# MIXED HEXAHEDRAL FINITE ELEMENTS FOR DARCY FLOW CALCULATION

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Abstract

The Kuznetsov-Repin mixed finite element method is designed to handle nonrectangular hexahedral meshes for Darcy flow calculations. In this situation, the standard mixed finite element method does not converge. Numerical experiments show the convergence of the new method and it is applied to a flow calculation around a nuclear waste disposal.

## 1. Introduction

The Darcy flow equation is an elliptic equation coupling a conservation equation with Darcy's law. As the Darcy velocity is the unknown of interest and we are concerned with problems with large changes in the permeability coefficient, we use a mixed finite element method. However standard mixed finite elements do not work on general hexahedral grids because the space of discrete velocities does not contain the constant velocities [8]. To correct this situation a solution was proposed in two dimensions in [10] with a discrete velocity space including a bubble function. But it is not known how to extend this method to three dimensions. Still in two dimensions, another solution was given in [1, 2] with a method consisting in adding two degrees of freedom which are the moments of order 1 in $x$ and $y$. However extending the Arnold-Boffi-Falk's method to three dimensions is very complicated since it requires very many degrees of freedom [6].

We will instead use a new mixed finite element method for hexahedrons proposed by Yu. Kuznetzov and S. Repin [4].

Let $\Omega$ be a convex polyhedral domain in $\mathbb{R}^3$ with boundary $\partial\Omega$. We consider for example the elliptic problem given in mixed form:

$$\begin{array}{rcll} \text{div } \vec{\mathbf{u}} &=& f & \text{in } \Omega \\ \vec{\mathbf{u}} &=& -K\ \nabla p & \text{in } \Omega \\ \vec{\mathbf{u}}\cdot\vec{n} &=& 0 & \text{on } \partial\Omega. \end{array}$$

The weak formulation of the problem is

$$\begin{array}{lrcl} & \multicolumn{3}{l}{\text{Find } (\mathbf{u},p)\in(\mathcal{W},\mathcal{M}) \text{ such that}} \\ (\mathcal{P}) & a(\mathbf{u},\mathbf{v})-b(\mathbf{v},p) &=& 0 \quad \forall \mathbf{v}\in\mathcal{W} \\ & b(\mathbf{u},q) &=& l_f(q) \quad \forall q\in\mathcal{M}, \end{array}$$

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where $\mathcal{M}$ and $\mathcal{W}$ are the Hilbert spaces $L^2(\Omega)$ and $\mathbf{H}(\mathrm{div};\Omega)$, respectively, the continuous bilinear forms $a$ and $b$ are defined by

$$\begin{aligned} a(\mathbf{u},\mathbf{v}) &= \int_\Omega K^{-1}\mathbf{u}\cdot\mathbf{v}\,dx \qquad \forall \mathbf{u},\mathbf{v}\in\mathcal{W} \\ b(\mathbf{u},q) &= \int_\Omega \mathrm{div}\,\mathbf{u}\,q\,dx \qquad \forall \mathbf{u}\in\mathcal{W},\quad \forall q\in\mathcal{M}, \end{aligned}$$

and the continuous linear form $l_f$ is given by

$$l_f(q) = \int_\Omega f q dx \quad \forall q\in\mathcal{M}.$$

It is well known that problem $(\mathcal{P})$ has a unique solution. See [3, 7].

## 2. The Kuznetsov-Repin mixed finite element

Let $\mathcal{T}_h$ be a mesh made up of general hexahedral cells $E$ and let $\mathcal{F}_h$ be the set of faces of elements of $\mathcal{T}_h$. $h$ is the largest diameter of the elements. The objective is to define an approximation space $\mathbf{W}_h \subset \mathcal{W}$ such that an element $u_h \in \mathbf{W}_h$

- 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 Raviart-Thomas-Nedelec mixed finite element approximation space of lowest-order for a tetrahedral or a parallelepiped mesh.

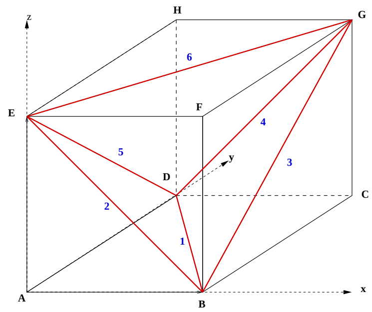


Figure 1. The macroelement

Toward this end, we construct a macroelement by subdividing each hexahedron $E$ into 5 tetrahedra $T_j^E, \quad j = 1,\cdots,5$ as indicated in Figure 1.

$$E \;=\; T_1^E \cup T_2^E \cup T_3^E \cup T_4^E \cup T_5^E$$

with

$$T_1^E = ABDE, \quad T_2^E = BEFG, \quad T_3^E = BCGD, \quad T_4^E = DEHG, \quad T_5^E = BEDG.$$

Each of the first four tetrahedra, $T_j^E \quad j = 1, \cdots, 4$, 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 $T_5^E$.

For a given $E \in \mathcal{T}_h$ we construct a space $\mathcal{W}_E$ of vector functions $v \in \mathbf{H}(\mathrm{div}; E)$ satisfying the following conditions:

$$v_{|T_j^E} \in \mathbf{RTN}_0(T_j^E), \quad j = 1, \cdots, 5 \tag{1}$$

$$\mathrm{div}\, v \quad \text{is a constant over E} \tag{2}$$

$$v \cdot n_E \quad \text{is constant on each face of E} \tag{3}$$

so that

$$\mathcal{W}_E = \{v \in \mathbf{H}(\mathrm{div}; E) \quad \text{satisfying} \quad (1), (2) \text{ and } (3)\} \tag{4}$$

The space $\mathcal{W}_E$ is a subspace of the space $\tilde{\mathcal{W}}_E$ defined by

$$\tilde{\mathcal{W}}_E = \{\tilde{v} \in \mathbf{H}(\mathrm{div}; E) \quad \text{satisfying} \quad (1)\} \tag{5}$$

which is just the lowest order Raviart-Thomas-Nédelec space over $E$ associated with the triangulation $\mathcal{T}_E = \{T_j^E : j = 1, \cdots, 5\}$. It is clear that

$$\mathcal{W}_E \subset \tilde{\mathcal{W}}_E.$$

Let us check that a function $v$ of $\mathcal{W}_E$ is uniquely defined by its normal traces through the 6 faces of $E$. For a function $v \in \mathcal{W}_E$ let $v_j$, $j = 1, \cdots, 5$ denote its restruction to $T_j^E$. Then by condition (1) $v_j$ is of the form

$$v_j \;=\; a_j \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} b_j \\ c_j \\ d_j \end{pmatrix}, \quad a_j, b_j, c_j, d_j \in \mathbb{R}, j = 1, \cdots, 5 \tag{6}$$

Thus v is determined by 20 coefficients. Since $v \in \mathbf{H}(\mathrm{div}; E)$ its normal components through the 4 internal faces of the macroelement must be continuous which imposes 4 constrains. Condition (2) gives 4 more constrains and the condition (3) gives 6 others. That leaves 6 coefficients to determine which correspond to the values of $\mathbf{v} \cdot \mathbf{n}$ on the six faces of $E$. To see this it suffices to remark that the basis element $\omega_i$ of $\mathcal{W}_E$ having normal component equal to 1 on the face $F_i$ and normal component equal to 0 on each other face of $E$ is the first component of a solution to the problem

Find $(\mathbf{u}, p) \in (\tilde{\mathcal{W}}_E^{g_i}, \tilde{\mathcal{M}}_E)$ such that

$$(\mathcal{P}_E) \qquad \begin{array}{rcll} a(\mathbf{u}, \mathbf{v}) - b(\mathbf{v}, p) & = & 0 & \forall \mathbf{v} \in \tilde{\mathcal{W}}_E^0 \\ b(\mathbf{u}, q) & = & \dfrac{|F_i|}{|E|} & \forall q \in \tilde{\mathcal{M}}_E, \end{array}$$

where $\tilde{\mathcal{W}}_E^{g_i}$, respectively $\tilde{\mathcal{W}}_E^0$, is the subspace of $\tilde{\mathcal{W}}_E$ consisting of those elements whose normal traces agree with $g_i$, respectively are equal to 0, on the boundary of $E$, and $\mathcal{M}_E$ is the space of functions which are constant on each tetrahedra $T_j^E$, $j = 1, \cdots, 5$. Note that while this Neumann problem determines $p$ only up to a constant, it determines $\mathbf{v}$ uniquely so that $\omega_i$ is well defined.

These 6 degrees of freedom, by hexahedron, are determined by the equations given by the discrete system of the mixed finite element method.

**Remark 1.** *It would 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 $6 * 4 = 24$ coefficients to determine with 6 constraints imposed by the fact that the function belongs to $\mathbf{H}(div; E)$. Conditions (2) and (3) impose 5 and 6 constraints respectively leaving 7 degrees of freedom to calculate. The macroelement would not be unisolvant.*

The pressure function is still calculated in

$$\mathcal{M}_h = \{q_h \in \mathcal{M} \quad | \quad q_h|_E \in \mathbb{R} \quad \forall E \in \mathcal{T}_h\},$$

the space of piece wise constant functions.

The discrete problem associated with the macroelement space $\mathbf{W}_h$ is the following:

$$\text{Find } (\mathbf{u}_h, p_h) \in (\mathbf{W}_h, \mathcal{M}_h) \text{ such that}$$

$$(\mathcal{P}_h) \qquad \begin{aligned} a(\mathbf{u}_h, \mathbf{v}_h) - b(\mathbf{v}_h, p_h) &= 0 \quad \forall \mathbf{v}_h \in \mathbf{W}_h \\ b(\mathbf{u}_h, q_h) &= \int_\Omega f q_h \quad \forall q_h \in \mathcal{M}_h. \end{aligned}$$

Existence and uniqueness of the solution for this problem is shown in [5, 9]. In the same papers the authors show the convergence of the approximate solution to the continuous solution with a rate of $h$.

## 3. Numerical experiment

First we present numerical convergence results for the analytical solution

$$p = sin(\pi x) sin(\pi y) sin(\pi z) + x(1-x)y^2(1-y)^2 z(1-z)$$

on meshes which are deformations of a uniform cubic mesh $n \times n \times n$ for $n = 4, 8, 16, 32, 64$. Figure 2 shows three $8 \times 8 \times 8$ meshes corresponding to an increasing deformation. The deformation consists in moving the vertices in the horizontal plane in order to obtain for the cells the form of truncated pyramids.

The following tables show errors for the pressure and the velocity using respectively the Raviart-Thomas-Nédélec (RTN) and the Kuznetsov-Repin (KR) mixed finite elements.

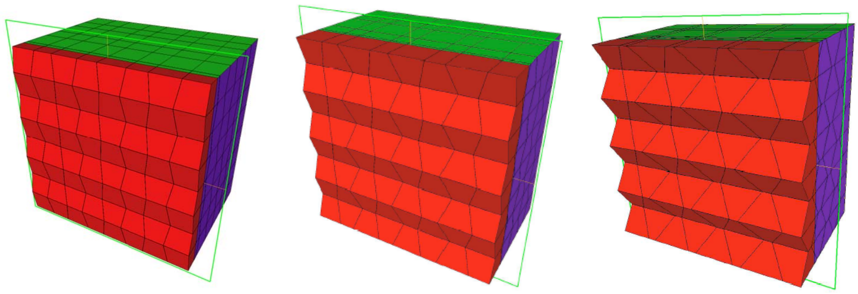

FIGURE 2. Hexahedral meshes for the error calculations: meshD1, meshD2, meshD3 from left to right

This tables confirm theoretical results stating that the RTN method is not converging on general hexahedrons while the KR method is.

Once the Kuznetsov-Repin mixed finite element method was proven to be convergent, it was used to calculate the pressure and velocity field around a nuclear waste disposal. Figure 3 shows the domain of calculation on the left. It is made up of 13 geological subdomains with permeabilities changing with three orders of magnitude. On the right in Figure 3 the calculated pressure field is shown. Both figures are blown up 30 times in the $z$-direction in order to visualize the results.

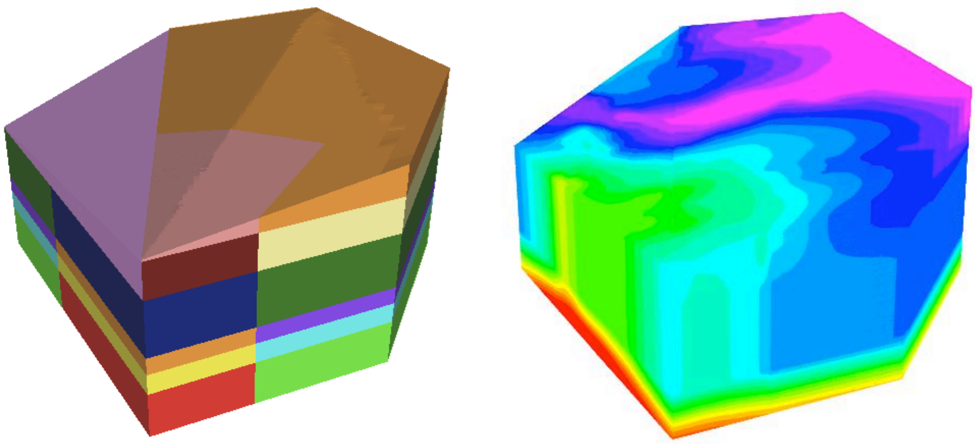

FIGURE 3. The domain of calculation (left) and the calculated pressure field (right)

3.1. **Conclusion.** The Kuznetsov-Repin mixed finite element method is an elegant and simple to implement solution to the problem of finding a suitable mixed finite element method for general hexahedral discretizations.

| | RTN finite element | | | | KR finite element | | | |
|---|---|---|---|---|---|---|---|---|
| n | $\|\| p_h - \pi_h p \|\|_{0,\Omega}$ | | $\|\| u_h - \Pi_h u \|\|_{0,\Omega}$ | | $\|\| p_h - \pi_h p \|\|_{0,\Omega}$ | | $\|\| u_h - \Pi_h u \|\|_{0,\Omega}$ | |
| | error | rate | error | rate | error | rate | error | rate |
| 4 | 0.01716 | | 0.07885 | | 0.016072 | | 0.039495 | |
| 8 | 0.00565 | 1.6 | 0.04048 | 0.96 | 0.00423 | 1.92 | 0.01319 | 1.58 |
| 16 | 0.00294 | 0.62 | 0.02632 | 0.62 | 0.00106 | 1.99 | 0.00421 | 1.64 |
| 32 | 0.00238 | 0.3 | 0.02343 | 0.16 | 0.00026 | 2. | 0.00136 | 1.62 |
| 64 | 0.00226 | 0.08 | 0.02289 | 0.03 | 6.5e-5 | 2.01 | 0.00046 | 1.32 |

TABLE 1. Pressure and velocity errors for the RTN and the KR mixed finite elements on the sequence of meshes meshD1

| | RTN finite element | | | | KR finite element | | | |
|---|---|---|---|---|---|---|---|---|
| n | $\|\| p_h - \pi_h p \|\|_{0,\Omega}$ | | $\|\| u_h - \Pi_h u \|\|_{0,\Omega}$ | | $\|\| p_h - \pi_h p \|\|_{0,\Omega}$ | | $\|\| u_h - \Pi_h u \|\|_{0,\Omega}$ | |
| | error | order | error | rate | error | rate | error | rate |
| 4 | 0.0206 | | 0.1773 | | 0.01519 | | 0.0785 | |
| 8 | 0.0119 | 0.79 | 0.116 | 0.61 | 0.0036 | 2.075 | 0.0265 | 1.56 |
| 16 | 0.01 | 0.25 | 0.0994 | 0.22 | 0.00083 | 2.1 | 0.0088 | 1.57 |
| 32 | 0.0095 | 0.08 | 0.0967 | 0.04 | 0.000199 | 2.06 | 0.00318 | 1.48 |
| 64 | 00.0093 | 0.022 | 0.0961 | 0.008 | 4.87e-5 | 2.03 | 0.00126 | 1.32 |

TABLE 2. Pressure and velocity errors for the RTN and the KR mixed finite elements on the sequence of meshes meshD2

| | RTN finite element | | | | KR finite element | | | |
|---|---|---|---|---|---|---|---|---|
| n | $\|\| p_h - \pi_h p \|\|_{0,\Omega}$ | | $\|\| u_h - \Pi_h u \|\|_{0,\Omega}$ | | $\|\| p_h - \pi_h p \|\|_{0,\Omega}$ | | $\|\| u_h - \Pi_h u \|\|_{0,\Omega}$ | |
| | error | rate | error | rate | error | rate | error | rate |
| 4 | 0.04736 | | 0.5234 | | 0.0135291 | | 0.167089 | |
| 8 | 0.047977 | -0.01 | 0.477 | 0.133 | 0.0023 | 2.548 | 0.0699 | 1.25 |
| 16 | 0.04588 | 0.064 | 0.472681 | 0.01 | 0.000368 | 2.68 | 0.0319 | 1.12 |
| 32 | 0.04487 | 0.03 | 0.4733 | -0.001 | 6.98e-5 | 2.36 | 0.01547 | 1.04 |
| 64 | 0.04457 | 0.009 | 0.4731 | 0.0005 | 1.6e-5 | 2.12 | 0.00766 | 1.01 |

TABLE 3. Pressure and velocity errors for the RTN and the KR mixed finite elements on the sequence of meshes meshD3

## 4. Aknowledgements

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