Benchmark 3D: A Composite Hexahedral Mixed Finite Element

Ibtihel Ben Gharbia, Jérôme Jaffré, N. Suresh Kumar, and Jean E. Roberts

1 The Numerical Scheme

The numerical method used here (see [6]) is a mixed finite element method based on the weak formulation of the problem:

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

Straightforward extensions of the Raviart-Thomas-Nédelec mixed finite elements [3, 5] to hexahedral meshes do not converge. Therefore in [6] a composite mixed finite element was introduced and analyzed.

Given a discretization $\mathscr{T}_h$ of Ω into hexahedra (with planar faces) we solve the following system:

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$$\text{Find } (p_h, \boldsymbol{u}_h) \in M_h \times \boldsymbol{W}_h \text{ such that}$$
$$\int_\Omega \boldsymbol{K}^{-1}\boldsymbol{u}_h \cdot \boldsymbol{v}_h - \int_\Omega p_h \text{div}\boldsymbol{v}_h = -\int_{\Gamma_D} \bar{p}\boldsymbol{v}_h \cdot \boldsymbol{n} \quad \forall \boldsymbol{v}_h \in \boldsymbol{W}_h, \tag{2}$$
$$\int_\Omega \text{div}\boldsymbol{v}_h\, q_h = \int_\Omega f q_h \quad \forall q_h \in M_h,$$

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). The space $\boldsymbol{W}_h \subset H(\text{div}; \Omega)$ is constructed following ideas of Kuznetsov and Repin see [4]. It 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):

- $\boldsymbol{W}_h \subset H(\text{div}; \Omega)$; i.e. elements of $\boldsymbol{W}_h$ are locally in $H(\text{div}; T)$; $\forall T \in \mathscr{T}_h$, 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 $\mathscr{T}_h$.
- $\text{div}\boldsymbol{W}_h \subset M_h$; 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 $H(\text{div}; \Omega)$ 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.

The collection of tetrahedra $\mathscr{T}_T = \{S_i : i = 0, 1, \cdots, 4\}$ is a discretization of T by tetrahedra, and we denote by $\widetilde{\boldsymbol{W}}_T$ the Raviart-Thomas-Nédelec 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

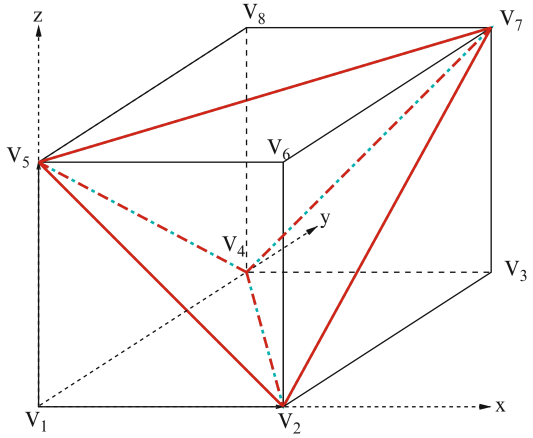

Fig. 1 A partition of the reference hexahedron into 5 tetrahedra: one tetrahedron lies in the interior of T and is determined by the vertices V_2, V_4, V_5, V_7. The four other tetrahedra have each three faces on the surface of T and each contains one of the vertices V_1, V_3, V_6, V_8. There are two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

equal to $\frac{1}{|F|}$ on F, we define $\boldsymbol{v}_F$ to be the second component of the solution of the problem

$$
\begin{aligned}
&\text{Find}(q_F, \boldsymbol{v}_F) \in \widetilde{M}_T \times \widetilde{\boldsymbol{W}}_{T,F} \text{ such that} \\
&\int_T \boldsymbol{v}_F \cdot \boldsymbol{v}_h - \int_T q_F \text{div} \boldsymbol{v}_h = 0, \quad \forall \boldsymbol{v}_h \in \widetilde{\boldsymbol{W}}_{T,0}, \\
&\int_T \text{div} \boldsymbol{v}_F \, q_h = \frac{1}{|T|} \int_T q_h \quad \forall q_h \in \widetilde{M}_T.
\end{aligned}
\tag{3}
$$

The pure Neumann problem (3) has a solution since 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 (3), 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

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

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

Remark 1. We point out that there are two possible choices for $\mathcal{T}_T$ (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 2. This method is not appropriate for meshes containing deformed cubes which are not true hexahedra; i.e. for meshes containing deformed cubes with nonplanar "faces". In applications nonplanar "faces" arise when a cube is deformed in such a way that four vertices defining a face of the cube are moved so that they are no longer planar. However any three of the vertices remain planar so for either choice of the decomposition into five tetrahedra the nonplanar "face" is divided into two (planar) triangles so that one obtains a polyhedron (with planar faces) of from seven to twelve sides depending on how many nonplanar "faces" the original "hexahedron" had. Thus the new polyhedron is divided into five tetrahedra and one could generalize the method used here to include this case. However, as mentioned above it may not be possible to choose the divisions of the hexahedra into five tetrahedra in such a way that the resulting collection of tetrahedra forms a finite element mesh; i. e. in such a way that the resulting division of the quadrilateral interior faces into two triangles is compatible for each pair of adjacent "hexahedra". The resulting pair of adjacent polyhedra may then either overlap or leave a void space between the two polyhedra. A new composite mixed finite element is now under development to treat the case of nonplanar faces.

Remark 3. One could in a perhaps more natural way divide each of the hexahedra into 6 tetrahedra (all of equal volume 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 (2) 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-Nédelec 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 [6]. Following [1] we define the notion of shape regularity for a family of meshes of hexahedra.

Definition 1. 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 [6] it is shown that if $(p, \boldsymbol{u}) \in L^2(\Omega) \times H(\text{div}; \Omega)$ is the solution of problem (1) and $(p_h, \boldsymbol{u}_h) \in M_h \times \boldsymbol{W}_h$ is the solution of problem (2) 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

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

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-Nédelec 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 $L^2(\Omega) \times H(\text{div}; \Omega)$ 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-Nédelec elements for grids of rectangular solids (when the problem has full tensor coefficients). As in [2] we can relax the condition that the approximate solution be sought in a subspace of $H(\text{div}; \Omega)$ 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:

Find $(p_h^*, \boldsymbol{u}_h^*, \lambda_h) \in M_h \times \boldsymbol{W}_h^* \times \Lambda_h$ such that

$$\sum_{T \in \mathscr{T}_h} \int_T \boldsymbol{K}^{-1} \boldsymbol{u}_h^* \cdot \boldsymbol{v}_h - \sum_{T \in \mathscr{T}_h} \int_T p_h^* \text{div}\boldsymbol{v}_h - \sum_{F \in \mathscr{F}_h} \int_F \lambda_F [\boldsymbol{v}_h \cdot \boldsymbol{n}_F] = -\int_{\Gamma_D} \bar{p} \boldsymbol{v}_h \cdot \boldsymbol{n} \quad \forall \boldsymbol{v}_h \in \boldsymbol{W}_h^*,$$

$$\sum_{T \in \mathscr{T}_h} \text{div}\boldsymbol{u}_h^*\, q_h = \int_\Omega f q_h \quad \forall q_h \in M_h,$$

$$\sum_{F \in \mathscr{F}_h} \int_F [\boldsymbol{u}_h^* \cdot \boldsymbol{n}_F] \mu_F = 0, \quad \forall \mu_h \in \Lambda_h,$$

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-Nédelec 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 (4). One shows easily that $\boldsymbol{u}_h^*$ is in fact in $\boldsymbol{W}_h$ and is equal to $\boldsymbol{u}_h$ and that $p_h^* = p_h$.

2 Numerical experiments

The data are provided by the *FVCA6 3D anisotropic benchmark* . We have chosen to do the first test case with mild anisotropy and Kershaw grids.Table 1 gives results obtained for the 4 Kershaw meshes which were proposed in the benchmark. The index i, i $= 1, 2, 3, 4$, denotes the mesh index for the $8 \times 8 \times 8$, the $16 \times 16 \times 16$, the $32 \times 32 \times 32$, and the $64 \times 64 \times 64$ Kershaw meshes respectively. As 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. From λ_h local calculations yield the cell pressure unknowns of p_h and the fluxes across the faces of the velocity $\boldsymbol{u}_h$.

In Table 1 nu, the number of unknowns of the linear system, is the number of degrees of freedom for λ_h which is the number of faces. The number of matrix nonzeros, nmat, is given in the table for the full matrix (not the upper or lower halves). umin, uemin, λmin (resp. umax, uemax, λmax) the minimum (resp. maximum) of p_h, p and λ_h.

The function p_h is constant inside each hexahedral cell, so the L^2 error erl2 between p and p_h is calculated as

$$\text{erl2} = \frac{\sqrt{\int_\Omega (p - p_h)^2}}{\sqrt{\int_\Omega p^2}}$$

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

The mixed finite element method calculates also the velocity $\boldsymbol{u}_h$ approximating the vector unknown $\boldsymbol{u} = -\boldsymbol{K}\nabla p$ as a piecewise polynomial vector function. The usual error calculated with the mixed method is the L^2 error for $\boldsymbol{u}_h$ in addition to the L^2 error for p_h. However in this benchmark the errors for p_h in the H^1 seminorm and in the energy norm are asked for. These norms are actually equivalent to the

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

i	nu	nmat	umin	uemin	umax	uemax	normg
1	576	2496	-0.03255	0.	1.94685	2.	1.84064
2	4352	32512	-0.04618	0.	1.99488	2.	1.85063
3	33792	310272	-0.03621	0.	2.00028	2.	1.85242
4	266240	2682880	-0.00837	0.	2.00061	2.	1.84036

i	nu	erl2	ratiol2	ergrad	ratiograd	ener	ratioener
1	576	0.063751		1.63849		1.49726	
2	4352	0.038971	0.73	0.96309	0.79	0.86755	0.81
3	33792	0.019424	1.02	0.51181	0.92	0.44853	0.97
4	266240	0.009148	1.09	0.25421	1.02	0.21819	1.05

L^2 norm of $\boldsymbol{u}$. Indeed we have $|\nabla p|^2 = |\boldsymbol{K}^{-1}\boldsymbol{u}|^2$ and $(\boldsymbol{K}\nabla p) \cdot \nabla p = (\boldsymbol{K}^{-1}\boldsymbol{u}) \cdot \boldsymbol{u}$. Therefore we calculate the error for the gradient and the error in the energy norm with the formula

$$\text{ergrad} = \frac{\sqrt{\int_\Omega |\boldsymbol{K}^{-1}(\boldsymbol{u}-\boldsymbol{u}_h)|^2}}{\sqrt{\int_\Omega |\boldsymbol{K}^{-1}\boldsymbol{u}|^2}}, \quad \text{ener} = \frac{\sqrt{\int_\Omega (\boldsymbol{K}^{-1}(\boldsymbol{u}-\boldsymbol{u}_h)) \cdot (\boldsymbol{u}-\boldsymbol{u}_h)}}{\sqrt{\int_\Omega (\boldsymbol{K}^{-1}\boldsymbol{u}) \cdot \boldsymbol{u}}}$$

where again the integrals in the numerator were calculated with an integration formula exact for polynomials of degree 2 inside each cell.

Similarly the L^1 norm of the gradient of p_h was calculated as

$$\text{normgrad} = \int_\Omega |\boldsymbol{K}^{-1}\boldsymbol{u}_h|.$$

The rates of convergence ratiol2, ratioener and ratiograd are calculated as required by the benchmark by comparing the errors erl2, ergrad and ener obtained on meshes i and i-1 using the formula

$$\text{ratio(i)} = -3\frac{\log(\text{error(i)}/\text{error(i-1)})}{\log(\text{nu(i)}/\text{nu(i-1)})}.$$

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

3 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 pressure as well as for the velocity, as it was predicted by the analysis of the method.

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The paper is in final form and no similar paper has been or is being submitted elsewhere.