstructure for a rotationally invariant, double well energy density</td>
</tr>
<tr>
<td>1326</td>
<td>Rakesh &amp; P. Sacks</td>
<td>Impedance inversion from transmission data for the wave equation</td>
</tr>
<tr>
<td>1327</td>
<td>O. Lafitte</td>
<td>Diffraction for a Neumann boundary condition</td>
</tr>
<tr>
<td>1328</td>
<td>E. Sobel, K. Lange, J.R. O’Connell &amp; D.E. Weeks</td>
<td>Haplotyping algorithms</td>
</tr>
<tr>
<td>1329</td>
<td>B. Cockburn, D.A. Jones &amp; E.S. Titi</td>
<td>Estimating the number of asymptotic degrees of freedom for nonlinear dissipative systems</td>
</tr>
<tr>
<td>1330</td>
<td>T. Aktosun</td>
<td>Inverse Schrödinger scattering on the line with partial knowledge of the potential</td>
</tr>
<tr>
<td>1331</td>
<td>T. Aktosun &amp; C. van der Mee</td>
<td>Partition of the potential of the one-dimensional Schrödinger equation</td>
</tr>
<tr>
<td>1332</td>
<td>B. Engquist &amp; E. Luo</td>
<td>Convergence of the multigrid method with a wavelet coarse grid operator</td>
</tr>
<tr>
<td>1333</td>
<td>V. Jakšić &amp; C.-A. Pillet</td>
<td>Ergodic properties of the Spin-Boson system</td>
</tr>
<tr>
<td>1334</td>
<td>S.K. Patch</td>
<td>Recursive solution for diffuse tomographic systems of arbitrary size</td>
</tr>
<tr>
<td>1335</td>
<td>J.C. Bronski</td>
<td>Semiclassical eigenvalue distribution of the non self-adjoint Zakharov-Shabat eigenvalue problem</td>
</tr>
<tr>
<td>1336</td>
<td>J.C. Cockburn</td>
<td>Bitangential structured interpolation theory</td>
</tr>
<tr>
<td>1337</td>
<td>S. Kichenassamy</td>
<td>The blow-up problem for exponential nonlinearities</td>
</tr>
<tr>
<td>1338</td>
<td>F.A. Grünbaum &amp; S.K. Patch</td>
<td>How many parameters can one solve for in diffuse tomography?</td>
</tr>
<tr>
<td>1339</td>
<td>R. Lipton</td>
<td>Reciprocal relations, bounds and size effects for composites with highly conducting interface</td>
</tr>
<tr>
<td>1340</td>
<td>H.A. Levine &amp; J. Serrin</td>
<td>A global nonexistence theorem for quasilinear evolution equations with dissipation</td>
</tr>
<tr>
<td>1341</td>
<td>A. Boutet de Monvel &amp; R. Purice</td>
<td>The conjugate operator method: Application to DIRAC operators and to stratified media</td>
</tr>
<tr>
<td>1342</td>
<td>G. Michele Graf</td>
<td>Stability of matter through an electrostatic inequality</td>
</tr>
<tr>
<td>1343</td>
<td>G. Avalos</td>
<td>Sharp regularity estimates for solutions of the wave equation and their traces with prescribed Neumann data</td>
</tr>
<tr>
<td>1344</td>
<td>G. Avalos</td>
<td>The exponential stability of a coupled hyperbolic/parabolic system arising in structural acoustics</td>
</tr>
<tr>
<td>1345</td>
<td>G. Avalos &amp; I. Lasiecka</td>
<td>A differential Riccati equation for the active control of a problem in structural acoustics</td>
</tr>
<tr>
<td>1346</td>
<td>G. Avalos</td>
<td>Well-posedness for a coupled hyperbolic/parabolic system seen in structural acoustics</td>
</tr>
<tr>
<td>1347</td>
<td>G. Avalos &amp; I. Lasiecka</td>
<td>The strong stability of a semigroup arising from a coupled hyperbolic/parabolic system</td>
</tr>
<tr>
<td>1348</td>
<td>A.V. Fursikov</td>
<td>Certain optimal control problems for Navier-Stokes system with distributed control function</td>
</tr>
<tr>
<td>1349</td>
<td>F. Gesztesy, R. Nowell &amp; W. Pötz</td>
<td>One-dimensional scattering theory for quantum systems with nontrivial spatial asymptotics</td>
</tr>
<tr>
<td>1350</td>
<td>F. Gesztesy &amp; H. Holden</td>
<td>On trace formulas for Schrödinger-type operators</td>
</tr>
<tr>
<td>1351</td>
<td>X. Chen</td>
<td>Global asymptotic limit of solutions of the Cahn-Hilliard equation</td>
</tr>
<tr>
<td>1352</td>
<td>X. Chen</td>
<td>Lorenz equations, Part I: Existence and nonexistence of homoclinic orbits</td>
</tr>
<tr>
<td>1353</td>
<td>X. Chen</td>
<td>Lorenz equations Part II: “Randomly” rotated homoclinic orbits and chaotic trajectories</td>
</tr>
<tr>
<td>1354</td>
<td>X. Chen</td>
<td>Lorenz equations, Part III: Existence of hyperbolic sets</td>
</tr>
<tr>
<td>1356</td>
<td>C. Liu</td>
<td>The Helmholtz equation on Lipschitz domains</td>
</tr>
<tr>
<td>1357</td>
<td>G. Avalos &amp; I. Lasiecka</td>
<td>Exponential stability of a thermoelastic system without mechanical dissipation</td>
</tr>
<tr>
<td>1358</td>
<td>R. Lipton</td>
<td>Heat conduction in fine scale mixtures with interfacial contact resistance</td>
</tr>
<tr>
<td>1359</td>
<td>V. Odisharia &amp; J. Peradze</td>
<td>Solvability of a nonlinear problem of Kirchhoff shell</td>
</tr>
<tr>
<td>1360</td>
<td>P.J. Olver, G. Sapiro &amp; A. Tannenbaum</td>
<td>Affine invariant edge maps and active contours</td>
</tr>
<tr>
<td>1361</td>
<td>R.D. James</td>
<td>Hysteresis in phase transformations</td>
</tr>
<tr>
<td>1362</td>
<td>A. Sei &amp; W. Symes</td>
<td>A note on consistency and adjointness for numerical schemes</td>
</tr>
<tr>
<td>1363</td>
<td>A. Friedman &amp; B. Hu</td>
<td>Head-media interaction in magnetic recording</td>
</tr>
<tr>
<td>1364</td>
<td>A. Friedman &amp; J.J.L. Velázquez</td>
<td>Time-dependent coating flows in a strip, part I: The linearized problem</td>
</tr>
<tr>
<td>1365</td>
<td>X. Ren &amp; M. Winter</td>
<td>Young measures in a nonlocal phase transition problem</td>
</tr>
<tr>
<td>1366</td>
<td>K. Bhattacharya &amp; R.V. Kohn</td>
<td>Elastic energy minimization and the recoverable strains of polycrystalline shape-memory materials</td>
</tr>
<tr>
<td>1367</td>
<td>G.A. Chechkin</td>
<td>Operator pencil and homogenization in the problem of vibration of fluid in a vessel with a fine net on the surface</td>
</tr>
<tr>
<td>1368</td>
<td>M. Carme Calderer &amp; B. Mukherjee</td>
<td>On Poiseuille flow of liquid crystals</td>
</tr>
<tr>
<td>1369</td>
<td>M.A. Pinsky &amp; M.E. Taylor</td>
<td>Pointwise Fourier inversion: A wave equation approach</td>
</tr>
<tr>
<td>1370</td>
<td>D. Brandon &amp; R.C. Rogers</td>
<td>Order parameter models of elastic bars and precursor oscillillations</td>
</tr>
<tr>
<td>1371</td>
<td>H.A. Levine &amp; B.D. Sleeman</td>
<td>A system of reaction diffusion equations arising in the theory of reinforced random walks</td>
</tr>
<tr>
<td>1372</td>
<td>B. Cockburn &amp; P.-A. Gremaud</td>
<td>A priori error estimates for numerical methods for scalar conservation laws. Part II: Flux-splitting monotone schemes on irregular Cartesian grids</td>
</tr>
</tbody>
</table>
1373 B. Li & M. Luskin, Finite element analysis of microstructure for the cubic to tetragonal transformation
1374 M. Luskin, On the computation of crystalline microstructure
1375 J.P. Matos, On gradient young measures supported on a point and a well
1376 M. Nitsche, Scaling properties of vortex ring formation at a circular tube opening
1377 J.L. Bona & Y.A. Li, Decay and analyticity of solitary waves
1378 V. Isakov, On uniqueness in a lateral cauchy problem with multiple characteristics
1379 M.A. Kouritzin, Averaging for fundamental solutions of parabolic equations
1380 T. Aktosun, M. Klaus & C. van der Mee, Integral equation methods for the inverse problem with discontinuous wavespeed
1381 P. Morin & R.D. Spies, Convergent spectral approximations for the thermomechanical processes in shape memory allows
1382 D.N. Arnold & X. Liu, Interior estimates for a low order finite element method for the Reissner-Mindlin plate model
1383 D.N. Arnold & R.S. Falk, Analysis of a linear-linear finite element for the Reissner-Mindlin plate model
1384 D.N. Arnold, R.S. Falk & R. Winther, Preconditioning in $H(div)$ and applications
1385 M. Lavrentiev, Nonlinear parabolic problems possessing solutions with unbounded gradients
1386 O.P. Bruno & P. Laurence, Existence of three-dimensional toroidal MHD equilibria with nonconstant pressure
1387 O.P. Bruno, F. Reitich, & P.H. Leo, The overall elastic energy of polycrystalline martensitic solids
1388 M. Fila & H.A. Levine, On critical exponents for a semilinear parabolic system coupled in an equation and a boundary condition
1390 J.M. Berg & H.G. Kwatny, Unfolding the zero structure of a linear control system
1391 A. Sei, High order finite-difference approximations of the wave equation with absorbing boundary conditions: A stability analysis
1392 A.V. Coward & Y.Y. Renardy, Small amplitude oscillatory forcing on two-layer plane channel flow
1393 V.A. Pliss & G.R. Sell, Approximation dynamics and the stability of invariant sets
1394 J.G. Cao & P. Roblin, A new computational model for heterojunction resonant tunneling diode
1395 C. Liu, Inverse obstacle problem: Local uniqueness for rougher obstacles and the identification of a ball
1396 K.A. Pericak-Spector & S.J. Spector, Dynamic cavitation with shocks in nonlinear elasticity
1397 G. Avalos & I. Lasiecka, Exponential stability of a thermoelastic system without mechanical dissipation II: The case of simply supported boundary conditions
1398 B. Brighi & M. Chipot, Approximation of infima in the calculus of variations
1399 G. Avalos, Concerning the well-posedness of a nonlinearly coupled semilinear wave and beam-like equation
1400 R. Lipton, Variational methods, bounds and size effects for composites with highly conducting interface
1401 B.T. Hayes & P.G. LeFloch, Non-classical shock waves in scalar conservation laws
1402 K.T. Joseph & P.G. LeFloch, Boundary layers in weak solutions to hyperbolic conservation laws
1403 Y. Diao, C. Ernst, & E.J.J. Van Rensburg, Energies of knots
1404 Xiaofeng Ren, Multi-layer local minimum solutions of the bistable equation in an infinite tube
1405 Vlastimil Pták, Krylov sequences and orthogonal polynomials
1406 T. Aktosun, M. Klaus, & C. van der Mee, Factorization of scattering matrices due to aptioning of potentials in one-dimensional Schrödinger-type equations
1408 D.N. Arnold, R.S. Falk, & R. Winther, Preconditioning discrete approximations of the Reissner-Mindlin plate model
1409 M.A. Kouritzin, On exact filters for continuous signals with discrete observations
1410 R. Lipton, The second Stekloff eigenvalue and energy dissipation inequalities for functionals with surface energy
1411 R. Lipton, The second Stekloff eigenvalue of an inclusion and new size effects for composites with imperfect interface
1412 W. Littman & B. Liu, The regularity and singularity of solutions of certain elliptic problems on polygonal domains
1413 C.R. Collins, Spurious oscillations are not fatal in computing microstructures
1414 M.A. Horn, Sharp trace regularity for the solutions of the equations of dynamic elasticity
1415 A. Friedman, B. Hu & Y. Liu, A boundary value problem for the Poisson equation with multi-scale oscillating boundary
1416 P. Baumann, D. Phillips & Q. Tang, Stable nucleation for the Ginzburg-Landau system with an applied magnetic field
1417 J.M. Berg, A strain profile for robust control of microstructure using dynamic recrystallization
1418 P. Klouček, Toward the computational modeling of nonequilibrium thermodynamics of the Martensitic transformations
1419 S. Chawla & S.M. Lenhart, Application of optimal control theory to in situ bioremediation
1420 B. Li & M. Luskin, Nonconforming finite element approximation of crystalline microstructure
1421 H. Kang & J.K. Seo, Inverse conductivity problem with one measurement: Uniqueness of balls in $\mathbb{R}^3$