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A COMPOSITE MIXED FINITE ELEMENT FOR HEXAHEDRAL GRIDS*

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Abstract. A new mixed finite element method on three-dimensional hexahedral meshes for second order elliptic problems is proposed. This finite element is a composite element. It is shown to have optimal convergence properties, and it is applied to a hydrogeology problem.

Key words. mixed finite element, hexahedral grid, flow in porous media

AMS subject classifications. 65N12, 65N15, 65N30, 76S05

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1. Introduction.

Single phase incompressible flow in a porous medium is governed by the Darcy flow equation, an elliptic equation coupling a conservation equation with Darcy's law. If gravity is neglected, the mixed form of this equation becomes the system

$$\begin{aligned} \mathbf{u} &= -K \,\mathrm{grad}\, p \quad && \text{in } \Omega, \\ \mathrm{div}\ \mathbf{u} &= f && \text{in } \Omega, \end{aligned}$$

where the primary unknown p is the fluid pressure, the secondary unknown $\mathbf{u}$ is the Darcy flow velocity, the coefficient K is a symmetric positive definite tensor, and f is a source term. It has been known since the early 1980s that mixed finite element methods are particularly useful for the numerical simulation of this system of equations. There are several reasons why this is so. First of all, with a mixed method the Darcy velocity $\mathbf{u}$ is calculated simultaneously with the pressure p and to the same order of accuracy. Also in many applications the permeability K is discontinuous and can vary over several orders of magnitude from one geological region to another, and mixed methods are particularly well suited to handling this difficulty. Another advantage of mixed methods is that they can easily handle tetrahedral as well as rectangular meshes and nondiagonal tensors K. Finally, equally important is the fact that mixed methods are conservative and even locally conservative, and for most geophysical applications this is an essential feature.

Many mixed methods for second order elliptic problems have been introduced. Among the most well known of these are [19], [16], [17], [5], [4], and [3]. These elements are all based on triangular or rectangular elements in two dimensions and on tetrahedral, parallelepiped, or prismatic elements in three dimensions. For large calculations, regular meshes of rectangular or parallelepipedic elements are particularly efficient. However, for geophysical applications, the porous medium is a geological structure and is not always well suited to a regular mesh of rectangular elements. A natural idea is to deform a regular rectangular mesh so that the elements are convex quadrilaterals or hexahedra and to construct finite elements on the mesh by using multilinear mappings to a reference rectangle or rectangular solid. The approximation space on the

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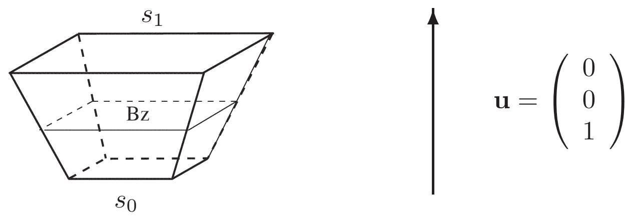

Fig. 1.1. *A hexahedron in the form of a truncated pyramid and a constant flow field.*

deformed element is the image under the Piola transformation (see [14]) of the approximation space on the reference element. However, unless the new elements are parallelograms or parallelepipeds, so that the multilinear maps are actually affine, the classical scaling arguments break down and interpolation accuracy is lost. Though there remain problems for two-dimensional elements, see [2], the problem is particularly evident for three-dimensional elements. We describe an example due to Russell given in [15] to show that if the approximation space on the reference element is $\mathbf{RTN}_0$, the lowest order Raviart–Thomas–Nédélec space, cf. [16], [20], the resulting approximation space does not even contain the constant functions. We will refer to this construction as the extended RTN mixed finite element method, but it should be pointed out that neither Raviart, Thomas nor Nédélec ever claimed that the RTN construction on rectangular and parallelepipedic elements could be extended to hexahedrons.

Consider the truncated pyramid E of unit height and with square horizontal bases of extents $s_0 \times s_0$ and $s_1 \times s_1$, shown in Figure 1.1, and suppose that the constant vector field $\mathbf{u}(x) = (0,0,1)^t \; \forall x \in E$ does belong to the approximation space. The exact flux through a horizontal section B_z, for $0 \leq z \leq 1$, is equal to the area of this section

$$\int_{B_z} \mathbf{u} \cdot \mathbf{n}_z = ((1-z)s_0 + zs_1)^2.$$

However, the flux of any $\mathbf{v} \in \mathbf{RTN}_0$ of the unit reference cube through a horizontal section $\hat{B}_z$ varies linearly with z:

$$\int_{\hat{B}_z} \mathbf{v} \cdot \mathbf{n}_z = (1-z)s_0^2 + zs_1^2.$$

Since the Piola transformation preserves flux through any section, the constant field $\mathbf{u}$ cannot be the image of any vector field in $\mathbf{RTN}_0$.

To show the effect in an actual computation we show a calculation carried out by Prosi [18]. The calculation domain is a right circular cylinder. The permeability is constant, and the source term is null. The boundary conditions imposed on the sides of the cylinder are so-called no flow conditions, i.e., homogeneous Neumann conditions, and a constant pressure is given on each of the two bases of the cylinder with a pressure drop from one end to the other. Thus for the analytic solution the pressure is constant on each cross section parallel to the axis and it varies linearly from one end to the other, while the flow field is constant and is parallel to the axis of the cylinder. The results shown in Figure 1.2 were obtained with the RTN elements extended to hexahedrons. The pressure result is correct, but the flow field is not constant.

Several articles have addressed the problem of defining a mixed finite element on a distorted, nonparallelogram rectangle or on a distorted, nonparallelepiped rectangular solid at least for lowest order elements. In [22] and [1], [2] elements are introduced for

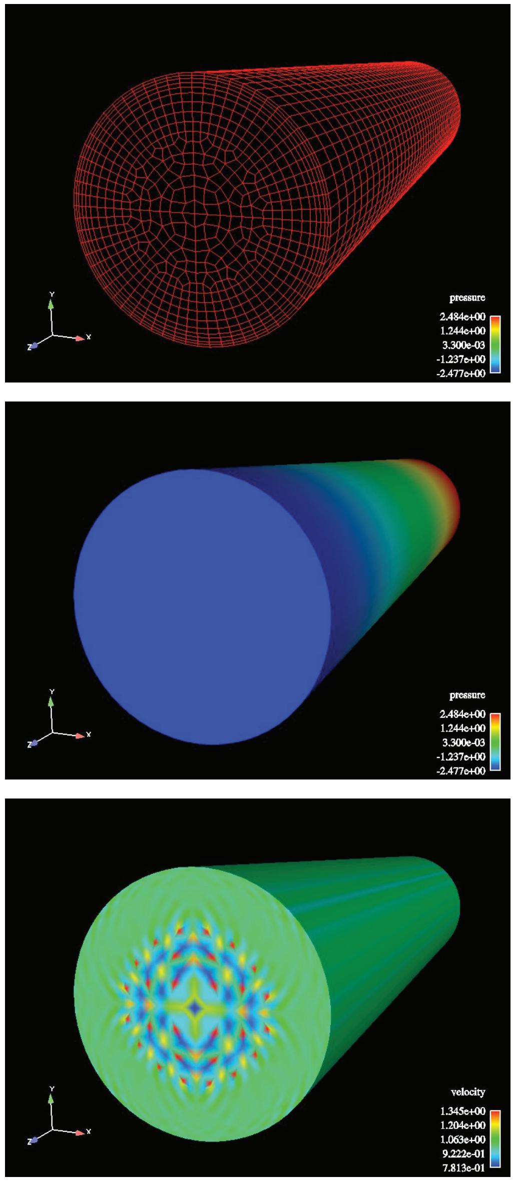

FIG. 1.2. *Difficulty for a mesh of nonparallelepiped hexahedra.*

convex quadrilateral elements, i.e., two-dimensional elements, but neither of these has a satisfactory extension to convex hexahedral elements, or three-dimensional elements. Recently a solution requiring higher order polynomials was published [8].

In [12] a composite element was introduced for convex quadrilaterals in which the quadrilateral was subdivided into two triangles. The space of functions corresponding to the subdivided quadrilateral was the space of $\mathbf{H}(\text{div})$-functions on the quadrilateral such that the restriction to each of the two triangles was in $\mathbf{RTN}_0$ of the triangle and such that the divergence of the function was constant over the entire quadrilateral. In a paper of Kuznetsov and Repin [13] this idea was extended in a general way to elements that are three-dimensional polygons.

In this article, we use hexahedrons with their original definition which requires that they have planar faces, and, following the ideas of Kuznetsov and Repin, we develop a composite element specifically for a convex hexahedron. This element is obtained by dividing the hexahedron into five tetrahedra, and it is shown to have optimal convergence properties. In particular, unlike in [13], no extra regularity on the solution is needed. Also, unlike in [13], the analysis given here does not require that the set of all tetrahedra obtained from dividing the hexahedra form a mesh. This is important because it is not always possible to obtain a tetrahedral mesh from a general hexahedral mesh by subdividing the hexahedrons into five tetrahedra. In certain cases to obtain a tetrahedral mesh some of the hexahedra must be divided into six tetrahedra.

Let Ω denote a bounded domain in $\mathbb{R}^3$. The boundary $\partial\Omega$ of Ω is made up of a nonempty part Γ_D on which a Dirichlet boundary condition is imposed, and on the remainder of the boundary Γ_N, a homogeneous Neumann condition has been imposed. Thus we consider the problem

$$(1.1)\qquad (\mathcal{P})\quad \begin{aligned} \mathbf{u} &= -K\,\mathrm{grad}\,p && \text{in} \quad \Omega,\\ \mathrm{div}\,\mathbf{u} &= f && \text{in} \quad \Omega,\\ p &= p_d && \text{on} \quad \Gamma_D,\\ \mathbf{u}\cdot\mathbf{n}_\Omega &= 0 && \text{on} \quad \Gamma_N, \end{aligned}$$

where $\mathbf{n}_\Omega$ is the unit outward normal vector on the boundary of Ω. Throughout we will use the notation $\mathbf{n}_X$ for the unit outward pointing normal vector field on the boundary of a domain $X \subset \mathbb{R}^3$. If Y is a surface in $\mathbb{R}^3$, then $\mathbf{n}_Y$ denotes one of the two unit normal vector fields on Y.

In section 2 we recall some of the theory for mixed finite elements methods. The new mixed finite element approximation is developed in section 3. Section 4 is devoted to the interpolation error. In section 5 we present some numerical results.

2. Numerical analysis for mixed methods. In this section we recall some well known results for mixed finite element methods.

In [7] it is shown that if $\mathcal{W}$ and $\mathcal{M}$ are Hilbert spaces and if $a : \mathcal{W}\times\mathcal{W} \longrightarrow \mathbb{R}$ and $b : \mathcal{W}\times\mathcal{M} \longrightarrow \mathbb{R}$ are continuous bilinear forms satisfying the following two conditions

(2.1) (i) a is $\mathcal{V}$-elliptic, where $\mathcal{V} = \{\mathbf{v}\in\mathcal{W} : b(\mathbf{v},q) = 0 \quad \forall q\in\mathcal{M}\}$, i.e.,

$$\exists\alpha > 0 \text{ such that } \forall\mathbf{v}\in\mathcal{V},\quad a(\mathbf{v},\mathbf{v}) \geq \alpha\|\mathbf{v}\|^2_{H(\mathrm{div};\Omega)},$$

(2.2) (ii) b satisfies the inf sup condition on $\mathcal{W}\times\mathcal{M}$, i.e.,

$$\exists\beta > 0 \text{ such that } \inf_{q\in\mathcal{M}}\sup_{\mathbf{v}\in\mathcal{W}} b(\mathbf{v},q) \geq \beta\|\mathbf{v}\|_{H(\mathrm{div};\Omega)}\|q\|_{L^2(\Omega)},$$

then if $\mathcal{L}_\mathcal{W} : \mathcal{W} \longrightarrow \mathbb{R}$ and $\mathcal{L}_\mathcal{M} : \mathcal{M} \longrightarrow \mathbb{R}$ are continuous linear forms, there exists a unique solution ($\mathbf{u}$, p) to the problem

$$(2.3)\qquad (\mathcal{P}_w)\quad \begin{aligned} &\text{find } \mathbf{u}\in\mathcal{W} \text{ and } p\in\mathcal{M} \text{ such that}\\ &a(\mathbf{u},\mathbf{v}) - b(\mathbf{v},p) = \mathcal{L}_\mathcal{W}(\mathbf{v}) \quad \forall\mathbf{v}\in\mathcal{W},\\ &b(\mathbf{u},q) = \mathcal{L}_\mathcal{M}(q) \quad \forall q\in\mathcal{M}. \end{aligned}$$

If also $\mathcal{W}_h$ and $\mathcal{M}_h$ are finite element subspaces of $\mathcal{W}$ and $\mathcal{M}$, respectively, and the bilinear forms a and b are such that

(2.4) (i) a is $\mathcal{V}_h$-elliptic, where $\mathcal{V}_h = \{\mathbf{v} \in \mathcal{W}_h : b(\mathbf{v}, q) = 0 \quad \forall q \in \mathcal{M}_h\}$, i.e.,

$$\exists \alpha_h > 0 \text{ such that } \forall \mathbf{v} \in \mathcal{V}_h, \quad a(\mathbf{v}, \mathbf{v}) \geq \alpha_h \|\mathbf{v}\|^2_{H(\text{div};\Omega)},$$

(2.5) (ii) b satisfies the inf sup condition on $\mathcal{W}_h \times \mathcal{M}_h$, i.e.,

$$\exists \beta_h > 0 \text{ such that } \inf_{q \in \mathcal{M}_h} \sup_{\mathbf{v} \in \mathcal{W}_h} b(\mathbf{v}, q) \geq \beta_h \|\mathbf{v}\|_{H(\text{div};\Omega)} \|q\|_{L^2(\Omega)},$$

then the discretized problem

$$(2.6) \qquad (\mathcal{P}_h) \quad \begin{array}{l} \text{find } \mathbf{u} \in \mathcal{W}_h \text{ and } p \in \mathcal{M}_h \text{ such that} \\ a(\mathbf{u}, \mathbf{v}) - b(p, \mathbf{v}) = \mathcal{L}_{\mathcal{W}}(\mathbf{v}) \quad \forall \mathbf{v} \in \mathcal{W}_h, \\ b(q, \mathbf{u}) = \mathcal{L}_{\mathcal{M}}(q) \quad \forall q \in \mathcal{M}_h \end{array}$$

admits a unique solution $(\mathbf{u}_h, p_h)$, and

$$\|p - p_h\|^2_{L^2(\Omega)} + \|\mathbf{u} - \mathbf{u}_h\|^2_{H(\text{div};\Omega)} \leq C \left\{ \inf_{q_h \in \mathcal{M}_h} \|p - q_h\|^2_{L^2(\Omega)} + \inf_{\mathbf{v}_h \in \mathcal{W}_h} \|\mathbf{u} - \mathbf{v}_h\|^2_{H(\text{div};\Omega)} \right\}$$

with a constant C which depends only on the constants of continuity of the bilinear forms a and b and the constants α_h and β_h.

With $\mathcal{W} = \mathbf{H}(\text{div};\Omega)$ and $\mathcal{M} = L^2(\Omega)$ and

$$a(\mathbf{u}, \mathbf{v}) = \int_\Omega \left(K^{-1}\mathbf{v}\right) \cdot \mathbf{u} \qquad \text{and} \qquad b(\mathbf{u}, q) = \int_\Omega q \operatorname{div} \mathbf{v},$$

problem $(\mathcal{P}_w)$ is the weak form of $(\mathcal{P})$ where the forms $\mathcal{L}_{\mathcal{W}} : \mathcal{W} \longrightarrow \mathbb{R}$ and $\mathcal{L}_{\mathcal{M}} : \mathcal{M} \longrightarrow \mathbb{R}$ are determined by the source term and the Dirichlet boundary data, respectively:

$$\mathcal{L}_{\mathcal{W}}(\mathbf{v}) = \int_{\Gamma_D} p_d \mathbf{v} \cdot \mathbf{n}_\Omega, \quad \mathcal{L}_{\mathcal{M}}(q) = \int_\Omega f q.$$

Further a and b satisfy the conditions (2.1) and(2.2) so there is a unique solution $(\mathbf{u}, p)$ to problem $(\mathcal{P})$.

Thus to see that a pair of spaces $(\mathcal{W}_h, \mathcal{M}_h)$ is suitable for a mixed method it suffices to show that the two conditions (2.4) and (2.5) are satisfied, with contants α_h and β_h independent of h, and to estimate interpolation errors.

For the spaces $(\mathcal{W}_h, \mathcal{M}_h)$ that we shall construct in section 3, it is easy to see that condition (2.4) is satisfied because we will have $\mathcal{V}_h \subset \mathcal{V}$ so that α_h may be taken to be α. For condition (2.5), we will have that $\mathcal{M}_h \subset \mathcal{M}$ and that b satisfies (2.2) for the spaces $(\mathcal{W}, \mathcal{M})$. Thus given $q_h \in \mathcal{M}_h$ there is an element $\mathbf{v} \in \mathcal{W}$ such that $b(\mathbf{v}, q_h) \geq \beta \|\mathbf{v}\|_{H(\text{div};\Omega)} \|q_h\|_{L^2(\Omega)}$. However, one can also show that there exists $\widetilde{\mathbf{v}} \in (H^1(\Omega))^3$ such that $b(\widetilde{\mathbf{v}}, q_h) \geq \beta \|\widetilde{\mathbf{v}}\|_{H^1(\Omega)} \|q_h\|_{L^2(\Omega)}$ (see [20, proof of Theorem 13.2, p. 582]). Thus it suffices to show that there exists a continuous projection operator Π_h from $(H^1(\Omega))^3$ onto $\mathcal{W}_h$ such that $b(\Pi_h \mathbf{v}, q_h) = b(\mathbf{v}, q_h)$ $\forall q_h \in \mathcal{M}_h$ and such that $\|\Pi_h \mathbf{v}\|_{H(\text{div};\Omega)} \leq \gamma \|\mathbf{v}\|_{H^1(\Omega)}$ and with γ independent of h (for h sufficiently small). The operator Π_h is defined in section 4.2, and the fact that it has the desired properties follows from the commuting diagram property (4.14) and inequality (4.15). We will also give interpolation estimates in the same section.

3. The approximation spaces. Suppose that Ω is a convex polyhedral domain in $\mathbb{R}^3$, and let $\mathcal{M} = L^2(\Omega)$ and $\mathcal{W} = \{\mathbf{u} \in \mathbf{H}(\mathrm{div};\Omega) \ : \ \mathbf{u}\cdot\mathbf{n}_\Omega = 0 \text{ on } \Gamma_N\}$. Let $\mathcal{T}_h$ be a mesh made up of general convex hexahedral cells E with planar faces such that the permeability K is constant on each cell E. Let $\mathcal{F}_h$ be the set of faces F (quadrilaterals) of elements of $\mathcal{T}_h$. Let $\mathcal{M}_h \subset \mathcal{M}$ be the space of L^2 functions on Ω that are constant on each cell $E \in \mathcal{T}_h$. The object of this section is to define an approximation space $\mathcal{W}_h \subset \mathcal{W}$ such that the pair $(\mathcal{W}_h, \mathcal{M}_h)$ yields a pair of approximation spaces appropriate for mixed finite element approximation in the sense that both Brezzi conditions are satisfied and that the spaces permit order h approximation of sufficiently regular functions.

The approximation space $\mathcal{W}_h \subset \mathcal{W}$ will be defined such that an element $\mathbf{u}_h \in \mathcal{W}_h$

- has constant divergence in each hexahedron $E \in \mathcal{T}_h$,
- has constant normal component on each face $F \in \mathcal{F}_h$,
- is uniquely determined by its normal traces on the faces $F \in \mathcal{F}_h$

as is the case for elements of the Raviart–Thomas–Nédélec mixed finite element approximation space of lowest order for a tetrahedral or a parallelepiped mesh. Toward this end, we construct a composite element by subdividing each hexahedron E into 5 tetrahedra $T_j^E, j = 1, \ldots, 5$.

We define a space $\mathcal{W}_E$ for each E in $\mathcal{T}_h$, and we will define $\mathcal{W}_h$ to be the space of $\mathbf{H}(\mathrm{div};\Omega)$-functions that are locally in $\mathcal{W}_E$. Thus the pair of approximation spaces is defined by

$$\begin{aligned} \mathcal{M}_h &= \{q \in \mathcal{M} \ : \ q_{|E} \text{ is constant } \forall E \in \mathcal{T}_h\}, \\ \mathcal{W}_h &= \{\mathbf{u} \in \mathcal{W} \ : \ \mathbf{u}_{|E} \in \mathcal{W}_E \ \forall E \in \mathcal{T}_h\}. \end{aligned}$$

3.1. A composite element. One begins by choosing either set of four of the eight vertices for which no pair is joined by an edge of a face of E; i.e., one chooses any of the eight vertices together with the three vertices which share a face with the original vertex but are not joined to it by an edge. These four points determine a tetrahedron T_5^E whose faces are in the interior of E, and $E \setminus T_5^E$ is made up of four disjoint tetrahedra $T_j^E, j = 1, \ldots, 4$,

$$\begin{aligned} E = T_1^E \cup T_2^E \cup T_3^E \cup T_4^E \cup T_5^E, \quad & T_1^E = V_1V_2V_4V_5, \\ T_2^E = V_6V_7V_2V_5, \quad & T_3^E = V_3V_4V_2V_7, \\ T_4^E = V_8V_7V_5V_4, \quad & T_5^E = V_2V_4V_5V_7 \end{aligned}$$

as shown in Figure 3.1. Each of the first four tetrahedra $T_j^E, j = 1, \ldots, 4$, has three triangular faces which are contained in the boundary of E and one internal face. (In fact if E is a cube, these four tetrahedra are similar.) The four internal faces of these four tetrahedra form the boundary of the fifth tetrahedron T_5^E. Note that for a given hexahedron there are exactly two ways to subdivide it in such a manner.

We denote by $\widetilde{\mathcal{T}}_E$ one of the triangulations of E made up of these 5 tetrahedra:

$$\widetilde{\mathcal{T}}_E = \{T_j^E : j = 1, \ldots, 5\}.$$

We will also use the notation $\mathcal{F}_E$ for the set of faces F (quadrilaterals) of the hexahedron E and $\widetilde{\mathcal{F}}_E$ for the set of faces $\widetilde{F}$ (triangles) of the tetrahedra $T \in \widetilde{\mathcal{T}}_E$:

$$\begin{aligned} \mathcal{F}_E &= \{F \in \mathcal{F}_h \ : \ F \text{ is a face of } E\}, \\ \widetilde{\mathcal{F}}_E &= \left\{\widetilde{F} \ : \ \widetilde{F} \text{ is a face of } T_j^E \text{ for some } j, \ j = 1, \ldots 5\right\}. \end{aligned}$$

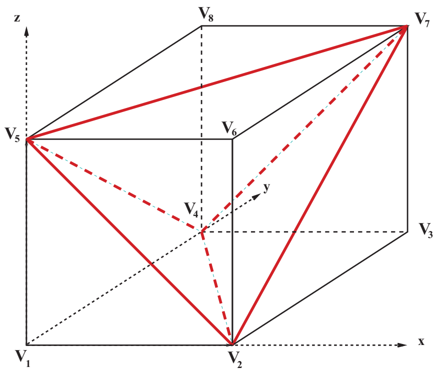

FIG. 3.1. *One partition of the reference hexahedron into* 5 *tetrahedra.*

Note that $\mathcal{F}_E$ has 6 elements and $\widetilde{\mathcal{F}}_E$ 16 elements, 12 of which are on the boundary of E and 4 of which lie in the interior of E.

3.2. Local approximation spaces. Here we define several local approximation spaces both for scalar functions and for vector valued functions. For a given hexahedron $E \in \mathcal{T}_h$ define the space $\mathcal{M}_E$ to be the space of scalar functions q that are constant on E and let $\widetilde{\mathcal{M}}_E$ denote the space of piecewise constant functions on E that are constant on each tetrahedra of $\widetilde{\mathcal{T}}_E$:

$$\mathcal{M}_E = \left\{ q \in L^2(E) \ : \ q_{|E} \text{ is constant } \right\},$$
$$\widetilde{\mathcal{M}}_E = \left\{ q \in L^2(E) \ : \ q_{|T_j^E} \text{ is constant, } j = 1, \ldots, 5 \right\},$$

and note that

$$\mathcal{M}_E \subset \widetilde{\mathcal{M}}_E.$$

An element of $\mathcal{M}_E$ is determined by its constant value on E, and an element of $\widetilde{\mathcal{M}}_E$ is determined by its constant values on the 5 tetrahedra of $\widetilde{\mathcal{T}}_E$.

The space associated with the composite element is $\mathcal{W}_E$, the space of vector functions $\mathbf{v} \in \mathbf{H}(\mathrm{div}; E)$ satisfying the following conditions:

$$\mathbf{v}_{|T_j^E} \in \mathbf{RTN}_0 \left(T_j^E \right), \quad j = 1, \ldots, 5, \tag{3.1}$$

$$\mathrm{div}\ \mathbf{v} \quad \text{is a constant over E}, \tag{3.2}$$

$$\mathbf{v} \cdot \mathbf{n}_E \quad \text{is constant on each face of E}. \tag{3.3}$$

We denote by $\widetilde{\mathcal{W}}_E$ the lowest order Raviart–Thomas–Nédélec space over E associated with the discretization $\widetilde{\mathcal{T}}_E$ of E and define the intermediate space $\widehat{\mathcal{W}}_E$ to be the elements of $\widetilde{\mathcal{W}}_E$ having constant divergence so that

$$\widetilde{\mathcal{W}}_E = \left\{ \mathbf{v} \in \mathbf{H}(\mathrm{div}; E) \ : \ \mathbf{v}_{|T_j^E} \in \mathbf{RTN}_0 \left(T_j^E \right), \quad j = 1, \ldots, 5 \right\},$$

$$\widehat{\mathcal{W}}_E = \left\{ \tilde{\mathbf{v}} \in \widetilde{\mathcal{W}}_E \ : \ \mathrm{div}\ \tilde{\mathbf{v}}|_E \text{ is constant} \right\},$$

$$\mathcal{W}_E = \left\{ \widehat{\mathbf{v}} \in \widehat{\mathcal{W}}_E \ : \ \widehat{\mathbf{v}} \cdot \mathbf{n}_{E\,|F} \text{ is constant } \forall F \in \mathcal{F}_E \right\},$$

and

$$\mathcal{W}_E \subset \widehat{\mathcal{W}}_E \subset \widetilde{\mathcal{W}}_E.$$

It is well known that an element of $\widetilde{\mathcal{W}}_E$ is uniquely determined by the constant values of the normal fluxes through the faces $\widetilde{F} \in \widetilde{\mathcal{F}}_E$ and that a basis for $\widetilde{\mathcal{W}}_E$ consists of the set of functions $\tilde{\omega}_{\tilde{F}_i}$, $\widetilde{F}_i \in \widetilde{\mathcal{F}}_E$, having constant normal component on the face $\widetilde{F}_j$ equal to $\delta_{i,j}, j = 1, \dots, 16$.

To check that a function $\mathbf{v}$ of $\mathcal{W}_E$ is uniquely defined by its normal traces through the 6 faces of E, first note that it is also in $\widetilde{\mathcal{W}}_E$, and so it is determined by the 16 degrees of freedom which are its normal traces on the faces in $\widetilde{\mathcal{F}}_E$. However, since its normal traces on the faces in $\mathcal{F}_E$ are constant, the number of degrees of freedom is reduced to 10. (Each (quadrilateral) face in $\mathcal{F}_E$ is made up of 2 (triangular) faces in $\widetilde{\mathcal{F}}_E$.) Since the divergence of the element is the same on each of the 5 tetrahedra in $\widetilde{\mathcal{T}}_E$, the number of degrees of freedom is reduced again by 4. Thus there remain 6 degrees of freedom to be determined. To check for unisolvence it suffices to note that with g_i denoting the function defined on the boundary of E by $g_{i\,|F_j} = \delta_{i,j}$ for each face $F_j, j = 1, \dots, 6$, of E, ω_i is defined to be the component $\mathbf{u}$ of the solution $(\mathbf{u}, p)$ to the mixed finite element problem

$$(\mathcal{P}_E) \quad \begin{aligned} &\text{find } (\mathbf{u}, p) \in \left(\widetilde{\mathcal{W}}_E^{g_i}, \widetilde{\mathcal{M}}_E\right) \text{ such that} \\ &a(\mathbf{u}, \mathbf{v}) - b(\mathbf{v}, p) = 0 \qquad \forall \mathbf{v} \in \widetilde{\mathcal{W}}_E^0, \\ &\qquad\qquad b(\mathbf{u}, q) = \frac{|F_i|}{|E|} \qquad \forall q \in \widetilde{\mathcal{M}}_E, \end{aligned}$$

where $\widetilde{\mathcal{W}}_E^{g_i}$, respectively, $\widetilde{\mathcal{W}}_E^0$, is the subspace of $\widetilde{\mathcal{W}}_E$ consisting of those elements whose normal traces agree with g_i, respectively, are equal to 0 on the boundary of E. Note that while this Neumann problem determines p only up to a constant, it determines $\mathbf{u}$ uniquely so that ω_i is well defined. To see that this is true suppose that ω_i' is a second such solution. Then the difference $\omega_i - \omega_i'$ is a solution to the problem $(\mathcal{P}_E)$ but with the boundary term g_i replaced by 0 and the source term $\frac{|F_i|}{|E|}$ replaced by 0. Thus the solution has zero divergence in each of the tetrahedra of $\widetilde{\mathcal{T}}_E$ and has zero normal component on all of the external faces of $\widetilde{\mathcal{F}}_E$. But each of the exterior tetrahedra $T_i^E, i = 1, \dots, 4$, has 3 faces on the boundary of E. Since the flux through each of these faces is null and since the divergence on the tetrahedron is null, the flux through the fourth face, the interior face, must also be null. Thus $\omega_i = \omega_i'$. The set of functions $\omega_i, i = 1, \dots, 6$, thus defined forms a basis of $\mathcal{W}_E$.

In the same way one can see that an element of $\widehat{\mathcal{W}}_E$ is determined by the values of its normal components on the 12 faces in $\widetilde{\mathcal{F}}_E$ that lie on the boundary of E and that a basis for $\widehat{\mathcal{W}}_E$ is made up of the 12 functions $\widehat{\omega}_i$ defined in the obvious maner.

Remark 1. It might seem more natural to use the canonical subdivision of the hexahedron into 6 tetrahedra (all of which are identical when the hexahedron is a cube). If, instead, the hexahedron were divided in this way into 6 tetrahedra, there would be 18 coefficients to determine corresponding to 18 tetrahedral faces. Conditions (3.2) and (3.3) impose 5 and 6 constraints, respectively, leaving 7 degrees of freedom to calculate. The macroelement would not be unisolvent. One could still solve a problem analogous to $(\mathcal{P}_E)$, but the element ω_i would no longer be uniquely determined, as with this alternative decomposition each tetrahedron would have 2 external faces and 2 internal faces. This decomposition introduces an edge which does not lie on the boundary of E and around which a divergence free flow could turn. As was suggested to us by Todd Arbogast, one could instead work with the rotation free subspace to obtain the right dimension for the approximation space.

Remark 2. Note that, while $\mathcal{W}_h$ and $\mathcal{M}_h$ are defined from the local spaces $\mathcal{W}_E$ and $\mathcal{M}_E$, global spaces $\widetilde{M}_h$, $\widetilde{W}_h$, and $\widehat{\mathcal{W}}_h$ cannot be defined since the decomposition of the elements E is not necessarily done in a way that makes the set of all T such that $T \in \mathcal{T}_E$ for some $E \in \mathcal{T}_h$ a triangulation of Ω.

Remark 3. Note that, given a hexahedral mesh, the finite element space $\mathcal{W}_h$ depends on the choice of the decomposition in tetrahedra (with N hexahedra there are 2^N possibilities for the space $\mathcal{W}_h$), and there is no obvious manner for specifying one of these possibilities. However, for a given set of data representing a mesh it is easy to prescribe a choice.

4. Interpolation error. As we saw in section 2 it follows from the Babuska–Brezzi theory that the errors committed in using the mixed finite element method with approximation spaces satisfying the two conditions (2.1) and (2.2) is of the same order as the error of interpolation:

$$\|p-p_h\|_{L^2(\Omega)}+\|\mathbf{u}-\mathbf{u}_h\|_{H(\mathrm{div};\Omega)} \leq C\left(\inf_{q_h\in\mathcal{M}_h}\|p-q_h\|_{L^2(\Omega)}+\inf_{\mathbf{v}_h\in\mathcal{W}_h}\|\mathbf{u}-\mathbf{v}_h\|_{H(\mathrm{div};\Omega)}\right).$$

This section is devoted to the estimation of this error. The goal is thus to show that

$$\inf_{q_h\in\mathcal{M}_h}\|p-q_h\|_{L^2(\Omega)} \leq ChN(p) \quad \text{and} \quad \inf_{\mathbf{v}_h\in\mathcal{W}_h}\|\mathbf{u}-\mathbf{v}_h\|_{H(\mathrm{div};\Omega)} \leq ChN(\mathbf{u}),$$

where C is a constant independent of both the mesh parameter h and the particular function being approximated and $N(p)$, respectively, $N(\mathbf{u})$ represents some norm of the function p, respectively, $\mathbf{u}$ being approximated. For the more classical approximation spaces, the usual technique is to define a projection operator into the approximation space and use a linear mapping to a reference element which commutes with the projection operator and then use a scaling argument. In the present case we define projection operators, but there is no linear mapping to a reference element. Such a mapping would be trilinear and would not produce the desired scaling argument. For both the scalar and the vector functions we define a projection operator which is factored through a projection into a classical approximation space. We then obtain the standard estimate.

To calculate interpolation errors we define, following [13], a norm on the four-dimensional spaces $\mathbf{RTN}_0(T)$, for T a tetrahedron, by

$$|[\mathbf{v}]|_T = \int_{\partial T} |\mathbf{v}_j \cdot \mathbf{n}_T| \quad \forall \mathbf{v} \in \mathbf{RTN}_0(T).$$

That this seminorm is in fact a norm is evident because, in $\mathbf{RTN}_0(T)$, an element with zero normal component on each face of T is the zero vector function. As $\mathbf{RTN}_0(T)$ is finite dimensional, any two norms are equivalent so there exist positive constants $\alpha_0(T)$ and $\alpha_1(T)$ such that

$$\alpha_0(T) \leq \frac{\|\mathbf{v}\|_{0,T}^2}{|[\mathbf{v}]|_T^2} \leq \alpha_1(T) \quad \forall \mathbf{v} \in \mathbf{RTN}_0(T).$$

DEFINITION 4.1. *For T a tetrahedron, let ρ_T and h_T be the radius of the inscribed sphere for T and the diameter of T, respectively. Following Arnold, Boffi, and Falk [2] we use the notion of shape regularity. To define the composite element for a hexahedron E, the hexahedron is divided into* 5 *tetrahedra. There are two possible ways to decompose E into tetrahedra in such a fashion, each resulting in* 5 *tetrahedra. Let ρ_E be the smallest radius of the inscribed spheres for these* 10 *tetrahedra, and let h_E be the diameter of E. Then the shape constant of E is defined to be $\sigma_E = \frac{h_E}{\rho_E}$. The shape* *constant for a mesh $\mathcal{T}_h$ consisting of convex hexahedra is the supremum of the shape constants σ_E for $E \in \mathcal{T}_h$. A family of meshes $\{\mathcal{T}_h \ : \ h \in \mathcal{H}\}$ is said to be shape regular if the shape constants for the meshes can be uniformly bounded.*

LEMMA 4.2. *If the family of discretizations $\{\mathcal{T}_h, h \in \mathcal{H}\}$ is shape regular, then there are constants β_0 and β_1, independent of T and h, such that $\forall T \in \widetilde{\mathcal{T}}_E,\ E \in \mathcal{T}_h,\ h \in \mathcal{H}$,*

$$\beta_0 \leq \frac{\|\mathbf{v}\|^2_{0,T} h_E^4}{|[\mathbf{v}]|^2_T |T|} \leq \beta_1. \tag{4.1}$$

Proof. The result follows from a scaling argument: if $\hat{T}$ is a reference tetrahedral element (for which we note $\hat{h} = h_{\hat{T}}$ and $\hat{\rho} = \rho_{\hat{T}}$) and T is the image of $\hat{T}$ under a bijective affine mapping G and if $\forall \hat{\mathbf{v}} \in \mathbf{RTN}_0(\hat{T}), \mathbf{v}$ denotes the image of $\hat{\mathbf{v}}$ under the Piola transformation, then $|[\mathbf{v}]|_T = |[\hat{\mathbf{v}}]|_{\hat{T}}$. The following inequalities hold [6]:

$$\frac{1}{|J|\|DG^{-1}\|^2}\|\hat{\mathbf{v}}\|^2_{0,\hat{T}} \leq \|\mathbf{v}\|^2_{0,T} \leq \frac{1}{|J|}\|DG\|^2\|\hat{\mathbf{v}}\|^2_{0,\hat{T}},$$

where DG is the linear part of G and J is its determinant. Thus

$$\frac{1}{|J|\|DG^{-1}\|^2}\frac{\|\hat{\mathbf{v}}\|^2_{0,\hat{T}}}{|[\hat{\mathbf{v}}]|_{\hat{T}}} \leq \frac{\|\mathbf{v}\|^2_{0,T}}{|[\mathbf{v}]|_T} \leq \frac{1}{|J|}\|DG\|^2\frac{\|\hat{\mathbf{v}}\|^2_{0,\hat{T}}}{|[\hat{\mathbf{v}}]|_{\hat{T}}}$$

and

$$\frac{|\hat{T}|^2}{|T|^2}\frac{\rho_T^2}{\hat{h}^2}\frac{\|\hat{\mathbf{v}}\|^2_{0,\hat{T}}}{|\hat{T}||[\hat{\mathbf{v}}]|_{\hat{T}}} \leq \frac{\|\mathbf{v}\|^2_{0,T}}{|T||[\mathbf{v}]|_T} \leq \frac{|\hat{T}|^2}{|T|^2}\frac{h_T^2}{\hat{\rho}^2}\frac{\|\hat{\mathbf{v}}\|^2_{0,\hat{T}}}{|\hat{T}||[\hat{\mathbf{v}}]|_{\hat{T}}},$$

regrouping and multiplying by h_E^4

$$\frac{\rho_T^2 h_E^4}{|T|^2}\frac{|\hat{T}|\|\hat{\mathbf{v}}\|^2_{0,\hat{T}}}{\hat{h}^2|[\hat{\mathbf{v}}]|_{\hat{T}}} \leq \frac{h_E^4\|\mathbf{v}\|^2_{0,T}}{|T||[\mathbf{v}]|_T} \leq \frac{h_T^2 h_E^4}{|T|^2}\frac{|\hat{T}|\|\hat{\mathbf{v}}\|^2_{0,\hat{T}}}{\hat{\rho}^2|[\hat{\mathbf{v}}]|_{\hat{T}}}$$

using norm equality

$$\frac{\rho_T^2 h_E^4}{|T|^2}\alpha_0\left(\hat{T}\right)\frac{|\hat{T}|}{\hat{h}^2} \leq \frac{h_E^4\|\mathbf{v}\|^2_{0,T}}{|T||[\mathbf{v}]|_T} \leq \frac{h_T^2 h_E^4}{|T|^2}\alpha_1\left(\hat{T}\right)\frac{|\hat{T}|}{\hat{\rho}^2}$$

or

$$\frac{\rho_T^2 h_E^4}{|T|^2}\hat{\alpha}_0 \leq \frac{h_E^4\|\mathbf{v}\|^2_{0,T}}{|T||[\mathbf{v}]|_T} \leq \frac{h_T^2 h_E^4}{|T|^2}\hat{\alpha}_1,$$

where $\hat{\alpha}_0 = \alpha_0(\hat{T})\frac{|\hat{T}|}{\hat{h}^2}$ and $\hat{\alpha}_1 = \alpha_1(\hat{T})\frac{|\hat{T}|}{\hat{\rho}^2}$. To conclude it suffices to use the shape regularity of the family $\{\mathcal{T}_h :\ h \in \mathcal{H}\}$. ◻

4.1. Local interpolation operators and error estimates. Estimates for the scalar function spaces. We denote by π_E, respectively, $\tilde{\pi}_E$, the L^2-projection operator from $L^2(E)$ onto $\mathcal{M}_E$, respectively, $\widetilde{\mathcal{M}}_E$:

$$\pi_E(q) = \frac{1}{|E|}\int_E q(x)dx \quad \forall E \in \mathcal{T}_E\ \forall q \in L^2(E),$$
$$(\tilde{\pi}_E(q))_{|T} = \frac{1}{|T|}\int_T q(x)dx \quad \forall T \in \widetilde{\mathcal{T}}_E\ \forall q \in L^2(E).$$

It is well known [7], [9] that the following approximation results hold:

$$\|q-\tilde{\pi}_E(q)\|_{0,E} \leq Ch^m|q|_{m,E}, \quad \|q-\pi_E(q)\|_{0,E} \leq Ch^m|q|_{m,E} \quad \forall q \in H^m(E), \quad m = 0, 1. \tag{4.2}$$

Estimates for the vector function spaces. The Raviart–Thomas–Nédélec projection operator $\widetilde{\Pi}_E$ from $(H^1(E))^3$ onto $\widetilde{\mathcal{W}}_E$ is defined by

$$\int_{\widetilde{F}} \widetilde{\Pi}_E(\mathbf{v}) \cdot \mathbf{n}_{\widetilde{F}} \, ds = \int_{\widetilde{F}} \mathbf{v} \cdot \mathbf{n}_{\widetilde{F}} \, ds \quad \forall \widetilde{F} \in \widetilde{\mathcal{F}}_E \; \forall \mathbf{v} \in \left(H^1(E)\right)^3,$$

where, for each $\widetilde{F} \in \widetilde{\mathcal{F}}_E$, $\mathbf{n}_{\widetilde{F}}$ is a unit vector normal to $\widetilde{F}$. It is known [7] that

$$\|\mathbf{v} - \widetilde{\Pi}_E(\mathbf{v})\|_{0,E} \leq Ch|\mathbf{v}|_{1,E} \quad \forall \mathbf{v} \in \left(H^1(E)\right)^3 \tag{4.3}$$

and that the interpolation operators $\widetilde{\Pi}_E$ and $\tilde{\pi}_E$ satisfy the property

$$\tilde{\pi}_E \text{div } \mathbf{v} = \text{div } \widetilde{\Pi}_E \mathbf{v} \quad \forall \mathbf{v} \in \left(H^1(E)\right)^3 \tag{4.4}$$

so that

$$\begin{aligned} \left\|\text{div } \left(\mathbf{v} - \widetilde{\Pi}_E(\mathbf{v})\right)\right\|_{0,E} &= \|\text{div } \mathbf{v} - \tilde{\pi}_E(\text{div } \mathbf{v})\|_{0,E} \leq Ch^m |\text{div } \mathbf{v}|_{m,E} \\ &\qquad \forall \mathbf{v} \in \left(H^m(E)\right)^3, \quad m = 0, 1. \end{aligned} \tag{4.5}$$

Similarly one may define the interpolation operator $\widehat{\Pi}_E$ from $(H^1(E))^3$ onto $\widehat{\mathcal{W}}_E$ by

$$\int_{\widetilde{F}} \widehat{\Pi}_E(\mathbf{v}) \cdot \mathbf{n}_{\widetilde{F}} \, ds = \int_{\widetilde{F}} \mathbf{v} \cdot \mathbf{n}_{\widetilde{F}} \, ds \quad \forall \widetilde{F} \in \widetilde{\mathcal{F}}_E, \widetilde{F} \subset \partial E,$$

and the interpolation operator Π_E from $(H^1(E))^3$ onto $\mathcal{W}_E$ by

$$\int_F \Pi_E(\mathbf{v}) \cdot \mathbf{n}_F \, ds = \int_F \mathbf{v} \cdot \mathbf{n}_F \, ds \quad \forall F \in \mathcal{F}_E.$$

One can show that

$$\pi_E \text{div } \mathbf{v} = \text{div } \widehat{\Pi}_E \mathbf{v} = \text{div } \Pi_E \mathbf{v} \quad \forall \mathbf{v} \in (H^1(E))^3 \tag{4.6}$$

so that if $\mathbf{v}$ is sufficiently regular, using (4.2), we have

$$\begin{aligned} \|\text{div } (\mathbf{v} - \Pi_E(\mathbf{v}))\|_{0,E}^2 &= \left\|\text{div } \left(\mathbf{v} - \widehat{\Pi}_E(\mathbf{v})\right)\right\|_{0,E}^2 = \|\text{div } \mathbf{v} - \pi_E(\text{div } \mathbf{v})\|_{0,E}^2 \\ &\leq Ch^{2m} |\text{div } \mathbf{v}|_{m,E}^2 \quad \forall \mathbf{v} \in (H^m(E))^3, \quad m = 0, 1. \end{aligned} \tag{4.7}$$

We note that $\Pi_E(\mathbf{v})$ is also determined by

$$\forall F \in \mathcal{F}_E \int_F \Pi(\mathbf{v})_E \cdot \mathbf{n}_F ds = \sum_{j=1}^{2} \int_{\widetilde{F}_j} \widehat{\Pi}_E(\mathbf{v}) \cdot \mathbf{n}_F, \;\; \text{where} \;\; F = \widetilde{F}_1 \cup \widetilde{F}_2 \;\; \text{with} \;\; \widetilde{F}_1, \widetilde{F}_2 \in \widetilde{\mathcal{F}}_E.$$

To obtain an estimate for $\|\mathbf{v} - \Pi_E(\mathbf{v})\|_{0,E}$ we write

$$\|\mathbf{v} - \Pi_E(\mathbf{v})\|_{0,E}^2 \leq \left\|\mathbf{v} - \widetilde{\Pi}_E(\mathbf{v})\right\|_{0,E}^2 + \left\|\widetilde{\Pi}_E(\mathbf{v}) - \widehat{\Pi}_E(\mathbf{v})\right\|_{0,E}^2 + \left\|\widehat{\Pi}_E(\mathbf{v}) - \Pi_E(\mathbf{v})\right\|_{0,E}^2. \tag{4.8}$$

Since we have (4.3), there remains to estimate the last two terms on the right-hand side.

First, however, we number the faces of $F \in \mathcal{F}_E$ arbitrarily and then number the faces $\widetilde{F} \in \widetilde{\mathcal{F}}_E$ as follows: let $\widetilde{F}_i = T_i^E \cap T_5^E$ be the interior faces of T_i^E, $i = 1, \ldots, 4$, and let the remaining faces, the exterior faces, be numbered such that $F_i = \widetilde{F}_{2i+3} \cup \widetilde{F}_{2i+4}, i = 1, \ldots, 6$.

Recall that, for $i = 1, \ldots, 16$, $\tilde{\omega}_i$ denotes the basis element of $\widetilde{\mathcal{W}}_E$ whose constant normal component on the face $\widetilde{F}_j$ is $\delta_{i,j}, j = 1, \ldots, 16$. Also, for $i = 5, \ldots, 16$, $\widehat{\omega}_i$ denotes the basis element of $\widehat{\mathcal{W}}_E$ whose constant normal component on the face $\widetilde{F}_j$ is $\delta_{i,j}, j = 5, \ldots, 16$. For $i = 1, \ldots, 6$, ω_i denotes the basis element of $\mathcal{W}_E$ whose constant normal component on the face F_j is $\delta_{i,j}, j = 1, \ldots, 6$. Similarly let χ_E be the constant function of value one on E, and for $j = 1, \ldots, 5$, let χ_j be the characteristic function of T_j^E defined on E. Then we have

(4.9)

$$\begin{aligned}
\widetilde{\Pi}_E \mathbf{v} &= \sum_{i=1}^{16} \tilde{\phi}_i \tilde{\omega}_i, \quad \text{where} \quad \tilde{\phi}_i = \frac{1}{|\widetilde{F}_i|} \int_{\widetilde{F}_i} \widetilde{\Pi}_E \mathbf{v} \cdot \mathbf{n}_{\widetilde{F}_i} = \frac{1}{|\widetilde{F}_i|} \int_{\widetilde{F}_i} \mathbf{v} \cdot \mathbf{n}_{\widetilde{F}_i}, \quad i = 1, \ldots, 16, \\
\operatorname{div} \widetilde{\Pi}_E \mathbf{v} &= \sum_{j=1}^{5} \tilde{\psi}_j \tilde{\chi}_j, \quad \text{where} \quad \tilde{\psi}_j = \frac{1}{|T_j^E|} \int_{T_j^E} \operatorname{div} \widetilde{\Pi}_E \mathbf{v} = \frac{1}{|T_j^E|} \int_{T_j^E} \operatorname{div} \mathbf{v}, \quad j = 1, \ldots, 5, \\
\widehat{\Pi}_E \mathbf{v} &= \sum_{i=5}^{16} \widehat{\phi}_i \widehat{\omega}_i, \quad \text{where} \quad \widehat{\phi}_i = \frac{1}{|\widetilde{F}_i|} \int_{\widetilde{F}_i} \widehat{\Pi}_E \mathbf{v} \cdot \mathbf{n}_{\widetilde{F}_i} = \frac{1}{|\widetilde{F}_i|} \int_{\widetilde{F}_i} \mathbf{v} \cdot \mathbf{n}_{\widetilde{F}_i}, \quad i = 5, \ldots, 16, \\
\operatorname{div} \widehat{\Pi}_E \mathbf{v} &= \widehat{\psi} \chi_E, \quad \text{where} \quad \widehat{\psi} = \frac{1}{|E|} \int_E \operatorname{div} \widehat{\Pi}_E \mathbf{v} = \frac{1}{|E|} \int_E \operatorname{div} \mathbf{v}, \\
\Pi_E \mathbf{v} &= \sum_{i=1}^{6} \phi_i \omega_i, \quad \text{where} \quad \phi_i = \frac{1}{|F_i|} \int_{F_i} \Pi_E \mathbf{v} \cdot \mathbf{n}_{F_i} = \frac{1}{|F_i|} \int_{F_i} \mathbf{v} \cdot \mathbf{n}_{F_i}, \quad i = 1, \ldots, 6, \\
\operatorname{div} \Pi_E \mathbf{v} &= \psi \chi_E, \quad \text{where} \quad \psi = \frac{1}{|E|} \int_E \operatorname{div} \Pi_E \mathbf{v} = \frac{1}{|E|} \int_E \operatorname{div} \mathbf{v}.
\end{aligned}$$

Also let

$$\widehat{\phi}_i = \frac{1}{|\widetilde{F}_i|} \int_{\widetilde{F}_i} \widehat{\Pi}_E \mathbf{v} \cdot \mathbf{n}_{\widetilde{F}_i} \quad \left(\neq \frac{1}{|\widetilde{F}_i|} \int_{\widetilde{F}_i} \mathbf{v} \cdot \mathbf{n}_{\widetilde{F}_i} \right), \quad i = 1, \ldots, 4.$$

Note that $\tilde{\phi}_i = \widehat{\phi}_i,\ i = 5, \ldots, 16, \widehat{\psi} = \psi$, but $\tilde{\phi}_i \neq \widehat{\phi}_i,\ i = 1, \ldots, 4$.

Since the normal components of the functions $\widehat{\Pi}_E \mathbf{v}$ and $\widetilde{\Pi}_E \mathbf{v}$ are the same on ∂E but may differ on the internal faces, we have

$$\begin{aligned}
&\int_{\partial T_j^E \setminus \widetilde{F}_j} \widetilde{\Pi}_E \mathbf{v} \cdot \mathbf{n} + \tilde{\phi}_j |\widetilde{F}_j| = |T_j^E| \tilde{\psi}_j, \quad j = 1, \ldots, 4, \qquad -\sum_{j=1}^{4} \tilde{\phi}_j |\widetilde{F}_j| = |T_5^E| \tilde{\psi}_5, \\
&\int_{\partial T_j^E \setminus \widetilde{F}_j} \widehat{\Pi}_E \mathbf{v} \cdot \mathbf{n} + \widehat{\phi}_j |\widetilde{F}_j| = |T_j^E| \widehat{\psi}, \quad j = 1, \ldots, 4, \qquad -\sum_{j=1}^{4} \widehat{\phi}_j |\widetilde{F}_j| = |T_5^E| \widehat{\psi},
\end{aligned}$$

and subtracting, we obtain

(4.10)

$$\left(\tilde{\phi}_j - \widehat{\phi}_j\right) |\widetilde{F}_j| = |T_j^E| \left(\tilde{\psi}_j - \widehat{\psi}\right), \ j = 1, \ldots, 4, \quad \sum_{j=1}^{4} \left(\tilde{\phi}_j - \widehat{\phi}_j\right) |\widetilde{F}_j| = |T_5^E| \left(\widehat{\psi} - \tilde{\psi}_5\right).$$

Now, to estimate the second term on the right-hand side of (4.8) $\| \widetilde{\Pi}_E \mathbf{v} - \widehat{\Pi}_E \mathbf{v} \|_{0,E}^2$, we use the norm equivalence (4.1) together with (4.9) and (4.10) to obtain

$$
\begin{aligned}
\left\|\widetilde{\Pi}_E\mathbf{v}-\widehat{\Pi}_E\mathbf{v}\right\|_{0,E}^2 &= \sum_{j=1}^{5}\left\|\widetilde{\Pi}_E\mathbf{v}-\widehat{\Pi}_E\mathbf{v}\right\|_{0,T_j^E}^2\\
&\le \frac{\beta_1}{h_E^4}\sum_{j=1}^{5}\left|T_j^E\right|\left|\left[\widetilde{\Pi}_E\mathbf{v}-\widehat{\Pi}_E\mathbf{v}\right]\right|_{T_j^E}^2\\
&= \frac{\beta_1}{h_E^4}\left\{\sum_{j=1}^{4}\left|T_j^E\right|\left(\int_{\partial T_j^E}\left|\widetilde{\Pi}_E\mathbf{v}\cdot\mathbf{n}_{T_j^E}-\widehat{\Pi}_E\mathbf{v}\cdot\mathbf{n}_{T_j^E}\right|\right)^2\right.\\
&\qquad\left.+\left|T_5^E\right|\left(\int_{\partial T_5^E}\left|\widetilde{\Pi}_E\mathbf{v}\cdot\mathbf{n}_{T_5^E}-\widehat{\Pi}_E\mathbf{v}\cdot\mathbf{n}_{T_5^E}\right|\right)^2\right\}\\
&= \frac{\beta_1}{h_E^4}\left\{\sum_{j=1}^{4}\left|T_j^E\right|\left|\tilde{\phi}_j-\widehat{\phi}_j\right|^2\left|\widetilde{F}_j\right|^2+\left|T_5^E\right|\left(\sum_{j=1}^{4}\left|\tilde{\phi}_j-\widehat{\phi}_j\right|\left|\widetilde{F}_j\right|\right)^2\right\}\\
&\le \frac{\beta_1}{h_E^4}\left\{\sum_{j=1}^{4}\left|T_j^E\right|\left|\tilde{\psi}_j-\widehat{\psi}\right|^2\left|T_j^E\right|^2+\left|T_5^E\right|\left(\sum_{j=1}^{4}\left|\tilde{\psi}_j-\widehat{\psi}\right|\ \left|T_j^E\right|\right)^2\right\}\\
&\le \frac{\beta_1}{h_E^4}\left\{\sum_{j=1}^{4}\left|T_j^E\right|\left|\tilde{\psi}_j-\widehat{\psi}\right|^2\left|T_j^E\right|^2+4\left|T_5^E\right|\sum_{j=1}^{4}\left|\tilde{\psi}_j-\widehat{\psi}\right|^2\left|T_j^E\right|^2\right\}\\
&\le 5\beta_1\frac{|E|^2}{h_E^4}\sum_{j=1}^{4}\left|\tilde{\psi}_j-\widehat{\psi}\right|^2\left|T_j^E\right|\\
&= 5\beta_1\frac{|E|^2}{h_E^4}\sum_{j=1}^{4}\left|\frac{1}{\left|T_j^E\right|}\int_{T_j^E}\operatorname{div}\ \left(\widetilde{\Pi}_E\mathbf{v}-\widehat{\Pi}_E\mathbf{v}\right)\right|^2\left|T_j^E\right|\\
&\le 5\beta_1\frac{|E|^2}{h_E^4}\sum_{j=1}^{4}\left\|\operatorname{div}\ \left(\widetilde{\Pi}_E\mathbf{v}-\widehat{\Pi}_E\mathbf{v}\right)\right\|_{0,T_j^E}^2\\
&\le 5\beta_1 h_E^2\left\|\operatorname{div}\ \widetilde{\Pi}_E\mathbf{v}-\operatorname{div}\ \widehat{\Pi}_E\mathbf{v}\right\|_{0,E}^2\\
&\le 5\beta_1 h_E^2\left\|\operatorname{div}\ \widetilde{\Pi}_h\mathbf{v}-\operatorname{div}\ \widehat{\Pi}_h\mathbf{v}\right\|_{0,E}^2\\
&\le 5\beta_1 h_E^2\left\|\tilde{\pi}_h\operatorname{div}\ \mathbf{v}-\pi_h\operatorname{div}\ \mathbf{v}\right\|_{0,E}^2\\
&\le 5\beta_1 h_E^2\left\|\tilde{\pi}_h\operatorname{div}\ \mathbf{v}-\pi_h(\tilde{\pi}_h\operatorname{div}\ \mathbf{v})\right\|_{0,E}^2.
\end{aligned}
$$

Since

$$\|\ (I-\pi_h)\tilde{\pi}_h\operatorname{div}\ \mathbf{v}\ \|_{0,E}^2\le 2\ \|\ \tilde{\pi}_h\operatorname{div}\ \mathbf{v}\ \|_{0,E}^2+2\ \|\ \pi_h\tilde{\pi}_h\operatorname{div}\ \mathbf{v}\ \|_{0,E}^2\le 4\ \|\ \tilde{\pi}_h\operatorname{div}\ \mathbf{v}\ \|_{0,E}^2,$$

we obtain

$$\left\|\widetilde{\Pi}_h\mathbf{v}-\widehat{\Pi}_h\mathbf{v}\right\|_{0,E}^2\le 20\beta_1 h_E^2\left\|\tilde{\pi}_h\operatorname{div}\ \mathbf{v}\right\|_{0,E}^2\le 20\beta_1 h_E^2\ \|\ \operatorname{div}\ \mathbf{v}\ \|_{0,E}^2\ . \tag{4.11}$$

To estimate the third and final term $\| \widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v} \|_{0,E}$ of (4.8) we use the fact that for each exterior tetrahedra $T_j^E, \quad j = 1, \ldots, 4$,

$$\text{div } \left(\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right)_{|T_j^E} = 0, \quad \int_{\partial T_j^E} \left(\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right) \cdot \mathbf{n}_{T_j^E} = 0, \quad j = 1, \ldots, 4.$$

Then for $\mathbf{w} = \widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}$

$$\int_{\widetilde{F}_j} \mathbf{w} \cdot \mathbf{n}_{T_j^E} = - \int_{\partial T_j^E \setminus \widetilde{F}_j} \mathbf{w} \cdot \mathbf{n}_{T_j^E}, \quad j = 1, \ldots, 4,$$

and

$$\int_{\widetilde{F}_j} |\mathbf{w} \cdot \mathbf{n}_{T_j^E}| = \left| \int_{\widetilde{F}_j} \mathbf{w} \cdot \mathbf{n}_{T_j^E} \right| = \left| \int_{\partial T_j^E \setminus \widetilde{F}_j} \mathbf{w} \cdot \mathbf{n}_{T_j^E} \right| \leq \int_{\partial T_j^E \setminus \widetilde{F}_j} |\mathbf{w} \cdot \mathbf{n}_{T_j^E}|, \quad j = 1, \ldots, 4,$$

so we obtain

$$\sum_{j=1}^{4} \int_{\widetilde{F}_j} |\mathbf{w} \cdot \mathbf{n}_{T_j^E}| \leq \sum_{j=1}^{4} \int_{\partial T_j^E \setminus \widetilde{F}_j} |\mathbf{w} \cdot \mathbf{n}_{T_j^E}| = \sum_{i=5}^{16} \int_{\widetilde{F}_i} |\mathbf{w} \cdot \mathbf{n}_{\widetilde{F}_i}|.$$

Then we have

$$\begin{aligned}
\left\|\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right\|_{0,E}^2 &= \sum_{j=1}^{5} \left\|\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right\|_{0,T_j^E}^2 \\
&\leq \frac{\beta_1}{h_E^4} \sum_{j=1}^{5} \left|T_j^E\right| \left| \left[\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right] \right|_{\partial T_j^E}^2 \\
&\leq \frac{\beta_1}{h_E^4} |E| \Bigg\{ \sum_{j=1}^{4} \left(\int_{\partial T_j^E} \left| \left(\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right) \cdot \mathbf{n}_{T_j^E} \right| \right)^2 \\
&\qquad + \left(\int_{\partial T_5^E} \left| \left(\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right) \cdot \mathbf{n}_{T_5^E} \right| \right)^2 \Bigg\} \\
&\leq \frac{\beta_1}{h_E^4} |E| \Bigg\{ 8 \sum_{i=1}^{4} \left(\int_{\widetilde{F}_i} \left| \left(\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right) \cdot \mathbf{n}_{\widetilde{F}_i} \right| \right)^2 \\
&\qquad + 4 \sum_{i=5}^{16} \left(\int_{\widetilde{F}_i} \left| \left(\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right) \cdot \mathbf{n}_{\widetilde{F}_i} \right| \right)^2 \Bigg\} \\
&\leq C \frac{\beta_1}{h_E^4} |E| \left\{ \sum_{i=5}^{16} \left(\int_{\widetilde{F}_i} \left| \left(\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right) \cdot \mathbf{n}_{\widetilde{F}_i} \right| \right)^2 \right\} \\
&\leq C \frac{\beta_1}{h_E^4} |E| \left\{ \sum_{i=5}^{16} \left|\widetilde{F}_i\right| \left\| \left(\widehat{\Pi}_E \mathbf{v} - \Pi_E \mathbf{v}\right) \cdot \mathbf{n}_{\widetilde{F}_i} \right\|_{0,\widetilde{F}_i}^2 \right\} \\
&\leq C h_E \left\{ \sum_{i=5}^{16} \left\| \left(\widehat{\Pi}_E \mathbf{v} - \mathbf{v}\right) \cdot \mathbf{n}_{\widetilde{F}_i} \right\|_{0,\widetilde{F}_i}^2 + \sum_{l=1}^{6} \|(\Pi_E \mathbf{v} - \mathbf{v}) \cdot \mathbf{n}_{F_l}\|_{0,F_l}^2 \right\}.
\end{aligned}$$

Since $\widehat{\Pi}_E$ and Π_E can be interpreted as L^2-projections of the scalar function $\mathbf{v}\cdot\mathbf{n}$ on the faces $\widetilde{F}_i$ and F_i, respectively, we have the approximation estimates

$$\left\|\left(\widehat{\Pi}_E\mathbf{v}-\mathbf{v}\right)\cdot\mathbf{n}_{\widetilde{F}_i}\right\|_{0,\widetilde{F}_i}\le Ch^{1/2}\parallel\mathbf{v}\parallel_{1/2,\widetilde{F}_i}\quad\forall\mathbf{v}\in\left(H^1(E)\right)^3,$$
$$\|(\Pi_E\mathbf{v}-\mathbf{v})\cdot\mathbf{n}_{F_l}\|_{0,F_l}\le Ch^{1/2}\parallel\mathbf{v}\parallel_{1/2,F_l}\quad\forall\mathbf{v}\in\left(H^1(E)\right)^3.$$

From a standard trace theorem [10] $\parallel\mathbf{v}\parallel_{1/2,\widetilde{F}_i}\le C\parallel\mathbf{v}\parallel_{1,E}$, so

$$\begin{aligned}\sum_{i=5}^{16}\left\|\left(\widehat{\Pi}_E\mathbf{v}-\mathbf{v}\right)\cdot\mathbf{n}_{\widetilde{F}_i}\right\|^2_{0,\widetilde{F}_i}+\sum_{l=1}^{6}\parallel(\Pi_E\mathbf{v}-\mathbf{v})\cdot\mathbf{n}_{F_l}\parallel^2_{0,F_l}&\le Ch\sum_{i=5}^{16}\parallel\mathbf{v}\parallel^2_{1/2,\widetilde{F}_i}\\&\quad+Ch\sum_{l=1}^{6}\parallel\mathbf{v}\parallel^2_{1/2,F_l}\\&\le Ch\parallel\mathbf{v}\parallel^2_{1,E},\end{aligned}$$

and we obtain

$$\left\|\widehat{\Pi}_E\mathbf{v}-\Pi_E\mathbf{v}\right\|^2_{0,E}\le Ch^2\parallel\mathbf{v}\parallel^2_{1,E}\,. \tag{4.12}$$

Now summing up the three terms (4.3), (4.11), and (4.12) we obtain

$$\begin{aligned}\parallel\mathbf{v}-\Pi_E\mathbf{v}\parallel^2_{0,E}&=\left\|\mathbf{v}-\widetilde{\Pi}_E\mathbf{v}\right\|^2_{0,E}+\left\|\widetilde{\Pi}_E\mathbf{v}-\widehat{\Pi}_E\mathbf{v}\right\|^2_{0,E}+\left\|\widehat{\Pi}_E\mathbf{v}-\Pi_E\mathbf{v}\right\|^2_{0,E}\\&\le Ch^2\left(|\mathbf{v}|^2_{1,E}+\parallel\operatorname{div}\mathbf{v}\parallel^2_{0,E}+\parallel\mathbf{v}\parallel^2_{1,E}\right)\\&\le Ch^2\parallel\mathbf{v}\parallel^2_{1,E},\end{aligned}$$

and by using (4.7) we obtain that

$$\|\mathbf{v}-\Pi_E(\mathbf{v})\|^2_{H(\operatorname{div};E)}\le Ch^{2m}(\parallel\operatorname{div}\mathbf{v}\parallel^2_{m,E}+\parallel\mathbf{v}\parallel^2_{1,E}),\quad m=0,1. \tag{4.13}$$

4.2. Global interpolation error estimates. Let π_h be the L^2-projection operator from $L^2(\Omega)$ onto $\mathcal{M}_h$

$$\pi_h(q)(x)=\pi_E(q)(x)\quad\text{if}\quad x\in E,$$

and let Π_h be the interpolation operator from $(H^1(\Omega))^3$ onto $\mathcal{W}_h$ defined by

$$\Pi_h(\mathbf{v})(x)=\Pi_E(\mathbf{v})(x)\quad\text{if}\quad x\in E.$$

It then follows from (4.6) that

$$\pi_h\operatorname{div}\mathbf{v}=\operatorname{div}\Pi_h\mathbf{v}\quad\forall\mathbf{v}\in(H^1(\Omega))^3. \tag{4.14}$$

By summing (4.2) over the cells $E\in\mathcal{T}_h$ we obtain

$$\|q-\pi_h(q)\|^2_{0,\Omega}\le Ch^2|q|^2_{1,\Omega}.$$

Then summing (4.13) over all the cells E gives

$$\|\mathbf{v}-\Pi_h(\mathbf{v})\|^2_{H(\operatorname{div};\Omega)}\le Ch^{2m}(\parallel\operatorname{div}\mathbf{v}\parallel^2_{m,\Omega}+\parallel\mathbf{v}\parallel^2_{1,\Omega}),\quad m=0,1. \tag{4.15}$$

Finally, we obtain that the approximation errors are of order one:

$$\|q-\pi_h(q)\|^2_{0,\Omega}+\|\mathbf{v}-\Pi_h(\mathbf{v})\|^2_{H(\operatorname{div};\Omega)}\le Ch^2\left(|q|^2_{1,\Omega}+\parallel\operatorname{div}\mathbf{v}\parallel^2_{1,\Omega}+\parallel\mathbf{v}\parallel^2_{1,\Omega}\right).$$

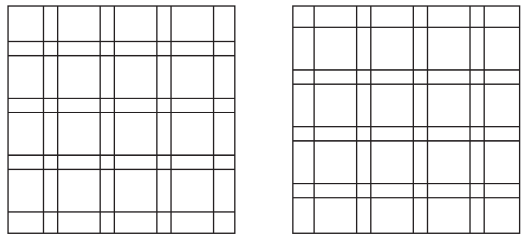

FIG. 5.1. *Horizontal cross sections $z = kh_z$ and $z = (k+1)h_z$ in a deformed mesh ($n = 8$).*

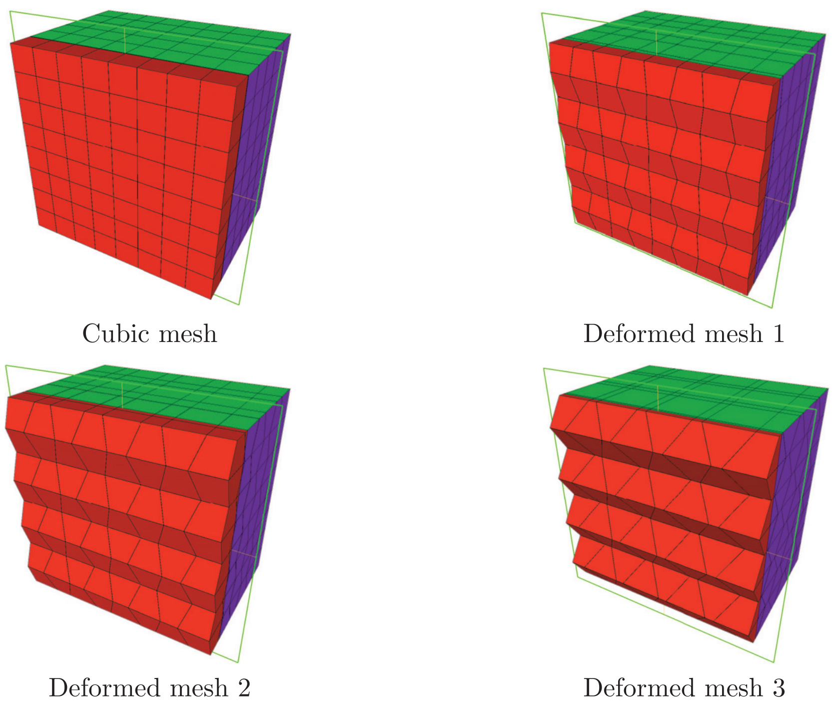

FIG. 5.2. *An $8 \times 8 \times 8$ cubic mesh with 3 deformed meshes with increasing deformation from the cubic mesh.*

5. Numerical experiment. In this section we consider two experiments: one for an academic case for which an analytical solution is known so that we can calculate errors and one for a more realistic case. The mixed method was implemented using the finite element library LifeV (http://www.lifev.org). Our implementation uses the LDL factorization instead of Cramer's formula for the inverse of K as recommended in [11].

First we present numerical convergence results for the analytical solution $p = x(1-x)y^2(1-y)^2z(1-z)$ on meshes which are deformations of an $n \times n \times n$ uniform cubic mesh for $n = 4, 8, 16, 32, 64$.

The deformation consists in moving the vertices in horizontal cross sections as shown in Figure 5.1 in order to obtain for the cells the form of truncated pyramids. Figure 5.2 shows four $8 \times 8 \times 8$ meshes, a cubic mesh with three deformed meshes with increasing degrees of deformation. The sequences of deformed meshes corresponding to $n = 4, 8, 16, 32, 64$ are not obtained by refining mesh n to obtain mesh $n+1$, but they are meshes that keep the same angle of deformation.

Table 5.1
Pressure and velocity errors for RTN and KR mixed finite elements on the sequence of cubic meshes.

	RTN finite element				KR finite element			
n	$\|\| p - p_h \|\|_{0,\Omega}$		$\|\| \mathbf{u} - \mathbf{u}_h \|\|_{0,\Omega}$		$\|\| p - p_h \|\|_{0,\Omega}$		$\|\| \mathbf{u} - \mathbf{u}_h \|\|_{0,\Omega}$	
	error	rate	error	rate	error	rate	error	rate
4	5.273e-4		2.492e-3		5.302e-4		3.492e-3	
8	2.690e-4	0.97	1.248e-3	1.00	2.697e-4	0.97	1.916e-3	0.86
16	1.352e-4	0.99	0.624e-3	1.00	1.354e-4	0.99	0.982e-3	0.96
32	0.677e-4	1.00	0.312e-3	1.00	0.678e-4	1.00	0.494e-3	0.99
64	0.388e-4	1.00	0.156e-3	1.00	0.339e-4	1.00	0.247e-3	1.00

Table 5.2
Pressure and velocity errors for extended RTN and KR finite elements on the sequence of deformed meshes 1.

	Extended RTN finite element				KR finite element			
n	$\|\| p - p_h \|\|_{0,\Omega}$		$\|\| \mathbf{u} - \mathbf{u}_h \|\|_{0,\Omega}$		$\|\| p - p_h p \|\|_{0,\Omega}$		$\|\| \mathbf{u} - \mathbf{u}_h \|\|_{0,\Omega}$	
	error	rate	error	rate	error	rate	error	rate
4	5.288e-4		2.759e-3		5.319e-4		3.566e-3	
8	2.702e-4	0.97	1.767e-3	0.64	2.710e-4	0.97	1.974e-3	0.85
16	1.362e-4	0.99	1.387e-3	0.35	1.362e-4	0.99	1.015e-3	0.96
32	0.686e-4	0.99	1.270e-3	0.13	0.682e-4	1.00	0.511e-3	0.99
64	0.351e-4	0.97	1.239e-3	0.04	0.341e-4	1.00	0.256e-3	1.00

Table 5.3
Pressure and velocity errors for extended RTN and KR finite elements on the sequence of deformed meshes 2.

	Extended RTN finite element				KR finite element			
n	$\|\| p - p_h \|\|_{0,\Omega}$		$\|\| \mathbf{u} - \mathbf{u}_h \|\|_{0,\Omega}$		$\|\| p - p_h \|\|_{0,\Omega}$		$\|\| \mathbf{u} - \mathbf{u}_h \|\|_{0,\Omega}$	
	error	order	error	rate	error	rate	error	rate
4	5.337e-4		3.339e-3		5.369e-4		3.796e-3	
8	2.757e-4	0.95	2.732e-3	0.31	2.751e-4	0.96	2.148e-3	0.82
16	1.425e-4	0.95	2.468e-3	0.15	1.385e-4	0.99	1.114e-3	0.95
32	0.777e-4	0.87	2.378e-3	0.05	0.694e-4	1.00	0.563e-3	0.98
64	0.494e-4	0.65	2.348e-3	0.02	0.348e-4	1.00	0.283e-3	0.99

Table 5.4
Pressure and velocity errors for extended RTN and KR finite elements on the sequence of deformed meshes 3.

	Extended RTN finite element				KR finite element			
n	$\|\| p - p_h \|\|_{0,\Omega}$		$\|\| \mathbf{u} - \mathbf{u}_h \|\|_{0,\Omega}$		$\|\| p - p_h \|\|_{0,\Omega}$		$\|\| \mathbf{u} - \mathbf{u}_h \|\|_{0,\Omega}$	
	error	rate	error	rate	error	rate	error	rate
4	5.664e-4		5.763e-3		5.557e-4		4.878e-3	
8	3.332e-4	0.76	5.601e-3	0.04	2.913e-4	0.93	2.942e-3	0.73
16	2.241e-4	0.57	5.185e-3	0.11	1.481e-4	0.98	1.561e-3	0.91
32	1.838e-4	0.29	4.952e-3	0.07	0.746e-4	0.99	0.798e-3	0.97
64	1.720e-4	0.10	4.842e-3	0.03	0.374e-4	0.99	0.403e-3	0.99

Tables 5.1, 5.2, 5.3, and 5.4 show errors for the pressure and the velocity using, respectively, the RTN method extended to general hexahedra (denoted extended RTN) and the new method (denoted KR). These tables confirm theoretical results stating that the extended RTN method does not converge on general hexahedra while the KR method does. Even for the most highly deformed meshes (deformed meshes 3)

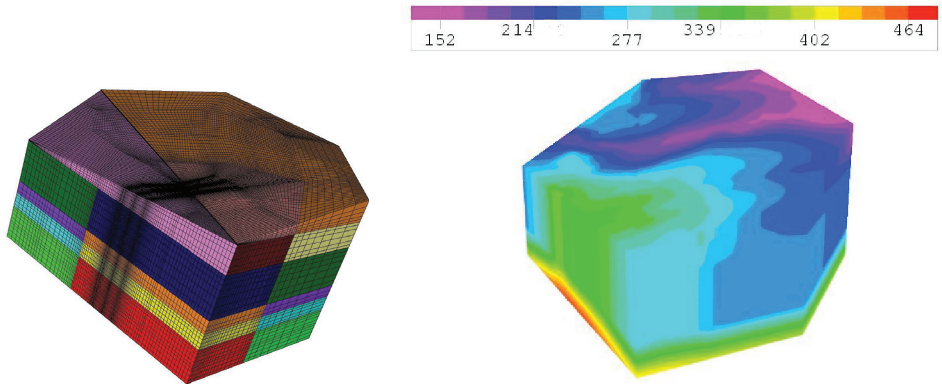

Fig. 5.3. *The domain of calculation (left) and the pressure field calculated on the boundary (right).*

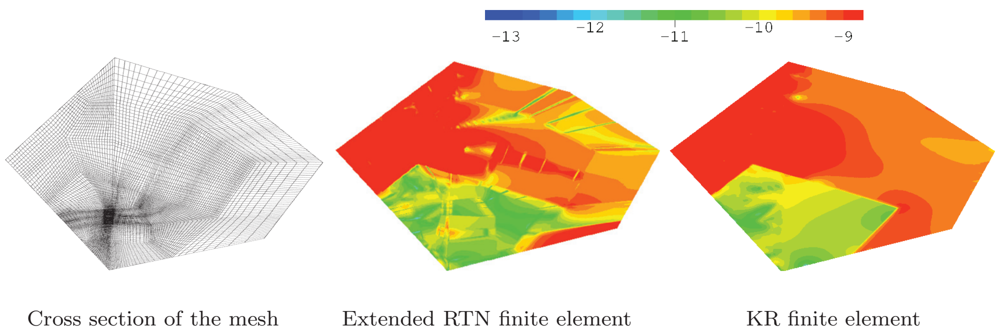

Fig. 5.4. *Horizontal cross section of the norm of the Darcy velocity for the extended RTN (center) and KR (right) mixed finite elements.*

which correspond to very large deformations, convergence is maintained. This shows the robustness of the method.

In the second experiment we calculate the pressure and velocity field around a nuclear waste disposal [21]. Figure 5.3 left shows the domain of calculation. It is made up of 13 geological subdomains, shown by different colors, with permeabilities changing with up to three orders of magnitude from one subdomain to the next.

The permeabilities of the geological layers have two principal characteristics: on the one hand, the values are extremely small, and, on the other hand, they are particularly heterogeneous. In Figure 5.3 left, the mesh is shown. It was provided by engineers from Andra (http://www.andra.fr) and is made of about 500,000 hexahedrons which for the most part are not parallelepipeds. On the right in Figure 5.3, the calculated pressure field calculated with KR mixed finite elements is shown. Both figures are blown up 30 times in the z-direction in order to visualize the mesh and results.

However, since the Darcy velocity is actually the important quantity that is needed for the transport, we show in Figure 5.4 the norm of the velocity on a horizontal cross section, the velocity calculated with extended RTN finite elements (center) and KR finite elements (right) and the corresponding cross section of the mesh (left). The scale on the color bar corresponds to powers of 10. As one can observe, there are significant differences in the calculated velocity. In particular the norm of the velocity calculated with extended RTN mixed finite elements shows a rough behavior which is clearly nonphysical for regions with constant permeabilities. This necessarily has a strong impact when this velocity is used in transport calculations. This mixed finite element method was also used to calculate diffusion in the transport problem around the waste disposal [21].

6. Conclusion. A new mixed finite element for hexahedral grids based on Kuznetsov's and Repin's general procedure for composite mixed finite elements has been constructed. This new mixed finite element provides an elegant and simple way to implement mixed finite elements for hexahedral discretizations. Theoretical convergence was proven, and numerical convergence was observed. The method is applied to the calculation of a Darcy velocity which will be used for the simulation of the transport of radionucides around a storage site.

It should be pointed out, however, that this element is not adapted to general distorted cubes with nonplanar faces. In the general case it is not possible to construct an unstructured mesh with hexahedra (distorted cubes with planar faces). Nevertheless in many cases, as in the example shown in Figure 5.3, engineers produce meshes with hexahedra or distorted cubes with almost planar faces, and our method can be used.

Appendix. Basis functions for the new finite element.

A.1. Geometry. The vertices of a hexahedron are denoted by $V_i, i = 1, \ldots, 8$, and its faces of a hexahedron E by $FE_i, i = 1, \ldots, 6$. Their numberings are shown in Figure A.1. The area of a face is denoted by $|FE_i|$. The volume of the hexahedron is denoted by $|E|$, and the numbering of the vertices in the hexahedron is shown in Figure A.1. The definition of the KR mixed finite element depends on the way the hexahedron is divided into tetrahedra. We here make a choice corresponding to Figure A.1, and the numbering of the vertices in the tetrahedra and the numbering of the tetrahedra are shown in Table A.1.

A.2. Basis functions. For each tetrahedron $T_\ell, \ell = 1, \ldots, 5$, in the chosen decomposition of the hexahedron E, the faces are denoted $FT_{\ell,i}, i = 1, \ldots, 4$, and the vertices $\mathbf{s}^{\ell,i}, i = 1, \ldots, 4$, where the numbering is such that $\mathbf{s}^{\ell,i}$ is the vertex opposite the face $FT_{\ell,i}$. Therefore if we denote the vertices of the tetrahedron T_ℓ, a standard

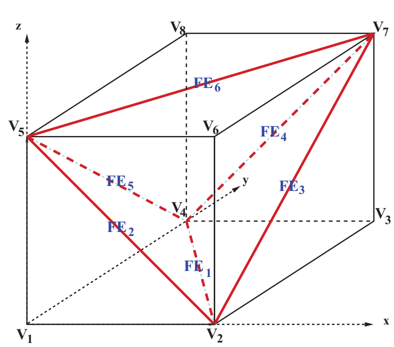

FIG. A.1. *Reference hexahedron with a numbering of its vertices and of its faces.*

Table A.1
Definition of the 5 *tetrahedra in the division shown in Figure* A.1.

Tetrahedron 1	Vertices	V_1	V_2	V_4	V_5
Tetrahedron 2	Vertices	V_6	V_7	V_2	V_5
Tetrahedron 3	Vertices	V_3	V_4	V_2	V_7
Tetrahedron 4	Vertices	V_8	V_7	V_5	V_4
Tetrahedron 5	Vertices	V_2	V_4	V_5	V_7

RTN_0 basis in this tetrahedron is

$$\mathbf{w}_{T_\ell,i} = \frac{|FT_{\ell,i}|}{3|T_\ell|}\left(\mathbf{x}-\mathbf{s}^{\ell,i}\right), \quad i=1,\dots,4, \quad \ell=1,\dots,5,$$

where $|FT_{\ell,i}|$ denotes the area of the face $FT_{\ell,i}$ and $|T_\ell|$ the volume of the tetrahedron T_ℓ. These basis functions are such that

$$\mathbf{w}_{T_\ell,i}\cdot\mathbf{n}_{\ell j} = \delta_{ij}, \quad i,j=1,2,3,4,$$

where $\mathbf{n}_{\ell j}$ denotes the unit outward normal to T_ℓ on the face $FT_{\ell,j}$. Therefore they satisfy also

$$\operatorname{div}\,\mathbf{w}_{T_\ell,i} = \frac{|FT_{\ell,i}|}{|T_\ell|}, \quad i=1,\dots,4, \quad \ell=1,\dots,5.$$

A basis for the new mixed finite element, denoted for a given hexahedron E by $\mathbf{w}_{Ei}, i=1,\dots,6$, is determined by

$$\int_{FE_j}\mathbf{w}_{Ei}\cdot\mathbf{n}_j = \delta_{ij}, \quad i,j=1,\dots,6,$$

where $\mathbf{n}_j$ denotes the unit outward normal to E on the face FE_j. These basis elements must be written tetrahedron by tetrahedron, and the restriction of $\mathbf{w}_{Ei}$ to the ℓth tetrahedron is denoted by $\mathbf{w}_{Ei,\ell}, i=1,\dots,6, \ell=1,\dots,5$. These basis functions are

Tetrahedron 1.

$$\mathbf{w}_{E1,1} = \left(\mathbf{w}_{T_1,4} + \frac{|T_1||FE_1|-|FT_{1,4}||E|}{|FT_{1,1}||E|}\mathbf{w}_{T_1,1}\right)\Big/|FE_1|,$$

$$\mathbf{w}_{E2,1} = \left(\mathbf{w}_{T_1,3} + \frac{|T_1||FE_2|-|FT_{1,3}||E|}{|FT_{1,1}||E|}\mathbf{w}_{T_1,1}\right)\Big/|FE_2|,$$

$$\mathbf{w}_{E3,1} = \frac{|T_1|}{|FT_{1,1}||E|}\mathbf{w}_{T_1,1},$$

$$\mathbf{w}_{E4,1} = \frac{|T_1|}{|FT_{1,1}||E|}\mathbf{w}_{T_1,1},$$

$$\mathbf{w}_{E5,1} = \left(\mathbf{w}_{T_1,2} + \frac{|T_1||FE_5|-|FT_{1,2}||E|}{|FT_{1,1}||E|}\mathbf{w}_{T_1,1}\right)\Big/|FE_5|,$$

$$\mathbf{w}_{E6,1} = \frac{|T_1|}{|FT_{1,1}||E|}\mathbf{w}_{T_1,1},$$

Tetrahedron 2.

$$
\begin{aligned}
\mathbf{w}_{E1,2} &= \frac{|T_2|}{|FT_{2,1}||E|}\mathbf{w}_{T_2,1},\\
\mathbf{w}_{E2,2} &= \left(\mathbf{w}_{T_2,2} + \frac{|T_2||FE_2| - |FT_{2,2}||E|}{|FT_{2,1}||E|}\mathbf{w}_{T_2,1}\right)\Big/|FE_2|,\\
\mathbf{w}_{E3,2} &= \left(\mathbf{w}_{T_2,4} + \frac{|T_2||FE_3| - |FT_{2,4}||E|}{|FT_{2,1}||E|}\mathbf{w}_{T_2,1}\right)\Big/|FE_3|,\\
\mathbf{w}_{E4,2} &= \frac{|T_2|}{|FT_{2,1}||E|}\mathbf{w}_{T_2,1},\\
\mathbf{w}_{E5,2} &= \frac{|T_2|}{|FT_{2,1}||E|}\mathbf{w}_{T_2,1},\\
\mathbf{w}_{E6,2} &= \left(\mathbf{w}_{T_2,3} + \frac{|T_2||FE_6| - |FT_{2,3}||E|}{|FT_{2,1}||E|}\mathbf{w}_{T_2,1}\right)\Big/|FE_6|,
\end{aligned}
$$

Tetrahedron 3.

$$
\begin{aligned}
\mathbf{w}_{E1,3} &= \left(\mathbf{w}_{T_3,4} + \frac{|T_3||FE_1| - |FT_{3,4}||E|}{|FT_{3,1}||E|}\mathbf{w}_{T_3,1}\right)\Big/|FE_1|,\\
\mathbf{w}_{E2,3} &= \frac{|T_3|}{|FT_{3,1}||E|}\mathbf{w}_{T_3,1},\\
\mathbf{w}_{E3,3} &= \left(\mathbf{w}_{T_3,2} + \frac{|T_3||FE_3| - |FT_{3,2}||E|}{|FT_{3,1}||E|}\mathbf{w}_{T_3,1}\right)\Big/|FE_3|,\\
\mathbf{w}_{E4,3} &= \left(\mathbf{w}_{T_3,3} + \frac{|T_3||FE_4| - |FT_{3,3}||E|}{|FT_{3,1}||E|}\mathbf{w}_{T_3,1}\right)\Big/|FE_4|,\\
\mathbf{w}_{E5,3} &= \frac{|T_3|}{|FT_{3,1}||E|}\mathbf{w}_{T_3,1},\\
\mathbf{w}_{E6,3} &= \frac{|T_3|}{|FT_{3,1}||E|}\mathbf{w}_{T_3,1},
\end{aligned}
$$

Tetrahedron 4.

$$
\begin{aligned}
\mathbf{w}_{E1,4} &= \frac{|T_4|}{|FT_{4,1}||E|}\mathbf{w}_{T_4,1},\\
\mathbf{w}_{E2,4} &= \frac{|T_4|}{|FT_{4,1}||E|}\mathbf{w}_{T_4,1},\\
\mathbf{w}_{E3,4} &= \frac{|T_4|}{|FT_{4,1}||E|}\mathbf{w}_{T_4,1},\\
\mathbf{w}_{E4,4} &= \left(\mathbf{w}_{T_4,3} + \frac{|T_4||FE_4| - |FT_{4,3}||E|}{|FT_{4,1}||E|}\mathbf{w}_{T_4,1}\right)\Big/|FE_4|,\\
\mathbf{w}_{E5,4} &= \left(\mathbf{w}_{T_4,2} + \frac{|T_4||FE_5| - |FT_{4,2}||E|}{|FT_{4,1}||E|}\mathbf{w}_{T_4,1}\right)\Big/|FE_5|,\\
\mathbf{w}_{E6,4} &= \left(\mathbf{w}_{T_4,4} + \frac{|T_4||FE_6| - |FT_{4,4}||E|}{|FT_{4,1}||E|}\mathbf{w}_{T_4,1}\right)\Big/|FE_6|,
\end{aligned}
$$

Tetrahedron 5.

$$\mathbf{w}_{E1,5} = \Bigg(-\frac{|T_1||FE_1| - |FT_{1,4}||E|}{|FT_{5,4}||E|}\mathbf{w}_{T_5,4} \quad -\frac{|T_2||FE_1|}{|FT_{5,2}||E|}\mathbf{w}_{T_5,2}$$
$$-\frac{|T_3||FE_1| - |FT_{3,4}||E|}{|FT_{5,3}||E|}\mathbf{w}_{T_5,3} \quad -\frac{|T_4||FE_1|}{|FT_{5,1}||E|}\mathbf{w}_{T_5,1}\Bigg) \Bigg/ |FE_1|,$$

$$\mathbf{w}_{E2,5} = \Bigg(-\frac{|T_1||FE_2| - |FT_{1,3}||E|}{|FT_{5,4}||E|}\mathbf{w}_{T_5,4} \quad -\frac{|T_2||FE_2| - |FT_{2,2}||E|}{|FT_{5,2}||E|}\mathbf{w}_{T_5,2}$$
$$-\frac{|T_3||FE_2|}{|FT_{5,3}||E|}\mathbf{w}_{T_5,3} \quad -\frac{|T_4||FE_2|}{|FT_{5,1}||E|}\mathbf{w}_{T_5,1}\Bigg) \Bigg/ |FE_2|,$$

$$\mathbf{w}_{E3,5} = \Bigg(-\frac{|T_1||FE_3|}{|FT_{5,4}||E|}\mathbf{w}_{T_5,4} \quad -\frac{|T_2||FE_3| - |FT_{2,3}||E|}{|FT_{5,2}||E|}\mathbf{w}_{T_5,2}$$
$$-\frac{|T_3||FE_3| - |FT_{3,2}||E|}{|FT_{5,3}||E|}\mathbf{w}_{T_5,3} \quad -\frac{|T_4||FE_3|}{|FT_{5,1}||E|}\mathbf{w}_{T_5,1}\Bigg) \Bigg/ |FE_3|,$$

$$\mathbf{w}_{E4,5} = \Bigg(-\frac{|T_1||FE_4|}{|FT_{5,4}||E|}\mathbf{w}_{T_5,4} \quad -\frac{|T_2||FE_4|}{|FT_{5,2}||E|}\mathbf{w}_{T_5,2}$$
$$-\frac{|T_3||FE_4| - |FT_{3,3}||E|}{|FT_{5,3}||E|}\mathbf{w}_{T_5,3} \quad -\frac{|T_4||FE_4| - |FT_{4,3}||E|}{|FT_{5,1}||E|}\mathbf{w}_{T_5,1}\Bigg) \Bigg/ |FE_4|,$$

$$\mathbf{w}_{E5,5} = \Bigg(-\frac{|T_1||FE_5| - |FT_{1,2}||E|}{|FT_{5,4}||E|}\mathbf{w}_{T_5,4} \quad -\frac{|T_2||FE_5|}{|FT_{5,2}||E|}\mathbf{w}_{T_5,2}$$
$$-\frac{|T_3||FE_5|}{|FT_{5,3}||E|}\mathbf{w}_{T_5,3} \quad -\frac{|T_4||FE_5| - |FT_{4,3}||E|}{|FT_{5,1}||E|}\mathbf{w}_{T_5,1}\Bigg) \Bigg/ |FE_5|,$$

$$\mathbf{w}_{E6,5} = \Bigg(-\frac{|T_1||FE_6|}{|FT_{5,4}||E|}\mathbf{w}_{T_5,4} \quad -\frac{|T_2||FE_6| - |FT_{2,3}||E|}{|FT_{5,2}||E|}\mathbf{w}_{T_5,2}$$
$$-\frac{|T_3||FE_6|}{|FT_{5,3}||E|}\mathbf{w}_{T_5,3} \quad -\frac{|T_4||FE_6| - |FT_{4,4}||E|}{|FT_{5,1}||E|}\mathbf{w}_{T_5,1}\Bigg) \Bigg/ |FE_6|.$$

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