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ANALYSIS OF A CLASS OF NONCONFORMING FINITE ELEMENTS FOR CRYSTALLINE MICROSTRUCTURES

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Abstract. An analysis is given for a class of nonconforming Lagrange-type finite elements which have been successfully utilized to approximate the solution of a variational problem modeling the deformation of martensitic crystals with microstructure. These elements were first proposed and analyzed in 1992 by Rannacher and Turek for the Stokes equation. Our analysis highlights the features of these elements which make them effective for the computation of microstructure. New results for superconvergence and numerical quadrature are also given.

1. Introduction

Recent years have seen the development of a continuum theory for martensitic crystals based on the minimization of the Ericksen-James elastic energy [2, 3, 13, 14, 17, 19]. The elastic energy density attains a minimum value at several symmetry-related deformation gradients. Thus, the deformations of energy-minimizing sequences often exhibit a microstructure—the simplest of which are fine-scale layers in which the deformation gradient is nearly constant and across which the deformation gradient oscillates between the energy wells—to allow the effective energy of a deformation to be that of a macroscopic or relaxed energy. Further, the parallel planes defining the layering in the microstructure are constrained by the symmetry of the energy density to be a member of a finite family of parallel planes.

If the deformation is constrained on the boundary, then the deformation cannot generally attain a minimum energy by forming a microstructure with layers of nonzero thickness [3]. Rather, minimizing sequences of deformations must be constructed from layers with a thickness which converges to zero. Such minimizing sequences define the solution to the variational problems. They can be described physically by the notion of microstructure and mathematically by the Young measure [2, 3, 17, 19].

When an energy minimizing deformation is sought in a finite element space, the fineness of the layers is limited not only by the mesh size, but also by the nature of the finite element used. The most accurate finite element spaces will be those which

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can approximate microstructures with the most fine-scale layers possible on meshes which are oriented arbitrarily with respect to the layers defining the microstructure.

Several approaches have been developed for the finite element approximation of microstructure. The most commonly used finite element spaces are the conforming spaces with continuous deformations which are either piecewise linear or multilinear with respect to some mesh. Although these spaces can approximate well microstructure with layers which are oriented with respect to the mesh, we have had difficulty approximating microstructure with these conforming spaces when the layers are not oriented with respect to the mesh. We have not generally been able to obtain solutions with conforming spaces which have a layer thickness of less than three elements if the grid is not oriented so that the planes across which the gradients of the deformations in the conforming finite element space are allowed to be discontinuous are not parallel to the layers.

Two alternative methods have been developed to allow microstructure to be approximated on meshes which are not aligned with the microstructure. The first method was that of reduced integration of the multilinear element [8, 9, 12]. This method has been effectively used to compute microstructure with fine-scale layers on meshes which are not oriented with respect to the microstructure. For Laplace's equation on a uniform grid, the deformation computed with this method can be shown to converge strongly, but the deformation gradients do not converge strongly. This would not be an effective method for the minimization of a quasi-convex energy, however this method can be used effectively with the nonconvex Ericksen-James energy since its energy-minimizing deformations converge strongly while its gradients do not converge strongly. Most importantly, numerical experiments indicate the convergence of the microstructure or Young measure for the piecewise constant projection of the gradients of the deformation.

The approach analyzed here is that given by a family of nonconforming finite elements. The use of nonconforming finite elements is intuitively appealing for problems with microstructure because the admissible deformations have more flexibility to approximate oscillatory functions. The nonconforming elements that we study in this paper were first proposed and analyzed by Rannacher and Turek for solving the Stokes problem [24]. Recently, we have used these finite elements to simulate the deformation of martensitic crystals with microstructure [18], and we found that with a suitable numerical quadrature they produce a very robust approximation method. Our analysis demonstrates that the deformation, as well as the deformation gradient, converges strongly for second-order, linear elliptic problems.

The first version of the considered elements is a finite element defined on rectangles (respectively, rectangular parallelepipeds) with degrees of freedom given by the values at midpoints of edges of the rectangles (respectively, the centers of the faces of the rectangular parallelepipeds). The second version is a finite element defined on rectangles (respectively, rectangular parallelepipeds) with the degrees of freedom given by the averages over the four edges of the rectangles (respectively, the six faces of the rectangular parallelepipeds).

Unlike most other nonconforming finite elements, these elements do not have any conforming counterparts. Consequently, the error analysis is nontrivial. We prove error estimates for these finite element approximations in both the H^1 and the L^2 norms. Our analysis contributes to the understanding of these elements by emphasizing their relation to the conforming multilinear elements. We also give new superconvergence estimates for the error of the deformation gradient. In view of practical computations, especially for the computation of material microstructures, we also give an analysis of the effect of the numerical integration.

The convergence of the approximation of the microstructure of the deformation gradient of a crystal by continuous, piecewise linear finite element methods has been proven in [10, 11] for one-dimensional model problems for norms which measure the weak convergence of nonlinear functions of the deformation gradient, and the convergence of the three-dimensional approximation of the microstructure of the magnetization in the micromagnetics model for ferromagnetics has been proven for related norms [22]. These norms are stronger than the L^2 norm, which does not control oscillations in the gradient, and are weaker than the H^1 norm, which does not allow oscillations in the gradient for convergent sequences. The above analyses and the multidimensional analysis in [5, 6] proceed by demonstrating that the deformation gradient (or magnetization in the micromagnetics problem) converges weakly and that the approximate deformation gradient (or magnetization) must lie in arbitrarily small neighborhoods of the minima of the energy density. Thus far, these techniques have not yet made possible the rigorous analysis of the numerical approximation of microstructure for realistic, multidimensional models for the deformation of crystals [2, 3, 9].

Throughout this paper we will mostly focus on the three-dimensional approximations, although similar results hold in two dimensions. For simplicity, let $\Omega = (0, L_1) \times (0, L_2) \times (0, L_3)$ be a rectangular parallelepiped with faces parallel to the coordinate planes. The points of Ω will be denoted by (x, y, z) or by (x_1, x_2, x_3) as appropriate. Results similar to those presented in this paper are valid for domains which are the union of rectangular parallelepipeds except that the rate of convergence in the L^2 norm may be reduced since the regularity of the solution of the dual problem with L^2 data may be reduced.

We consider the following divergence-type second-order elliptic boundary value problem,

$$
\begin{aligned}
\boldsymbol{\mathcal{L}} u \equiv -\frac{\partial}{\partial x}\left(a_1 \frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(a_2 \frac{\partial u}{\partial y}\right) - \frac{\partial}{\partial z}\left(a_3 \frac{\partial u}{\partial z}\right) + c\,u = f, &\qquad \text{in } \Omega, \\
u = 0, &\qquad \text{on } \partial\Omega,
\end{aligned} \tag{1.1}
$$

where $a_1, a_2, a_3 \in W^{1,\infty}(\Omega)$, $a_1, a_2, a_3 \geq a_0 = \text{constant} > 0$, a.e. Ω, $c \in L^\infty(\Omega)$, $c \geq 0$, a.e. Ω, $f \in L^2(\Omega)$. We define $a(\cdot,\cdot)$: $H^1(\Omega) \times H^1(\Omega) \longrightarrow \mathbb{R}$ by

$$
a(v, w) \equiv \int_\Omega \left(a_1 \frac{\partial v}{\partial x}\frac{\partial w}{\partial x} + a_2 \frac{\partial v}{\partial y}\frac{\partial w}{\partial y} + a_3 \frac{\partial v}{\partial z}\frac{\partial w}{\partial z} + cvw \right) dxdydz.
$$

It is obvious that $a(\cdot,\cdot)$ is symmetric, continuous and bilinear. Furthermore, by the Poincaré inequality, $a(\cdot,\cdot)$ is $H^1_0(\Omega)$-elliptic. We denote by $(\cdot,\cdot)$ the $L^2(\Omega)$ inner product. The existence and uniqueness of the solution to the problem (1.1) follow from the Lax-Milgram lemma. The following theorem gives the regularity of the solution [15, 16].

Theorem 1.1. *For any $f \in L^2(\Omega)$, there exists a unique $u \in H^1_0(\Omega) \cap H^2(\Omega)$ such that*

$$
a(u, v) = (f, v), \qquad \forall v \in H^1_0(\Omega). \tag{1.2}
$$

Furthermore, there holds the a priori estimate

$$\|u\|_{2,\Omega} \le C\|f\|_{0,\Omega}, \tag{1.3}$$

where $C = C(a_1, a_2, a_3, c, \Omega) > 0$ *is a constant.*

The rest of this paper is organized as follows. In §2 we define the finite elements and their corresponding finite element spaces based on a rectangular partition of Ω. We then prove a Poincaré-type inequality for the test functions. In §3 we give the error estimates in both the H^1 and the L^2 norms. In §4, we discuss the relation of the considered finite elements to multilinear finite elements. In §5, we give a superconvergence estimate for the gradients based on cubic partitions. Finally, in §6, we apply numerical quadrature to the finite element approximations, and we study the rates of convergence for several resulting schemes.

2. The finite elements

The first finite element is defined by the triple (Q, P_Q, Σ_Q^p), where $Q \equiv [a-r, a+r] \times [b-s, b+s] \times [c-t, c+t]$ is a rectangular parallelepiped with its center at (a, b, c) and the lengths of its edges $2r$, $2s$, $2t$, where $r, s, t > 0$,

$$P_Q = \mathrm{Span}\left\{ 1,\, x,\, y,\, z,\, \left(\frac{x}{r}\right)^2 - \left(\frac{y}{s}\right)^2, \left(\frac{x}{r}\right)^2 - \left(\frac{z}{t}\right)^2 \right\}, \tag{2.1}$$

$$\Sigma_Q^p = \{\, q(M_i) : i = 1, \ldots, 6 \,\}, \tag{2.2}$$

where M_i, $i = 1, \ldots, 6$, are the centers of the faces of Q. This Lagrange-type element is well defined since it is easy to verify that Σ_Q^p is P_Q-unisolvent, i.e., for any given $\alpha_i \in \mathbb{R}$, $i = 1, \ldots, 6$, there exists a unique $q \in P_Q$ such that

$$q(M_i) = \alpha_i, \qquad i = 1, \ldots, 6.$$

We define $\varphi_i = \varphi_i(x, y, z) \in P_Q$, $i = 1, \ldots, 6$, such that

$$\varphi_i(M_j) = \delta_{ij}, \qquad i, j = 1, \ldots, 6, \tag{2.3}$$

by permuting the terms $(x-a)/r$, $(y-b)/s$ and $(z-c)/t$ in the polynomial

$$\varphi(x, y, z) = -\frac{1}{6}\left(\frac{x-a}{r}\right)^2 - \frac{1}{6}\left(\frac{y-b}{s}\right)^2 + \frac{1}{3}\left(\frac{z-c}{t}\right)^2 + \epsilon\frac{z-c}{2t} + \frac{1}{6}, \tag{2.4}$$

where $\epsilon = \pm 1$. Thus, it follows that $\{\varphi_i\}_{i=1}^6$ is the standard basis for the finite element (Q, P_Q, Σ_Q^p). We then define the affine family of finite elements (R, P_R, Σ_R^p), where R is a rectangular parallelepiped. We note that in general $\nabla \cdot \nabla\phi \neq 0$ for $\phi \in P_Q$ unless $r = s = t$.

Next, we define the averaged version of the preceding finite element to be the triple (Q, P_Q, Σ_Q^a). The polynomial space P_Q is the same as defined in (2.1) and the set of degrees of freedom is defined by

$$\Sigma_Q^a = \left\{ \fint_{F_i} q\, dS : i = 1, \ldots, 6 \right\}, \tag{2.5}$$

where $F_i,\ i=1,\dots,6$, are the faces of the rectangular parallelepiped Q and

$$\fint_F \equiv \frac{1}{|F|}\int_F$$

for faces $F\subset\partial Q$, where $|F|$ denotes the area of the face F. This finite element is well defined since Σ_Q^a is P_Q-unisolvent. This can be easily checked by considering the six polynomials $\psi_i=\psi_i(x,y,z),\ i=1,\dots,6$, obtained by permuting the terms $(x-a)/r$, $(y-b)/s$ and $(z-c)/t$ in the polynomial

$$\psi(x,y,z)=-\frac{1}{4}\left(\frac{x-a}{r}\right)^2-\frac{1}{4}\left(\frac{y-b}{s}\right)^2+\frac{1}{2}\left(\frac{z-c}{t}\right)^2+\epsilon\frac{z-c}{2t}+\frac{1}{6}, \tag{2.6}$$

where $\epsilon=\pm1$. It is obvious that $\psi_i\in P_Q, i=1,\dots,6$, and it is easily checked that with a suitable labeling of the indices,

$$\fint_{F_i}\psi_j\,dS=\delta_{ij}. \tag{2.7}$$

Thus, $\{\psi_i\}_{i=1}^6$ is the standard basis for the finite element (Q,P_Q,Σ_Q^a). Again, we define the affine family of finite elements (R,P_R,Σ_R^a), where R is a rectangular parallelepiped.

To construct a rectangular partition τ_h of Ω, we define one-dimensional partitions of $[0,L_k]$, for $k=1,2,3$, by

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

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

$$R_{i_1,i_2,i_3}\equiv[x_1^{i_1-1},x_1^{i_1}]\times[x_2^{i_2-1},x_2^{i_2}]\times[x_3^{i_3-1},x_3^{i_3}],\qquad 1\le i_1\le m_1,\dots,1\le i_3\le m_3,$$

and the rectangular partition

$$\tau_h\equiv\{\,R_{i_1,i_2,i_3}:1\le i_1\le m_1,\dots,1\le i_3\le m_3\,\}$$

with the mesh size parameter h defined by $h=\max\{h_k:1\le k\le 3\}$, where $h_k\equiv\max\{x_k^i-x_k^{i-1}:1\le i\le m_k\}$ is the maximal discretization size in the kth coordinate direction for $k=1,2,3$.

For the first finite element, we define the set of nodal points N_h to be the set of all the centers of faces of elements in τ_h. The finite element spaces over the partition τ_h are then defined respectively to be

$$\begin{aligned}V_h^p\equiv\{\,&v_h\in L^2(\Omega)\,:\,v_h\big|_R\in P_R,\ \forall R\in\tau_h\,;\ \text{adjoining } v_h \text{ have the same}\\&\text{values at shared nodal points, i.e., } v_h \text{ is continuous on } N_h\,\},\\V_h^a\equiv\{\,&v_h\in L^2(\Omega)\,:\,v_h\big|_R\in P_R,\ \forall R\in\tau_h;\\&\int_F v_h\big|_{R'}\,dS=\int_F v_h\big|_{R''}\,dS,\ \forall \text{ faces } F=\partial R'\cap\partial R''\neq\emptyset,\ R',R''\in\tau_h\,\}.\end{aligned}$$

To solve the Dirichlet problem (1.1), we define

$$V_{0h}^p \equiv \{\, v_h \in V_h^p : v_h = 0 \text{ on } N_h \cap \partial\Omega \,\},$$
$$V_{0h}^a \equiv \left\{ v_h \in V_h^a : \int_F v_h \, dS = 0, \forall \, \text{faces}\, F \subset \partial R \cap \partial\Omega \neq \emptyset, R \in \tau_h \right\}.$$

It is obvious that all of the spaces V_h^p, V_{0h}^p, V_h^a and V_{0h}^a are finite-dimensional subspaces of $L^2(\Omega)$. They are also affine finite element spaces [7]. For $v_h \in V_h^p$ (or $V_{0h}^p, V_h^a, V_{0h}^a$), we have in general that $v_h \notin C(\bar{\Omega})$ since v_h is continuous necessarily only at centers (or at some other points in the case of the V_h^a-approximation) of faces of adjacent elements. Therefore, V_h^p (or $V_{0h}^p, V_h^a, V_{0h}^a$) $\not\subseteq C(\bar{\Omega})$, and, hence, V_h^p (or $V_{0h}^p, V_h^a, V_{0h}^a$) $\not\subseteq H^1(\Omega)$. Thus, in view of solving a second-order elliptic boundary value problem, the finite elements are nonconforming.

For convenience, we define for an integer $k \geq 0$ and $p \in [1, \infty]$ the space

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

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

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

where, for $R \in \tau_h$, $|\cdot|_{k,p,R}$ and $\|\cdot\|_{k,p,R}$ are the usual seminorm and norm on the Sobolev space $W^{k,p}(R)$ [1]. If $p = 2$ we write $H_h^k(\Omega)$ for $W_h^{k,p}(\Omega)$ and omit p in all the above seminorm and norm expressions.

Now it is obvious that $|\cdot|_{1,h}$ defines a norm on V_{0h}^p and V_{0h}^a. We next prove a Poincaré-type inequality for functions in the finite element spaces V_{0h}^p and V_{0h}^a. This inequality leads to the uniform V_{0h}^p- and V_{0h}^a-ellipticity, which is required in deriving the second Strang lemma [7, 25].

Theorem 2.1. *For any $v_h \in V_{0h}^p \cup V_{0h}^a$, we have*

$$\|v_h\|_{0,\Omega} \leq \sqrt{6}\; h \, |v_h|_{1,h} + \sqrt{2} L_k \left\| \frac{\partial v_h}{\partial x_k} \right\|_{0,h}, \qquad k = 1, 2, 3. \tag{2.8}$$

Proof. Let us fix $v \equiv v_h \in V_{0h}^p \cup V_{0h}^a$. For any $\bar{\boldsymbol{x}} = (\bar{x}_1, \bar{\boldsymbol{x}}') \in \Omega$, where $\bar{\boldsymbol{x}}' = (\bar{x}_2, \bar{x}_3)$, let $R = [x_1^{i_1-1}, x_1^{i_1}] \times R'$, where $R' = [x_2^{i_2-1}, x_2^{i_2}] \times [x_3^{i_3-1}, x_3^{i_3}]$, be such that $\bar{\boldsymbol{x}} \in R$. Without loss of generality, we assume $i_1 \geq 2$. Denote by v_j the restriction of v on $[x_1^{j-1}, x_1^j] \times R'$, for $j = 1, \ldots, m_1$. If $v \in V_{0h}^a$, we have

$$\int_{R'} v_1(x_1^0, \boldsymbol{x}') d\boldsymbol{x}' + \sum_{j=1}^{i_1-1} \left[\int_{R'} v_{j+1}(x_1^j, \boldsymbol{x}') d\boldsymbol{x}' - \int_{R'} v_j(x_1^j, \boldsymbol{x}') d\boldsymbol{x}' \right] = 0.$$

Consequently, there exists $\boldsymbol{z}' = (z_2', z_3') \in R'$ so that

$$v_1(x_1^0, \boldsymbol{z}') + \sum_{j=1}^{i_1-1} \left[v_{j+1}(x_1^j, \boldsymbol{z}') - v_j(x_1^j, \boldsymbol{z}') \right] = 0. \tag{2.9}$$

Observe that on each element in τ_h,

$$\frac{\partial v}{\partial x_k} \in \mathrm{Span}\{1, x_k\}, \qquad k = 1, 2, 3. \tag{2.10}$$

By (2.9) and (2.10), we have

$$\begin{aligned} v(\bar{\boldsymbol{x}}) &= v_{i_1}(\bar{x}_1, \bar{\boldsymbol{x}}') - v_{i_1}(x_1^{i_1-1}, \boldsymbol{z}') + \sum_{j=1}^{i_1-1} \left[v_j(x_1^j, \boldsymbol{z}') - v_j(x_1^{j-1}, \boldsymbol{z}') \right] \\ &= \sum_{k=1}^{3} \int_{z_k'}^{\bar{x}_k} \frac{\partial v_{i_1}(\boldsymbol{x})}{\partial x_k}\, dx_k + \sum_{j=1}^{i_1-1} \int_{x_1^{j-1}}^{x_1^j} \frac{\partial v_j(\boldsymbol{x})}{\partial x_1}\, dx_1, \end{aligned} \tag{2.11}$$

where $z_1' = x_1^{i_1-1}$. This is also true for $v \in V_{0h}^p$ if we choose $\boldsymbol{z}' \in R'$ so that $(x_1^0, \boldsymbol{z}')$ is the center of the face $\{x_1^0\} \times R'$ of the element $[x_1^0, x_1^1] \times R'$. It then follows from (2.11), (2.10) and the Cauchy-Schwarz inequality that

$$|v(\bar{\boldsymbol{x}})|^2 \le 6h \sum_{k=1}^{3} \int_{x_k^{i_k-1}}^{x_k^{i_k}} \left| \frac{\partial v_{i_1}(\boldsymbol{x})}{\partial x_k} \right|^2 dx_k + 2L_1 \sum_{j=1}^{m_1} \int_{x_1^{j-1}}^{x_1^j} \left| \frac{\partial v_j(\boldsymbol{x})}{\partial x_1} \right|^2 dx_1. \tag{2.12}$$

Integrating (2.12) over R and summing up the integrals over $R \in \tau_h$, we thus obtain (2.8) for $k = 1$. The same argument applies to $k = 2, 3$. $\square$

3. H_h^1 AND L^2 ERROR ESTIMATES

We define $a_h(\cdot,\cdot) : H_h^1(\Omega) \times H_h^1(\Omega) \longrightarrow \mathbb{R}$ by

$$a_h(v, w) \equiv \sum_{R \in \tau_h} \int_R \left(a_1 \frac{\partial v}{\partial x}\frac{\partial w}{\partial x} + a_2 \frac{\partial v}{\partial y}\frac{\partial w}{\partial y} + a_3 \frac{\partial v}{\partial z}\frac{\partial w}{\partial z} + cvw \right) dxdydz.$$

We also denote $V_h = V_h^p$ or V_h^a and $V_{0h} = V_{0h}^p$ or V_{0h}^a, respectively. It is clear that $a_h(\cdot,\cdot)$ is symmetric, continuous and bilinear. By Theorem 2.1, it is also uniform V_{0h}-elliptic, i.e., there exists a constant $\alpha > 0$, independent of h, such that

$$a_h(v_h, v_h) \ge \alpha \|v_h\|_{1,h}^2, \qquad \forall v_h \in V_{0h}. \tag{3.1}$$

Therefore, by the Lax-Milgram lemma, there exists a unique finite element approximation $u_h \in V_{0h}$ such that

$$a_h(u_h, v_h) = (f, v_h), \qquad \forall v_h \in V_{0h}. \tag{3.2}$$

In the sequel, the rectangular partitions τ_h are always assumed to be quasi-uniform, i.e., there exists a constant $\sigma > 0$, independent of h, such that

$$\min\{\, x_k^i - x_k^{i-1} : \, i = 1, \ldots, m_k, \; k = 1, 2, 3\} \ge \sigma h.$$

We denote the Lagrange interpolation operator $I_h : C(\bar{\Omega}) \longrightarrow V_h$ to be either $I_h^p : C(\bar{\Omega}) \longrightarrow V_h^p$ or $I_h^a : C(\bar{\Omega}) \longrightarrow V_h^a$, which are defined respectively for $I_h^p v \in V_h^p$ and $I_h^a v \in V_h^a$ by

$$\begin{aligned} I_h^p v(M) &= v(M), && \forall M \in N_h, \\ \int_F I_h^a v \, dS &= \int_F v \, dS, && \forall \, \text{faces}\, F \subset \partial R \text{ where } R \in \tau_h, \end{aligned}$$

for any $v \in C(\bar{\Omega})$. We also use the same notation I_h, I_h^p and I_h^a to denote the restrictions of these operators over an element of the partition τ_h.

We use the symbol C to denote a generic constant varying with the context. This constant is always assumed to be independent of all the trial and test functions, the solution u to (1.2) and the mesh size parameter h unless the dependence is otherwise stated.

Let us recall the following well-known results on the estimates for interpolation errors and the inverse estimates for later use [7].

Theorem 3.1. *For $k = 0, 1, 2$, we have*

$$\begin{aligned} \|I_h v - v\|_{k,R} &\le C h^{2-k} |v|_{2,R}, && \forall R \in \tau_h, \ \forall v \in H^2(R), \\ \|I_h v - v\|_{k,h} &\le C h^{2-k} |v|_{2,h}, && \forall v \in H_h^2(\Omega). \end{aligned}$$

Theorem 3.2. *Let k and l be two integers such that $0 \le k \le l \le 2$. Then for any $R \in \tau_h$ and any $v_h \in V_h$ we have*

$$\begin{aligned} |v_h|_{l,R} &\le C h^{k-l} |v_h|_{k,R}, \\ |v_h|_{l,h} &\le C h^{k-l} |v_h|_{k,h}, \\ |v_h|_{l,\infty,R} &\le C h^{k-l-\frac{3}{2}} |v_h|_{k,R}, \\ |v_h|_{l,\infty,h} &\le C h^{k-l-\frac{3}{2}} |v_h|_{k,h}. \end{aligned}$$

Our main results in this section are the error estimates for the finite element approximations in the $H_h^1(\Omega)$ and the $L^2(\Omega)$ norms.

Theorem 3.3. *Let $u \in H_0^1(\Omega) \cap H^2(\Omega)$ and $u_h \in V_{0h}$ be the solutions to* (1.2) *and* (3.2)*, respectively. We have*

$$\|u - u_h\|_{m,h} \le C h^{2-m} \|u\|_{2,\Omega}, \qquad m = 0, 1. \tag{3.3}$$

To prove the theorem, we need some auxiliary lemmas.

Lemma 3.4. *Let $R \in \tau_h$ and $F \subset \partial R$ be a face of R and let $P_0 \in R$ be an arbitrary point. Then the following estimates hold:*

$$\left| w(P_0) - \frac{1}{|R|}\int_R w \, dxdydz \right| \le C h \, |w|_{1,\infty,R}, \qquad \forall w \in W^{1,\infty}(R), \tag{3.4}$$

$$\int_F \left| w - \frac{1}{|F|}\int_F w \, dS \right|^p dS \le C h^{2-\frac{p}{2}} \, |w|_{1,R}^p, \qquad \forall w \in H^1(R), \ p = 1, 2, \tag{3.5}$$

$$\int_{\partial R} w^2 \, dS \le \frac{C}{h} |w|_{0,R}^2 + C h |w|_{1,R}^2, \qquad \forall w \in H^1(R). \tag{3.6}$$

Proof. The inequality (3.4) follows easily from the estimate

$$\begin{aligned}\left|w(P_0) - \fint_R w\,dxdydz\right| &= \left|\fint_R [w(P_0) - w(x,y,z)]\,dxdydz\right| \\ &\le \fint_R |w(P_0) - w(x,y,z)|\,dxdydz \\ &\le \fint_R |P_0 - (x,y,z)||w|_{1,\infty,R}\,dxdydz\end{aligned}$$

for $w \in W^{1,\infty}(R)$.

Next, let $R = [a-r, a+r] \times [b-s, b+s] \times [c-t, c+t]$ and assume without loss of generality that $F = \{a+r\} \times [b-s, b+s] \times [c-t, c+t]$. Denote $\hat{R} = [-1,1] \times [-1,1] \times [-1,1]$ and $\hat{F} = \{1\} \times [-1,1] \times [-1,1]$, and define the affine mapping $K_R : \hat{R} \longrightarrow R$ by $K(\xi, \eta, \zeta) = (x, y, z)$, where

$$x = r\xi + a, \qquad y = s\eta + b, \qquad z = t\zeta + c. \tag{3.7}$$

For any function $w = w(P)$, $P \in R$, set $\hat{w} = w \circ K_R$. Now by the quasi-uniformity of τ_h and the trace theorem [1] we get that

$$\int_F \left| w - \fint_F w\,dS \right|^p dS = st \int_{\hat{F}} \left| \hat{w} - \fint_{\hat{F}} \hat{w}\,d\hat{S} \right|^p d\hat{S} \le Ch^2 \|\hat{w}\|^p_{1,\hat{R}}. \tag{3.8}$$

Replacing w by $w + c$ in (3.8) with c any constant, we have by the Bramble-Hilbert lemma [7, Theorem 4.1.3] that

$$\int_F \left| w - \fint_F w\,dS \right|^p dS \le Ch^2 \inf_{\hat{c}=\text{constant}} \|\hat{w} + \hat{c}\|^p_{1,\hat{R}} \le Ch^2 |\hat{w}|^p_{1,\hat{R}} \le Ch^{2-\frac{p}{2}}\, |w|^p_{1,R}.$$

This proves (3.5).

Finally, by the transformation (3.7), the quasi-uniformity of τ_h and the trace theorem, we have

$$\begin{aligned}\int_{\partial R} w^2\,dS \le Ch^2 \int_{\partial\hat{R}} \hat{w}^2\,d\hat{S} &\le Ch^2 \left[\int_{\hat{R}} \hat{w}^2\,d\xi d\eta d\zeta + \int_{\hat{R}} |\nabla\hat{w}|^2\,d\xi d\eta d\zeta\right] \\ &\le Ch^2 \left[h^{-3} \int_R w^2\,dxdydz + h^{-1} \int_R |\nabla w|^2\,dxdydz\right],\end{aligned}$$

leading to (3.6). □

In what follows, for $R \in \tau_h$ and a face $F \subset \partial R$, we define the functional T_F by either $T_F(w) = w(M_F)$ for $w \in C(F)$, where M_F is the center of the face F, when considering the V_h^p-approximation, or by $T_F(w) = \fint_F w\,dS$ for $w \in L^2(F)$ when considering the V_h^a-approximation.

Lemma 3.5. *For any $R \in \tau_h$ and any face $F \subset \partial R$, we have*

$$\int_F [v_h - T_F(v_h)]^2\,dS \le Ch|v_h|^2_{1,R}, \qquad \forall v_h \in V_h.$$

Proof. Without loss of generality, we assume that $F = \{a+r\} \times [b-s, b+s] \times [c-t, c+t]$. Let $P_F \equiv (a+r, \bar{y}, \bar{z}) \in F$ be such that $T_F(v_h) = v_h(P_F)$. Now, by the Cauchy-Schwarz inequality, the fact (2.10) that $\frac{\partial v_h}{\partial y}$ (respectively, $\frac{\partial v_h}{\partial z}$) depends only on y (respectively, z), and the quasi-uniformity of the partitions τ_h, we have

$$\begin{aligned}
\int_F [v_h - T_F(v_h)]^2 \, dS = & \int_{b-s}^{b+s} \int_{c-t}^{c+t} [v_h(a+r,y,z) - v_h(a+r,\bar{y},\bar{z})]^2 \, dydz \\
= & \int_{b-s}^{b+s} \int_{c-t}^{c+t} \left[\int_{\bar{y}}^{y} \frac{\partial v_h(a+r,y',z)}{\partial y'} \, dy' + \int_{\bar{z}}^{z} \frac{\partial v_h(a+r,\bar{y},z')}{\partial z'} \, dz' \right]^2 dydz \\
\le & \int_{b-s}^{b+s} \int_{c-t}^{c+t} \left\{ 2 \left[\int_{\bar{y}}^{y} \frac{\partial v_h(a+r,y',z)}{\partial y'} \, dy' \right]^2 \right. \\
& \left. \qquad + 2 \left[\int_{\bar{z}}^{z} \frac{\partial v_h(a+r,\bar{y},z')}{\partial z'} \, dz' \right]^2 \right\} dydz \\
\le & \int_{b-s}^{b+s} \int_{c-t}^{c+t} \left\{ 2\,|y-\bar{y}| \left| \int_{\bar{y}}^{y} \left| \frac{\partial v_h(a+r,y',z)}{\partial y'} \right|^2 dy' \right| \right. \\
& \left. \qquad + 2\,|z-\bar{z}| \left| \int_{\bar{z}}^{z} \left| \frac{\partial v_h(a+r,\bar{y},z')}{\partial z'} \right|^2 dz' \right| \right\} dydz \\
\le & \int_{b-s}^{b+s} \int_{c-t}^{c+t} \left\{ 4s \int_{b-s}^{b+s} \left| \frac{\partial v_h}{\partial y} \right|^2 dy + 4t \int_{c-t}^{c+t} \left| \frac{\partial v_h}{\partial z} \right|^2 dz \right\} dydz \\
\le & \; 4st \left(4s \int_{b-s}^{b+s} \left| \frac{\partial v_h}{\partial y} \right|^2 dy + 4t \int_{c-t}^{c+t} \left| \frac{\partial v_h}{\partial z} \right|^2 dz \right) \le \; Ch |v_h|^2_{1,R},
\end{aligned}$$

completing the proof. □

Lemma 3.6. *Let $R \in \tau_h$ and let $F \subset \partial R$ be a face of R. Then, for any trilinear function $w = w(x,y,z)$ on R, we have*

$$\int_F (w - I_h w) \, dS = 0 \qquad \textit{and} \qquad T_F(w - I_h w) = 0. \tag{3.9}$$

Proof. Without loss of generality, let $R \in \tau_h$ and $F \subset \partial R$ be the same as in the proof of Lemma 3.5. If $w = 1, x, y$ or z, then $I_h w = w$. Hence, (3.9) holds trivially. Now if w is not linear but multilinear with respect to the variables $x-a$, $y-b$, and $z-c$, then a simple calculation shows that $I_h w = 0$, $T_F(w) = 0$, and (3.9) is true as well. Our proof is complete since all the trilinear functions are linear combinations of those functions tested above. □

Now we are in a position to prove our theorem.

Proof of the H_h^1 error estimate. By Theorem 2.1, $a_h(\cdot,\cdot)$ is uniformly V_{0h}-elliptic. Hence, by the second Strang lemma [7, 25], we have

$$\|u - u_h\|_{1,h} \le C \left[\inf_{v_h \in V_{0h}} \|u - v_h\|_{1,h} + \sup_{0 \ne v_h \in V_{0h}} \frac{|d_h(u, v_h)|}{\|v_h\|_{1,h}} \right], \tag{3.10}$$

where $d_h : H^2(\Omega) \times H_h^1(\Omega) \longrightarrow \mathbb{R}$ is the nonconforming error functional defined by

$$d_h(\varphi, v) = a_h(\varphi, v) - (\boldsymbol{\mathcal{L}}\varphi, v), \qquad \varphi \in H^2(\Omega),\ v \in H_h^1(\Omega), \tag{3.11}$$

and where $\boldsymbol{\mathcal{L}}$ is the differential operator defined in (1.1). Since $u = 0$ on $\partial\Omega$, and $u \in H^2(\Omega) \hookrightarrow C(\bar{\Omega})$, we have that $I_h u \in V_{0h}$. Thus, Theorem 3.1 leads to the estimate

$$\inf_{v_h \in V_{0h}} \|u - v_h\|_{1,h} \le \|u - I_h u\|_{1,h} \le Ch\|u\|_{2,\Omega}. \tag{3.12}$$

To estimate the error functional $d_h(\cdot,\cdot)$, we fix an arbitrary function $v = v_h \in V_{0h}$. Since $u \in H_0^1(\Omega) \cap H^2(\Omega)$ is the solution to (1.2), by integration by parts, we get

$$\begin{aligned} d_h(u, v) &= \sum_{R\in\tau_h} \int_R \left(a_1 \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + a_2 \frac{\partial u}{\partial y}\frac{\partial v}{\partial y} + a_3 \frac{\partial u}{\partial z}\frac{\partial v}{\partial z} + cuv - fv \right) dxdydz \\ &= \sum_{R\in\tau_h} \int_{\partial R} a_1 \frac{\partial u}{\partial x} v n_1\, dS + \sum_{R\in\tau_h} \int_{\partial R} a_2 \frac{\partial u}{\partial y} v n_2\, dS + \sum_{R\in\tau_h} \int_{\partial R} a_3 \frac{\partial u}{\partial z} v n_3\, dS \\ &\equiv I_1 + I_2 + I_3, \end{aligned} \tag{3.13}$$

where $n = (n_1, n_2, n_3)$ is the unit outer normal to the boundary ∂R of an element $R \in \tau_h$.

By virtue of the definition of the V_h^p- and V_h^a-approximations, we have

$$\begin{aligned} I_1 &\equiv \sum_{R\in\tau_h} \int_{\partial R} a_1 \frac{\partial u}{\partial x} v n_1\, dS \\ &= \sum_{R\in\tau_h} \sum_{\text{face } F\subset\partial R} \int_F a_1 \frac{\partial u}{\partial x} \left[v - T_F(v)\right] n_1 dS \\ &= \sum_{R\in\tau_h} \sum_{\text{face } F\subset\partial R} \int_F \left(a_1 - \fint_R a_1 dxdydz \right) \frac{\partial u}{\partial x} \left[v - T_F(v)\right] n_1 dS \\ &\quad + \sum_{R\in\tau_h} \sum_{\text{face } F\subset\partial R} \left(\fint_R a_1 dxdydz \right) \int_F \frac{\partial u}{\partial x} \left[v - T_F(v)\right] n_1 dS \\ &\equiv I_4 + I_5. \end{aligned} \tag{3.14}$$

It follows from the Cauchy-Schwarz inequality, Lemma 3.4 and Lemma 3.5 that

$$\begin{aligned} |I_4| &\equiv \left| \sum_{R\in\tau_h} \sum_{\text{face } F\subset\partial R} \int_F \left(a_1 - \fint_R a_1 dxdydz \right) \frac{\partial u}{\partial x} \left[v - T_F(v)\right] n_1 dS \right| \\ &\le Ch\, \|u\|_{2,\Omega} \|v\|_{1,h}. \end{aligned} \tag{3.15}$$

To estimate I_5, we first consider the V_h^a-approximation. In this case, since $T_F(v) = \fint_F v\, dS$, by the Cauchy-Schwarz inequality and Lemma 3.4, we have

$$\begin{aligned} |I_5| &\equiv \left| \sum_{R\in\tau_h} \sum_{\text{face } F\subset\partial R} \left(\fint_R a_1 dxdydz \right) \int_F \frac{\partial u}{\partial x} \left[v - T_F(v)\right] n_1 dS \right| \\ &= \left| \sum_{R\in\tau_h} \sum_{F\subset\partial R} \left(\fint_R a_1 dxdydz \right) \int_F \left[\frac{\partial u}{\partial x} - T_F(\frac{\partial u}{\partial x}) \right] \left[v - T_F(v)\right] n_1 dS \right| \\ &\le Ch\, \|u\|_{2,\Omega} \|v\|_{1,h}. \end{aligned} \tag{3.16}$$

In the case of the V_h^p-approximation, we fix an element $R = [a-r, a+r] \times [b-s, b+s] \times [c-t, c+t] \in \tau_h$ and consider its two opposite faces $F_\pm = \{a \pm r\} \times [b-s, b+s] \times [c-t, c+t]$ with $n_1 = n_\pm = \pm 1$. We then have by (2.10), by the Cauchy-Schwarz inequality, and by the quasi-uniformity of the partitions τ_h that

$$
\begin{aligned}
&\left| \int_{F_+} \frac{\partial u}{\partial x} \left[v - T_{F_+}(v) \right] n_+ dS + \int_{F_-} \frac{\partial u}{\partial x} \left[v - T_{F_-}(v) \right] n_- dS \right| \\
&\quad = \left| \int_{b-s}^{b+s} \int_{c-t}^{c+t} \frac{\partial u(a+r,y,z)}{\partial x} \left[v(a+r,y,z) - v(a+r,b,c) \right] dydz \right. \\
&\qquad \left. - \int_{b-s}^{b+s} \int_{c-t}^{c+t} \frac{\partial u(a-r,y,z)}{\partial x} \left[v(a-r,y,z) - v(a-r,b,c) \right] dydz \right| \\
&\quad = \left| \int_{b-s}^{b+s} \int_{c-t}^{c+t} \left[\frac{\partial u(a+r,y,z)}{\partial x} - \frac{\partial u(a-r,y,z)}{\partial x} \right] \right. \\
&\qquad \left. \cdot \left[\int_b^y \frac{\partial v(a+r,y',z)}{\partial y} dy' + \int_c^z \frac{\partial v(a+r,b,z')}{\partial z} dz' \right] dydz \right| \\
&\quad \le Ch^{-2} \|u\|_{2,1,R} \|v\|_{1,1,R} \le Ch \|u\|_{2,R} \|v\|_{1,R}.
\end{aligned} \tag{3.17}
$$

Consequently, by rearranging the terms in the summation I_5, we obtain the estimate for the V_h^p-approximation

$$
|I_5| \le Ch \|u\|_{2,\Omega} \|v\|_{1,h}. \tag{3.18}
$$

It follows from (3.14)–(3.18) that

$$
|I_1| \le Ch \|u\|_{2,\Omega} \|v\|_{1,h}.
$$

Similar estimates hold for I_2 and I_3. We then obtain by (3.11) and (3.13) the following estimate

$$
\begin{aligned}
|d_h(u, v_h)| &\equiv |a_h(u, v_h) - (\boldsymbol{\mathcal{L}} u, v_h)| \\
&\le Ch \|u\|_{2,\Omega} \|v_h\|_{1,h}, \qquad \forall v_h \in V_{0h}.
\end{aligned} \tag{3.19}
$$

This, together with (3.10) and (3.12), leads to (3.3) with $m = 1$. The first part of the proof of the theorem is finished.

Proof of the L^2 error estimate. We follow the nonconforming version of the Aubin-Nitsche argument [21, 23]. Let $g \in L^2(\Omega)$. By Theorem 1.1, there exists a unique $\varphi_g \in H_0^1(\Omega) \cap H^2(\Omega)$ such that

$$
\begin{aligned}
L\varphi_g &= g, &&\text{in } \Omega, \\
u &= 0, &&\text{on } \partial\Omega,
\end{aligned} \tag{3.20}
$$

which by Theorem 1.1 satisfies

$$
\|\varphi_g\|_{2,\Omega} \le C \|g\|_{0,\Omega}. \tag{3.21}
$$

It is easy to verify, for any $\psi_h \in V_{0h}$, that

$$(u-u_h, g) = a_h(u-u_h, \varphi_g - \psi_h) - d_h(u, \varphi_g - \psi_h) - d_h(\varphi_g, u-u_h).$$

Consequently,

(3.22)

$$\begin{aligned}\|u-u_h\|_{0,\Omega} &= \sup_{0\neq g\in L^2(\Omega)} \frac{(u-u_h,g)}{\|g\|_{0,\Omega}} \\ &\leq \sup_{0\neq g\in L^2(\Omega)} \frac{1}{\|g\|_{0,\Omega}} \inf_{\psi_h\in V_{0h}} \big[|a_h(u-u_h,\varphi_g-\psi_h)| \\ &\qquad + |d_h(u,\varphi_g-\psi_h)| + |d_h(\varphi_g,u-u_h)|\,\big].\end{aligned}$$

Fix $g \in L^2(\Omega)$. Let $W_{0h} \subset C(\bar{\Omega}) \cap H_0^1(\Omega)$ be the trilinear finite element space over the partition τ_h. Denote by $Q_h : C(\bar{\Omega}) \longrightarrow W_{0h}$ the corresponding trilinear interpolation operator. We choose $\psi_h = I_h(Q_h\varphi_g) \in V_{0h}$. By the H_h^1 error estimate, Theorem 3.1, the well-known interpolation properties of the operator Q_h [7], and (3.21), we have

$$\begin{aligned}|a_h(u-u_h,\varphi_g-\psi_h)| &\leq C\,\|u-u_h\|_{1,h}\,\|\varphi_g-\psi_h\|_{1,h} \\ &\leq Ch\,\|u\|_{2,\Omega}\Big(\|\varphi_g-Q_h\varphi_g\|_{1,\Omega} + \|Q_h\varphi_g - I_h(Q_h\varphi_g)\|_{1,h}\Big) \\ &\leq Ch^2\|u\|_{2,\Omega}\Big(\|\varphi_g\|_{2,\Omega} + \|Q_h\varphi_g\|_{2,h}\Big) \leq\ Ch^2\,\|u\|_{2,\Omega}\,\|g\|_{0,\Omega}. \qquad (3.23)\end{aligned}$$

Since $Q_h\varphi_g \in H_0^1(\Omega)$ and $u \in H_0^1(\Omega)\cap H^2(\Omega)$ is the solution to (1.2), by denoting $\chi_h = Q_h\varphi_g - \psi_h$, we have

$$\begin{aligned}d_h(u,\varphi_g-\psi_h) &= d_h(u,Q_h\varphi_g-\psi_h) \\ &= \sum_{R\in\tau_h}\int_{\partial R}\left[a_1\frac{\partial u}{\partial x}\chi_h n_1 + a_2\frac{\partial u}{\partial y}\chi_h n_2 + a_3\frac{\partial u}{\partial z}\chi_h n_3\right] dS \qquad (3.24)\\ &\equiv J_1 + J_2 + J_3.\end{aligned}$$

On a face $F \subset \partial R$ for an element $R \in \tau_h$, we have by (3.9) that $⨍_F \chi_h dS = 0$. Hence, since $Q_h\varphi_g \in C(\bar{\Omega})$, by the same argument as in the proof of the H_h^1 error estimate (cf. (3.14), (3.16)) we have

$$\begin{aligned}J_1 &\equiv \sum_{R\in\tau_h}\int_{\partial R} a_1\frac{\partial u}{\partial x}\chi_h n_1\,dS = \sum_{R\in\tau_h}\sum_{\text{face } F\subset\partial R}\int_F a_1\frac{\partial u}{\partial x}\,\chi_h n_1\,dS \\ &= \sum_{R\in\tau_h}\sum_{\text{face } F\subset\partial R}\int_F\left(a_1-\bar{a}_1^R\right)\frac{\partial u}{\partial x}\chi_h n_1\,dS \\ &\quad + \sum_{R\in\tau_h}\sum_{\text{face } F\subset\partial R}\bar{a}_1^R\int_F\left(\frac{\partial u}{\partial x} - ⨍_F\frac{\partial u}{\partial x}\,dS\right)\chi_h n_1\,dS \\ &= \sum_{R\in\tau_h}\sum_{\text{face } F\subset\partial R}\int_F\left(a_1-\bar{a}_1^R\right)\frac{\partial u}{\partial x}\left(\chi_h - ⨍_F\chi_h\,dS\right)n_1\,dS \\ &\quad + \sum_{R\in\tau_h}\sum_{\text{face } F\subset\partial R}\bar{a}_1^R\int_F\left(\frac{\partial u}{\partial x} - ⨍_F\frac{\partial u}{\partial x}\,dS\right)\left(\chi_h - ⨍_F\chi_h\,dS\right)n_1\,dS\end{aligned}$$

where

$$\bar{a}_1^R = \fint_R a_1 dxdydz.$$

Therefore, by Lemma 3.4, the Cauchy-Schwarz inequality, Theorem 3.1, the properties of the operator Q_h, and (3.21), we get

$$(3.25)\quad \begin{aligned} |J_1| &\le C \sum_{R\in\tau_h} \sum_{\text{face } F\in\partial R} \left(h\|\nabla u\|_{0,F} + \left\| \frac{\partial u}{\partial x} - \fint_F \frac{\partial u}{\partial x} dS \right\|_{0,F} \right) \left\| \chi_h - \fint_F \chi_h dS \right\|_{0,F} \\ &\le Ch\|u\|_{2,\Omega}\|\chi_h\|_{1,h} \le Ch^2\|u\|_{2,\Omega}\| \, \|\varphi_g\|_{2,\Omega} \le Ch^2\|u\|_{2,\Omega}\|g\|_{0,\Omega}. \end{aligned}$$

Similarly,

$$(3.26)\qquad |J_2| + |J_3| \le Ch^2\|u\|_{2,\Omega}\|g\|_{0,\Omega}.$$

Now it follows from the fact $Q_h u \in H_0^1(\Omega)$ that

$$(3.27)\quad d_h(\varphi_g, u - u_h) = d_h(\varphi_g, Q_h u - I_h Q_h u) + d_h(\varphi_g, I_h Q_h u - u_h) \equiv J_4 + J_5.$$

By the same argument used in estimating $d_h(u, \varphi_g - \psi_h)$ (cf. (3.24)–(3.26)), we obtain

$$(3.28)\quad \begin{aligned} |J_4| &\equiv |d_h(\varphi_g, Q_h u - I_h Q_h u)| \\ &\le Ch^2 \|\varphi_g\|_{2,\Omega} \|Q_h u\|_{2,h} \le Ch^2 \|g\|_{0,\Omega} \|u\|_{2,\Omega}. \end{aligned}$$

Denote $v = I_h Q_h u - u_h \in V_{0h}$. Replacing u by φ_g in (3.19), by the H_h^1 error estimate, Theorem 3.1, the known properties of the operator Q_h and (3.21), we then have

$$(3.29)\quad \begin{aligned} |J_5| &\equiv |d_h(\varphi_g, v)| \le Ch \|\varphi_g\|_{2,\Omega} \|v\|_{1,h} \\ &\le Ch\|g\|_{0,\Omega} (\|I_h Q_h u - Q_h u\|_{1,h} + \|Q_h u - u\|_{1,\Omega} + \|u - u_h\|_{1,h}) \\ &\le Ch^2 \|u\|_{2,\Omega} \|g\|_{0,\Omega}. \end{aligned}$$

Finally, the L^2 error estimate (3.3) with $m = 0$ is a direct consequence of (3.22)–(3.29). □

4. Connection with multilinear finite elements

In the previous proof, we made use of the piecewise linear function $I_h Q_h u$ several times as an approximation function of u. This makes some connection between the considered nonconforming elements and the conforming multilinear elements. Furthermore, it is in fact true that all the piecewise linear functions in V_{0h} approximate the solution u well enough.

To be more precise, let $W_{0h} \subset C(\bar{\Omega}) \cap H_0^1(\Omega)$ be again the trilinear finite element space over the mesh τ_h. By the proof of Lemma 3.6, we know that all the functions in the subspace $I_h W_{0h} \subset V_{0h}$ are piecewise linear functions. Furthermore, by taking the boundary condition into account, it is easy to see that the operator $I_h : W_{0h} \longrightarrow I_h W_{0h}$ is in fact one-to-one and onto. Thus, the subspace $I_h W_{0h} \subset V_{0h}$

has the same number of degrees of freedom as the trilinear finite element space W_{0h} does. Now by the Lax-Milgram lemma, there exists a unique $\bar{u}_h \in I_h W_{0h}$ such that

$$a_h(\bar{u}_h, v_h) = (f, v_h), \qquad \forall v_h \in I_h W_{0h}. \tag{4.1}$$

We realize that $\bar{u}_h$ is in fact the projection of the finite element solution $u_h \in V_{0h}$ into the subspace $I_h W_{0h}$, since by (3.2) and (4.1), we have

$$a_h(u_h - \bar{u}_h, v_h) = 0, \qquad \forall v_h \in I_h W_{0h}. \tag{4.2}$$

Now let us write the error

$$u - \bar{u}_h = \left(u - I_h u_h^t\right) + \left(I_h u_h^t - \bar{u}_h\right), \tag{4.3}$$

where $u_h^t \in W_{0h}$ is the trilinear finite element approximation of u, i.e.,

$$a\left(u_h^t, w_h\right) = (f, w_h), \qquad \forall w_h \in W_{0h}. \tag{4.4}$$

By the known results on this approximation u_h^t [7], and by Theorem 3.1, we get

$$\|u - I_h u_h^t\|_{1,h} \le \left\|u - u_h^t\right\|_{1,\Omega} + \left\|u_h^t - I_h u_h^t\right\|_{1,h} \le Ch\|u\|_{2,\Omega}. \tag{4.5}$$

Notice that $\lambda_h \equiv I_h u_h^t - \bar{u}_h \in I_h W_{0h} \subset V_{0h}$. By (3.1), (4.5), (3.19) and the known results on u_h^t, we have

$$\begin{aligned} \alpha\|\lambda_h\|_{1,h}^2 \le a_h(\lambda_h, \lambda_h) = {} & a_h\left(I_h u_h^t - u, \lambda_h\right) + a_h(u - \bar{u}_h, \lambda_h) \\ \le {} & C\left\|I_h u_h^t - u\right\|_{1,h} \|\lambda_h\|_{1,h} + |d_h(u, \lambda_h)| \le Ch\|u\|_{2,\Omega}\|\lambda_h\|_{1,h}. \end{aligned} \tag{4.6}$$

It follows from (4.3)–(4.6) that

$$\|u - \bar{u}_h\|_{1,h} \le Ch\|u\|_{2,\Omega}. \tag{4.7}$$

Now, by the definition of $d_h(\cdot,\cdot)$ (cf. (3.11)) and (4.2), we have for any $g \in L^2(\Omega)$ and any $\psi_h \in I_h W_{0h}$ that

$$\begin{aligned} (u - \bar{u}_h, g) = {} & (u - u_h, g) + (u_h - \bar{u}_h, g) \\ = {} & (u - u_h, g) + a_h(u_h - \bar{u}_h, \varphi_g - \psi_h) - d_h(\varphi_g, u_h - \bar{u}_h). \end{aligned} \tag{4.8}$$

Setting $\psi_h = I_h Q_h \varphi_g \in I_h W_{0h}$ in (4.8), we have

$$\begin{aligned} & |a_h(u_h - \bar{u}_h, \varphi_g - \psi_h)| \le C\|u_h - \bar{u}_h\|_{1,h} \|\varphi_g - I_h Q_h \varphi_g\|_{1,h} \\ & \le C\left(\|u_h - u\|_{1,h} + \|u - \bar{u}_h\|_{1,h}\right)\left(\|\varphi_g - Q_h\varphi_g\|_{1,h} + \|Q_h\varphi_g - I_h Q_h \varphi_g\|_{1,h}\right) \\ & \qquad \le Ch^2\|u\|_{2,\Omega}\left(\|\varphi_g\|_{2,\Omega} + \|Q_h\varphi_g\|_{2,\Omega}\right) \le Ch^2\|u\|_{2,\Omega}\|g\|_{0,\Omega}, \end{aligned} \tag{4.9}$$

where we used the known properties of Q_h, Theorem 3.1, Theorem 3.3, (4.7) and (3.21). Replacing u by φ_g in (3.19), we then get by (3.21), Theorem 3.1 and (4.7) that

$$\begin{aligned} |d_h(\varphi_g, u_h - \bar{u}_h)| & \le Ch\|\varphi_g\|_{2,\Omega}\|u_h - \bar{u}_h\|_{1,h} \\ & \le Ch\|g\|_{0,\Omega}(\|u_h - u\|_{1,h} + \|u - \bar{u}_h\|_{1,h}) \\ & \le Ch^2\|u\|_{2,\Omega}\|g\|_{0,\Omega}. \end{aligned} \tag{4.10}$$

We have in fact proved, by (4.7)–(4.10) and Theorem 3.3, the following

Theorem 4.1. *Let $u \in H_0^1(\Omega) \cap H^2(\Omega)$ and $\bar{u}_h \in I_h W_{0h}$ be the solutions to* (1.2) *and* (4.1)*, respectively. Then,*

$$\|u - \bar{u}_h\|_{0,\Omega} + h\|u - \bar{u}_h\|_{1,h} \le Ch^2\|u\|_{2,\Omega}.$$

5. A superconvergence estimate

We first give a superconvergence estimate for the interpolation error gradients. Denote by C_R the center of a rectangular element $R \in \tau_h$.

Lemma 5.1. *For any $R \in \tau_h$, we have*

$$|\nabla(v - I_h v)(C_R)| \leq Ch^2 |v|_{3,\infty,R}, \qquad \forall v \in W^{3,\infty}(R). \tag{5.1}$$

Proof. Let $\hat{R} = [-1,1] \times [-1,1] \times [-1,1]$. Define: $\hat{F} : W^{3,\infty}(\hat{R}) \longrightarrow \mathbb{R}$ by

$$\hat{F}(\hat{v}) = \partial_\xi(\hat{v} - \hat{I}\hat{v})(O), \qquad \hat{v} \in W^{3,\infty}(\hat{R}),$$

where $O = (0,0,0)$ and $\hat{I}$ is the interpolation operator over $\hat{R}$ for the considered elements. By the imbedding $W^{3,\infty}(\hat{R}) \hookrightarrow C^1(\hat{R})$, we have

$$\left|\hat{F}(\hat{v})\right| \leq C \left\|\hat{v}\right\|_{3,\infty,\hat{R}}, \qquad \hat{v} \in W^{3,\infty}(\hat{R}). \tag{5.2}$$

Now the basis functions for our elements over $\hat{R}$ can be easily obtained by setting $a = b = c = 0$ and $r = s = t = 1$ in (2.4) and (2.6), respectively. By their properties (cf. (2.3), (2.7)) and by the Taylor expansion, a series of calculations then lead to

$$\hat{F}(\hat{p}) = 0, \qquad \forall \hat{p} \in P_2(\hat{R}), \tag{5.3}$$

where $P_2(\hat{R})$ is the set of all polynomials over $\hat{R}$ with degrees at most 2. It follows from (5.2), (5.3) and the Bramble-Hilbert lemma that

$$\left|\hat{F}(\hat{v})\right| \leq C \left|\hat{v}\right|_{3,\infty,\hat{R}}, \qquad \hat{v} \in W^{3,\infty}(\hat{R}).$$

This, together with the affine transformation from $\hat{R}$ to R (cf. (3.7)), leads to

$$|\partial_x(v - I_h v)(C_R)| \leq Ch^{-1} \left|\hat{F}(\hat{v})\right| \leq Ch^2 \left|v\right|_{3,\infty,R}.$$

Similar estimates hold for $\partial_y(v - I_h v)$ and $\partial_z(v - I_h v)$. □

In the rest of this section, we will only consider the V_h^a-approximation, i.e., the averaged element approximation, to the solution of the model problem

$$\begin{aligned} -\Delta u &= f, \qquad \text{in } \Omega, \\ u &= 0, \qquad \text{on } \partial\Omega. \end{aligned} \tag{5.4}$$

The following result shows that the nonconforming error functional $d_h(\cdot,\cdot)$, as defined in (3.11), is of one order higher than usual. Hence the nonconformity, in this case, is weak.

Lemma 5.2. *Let $u \in H_0^1(\Omega) \cap W^{3,\infty}(\Omega)$ be the solution to* (5.4). *Then,*

$$|d_h(u, v_h)| \leq Ch^2 \|u\|_{3,\infty,\Omega} \|v_h\|_{1,h}, \qquad \forall v_h \in V_{0h}^a. \tag{5.5}$$

Proof. Fix $v = v_h \in V_{0h}^a$. We have as before that

$$d_h(u, v) = \sum_{R \in \tau_h} \int_{\partial R} \left(\frac{\partial u}{\partial x} v n_1 + \frac{\partial u}{\partial y} v n_2 + \frac{\partial u}{\partial z} v n_3 \right) dS \equiv K_1 + K_2 + K_3. \tag{5.6}$$

By virtue of the V_{0h}^a-approximation, we can further write

$$\begin{aligned} K_1 &\equiv \sum_{R \in \tau_h} \int_{\partial R} \frac{\partial u}{\partial x} v n_1 dS \\ &= \sum_{R \in \tau_h} \sum_{\text{face } F \in \partial R} \int_F \left[\frac{\partial u}{\partial x} - \frac{\partial u(M_F)}{\partial x} \right] \left[v - T_F(v) \right] n_1 dS, \end{aligned} \tag{5.7}$$

where M_F is the center of a face F. Fix $R = [a-r, a+r] \times [b-s, b+s] \times [c-t, c+t] \in \tau_h$ and consider its two opposite faces $F_\pm = \{a \pm r\} \times [b-s, b+s] \times [c-t, c+t]$ with $n_1 = n_\pm = \pm 1$. An application of the Bramble-Hilbert lemma leads to the estimate

$$\int_R \left[\frac{\partial^2 u(x,y,z)}{\partial x^2} - \frac{\partial^2 u(x,b,c)}{\partial x^2} \right]^2 dxdydz \leq Ch^5 \|u\|_{3,\infty,R}^2. \tag{5.8}$$

It then follows from (2.10), the Cauchy-Schwarz inequality, (5.8) and Lemma 3.5, that

$$\begin{aligned} &\left| \int_{F_+} \left[\frac{\partial u}{\partial x} - \frac{\partial u(M_{F_+})}{\partial x} \right] \left[v - T_{F_+}(v) \right] n_+ dS \right. \\ &\qquad \left. + \int_{F_-} \left[\frac{\partial u}{\partial x} - \frac{\partial u(M_{F_-})}{\partial x} \right] \left[v - T_{F_-}(v) \right] n_- dS \right| \\ &= \left| \int_{b-s}^{b+s} \int_{c-t}^{c+t} \left\{ \left[\frac{\partial u(a+r,y,z)}{\partial x} - \frac{\partial u(a+r,b,c)}{\partial x} \right] \right. \right. \\ &\qquad \left. \left. - \left[\frac{\partial u(a-r,y,z)}{\partial x} - \frac{\partial u(a-r,b,c)}{\partial x} \right] \right\} \left[v(a+r,y,z) - T_{F_+}(v) \right] dydz \right| \\ &= \left| \int_{b-s}^{b+s} \int_{c-t}^{c+t} \left\{ \int_{a-r}^{a+r} \left[\frac{\partial^2 u(x,y,z)}{\partial x^2} - \frac{\partial^2 u(x,b,c)}{\partial x^2} \right] dx \right\} \right. \\ &\qquad \left. \cdot \left[v(a+r,y,z) - T_{F_+}(v) \right] dydz \right| \\ &\leq Ch^{\frac{7}{2}} \|u\|_{3,\infty,\Omega} \|v\|_{1,R}. \end{aligned}$$

Consequently, by a rearrangement of the terms in the summation K_1, we have

$$|K_1| \leq Ch^{\frac{7}{2}} \|u\|_{3,\infty,\Omega} \sum_{R \in \tau_h} \|v\|_{1,R} \leq Ch^2 \|u\|_{3,\infty,\Omega} \|v\|_{1,h},$$

where we also used the Cauchy-Schwarz inequality and the fact that

$$|\tau_h| \equiv \sum_{R \in \tau_h} 1 \leq Ch^{-3}. \tag{5.9}$$

In the two-dimensional case, h^{-3} should be replaced by h^{-2}. Similar estimates hold for K_2 and K_3 as well. Hence, (5.5) follows. □

Lemma 5.3. *Let $u \in H_0^1(\Omega) \cap W^{3,\infty}(\Omega)$ be the solution to* (5.4) *and $u_h \in V_{0h}^a$ its V_{0h}^a-approximation. Assume that all the elements in τ_h are cubes. Then*

$$\|I_h u - u_h\|_{1,h} \le Ch^2 \|u\|_{3,\infty,\Omega}. \tag{5.10}$$

Proof. Denote $\gamma_h \equiv I_h u - u_h \in V_{0h}^a$. Since each element in τ_h is assumed to be a cube, it is easy to see that γ_h is piecewise harmonic. On the other hand, since $I_h = I_h^a$ is the interpolation operator for the V_h^a-approximation, we have

$$\int_F (I_h u - u)\, dS = 0, \qquad \forall \, \text{faces}\, F \subset \partial R, \, \forall R \in \tau_h.$$

It then follows from (2.10) that

$$\begin{aligned} a_h(I_h u - u, \gamma_h) &= \sum_{R \in \tau_h} \int_R \nabla(I_h u - u) \nabla \gamma_h dxdydz \\ &= \sum_{R \in \tau_h} \sum_{\text{face}\, F \in \partial R} \left[\int_F (I_h u - u) \frac{\partial \gamma_h}{\partial x} n_1 dS \right. \\ &\quad \left. + \int_F (I_h u - u) \frac{\partial \gamma_h}{\partial y} n_2 dS + \int_F (I_h u - u) \frac{\partial \gamma_h}{\partial z} n_3 dS \right] = 0. \end{aligned} \tag{5.11}$$

Now, by (3.1), (5.11) and Lemma 5.2, we have

$$\begin{aligned} \alpha \|\gamma_h\|_{1,h}^2 &\le a_h(\gamma_h, \gamma_h) = a_h(I_h u - u_h, \gamma_h) \\ &= a_h(u - u_h, \gamma_h) = d_h(u, \gamma_h) \le Ch^2 \|u\|_{3,\infty,\Omega} \|\gamma_h\|_{1,h}, \end{aligned}$$

leading to (5.10). □

Now we present the main result in this section.

Theorem 5.4. *With the same assumption as in Lemma* 5.3, *we have*

$$\left[\sum_{R \in \tau_h} |\nabla(u - u_h)(C_R)|^2 h^3 \right]^{\frac{1}{2}} \le Ch^2 \|u\|_{3,\infty,\Omega}. \tag{5.12}$$

Proof. By Lemma 5.1, Theorem 3.2 and Lemma 5.3, we have

$$\begin{aligned} &\left[\sum_{R \in \tau_h} |\nabla(u - u_h)(C_R)|^2 h^3 \right]^{\frac{1}{2}} \\ &\qquad \le C \left[\sum_{R \in \tau_h} |\nabla(u - I_h u)(C_R)|^2 h^3 + \sum_{R \in \tau_h} |\nabla(I_h u - u_h)(C_R)|^2 h^3 \right]^{\frac{1}{2}} \\ &\qquad \le C \left[h^4 \|u\|_{3,\infty,\Omega}^2 + h^3 \sum_{R \in \tau_h} \left(h^{-\frac{3}{2}} \|I_h u - u_h\|_{1,R} \right)^2 \right]^{\frac{1}{2}} \\ &\qquad \le Ch^2 \|u\|_{3,\infty,\Omega}, \end{aligned}$$

completing the proof. □

Now let us turn back to both the V_h^p- and V_h^a-approximations with general partitions of the solution to the general problem (1.1). Recall that $Q_h : C(\bar{\Omega}) \longrightarrow W_{0h}$ is the interpolation operator for the trilinear finite element. We can easily obtain, if the solution u is smooth, that

$$|\nabla (u - Q_h u)(C_R)| + |\nabla (u - I_h Q_h u)(C_R)| = O\left(h^2\right). \tag{5.13}$$

As discussed in §4, the considered elements are connected with the conforming multilinear finite elements through the subspace $I_h W_{0h}$. Thus, the estimate (5.13), Lemma 5.1 and the known superconvergence results (cf. [20]) on the multilinear elements naturally lead to a conjecture on the pointwise superconvergence estimates for the error of the gradient: if the solution u is smooth enough and the partitions τ_h are suitably regular, then

$$\max_{R\in\tau_h} |\nabla (u - u_h)(C_R)| = O\left(h^2\right). \tag{5.14}$$

In its discrete average form, the superconvergence estimate (5.12) for the simplest case makes the estimate (5.14) believable somewhat. However, compared with a recent work on higher-order error estimates on the nonconforming Wilson finite element [4], the proof or disproof of (5.14) will be more difficult since our elements do not have any conforming counterparts, though there is some connection between our elements and the conforming multilinear elements.

6. Effect of numerical integration

We define on the reference element $\hat{R} = [-1,1]\times[-1,1]\times[-1,1]$ the numerical integration scheme

$$\int_{\hat{R}} \hat{g}(\xi,\eta,\zeta)\, d\xi d\eta d\zeta \doteq \sum_{i=1}^{I} \hat{\omega}_i\, \hat{g}(\hat{Q}_i), \qquad \hat{g} \in C(\hat{R}), \tag{6.1}$$

where $\hat{\omega}_i > 0$, $\hat{Q}_i \equiv (\xi_i, \eta_i, \zeta_i) \in \hat{R}$, $i = 1, \ldots, I$, and I is a positive integer. Let us denote

$$\hat{P} = \mathrm{Span}\{\, 1, \xi,\, \eta,\, \zeta,\, \xi^2 - \eta^2,\, \xi^2 - \zeta^2 \,\}.$$

We shall assume that the quadrature scheme is exact on $\hat{P}$, i.e.,

$$\int_{\hat{R}} \hat{p}(\xi,\eta,\zeta)\, d\xi d\eta d\zeta = \sum_{i=1}^{I} \hat{\omega}_i \hat{p}(\hat{Q}_i), \qquad \hat{p} \in \hat{P}, \tag{6.2}$$

and that the set of quadrature points

$$\{\hat{Q}_i\}_{i=1}^{I} \text{ in (6.1) contains a } P_1(\hat{R})\text{-unsolvent subset}, \tag{6.3}$$

where $P_1(\hat{R})$ is the set of all linear polynomials over $\hat{R}$.

The conditions (6.2) and (6.3) are satisfied by the quadrature schemes

$$\begin{cases} \text{Scheme 1:} \quad I = 6, \text{ all } \hat{w}_i = \frac{4}{3}, \ \{\hat{Q}_i\}_{i=1}^6 = \{(\pm\hat{q}, 0, 0), (0, \pm\hat{q}, 0), (0, 0, \pm\hat{q})\}; \\ \text{Scheme 2:} \quad I = 8, \text{ all } \hat{w}_i = 1, \ \{\hat{Q}_i\}_{i=1}^8 = \{(\xi, \eta, \zeta) : \xi, \eta, \zeta = \pm\hat{q}\}, \end{cases}$$

where $0 < \hat{q} \le 1$. The computations for the dynamics of martensitic microstructure reported in [18] used Scheme 1 with $\hat{q} = 1$, in which case the nodes of the quadrature scheme are identical to the nodes of the finite element with respect to the V_h^p-approximation. Scheme 2 with $\hat{q} = 1/\sqrt{3}$ is the Gaussian quadrature over $\hat{R}$ with eight nodes of quadrature.

Now, for an element $R \equiv [a - r, a + r] \times [b - s, b + s] \times [c - t, c + t] \in \tau_h$, let $K_R : \hat{R} \longrightarrow R$ be the invertible affine mapping given by (3.7). Then, the quadrature scheme (6.1) induces automatically the following quadrature scheme over the element $R \in \tau_h$,

$$\int_R g(x, y, z)\, dxdydz \doteq \sum_{i=1}^{I} \omega_{i,R}\, g(Q_{i,R}), \qquad g \in C(R), \tag{6.4}$$

where

$$\omega_{i,R} = \det(\nabla K_R)\hat{w}_i, \quad Q_{i,R} = K_R(\hat{Q}_i), \qquad i = 1, \ldots, I. \tag{6.5}$$

To apply the numerical quadrature to the finite element formulation (3.2), in what follows we assume that in (1.1) $c \in C(\bar{\Omega})$ and $f \in C(\bar{\Omega})$. Let us now define $a_h^*(\cdot,\cdot) : V_h \times V_h \longrightarrow \mathbb{R}$ by

$$\begin{aligned} a_h^*(v_h, w_h) = \sum_{R\in\tau_h} \sum_{i=1}^{I} \omega_{i,R} \Bigg[\left(a_1 \frac{\partial v_h}{\partial x} \frac{\partial w_h}{\partial x} \right)(Q_{i,R}) + \left(a_2 \frac{\partial v_h}{\partial y} \frac{\partial w_h}{\partial y} \right)(Q_{i,R}) \\ + \left(a_3 \frac{\partial v_h}{\partial z} \frac{\partial w_h}{\partial z} \right)(Q_{i,R}) + (c v_h w_h)(Q_{i,R}) \Bigg], \quad v_h, w_h \in V_h, \end{aligned} \tag{6.6}$$

and define $f_h^* : V_h \longrightarrow \mathbb{R}$ by

$$f_h^*(v_h) = \sum_{R\in\tau_h} \sum_{i=1}^{I} \omega_{i,R}\, (f v_h)(Q_{i,R}), \qquad v_h \in V_h. \tag{6.7}$$

Obviously, $a_h^*(\cdot,\cdot)$ and $f_h^*(\cdot)$ are discrete approximations for $a_h(\cdot,\cdot)$ and $f_h(\cdot) \equiv (f, \cdot)$, respectively.

By the uniform V_{0h}-ellipticity of $a_h(\cdot,\cdot)$ given by (3.1) and the conditions (6.2) and (6.3), we have the following uniform V_{0h}-ellipticity of $a_h^*(\cdot,\cdot)$ (cf. Theorem 4.1.2 in [7]).

Lemma 6.1. *There exists a constant $\alpha^* > 0$, independent of h, such that*

$$a_h^*(v_h, v_h) \ge \alpha^* \|v_h\|_{1,h}^2, \qquad \forall v_h \in V_{0h}. \tag{6.8}$$

It is now a direct consequence of the Lax-Milgram lemma that there exists a unique $u_h^* \in V_{0h}$, the discrete solution to (1.2), such that

$$a_h^*(u_h^*, v_h) = f_h^*(v_h), \qquad \forall v_h \in V_{0h}. \tag{6.9}$$

Our main result in this section is that, with a certain smoothness of the coefficients in (1.1), the discrete solution $u_h^* \in V_{0h}$ converges to the exact solution $u \in H_0^1(\Omega) \cap H^2(\Omega)$ with the same rates as the solution $u_h \in V_{0h}$ does.

Theorem 6.2. *Assume that in* (1.1), *in addition,* $c \in W^{1,\infty}(\Omega)$ *and* $f \in W^{1,\infty}(\Omega)$. *Let* $u \in H_0^1(\Omega) \cap H^2(\Omega)$ *and* $u_h^* \in V_{0h}$ *be the solutions to* (1.2) *and* (6.9), *respectively. Then,*

$$\|u - u_h^*\|_{1,h} \le Ch\|f\|_{1,\infty,\Omega}. \tag{6.10}$$

Theorem 6.3. *If the coefficients* a_1, a_2, a_3, *and* c, *and the term* f *are all in* $W^{2,\infty}(\Omega)$, *then*

$$\|u - u_h^*\|_{0,\Omega} \le Ch^2\|f\|_{2,\infty,\Omega}. \tag{6.11}$$

To prove these two theorems, we need to estimate the errors induced by the quadrature schemes (6.1) and (6.4). Thus, we first define the quadrature error functionals

$$\hat{E}(\hat{g}) \equiv \int_{\hat{R}} \hat{g}\, d\xi d\eta d\zeta - \sum_{i=1}^{I} \hat{\omega}_i\, \hat{g}(\hat{Q}_i), \quad \hat{g} \in C(\hat{R}) \tag{6.12}$$

and

$$E_R(g) \equiv \int_R g\, dxdydz - \sum_{i=1}^{I} \omega_{i,R}\, g(Q_{i,R}), \quad g \in C(R),\ R \in \tau_h. \tag{6.13}$$

Obviously,

$$E_R(g) = \det(\nabla K_R)\hat{E}(\hat{g}), \qquad \hat{g} = g \circ K_R \in C(\hat{R}). \tag{6.14}$$

Recall that P_R is the finite element polynomial space over the element $R \in \tau_h$ (cf. (2.1)).

Lemma 6.4. *Let* a_1, a_2, a_3 *and* c *be given in* (1.1). *Suppose* $c \in W^{1,\infty}(\Omega)$. *Then, for any* $R \in \tau_h$ *and any* $v, w \in P_R$, *we have*

$$\begin{aligned} &\left|E_R\left(a_1 \frac{\partial v}{\partial x}\frac{\partial w}{\partial x}\right)\right| + \left|E_R\left(a_2 \frac{\partial v}{\partial y}\frac{\partial w}{\partial y}\right)\right| + \left|E_R\left(a_3 \frac{\partial v}{\partial z}\frac{\partial w}{\partial z}\right)\right| + |E_R(cvw)| \\ &\qquad \le\ Ch\|v\|_{2,R}\|w\|_{1,R}. \end{aligned} \tag{6.15}$$

Proof. Let $R \equiv [a-r, a+r] \times [b-s, b+s] \times [c-t, c+t]$. As before, let the mapping $K_R : \hat{R} \longrightarrow R$ be defined by (3.7). Write $\hat{\varphi} = \varphi \circ K_R$ for $\varphi \in W^{1,\infty}(R)$. Since the L^∞ and L^2 norms are equivalent on the finite-dimensional space $P_{\hat{R}}$, we have that

$$\left|\hat{E}(\hat{\varphi}\hat{p})\right| \le C\, \|\hat{\varphi}\|_{1,\infty,\hat{R}}\, \|\hat{p}\|_{0,\hat{R}}\,, \quad \forall \hat{\varphi} \in W^{1,\infty}(\hat{R}),\ \hat{p} \in P_{\hat{R}}. \tag{6.16}$$

Replacing $\hat{\varphi}$ in (6.16) by $\hat{\varphi} + \hat{c}$ with $\hat{c}$ an arbitrary constant, by (6.2) we obtain

$$\begin{aligned} \left|\hat{E}\left(\hat{\varphi}\hat{p}\right)\right| &\le C \inf_{\hat{c}=\text{constant}} \|\hat{\varphi} + \hat{c}\|_{1,\infty,\hat{R}}\, \|\hat{p}\|_{0,\hat{R}} \\ &\le\ C\, |\hat{\varphi}|_{1,\infty,\hat{R}}\, \|\hat{p}\|_{0,\hat{R}}\,, \qquad \forall \hat{\varphi} \in W^{1,\infty}(\hat{R}),\ \hat{p} \in P_{\hat{R}}. \end{aligned} \tag{6.17}$$

Now let $a \in \{a_1, a_2, a_3, c\}$, $q \in \{v, \frac{\partial v}{\partial x}, \frac{\partial v}{\partial y}\}$, and $p \in \{w, \frac{\partial w}{\partial x}, \frac{\partial w}{\partial y}\}$, where $v,\ w \in P_R$. Note that $\frac{\partial w}{\partial x}, \frac{\partial w}{\partial y} \in P_R$ if $w \in P_R$. Setting $\hat{\varphi} = \hat{a}\hat{q}$ in (6.17), by (6.14), (3.7) and Theorem 3.2, we get

$$\begin{aligned} |E_R(aqp)| &\le\ Ch^3 \left|\hat{E}\left(\hat{a}\hat{q}\hat{p}\right)\right| \le\ Ch^3\, |\hat{a}\hat{q}|_{1,\infty,\hat{R}}\, \|\hat{p}\|_{0,\hat{R}} \le\ Ch^{\frac{5}{2}}\, \|aq\|_{1,\infty,R}\|p\|_{0,R} \\ &\le\ Ch^{\frac{5}{2}}\|q\|_{1,\infty,R}\|p\|_{0,R} \le\ Ch\|q\|_{1,R}\|p\|_{0,R} \le\ Ch\|v\|_{2,R}\|w\|_{1,R}. \end{aligned} \tag{6.18}$$

This proves (6.15). □

Lemma 6.5. *Suppose $f \in W^{1,\infty}(\Omega)$. Then, for any $R \in \tau_h$ and any $v \in P_R$, we have*

$$|E_R(fv)| \le Ch^{\frac{5}{2}} \|f\|_{1,\infty,R} \|v\|_{1,R}. \tag{6.19}$$

Proof. Since $\hat{E}(\hat{\varphi}) = 0$ for any constant polynomial $\hat{\varphi}$, by the Bramble-Hilbert lemma we have

$$\left|\hat{E}\left(\hat{\varphi}\right)\right| \le C \left|\hat{\varphi}\right|_{1,\infty,\hat{R}}, \qquad \forall\, \hat{\varphi} \in W^{1,\infty}(\hat{R}).$$

Taking $\hat{\varphi} = \hat{f}\hat{v}$, by (6.14) and Theorem 3.2 we have

$$\begin{aligned} |E_R(fv)| &\le Ch^3 \left|\hat{E}\left(\hat{f}\hat{v}\right)\right| \le Ch^3 \left|\hat{f}\hat{v}\right|_{1,\infty\hat{R}} \le Ch^4 \left|fv\right|_{1,\infty,R} \\ &\le Ch^4 \|f\|_{1,\infty,R} \|v\|_{1,\infty,R} \le Ch^{\frac{5}{2}} \|f\|_{1,\infty,R} \|v\|_{1,R}, \end{aligned}$$

completing the proof. □

Lemma 6.6. *Let $R \in \tau_h$ and $a \in W^{2,\infty}(R)$. Then for any $v, w \in P_R$ we have*

$$|E_R(av)| \le Ch^{\frac{7}{2}} \|a\|_{2,\infty,R} \|v\|_{2,R}, \tag{6.20}$$

$$|E_R(avw)| \le Ch^2 \|a\|_{2,\infty,R} \|v\|_{2,R} \|w\|_{2,R}. \tag{6.21}$$

Proof. By (6.12) and the imbedding $H^2(\hat{R}) \hookrightarrow C(\hat{R})$, we have

$$\left|\hat{E}(\hat{a}\hat{v})\right| \le C \left\|\hat{a}\hat{v}\right\|_{2,\hat{R}}. \tag{6.22}$$

By (6.14), (6.2), the Bramble-Hilbert lemma, and (3.7), we thus get

$$|E_R(av)| \le Ch^3 \left|\hat{a}\hat{v}\right|_{2,\hat{R}} \le Ch^{\frac{7}{2}} |av|_{2,R} \le Ch^{\frac{7}{2}} \|a\|_{2,\infty,R} \|v\|_{2,R}, \tag{6.23}$$

obtaining (6.20). Now, replacing a in (6.20) by aw, we have, by Theorem 3.2, that

$$\begin{aligned} |E_R(avw)| &\le Ch^{\frac{7}{2}} \|aw\|_{2,\infty,R} \|v\|_{2,R} \le Ch^{\frac{7}{2}} \|a\|_{2,\infty,R} \|w\|_{2,\infty,R} \|v\|_{2,R} \\ &\le Ch^2 \|a\|_{2,\infty,R} \|v\|_{2,R} \|w\|_{2,R}, \end{aligned}$$

leading to (6.21). □

Notice that in the two-dimensional case, the orders $h^{\frac{5}{2}}$ in (6.19) and $h^{\frac{7}{2}}$ in (6.20) should be replaced by h^2 and h^3, respectively.

Proof of Theorem 6.2. By (6.8), (3.2), (6.9), Lemma 6.4, and Lemma 6.5, we have

$$\begin{aligned} \alpha^* \|u_h - u_h^*\|_{1,h}^2 &\le a_h^*\left(u_h - u_h^*, u_h - u_h^*\right) \\ &= \left[a_h^*\left(u_h, u_h - u_h^*\right) - a_h\left(u_h, u_h - u_h^*\right)\right] + \left[f_h\left(u_h - u_h^*\right) - f_h^*\left(u_h - u_h^*\right)\right] \\ &\le Ch \sum_{R \in \tau_h} \|u_h\|_{2,R} \|u_h - u_h^*\|_{1,R} + Ch^{\frac{5}{2}} \sum_{R \in \tau_h} \|f\|_{1,\infty,R} \|u_h - u_h^*\|_{1,R} \\ &\le Ch \left(\|u_h\|_{2,h} + \|f\|_{1,\infty,\Omega}\right) \|u_h - u_h^*\|_{1,h}, \end{aligned}$$

where we also used the Cauchy-Schwarz inequality and (5.9). It then follows from Theorem 3.1–Theorem 3.3 and Theorem 1.1 that

$$\begin{aligned}\|u-u_h^*\|_{1,h} &\le \|u-u_h\|_{1,h}+\|u_h-u_h^*\|_{1,h}\\ &\le Ch\|u\|_{2,\Omega}+Ch\left(\|u_h-I_hu\|_{2,h}+\|I_hu-u\|_{2,h}+\|f\|_{1,\infty,\Omega}\right)\\ &\le Ch\left(\|u\|_{2,\Omega}+\|f\|_{1,\infty,\Omega}\right)\le Ch\|f\|_{1,\infty,\Omega}.\end{aligned}$$

which is the result of Theorem 6.2. ☐

Proof of Theorem 6.3. For any $g\in L^2(\Omega)$, by (3.2) and (6.9), the following identity holds,

$$\begin{aligned}(u_h-u_h^*,g)&=a_h\left(u_h-u_h^*,\varphi_{g_h}-\psi_h\right)-\left[a_h\left(u_h^*,\psi_h\right)-a_h^*\left(u_h^*,\psi_h\right)\right]\\ &\quad+\left[f_h\left(\psi_h\right)-f_h^*\left(\psi_h\right)\right],\qquad \forall\psi_h\in V_{0h},\end{aligned}\tag{6.24}$$

where $\varphi_{g_h}\in V_{0h}$ satisfies

$$a_h\left(\varphi_{g_h},v_h\right)=(g,v_h),\qquad \forall v_h\in V_{0h},$$

and $\varphi_g\in H_0^1(\Omega)\cap H^2(\Omega)$ satisfies (3.20) and (3.21). Consequently,

$$\begin{aligned}\|u-u_h^*\|_{0,\Omega}&\le\|u-u_h\|_{0,h}+\sup_{0\neq g\in L^2(\Omega)}\frac{1}{\|g\|_{0,\Omega}}\inf_{\psi_h\in V_{0h}}\left[\,\left|a_h\left(u_h-u_h^*,\varphi_{g_h}-\psi_h\right)\right|\right.\\ &\quad\left.+\left|a_h\left(u_h^*,\psi_h\right)-a_h^*\left(u_h^*,\psi_h\right)\right|+\left|f_h\left(\psi_h\right)-f_h^*\left(\psi_h\right)\right|\,\right].\end{aligned}\tag{6.25}$$

Now let us fix $g\in L^2(\Omega)$ and choose $\psi_h=I_h\varphi_g$. By Theorem 3.1, Theorem 6.2, Theorem 3.3 and (3.21), we get

$$\begin{aligned}\left|a_h\left(u_h-u_h^*,\varphi_{g_h}-\psi_h\right)\right|&\le C\left\|u_h-u_h^*\right\|_{1,h}\left\|\varphi_{g_h}-\psi_h\right\|_{1,h}\\ &\le Ch^2\left\|f\right\|_{1,\infty,\Omega}\left\|g\right\|_{0,\Omega}.\end{aligned}\tag{6.26}$$

It follows from the definitions of $a_h(\cdot,\cdot)$, $a_h^*(\cdot,\cdot)$, and $E_R(\cdot)$ that

$$\begin{aligned}\left|a_h\left(u_h^*,\psi_h\right)-a_h^*\left(u_h^*,\psi_h\right)\right|&\le\sum_{R\in\tau_h}\left[\left|E_R\left(a_1\frac{\partial u_h^*}{\partial x}\frac{\partial\psi_h}{\partial x}\right)\right|+\left|E_R\left(a_2\frac{\partial u_h^*}{\partial y}\frac{\partial\psi_h}{\partial y}\right)\right|\right.\\ &\quad\left.+\left|E_R\left(a_3\frac{\partial u_h^*}{\partial z}\frac{\partial\psi_h}{\partial z}\right)\right|+\left|E_R\left(cu_h^*\psi_h\right)\right|\right].\end{aligned}$$

Notice that $\partial u_h^*\big|_R,\partial\psi_h\big|_R\in P_R$, for $R\in\tau_h$, where $\partial=\partial_x,\partial_y$ or ∂_z. Therefore, by Lemma 6.6, the Cauchy-Schwarz inequality, Theorem 6.2, (3.21) and (1.3), we have

$$\begin{aligned}\left|a_h\left(u_h^*,\psi_h\right)-a_h^*\left(u_h^*,\psi_h\right)\right|&\le Ch^2\sum_{R\in\tau_h}\|u_h^*\|_{2,R}\,\|\psi_h\|_{2,R}\le Ch^2\,\|u_h^*\|_{2,h}\,\|I_h\varphi_g\|_{2,h}\\ &\le Ch^2\left(\|u\|_{2,\Omega}+\|f\|_{1,\infty,\Omega}\right)\|g\|_{0,\Omega}\\ &\le Ch^2\left\|f\right\|_{1,\infty,\Omega}\left\|g\right\|_{0,\Omega}.\end{aligned}\tag{6.27}$$

By Lemma 6.6, (5.9), Theorem 3.1 and (3.21), we have

$$\begin{aligned}\left|f_h\left(\psi_h\right)-f_h^*\left(\psi_h\right)\right|&\le C\sum_{R\in\tau_h}\left|E_R\left(f\psi_h\right)\right|\le Ch^{\frac{7}{2}}\sum_{R\in\tau_h}\|f\|_{2,\infty,R}\,\|\psi_h\|_{2,R}\\ &\le Ch^2\|f\|_{2,\infty,\Omega}\,\|\psi_h\|_{2,h}\le Ch^2\|f\|_{2,\infty,\Omega}\,\|g\|_{0,\Omega}.\end{aligned}\tag{6.28}$$

Now (6.11) is a direct consequence of the combination of (6.24)–(6.28) and Theorem 3.3. The proof is complete. ☐

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