A Composite Hexahedral Mixed Finite Element with Kershaw meshes

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Abstract: A Composite Hexahedral Mixed Finite Element for hexahedral meshes is presented. This composite element is based on the decomposition of the hexahedron into five tetrahedrons. A diffusion equation with an anisotropic diffusion coefficient and a known exact solution is solved on Kershaw meshes. Error charts for the L^2-error in both the scalar and vector variables are shown.

Key-words: mixed finite element, hexahedral grid, flow in porous media, Kershaw mesh.

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Un élément fini mixte héxaèdrique composite sur des maillages de Kershaw

Résumé : Un élément fini mixte composite pour des maillages héxaèdriques est présenté. Cet élément composite est basé sur la décomposition de l'héxaèdre en cinq tétraèdres. En utilisant cet élément, nous résolvons une équation de diffusion avec un coefficient anisotropique et une solution exacte connue. Un tableau d'erreurs L^2 pour les variables scalaires et vectorielle rassemble les résultats.

Mots-clés : élément fini mixte, maillages héxaèdriques, écoulement en milieu poreux, maillages de Kershaw.

1 Introduction

We consider the mixed finite element method for hexahedral meshes presented in [17]. Like other mixed finite element methods of lowest order the method of [17] is similar to a cell-centered, locally conservative finite volume method in that it uses the same degrees of freedom for the approximation of the scalar variable (pressure) as do these finite volume methods, but it differs in the way in which the vector variable (velocity) is calculated in terms of the pressure degrees of freedom: there is no explicit expression to obtain velocity from pressure and a linear system must be solved.

As is well known, the classical Raviart-Thomas-Nédélec mixed finite element method [15, 14, 6, 16] is for meshes made up of tetrahedra and/or rectangular solids. For the lowest order spaces, which are the ones which interest us here, the scalar variable is approximated in L^2 by functions which are constant on each cell of the mesh whereas the vector functions are approximated in $H(\text{div})$ by functions that have constant normal traces on each edge of each element of the mesh and also have a constant divergence on each element of the mesh. This method gives approximations with errors of order h in both variables and is known to be particularly appropriate for problems with large discontinuities in the coefficients. Thus it is normal to try to extend this method to handle meshes made up of hexahedra for applications in which such meshes are preferred. This can be done in a natural way by the technique of passing to a reference element. However the demonstration of order of h convergence for the Raviart-Thomas-Nédélec spaces relies on the fact that the functions mapping the tetrahedra or rectangular solids to the reference element are linear, but with hexahedra this is no longer the case (unless the hexahedra are parallelepipeds), and the demonstration breaks down. Approximation accuracy is lost; as was pointed out in [13], the resulting approximation space does not even contain the constant functions. (See [17] for some numerical calculations carried out with this approximation space.)

The problem of extending from rectangular solid meshes to hexahedral meshes in 3D is present, though to a lesser degree, in 2D for extending from rectangles to general quadrilaterals, and several articles have dealt with this problem: see [2, 18], but neither of these approaches extends satisfactorily to the 3D problem. One response to the problem in 3D is given in [7], but higher order polynomials are used. The method in [17] uses composite elements and is based on ideas of Kuznetsov and Repin ; see [11].

Suppose that Ω is a domain of R^3 with boundary Γ which is decomposed into a part Γ_N with Neumann boundary condition and a part Γ_D with Dirichlet boundary conditions. The outward pointing unit normal vector field on Γ is denoted $\boldsymbol{n}$. For simplicity we will suppose that the Neumann condition is a homogeneous condition. A nonhomogeneous Neumann condition can be treated in the way that is standard for mixed finite element methods. We consider the second order elliptic problem

$$\text{div}(-\boldsymbol{K}\nabla p) = f, \ \text{in } \Omega; \qquad p = \bar{p}, \ \text{on } \Gamma_D; \qquad \boldsymbol{K}\nabla p \cdot \boldsymbol{n} = 0, \ \text{on } \Gamma_N, \tag{1}$$

where the coefficient $\boldsymbol{K}$ is a full symmetric tensor such that $\boldsymbol{Kx}\cdot\boldsymbol{x}$ is bounded above and below on Ω by positive constants. In mixed form we introduce the vector unknown (velocity) $\boldsymbol{u} = -\boldsymbol{K}\nabla p$ and the mixed weak form of the problem may be written

$$\text{Find } (p,\boldsymbol{u}) \in L^2(\Omega) \quad \times \quad H(\text{div};\Omega) \text{ such that}$$

$$\begin{aligned} \int_\Omega \boldsymbol{K}^{-1}\boldsymbol{u}\cdot\boldsymbol{v} - \int_\Omega p\,\mathrm{div}\boldsymbol{v} &= -\int_{\Gamma_D} \bar{p}\,\boldsymbol{v}\cdot\boldsymbol{n} \quad \forall \boldsymbol{v}\in H(\mathrm{div};\Omega) \\ \int_\Omega \mathrm{div}\boldsymbol{v}\,q &= \int_\Omega fq \quad \forall q\in L^2(\Omega). \end{aligned} \tag{2}$$

In Section 2, we describe our composite mixed finite element method for hexahedral meshes. And in Section 3, we present numerical results obtained using Kershaw meshes.

2 The Numerical Scheme

The numerical method used here (see [17]) is a mixed finite element method based on the weak formulation of the problem. Thus given a discretization $\mathscr{T}_h$ of Ω into hexahedra (with planar faces) we solve the following system:

$$\begin{aligned} \text{Find } (p_h,\boldsymbol{u}_h)\in M_h &\times \boldsymbol{W}_h \text{ such that} \\ \int_\Omega \boldsymbol{K}^{-1}\boldsymbol{u}_h\cdot\boldsymbol{v}_h - \int_\Omega p_h\mathrm{div}\boldsymbol{v}_h &= -\int_{\Gamma_D} \bar{p}\boldsymbol{v}_h\cdot\boldsymbol{n} \quad \forall \boldsymbol{v}_h\in \boldsymbol{W}_h, \\ \int_\Omega \mathrm{div}\boldsymbol{v}_h\,q_h &= \int_\Omega fq_h \quad \forall q_h\in M_h, \end{aligned} \tag{3}$$

where $M_h\subset L^2(\Omega)$ is the space of piecewise constant functions (just as in the lowest order Raviart-Thomas-Nedelec spaces for tetrahedra or for rectangular solids), and $\boldsymbol{W}_h\subset H(\mathrm{div};\Omega)$ is a space of composite elements satisfying the following 4 conditions (all of which are satisfied by the Raviart-Thomas-Nédelec elements when the underlying spatial discretization is made up of tetrahedra and/or rectangular solids):

- $\boldsymbol{W}_h\subset H(\mathrm{div};\Omega)$; i.e. elements of $\boldsymbol{W}_h$ are locally in $H(\mathrm{div};T)$; $\forall T\in\mathscr{T}_h$, and normal components of elements of $\boldsymbol{W}_h$ are continuous across edges of the hexahedra in $\mathscr{T}_h$.
- normal components of elements of $\boldsymbol{W}_h$ are constant on each face of an element of $\mathscr{T}_h$.
- $\mathrm{div}\boldsymbol{W}_h\subset M_h$; i.e. the divergence of an element of $\boldsymbol{W}_h$ is constant on each hexahedron of $\mathscr{T}_h$.
- an element of $\boldsymbol{W}_h$ is uniquely determined by its flux through the faces of elements of $\mathscr{T}_h$; i.e. $\boldsymbol{W}_h$ has a basis of functions $\{\boldsymbol{v}_F : F\in\mathscr{F}_h\}$, where $\mathscr{F}_h$ is the set of all faces of hexahedra in $\mathscr{T}_h$, not lying on Γ_N, and for $F\in\mathscr{F}_h$, $\boldsymbol{v}_F$ is the unique function in $\boldsymbol{W}_h$ having normal component with flux across the face $E\in\mathscr{F}_h$ equal to $\delta_{E,F}$.

The space $\boldsymbol{W}_h$ is constructed element by element: for an element $T\in\mathscr{T}_h$ we define the space $\boldsymbol{W}_T$ of functions on T, and then $\boldsymbol{W}_h$ is defined to be the subspace of $H(\mathrm{div};\Omega)$ consisting of those functions whose restriction to T is in $\boldsymbol{W}_T$ for each $T\in\mathscr{T}_h$. To construct $\boldsymbol{W}_T$ for an element $T\in\mathscr{T}_h$, T is subdivided into 5 tetrahedra as follows: starting from any vertex V_1 of T there are 3 vertices (say V_2,V_4, and V_5) of T that can be joined to V_1 by an edge of T, there are 3 other vertices (say V_3,V_6, and V_8) that lie on a face with V_1 (but not on an edge with V_1). The remaining vertex V_7 together with V_2, V_4, and V_5 forms a tetrahedron S_0 having no face lying on the boundary of T. Then $T \setminus S_0$ is made up of 4 tetrahedra S_1, S_2, S_3 and S_4, each of which has 3 faces lying on the surface of T and one face in common with S_0; see Fig. 1.

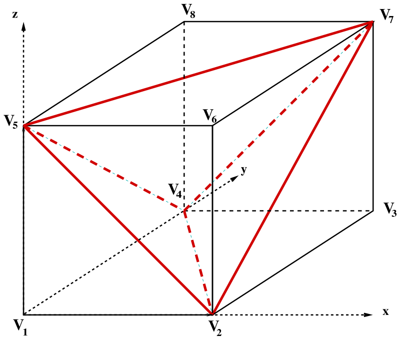

Figure 1: A partition of the reference hexahedron into 5 tetrahedra: one tetrahedron lies in the interior of T and is determined by the vertics V_2, V_4, V_5, V_7. The four other tetrahedra have each three faces on the surface of T and each contains one of the vertices V_1, V_3, V_6, V_8. There are two possible such constructions depending on which vertex is chosen as V_1.

The collection of tetrahedra $\mathscr{T}_T = \{S_i : i = 0, 1, \cdots, 4\}$ is a discretisation of T by tetrahedra, and we denote by $\widetilde{\boldsymbol{W}}_T$ the Raviart-Thomas-Nédélec space of lowest order associated with $\mathscr{T}_T$. We let $\widetilde{M}_T$ denote the set of functions constant on each of the five tetrahedra in $\mathscr{T}_T$, let $\widetilde{\boldsymbol{W}}_{T,0} \subset \widetilde{\boldsymbol{W}}_T$ denote the set of functions in $\widetilde{\boldsymbol{W}}_T$ whose normal traces vanish on all of ∂T, and let $|T|$ denote the volume of T. For each face F of T, letting $|F|$ denote the area of F and letting $\widetilde{\boldsymbol{W}}_{T,F} \subset \widetilde{\boldsymbol{W}}_T$ denote the set of functions in $\widetilde{\boldsymbol{W}}_T$ whose normal traces vanish on all of $\partial T \setminus F$ and are identically equal to $\frac{1}{|F|}$ on F, we define $\boldsymbol{v}_F$ to be the second component of the solution of the problem

$$\begin{aligned} \text{Find}(q_F, \boldsymbol{v}_F) \in \widetilde{M}_T \quad &\times \quad \widetilde{\boldsymbol{W}}_{T,F} \text{ such that} \\ \int_T \boldsymbol{v}_F \cdot \boldsymbol{v}_h - \int_T q_F \operatorname{div} \boldsymbol{v}_h \quad &= \quad 0, \quad \forall \boldsymbol{v}_h \in \widetilde{\boldsymbol{W}}_{T,0}, \\ \int_T \operatorname{div} \boldsymbol{v}_F \, q_h \quad &= \quad \frac{1}{|T|} \int_T q_h \quad \forall q_h \in \widetilde{M}_T. \end{aligned} \tag{4}$$

The pure Neumann problem (4) has a solution as the compatibility condition that the integral over ∂T of the Neumann data function be equal to the integral over T of the source term is satisfied. The second component $\boldsymbol{v}_F$ of the solution is uniquely determined: in the algebraic system associated with problem (4), the four equations corresponding to the four exterior tetrahedra, $S_1, \cdots, S_4$, determine $\boldsymbol{v}_F$, the equation associated with S_0 is redundant but is not a problem since the compatibility condition is satisfied. (The four equations associated with the internal faces, the four faces of S_0, imply that q_F is constant on all of T, but do not determine the value of the constant, but this is not needed here.) Then $\boldsymbol{W}_T \subset \widetilde{\boldsymbol{W}}_T$ is defined to be simply the six-dimensional subspace generated by the basis elements $\{\boldsymbol{v}_F : F \text{ is a face of } T\}$. Now defining $\boldsymbol{W}_h$ by

$$\boldsymbol{W}_h = \{\boldsymbol{v} \in H(\operatorname{div}; \Omega) : \boldsymbol{v}_{|T} \in \boldsymbol{W}_T, \quad \forall T \in \mathscr{T}_h\},$$

one can easily check that $\boldsymbol{W}_h$ satisfies the four conditions listed above.

Remark We point out that there are two possible choices for $\mathscr{T}_T$ (and thus for $\boldsymbol{W}_T$) depending on whether (in the notation used above) vertices $\{V_2, V_4, V_5, V_7\}$ or the vertices $\{V_1, V_3, V_6, V_8\}$ are used to form the interior tetrahedron. Also it is not always possible to choose the sets $\mathscr{T}_T$ is such a way that $\cup_{T\in\mathscr{T}_h}\mathscr{T}_T$ forms a finite element decomposition of Ω into tetrahedra.

Remark One could in a perhaps more natural way divide each of the hexahedra into 6 tetrahedra (all of equal area for the reference hexahedron) by adding a central edge between any single pair of vertices not belonging to a common face. The six tetrahedra would all have this edge in common and each would have two internal faces and two external faces. One could form a system similar to (3) for each of the six faces of T. The dimension of $\widetilde{M}_T$ would then be 6 instead of 5 and that of $\widetilde{\boldsymbol{W}}_{T,0}$ would be 6 instead of 4 as there would be 6 interior faces. The six equations of the linear system corresponding to one of the six tetrahedra would each only give a relation between the fluxes through the internal faces of the tetrahedron, so the second component of the solution would be determined only up to a (divergence free) flow going around the central edge. One would then need to impose a condition to make the macro elements rotational free (as are the Raviart-Thomas-Nédélec elements on tetrahedra and on rectangular solids as well as are those defined above on hexahedra using a decomposition into five tetrahedra). We have not further investigated this possibility.

Error estimates In this paragraph we briefly recall the error estimates obtained in [17]. Following [2] we define the notion of shape regularity for a family of meshes of hexahedra.

Definition For S a tetrahedron let ρ_S and h_S denote respectively the radius of the inscribed sphere of S and the diameter of S. Then for a hexahedron T, as seen earlier, there are two possible ways of decomposing T into five tetrahedra. Let ρ_T be the smallest of the ρ_S's for these 10 tetrahedra, let h_T be the diameter of T and let $\sigma_T = h_T/\rho_T$ be the shape constant of T. For a mesh $\mathscr{T}_h$ of hexahedra, the shape constant of $\mathscr{T}_h$ is the largest σ_T for $T \in \mathscr{T}_h$. A family $\{\mathscr{T}_h : h \in \mathscr{H}\}$ of meshes $\mathscr{T}_h$ made up of hexahedra is said to be *shape regular* if the shape constants for the meshes can be uniformly bounded.

In [17] it is shown that if $(p, \boldsymbol{u}) \in L^2(\Omega) \times H(\mathrm{div};\Omega)$ is the solution of problem (2) and $(p_h, \boldsymbol{u}_h) \in M_h \times \boldsymbol{W}_h$ is the solution of problem (3) and the family $\{\mathscr{T}_h : h \in \mathscr{H}\}$ of meshes $\mathscr{T}_h$ made up of hexahedra is shape regular then there is a constant C independent of h such that

$$\|p_h - p\|^2_{L^2(\Omega)} + \|\boldsymbol{u}_h - \boldsymbol{u}\|^2_{H(\mathrm{div};\Omega)} \leq C h^2 \left(|p|^2_{H^1(\Omega)} + \|\boldsymbol{u}\|^2_{H^1(\Omega)} + \|\mathrm{div}\boldsymbol{u}\|^2_{H^1(\Omega)} \right),$$

provided that p and $\boldsymbol{u}$ are sufficiently regular for the righthand side to be defined.

Mixed-hybrid finite elements and solution of the linear problem As with the Raviart-Thomas-Nédélec elements for tetrahedra and rectangular solids, the solution $(\boldsymbol{u}_h, p_h)$ is sought in a subspace $M_h \times \boldsymbol{W}_h$ of $L^2(\Omega) \times H(\mathrm{div};\Omega)$ in which the degrees of freedom are the average values of the pressure over the hexahedra of the grid and the fluxes through the faces of the grid. The resulting linear system then has exactly the same form as that for the Raviart-Thomas-Nédélec elements for grids of rectangular solids (when the problem has full tensor coefficients). As in [3] we can relax the condition that the approximate solution be sought in a subspace of $H(\mathrm{div};\Omega)$ and enforce this condition using Lagrange multipliers. We then define the approximation space $\boldsymbol{W}_h^*$ by

$$\boldsymbol{W}_h^* = \{\boldsymbol{v} \in (L^2(\Omega))^3 \,:\, \boldsymbol{v}_{|T} \in \boldsymbol{W}_T, \quad \forall T \in \mathscr{T}_h\},$$

and introduce a space of Lagrange multipliers $\Lambda_h = \{\lambda_h = \{\lambda_F\}_{F\in\mathscr{F}_h} \in R^{n_F}\}$ where n_F is the number of faces in $\mathscr{F}_h$. Then the following problem has a unique solution:

$$\begin{aligned}
&\text{Find } (p_h^*, \boldsymbol{u}_h^*, \lambda_h) \in M_h \times \boldsymbol{W}_h^* \times \Lambda_h \text{ such that}\\
&\sum_{T\in\mathscr{T}_h}\int_T \boldsymbol{K}^{-1}\boldsymbol{u}_h^*\cdot\boldsymbol{v}_h - \sum_{T\in\mathscr{T}_h}\int_T p_h^*\mathrm{div}\boldsymbol{v}_h - \sum_{F\in\mathscr{F}_h}\int_F \lambda_F[\boldsymbol{v}_h\cdot\boldsymbol{n}_F] = \\
&\qquad\qquad\qquad\qquad -\int_{\Gamma_D}\bar{p}\boldsymbol{v}_h\cdot\boldsymbol{n} \quad \forall \boldsymbol{v}_h \in \boldsymbol{W}_h^*,\\
&\sum_{T\in\mathscr{T}_h}\mathrm{div}\boldsymbol{u}_h^*\, q_h = \int_\Omega f q_h \quad \forall q_h \in M_h,\\
&\sum_{F\in\mathscr{F}_h}\int_F [\boldsymbol{u}_h^*\cdot\boldsymbol{n}_F]\mu_F = 0, \quad \forall \mu_h \in \Lambda_h,
\end{aligned} \tag{5}$$

where for $F \in \mathscr{F}_h$, $\boldsymbol{n}_F$ is a unit vector normal to F and for $\boldsymbol{v}_h \in \boldsymbol{W}_h^*$, $[\boldsymbol{v}_h\cdot\boldsymbol{n}_F]$ denotes the jump across F of $\boldsymbol{v}_h\cdot\boldsymbol{n}_F$ in the direction of $\boldsymbol{n}_F$. As with the Raviart-Thomas-Nédélec method it is now easy to eliminate first $\boldsymbol{u}_h^*$ and then p_h^* from the linear system and thus obtain a symmetric positive definite system with λ_h as the only unknown. For $F \in \mathscr{F}_h$ the multiplier λ_F enforcing continuity of $\boldsymbol{u}_h^*\cdot\boldsymbol{n}_F$ across F is in fact an approximation of the trace of the pressure p on F.

Once λ_h is found one can recover $\boldsymbol{u}_h^*$ and p_h^* through local calculations given by the first two equations of system (5). One shows easily that $\boldsymbol{u}_h^*$ is in fact in $\boldsymbol{W}_h$ and is equal to $\boldsymbol{u}_h$ and that $p_h^* = p_h$.

As with other mixed finite element methods, this method can be implemented as a nonconforming finite element method using pressure unknowns on the faces [3, 12, 1, 4].

3 Numerical experiments

The data are provided by the first test case of the *FVCA6 3D* anisotropic benchmark (cf. [9, 8]), a test case with anisotropy and Kershaw meshes [10]. An 8X8X8 Kershaw mesh is shown in Figure 2. The domain Ω is the unit cube in R^3, and the problem solved numerically is problem (1). Dirichlet conditions are given on the entire boundary: $\Gamma_D = \Gamma$. The permeability tensor $\boldsymbol{K}$ is

$$\boldsymbol{K} = \begin{pmatrix} 1 & \frac{1}{2} & 0 \\ \frac{1}{2} & 1 & \frac{1}{2} \\ 0 & \frac{1}{2} & 1 \end{pmatrix},$$

the source term f and the boundary data $\bar{p}$ are determined from the known exact solution p given by

$$p(x,y,z) = 1 + \sin(\pi x) + \sin\left(\pi\left(y + \frac{1}{2}\right)\right) + \sin\left(\pi\left(y + \frac{1}{3}\right)\right).$$

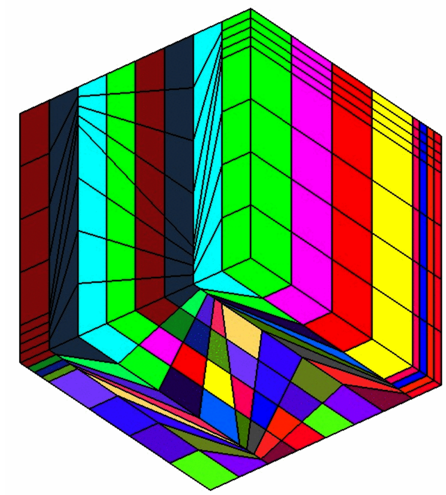

Figure 2: An 8X8X8 Kershaw mesh.

Table 1 gives results obtained with four Kershaw meshes. As was mentioned earlier the matrix of the linear system associated with the mixed-hybrid finite element after elimination of p_h^* and $\boldsymbol{u}_h^*$ is symmetric and positive definite, and the unknowns are the Lagrangian multipliers λ_h which are approximations of the averages of the trace of the scalar variable (pressure) over the faces. The number of matrix nonzeros given in the table is for the full matrix (not the upper or lower halves). From λ_h local calculations yield the cell pressure unknowns of p_h and the fluxes across the faces of the velocity $\boldsymbol{u}_h$. The mixed finite element method provides a piecewise polynomial representation of p_h and $\boldsymbol{u}_h$ inside the cells which allows a straightforward calculation of the L^2 errors :

$$|| \, p - p_h \, ||_0 = \frac{\sqrt{\int_\Omega (p - p_h)^2}}{\sqrt{\int_\Omega p^2}}, \quad || \, \boldsymbol{u} - \boldsymbol{u}_h \, ||_0 = \frac{\sqrt{\int_\Omega |\boldsymbol{u} - \boldsymbol{u}_h|^2}}{\sqrt{\int_\Omega |\boldsymbol{u}|^2}}.$$

The integrals are calculated using on each cell an integration formula exact for polynomials of degree 2 in 3D.

Then for the face pressures the error is

$$\| \lambda - \lambda_h \|_{0,h} = \frac{\sqrt{\sum_{F \in \mathscr{F}_h} \int_F (\lambda - \lambda_h)^2}}{\sqrt{\sum_{F \in \mathscr{F}_h} \int_F \lambda^2}}.$$

The face integrals are calculated using on each cell an integration formula exact for polynomials of degree 2 in 2D.

All errors behave as predicted by the theory and show an asymptotic rate of convergence of order 1. The exact solution is such that $0 \leq p \leq 2$ and the calculated solution has small undershoots which become smaller as the meshes are refined.

More error results can be found in [5].

Mesh		8X8X8	16X16X16	32X32X32	64X64X64
number of cells		512	4096	32768	262144
number of faces		576	4352	33792	266240
number of matrix unknowns		576	4352	33792	266240
number of matrix nonzeros		2496	32512	310272	2682880
$\| p - p_h \|_0$	error	0.0637513	0.038971	0.0194238	0.0091482
	rate		0.73	1.02	1.09
$\| \boldsymbol{u} - \boldsymbol{u}_h \|_0$	error	0.6979440	0.426929	0.216929	0.101924
	rate		0.729	0.991	1.10
$\| \lambda - \lambda_h \|_{0,h}$	error	0.088901	0.048125	0.024295	0.011245
	rate		0.91	1.00	1.12
min p_h		-0.03255	-0.04618	-0.03621	-0.00837
max p_h		1.94685	1.99488	2.00028	2.00061
min λ_h		-0.08554	-0.06291	-0.06571	0.00928
max λ_h		1.97834	2.06396	2.00166	2.00102

Table 1: Results obtained for a composite hexahedral mixed finite element on a sequence of Kershaw's meshes.

4 Conclusion

In spite of the bad aspect ratios of some of the hexahedra in the Kershaw meshes, the proposed composite hexahedral mixed finite element shows first order convergence for the scalar variable as well as for the vector variable.

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