Porous media flow calculations with hexahedral mixed finite elements

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Introduction

Incompressible Darcy flow

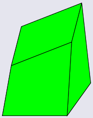
Find $\mathbf{u} \in \mathbf{H}(\mathrm{div}\,;\Omega)$ and $p \in \mathbf{L}^2(\Omega)$ such that

$$\begin{aligned} \mathbf{u} &= -\mathbf{K}\,\nabla\, p && \text{in } \Omega \\ \nabla\cdot\mathbf{u} &= f && \text{in } \Omega \\ p &= p_0 && \text{on } \partial\Omega \end{aligned}$$

Goal

A mixed finite element method

- 1 pressure per cell
- 1 flux per face



Extension for meshes with curved faces ?

Mixed finite elements

Weak formulation

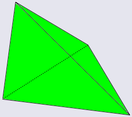
Find $\mathbf{u}_h \in \mathcal{W}_h$ and $p_h \in \mathcal{M}_h$ such that

$$\begin{aligned} \int_\Omega \mathbf{K}^{-1}\mathbf{u}_h \cdot \mathbf{v}_h - \int_\Omega p_h \nabla\cdot \mathbf{v}_h &= -\int_{\partial\Omega} p_0 \mathbf{v}_h \cdot \mathbf{n} \qquad &\forall \mathbf{v}_h \in \mathcal{W}_h \\ -\int_\Omega q_h \nabla\cdot \mathbf{u}_h &= -\int_\Omega f q_h \qquad &\forall q_h \in \mathcal{M}_h \end{aligned}$$

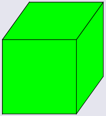
Define the approximation spaces $\mathcal{W}_h$ and $\mathcal{M}_h$

Mixed finite elements

$\mathbf{RTN}_0$ for tetrahedra and cubes (Raviart-Thomas-Nédélec)

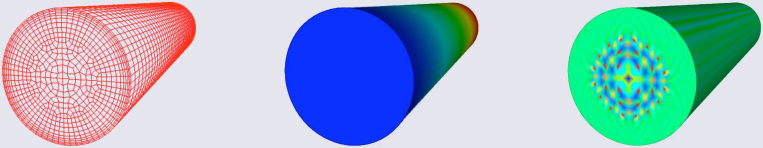


Tetrahedron



Cube

Constant velocity field in a cylinder with $\mathbf{RTN}_0$ extended to hexahedra

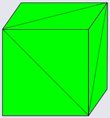


The constant velocity is not contained in the approximation space $\mathcal{W}_h$

Composite hexahedral mixed finite element

A first composite element with 5 tetrahedra [Sboui-Jaffré-Roberts]

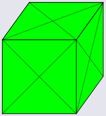
- Splitting is not unique
- Assume the faces are planar
- Tetrahedron do not make necessarily a conforming submesh



Cube split into 5 tetrahedra

Composite element with 24 tetrahedra

- Works with curved faces
- Splitting is unique
- Symmetry
- Conforming tetrahedral submesh



Cube split into 24 tetrahedra

Definition of the approximation spaces

Conditions to meet for the approximation spaces $\mathcal{W}_h$ and $\mathcal{M}_h$

$$\mathbf{u}_h \in \mathcal{W}_h \text{ and } p_h \in \mathcal{M}_h$$

- p_h must be constant on each hexahedron E of the mesh $\mathcal{T}_h$
- $\nabla \cdot \mathbf{u}_h$ must be constant on E
- $\mathbf{u}_h$ must be in the $\mathbf{RTN}_0$ space of the tetrahedral submesh $\mathcal{T}_E$
- $\mathbf{u}_h$ must be uniquely defined by this value on each face F of the mesh

Definition of the approximation spaces $\mathcal{W}_h$ and $\mathcal{M}_h$

$\mathcal{W}_h$ is defined locally inside each hexahedron E

$$\mathcal{M}_h = \{q \in \mathbf{L}^2(E) : q|_E \text{ is constant on } E, \forall E \in \mathcal{T}_h\}$$
$$\mathcal{W}_h = \{\mathbf{w} \in \mathbf{H}(\mathrm{div}\,;\Omega) : \mathbf{w}|_E \in \mathcal{W}_E, \forall E \in \mathcal{T}_h\}$$

Definition of the velocity approximation space

Definition of the local approximation space $\mathcal{W}_E$

- $\mathcal{F}_E$ is the set of faces of E

$$\mathcal{W}_E = \mathrm{Vect}\left\{\mathbf{w}_{E,F},\, F \in \mathcal{F}_E : \mathbf{w}_{E,F} \text{ solution of } (\mathcal{P}_{E,F})\right\}$$

- A local problem $(\mathcal{P}_{E,F})$ is defined to meet the conditions for each $\mathbf{w}_{E,F}$
- The basis function $\mathbf{w}_{E,F}$ will solve the local problem $(\mathcal{P}_{E,F})$ inside E

The local approximation spaces used to solve $(\mathcal{P}_{E,F})$

- $\mathcal{T}_E$ is the tetrahedral mesh of E
- $\widetilde{\mathcal{W}}_E$ and $\widetilde{\mathcal{M}}_E$ are the mixed finite elements spaces

$$\widetilde{\mathcal{M}}_E = \{q \in \mathbf{L}^2(E) : q|_T \text{ is constant on } T, \forall\, T \in \mathcal{T}_E\}$$

$$\widetilde{\mathcal{W}}_E = \{\mathbf{v} \in \mathbf{H}(\mathrm{div}\,; E) : \mathbf{v}|_T \in \mathbf{RTN}_0(T), \forall\, T \in \mathcal{T}_E\}$$

Definition of the basis functions

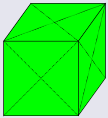
The local problem $(\mathcal{P}_{E,F})$ inside the composite element

Find $\mathbf{w}_{E,F} \in \widetilde{\mathcal{W}}_E$ with and $\widetilde{p}_{E,F} \in \widetilde{\mathcal{M}}_E$ such that

$$\begin{aligned} \int_E \mathbf{K}^{-1}\mathbf{w}_{E,F} \cdot \tilde{\mathbf{v}} - \int_E \widetilde{p}_{E,F}\, \nabla\cdot \tilde{\mathbf{v}} &= 0 \qquad \forall \tilde{\mathbf{v}} \in \widetilde{\mathcal{W}}_E, \tilde{\mathbf{v}} \cdot \mathbf{n}_E = 0 \\ -\int_E \widetilde{q}\, \nabla\cdot \mathbf{w}_{E,F} &= -\int_E \frac{1}{|E|}\widetilde{q} \qquad \forall \widetilde{q} \in \widetilde{\mathcal{M}}_E \end{aligned} \qquad (\mathcal{P}_{E,F})$$

$$\mathbf{w}_{E,F} \cdot \mathbf{n}_{F'} = \begin{cases} \frac{1}{|F|} & \text{if } F = F' \\ 0 & \text{else} \end{cases}$$

$$\int_E \widetilde{p}_{E,F} = 0$$



Cube split into 24 tetrahedra

- No explicit solution with 24 tetrahedra

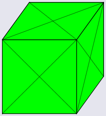
Numerical experiment

Convergence error

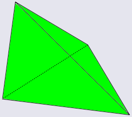
Exact solution inside the domain $\Omega = [0\,;1]^3$ with different meshes

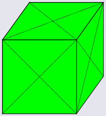
$$p = 2xz + \frac{y^2}{2} + z \qquad \mathbf{u} = -\begin{pmatrix} 2z \\ y \\ 2x+1 \end{pmatrix}$$

Composite method



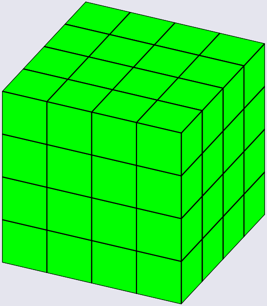
RTN_0 on the tetrahedral submesh



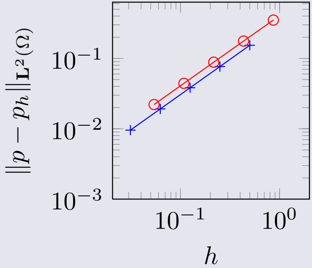


Numerical experiment on cubes

Regular mesh

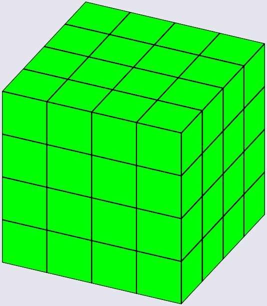


Pressure errors with standard refinement

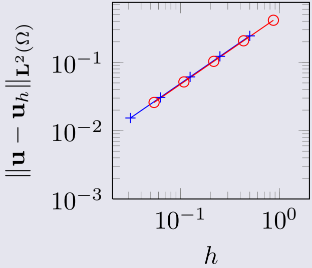


Numerical experiment on cubes

Regular mesh



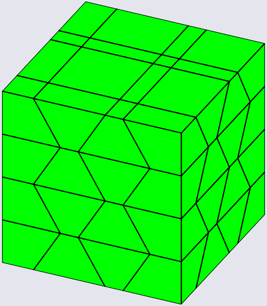
Velocity errors with standard refinement



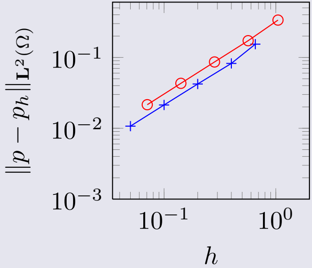
tetraedral $\mathbf{RTN}_0$ method
composite method

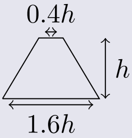
Numerical experiment on hexahedra with fixed aspect ratio

Hexahedral mesh



Pressure errors with finer meshes



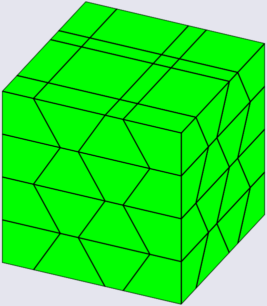


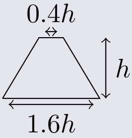
tetraedral $\mathbf{RTN}_0$ method

composite method

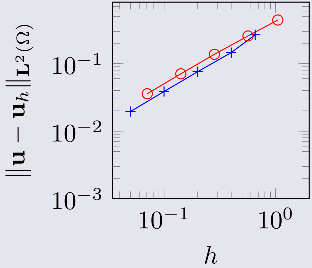
Numerical experiment on hexahedra with fixed aspect ratio

Hexahedral mesh





Velocity errors with finer meshes



tetraedral $\mathbf{RTN}_0$ method
composite method

Conclusion for hexahedra

Definition of the composite method

- $\mathcal{W}_E$ is spanned by the basis functions $\mathbf{w}_{E,F}$
- The basis function $\mathbf{w}_{E,F}$ solves a local problem $(\mathcal{P}_{E,F})$ inside E

Convergence errors

- Convergence is optimal for planar faces

Remark

- The composite method is similar to the 2 scale finite element method

CPU time for the composite method

- Time required to solve the problem is 30 times faster than $\mathbf{RTN}_0$
- Time required to build and solve the problem is 5 times faster than $\mathbf{RTN}_0$

The case of curved faces

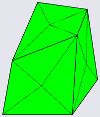
Problem with curved faces

Constant velocities do not lie in the approximation space $\mathcal{W}_h$

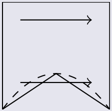
Proof [Nordbotten-Hægland]

- The curved face is approximated with F, the union of 4 subfaces F_i
- $\mathbf{n}_F = \mathbf{n}_{F_i}$ on the triangular subface F_i
- $\mathbf{u}$ is a constant velocity

$$\mathbf{u} \cdot \mathbf{n}_{F_i} \neq \mathbf{u} \cdot \mathbf{n}_{F_j}$$



Deformed cube



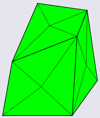
Constant velocity $\mathbf{u}$

Definition of the basis functions for curved faces

New Neumann conditions for $\mathbf{w}_{E,F}$

For a planar face F

$$\mathbf{w}_{E,F} \cdot \mathbf{n}_{F'} = \begin{cases} \frac{1}{|F|} & \text{if } F = F' \\ 0 & \text{else} \end{cases}$$



Deformed cube

$\bar{\mathbf{n}}_F$ is the mean of the normal $\mathbf{n}_{F_i}$

$$\bar{\mathbf{n}}_F = \frac{\sum_{i=1}^{4} |F_i| \mathbf{n}_{F_i}}{\| \sum_{i=1}^{4} |F_i| \mathbf{n}_{F_i} \|_{L^2}}$$

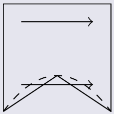
Neumann boundary condition for a curved face

$$\mathbf{w}_{E,F} \cdot \mathbf{n}_{F'_i} = \begin{cases} \dfrac{\bar{\mathbf{n}}_F \cdot \mathbf{n}_{F_i}}{\int_F \bar{\mathbf{n}}_F \cdot \mathbf{n}_F} & \text{if } F'_i \text{ is a subface of } F \\ 0 & \text{else} \end{cases}$$

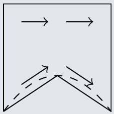
The case of curved faces

Approximate velocity with curved face

- $\mathbf{w}_{E,F}$ solves a local problem inside E
- $\mathbf{w}_{E,F} \cdot \mathbf{n}_{F_i'} = 0$ if $F \neq F'$



Constant velocity $\mathbf{u}$

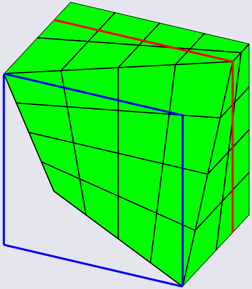


Approximate velocity $\mathbf{u}_h$

- The error is reduced when the mesh is refined

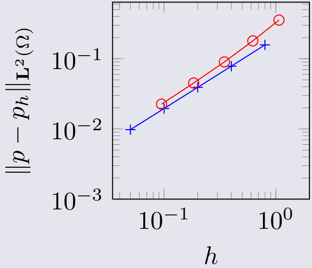
Numerical experiment on a mesh with curved faces

Deformed mesh



$y = 0.2$
$y = 0.8$

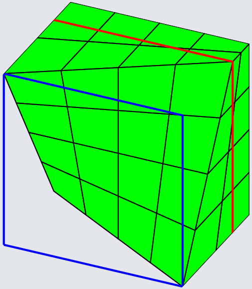
Pressure errors with standard refinement



tetraedral $\mathbf{RTN}_0$ method
composite method

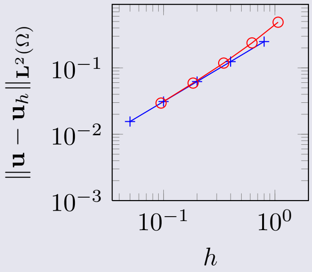
Numerical experiment on a mesh with curved faces

Deformed mesh



$y = 0.2$ (blue)
$y = 0.8$ (red)

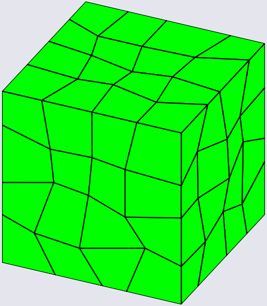
Velocity errors with standard refinement



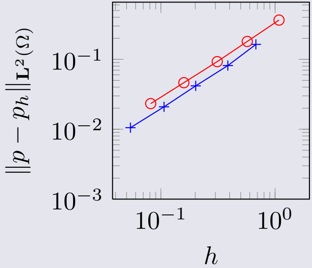
tetraedral $\mathbf{RTN}_0$ method
composite method

Numerical experiment on a mesh with fixed aspect ratio

Random mesh



Pressure errors with finer meshes

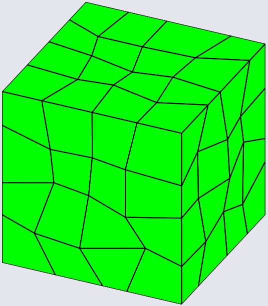


Shift randomly the vertices $\pm 0.3h$

tetraedral $\mathbf{RTN}_0$ method
composite method

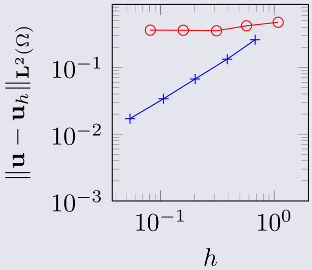
Numerical experiment on a mesh with fixed aspect ratio

Random mesh



Shift randomly the vertices $\pm 0.3h$

Velocity errors with finer meshes



tetraedral $\mathbf{RTN}_0$ method
composite method

Conclusion

Convergence errors for planar faces

- Convergence is optimal

Convergence errors for curved faces

- The method converges if the mesh is refined in a standard manner
- The velocity does not converge on meshes with fixed aspect ratio

Remarks

- The same methodology can be apply for prisms and pyramids
- Local and conforming refinement

A posteriori error estimation

Estimate the error of the approximate solution [Vohralík]

Bound the velocity error

$$|||\mathbf{u} - \mathbf{u}_h|||_* \leqslant \eta_h(p_h, \mathbf{u}_h, f, \mathbf{K}) \leqslant C|||\mathbf{u} - \mathbf{u}_h|||_*$$

with C a positive constant and the energy norm

$$|||\mathbf{v}|||_*^2 = \int_\Omega \mathbf{K}^{-1}\mathbf{v} \cdot \mathbf{v} \qquad |||\mathbf{v}|||_{*,T}^2 = \int_T \mathbf{K}^{-1}\mathbf{v} \cdot \mathbf{v}$$

$\eta_h(p_h, \mathbf{u}_h, f, \mathbf{K})$ is defined using the estimators for the $\mathbf{RTN}_0$ method

The error is evaluated locally inside each element E of $\mathcal{T}_h$

- Project the solutions into the $\mathbf{RTN}_0$ spaces of the tetrahedral mesh
- Estimate the error inside each tetrahedron
- Bound the error in the hexahedron with the tetrahedral estimators

A posteriori error estimation

Projection of the solution

$\widetilde{\mathcal{T}}_h$ is the conforming tetrahedral submesh of $\mathcal{T}_h$

- $\widetilde{\mathbf{u}}_h = \mathbf{u}_h$ which is already in $\mathbf{RTN}_0(\widetilde{\mathcal{T}}_h)$
- $\widetilde{p}_h$ is formed using p_h and the pressure variations $\widetilde{p}_{E,F}$'s in $(\mathcal{P}_{E,F})$

The potential estimator

- $\widetilde{p}_{h,2}$ is an approximation of the pressure in $\mathbf{P}^2(\widetilde{\mathcal{T}}_h) \bigcap \mathbf{H}_0^1(\Omega)$

$$\eta_{\mathrm{P},T} = |||\widetilde{\mathbf{u}}_h + \mathbf{K}\,\nabla\,\widetilde{p}_{h,2}|||_{*,T}$$

- $\widetilde{\mathcal{T}}_h$ is uniquely determined in the case of 24 tetrahedra

A posteriori error estimation

The residual estimator

- h_T is the diameter of T
- $c_{\mathrm{s},T}$ is the smallest eigenvalue of $\mathbf{K}$ on T
- C_{p} is the Poincaré inequality coefficient, $\frac{1}{\pi^2}$ on simplices
- $\tilde{\pi}$ is the projection operator from $\mathbf{L}^2(\Omega)$ into $\widetilde{\mathcal{M}}_E$

$$\eta_{\mathrm{R},T} = h_T \frac{C_{\mathrm{p}}^{1/2}}{c_{\mathrm{s},T}^{1/2}} \|f - \tilde{\pi} f\|_{\mathbf{L}^2(T)}$$

The error estimators

The local error estimator

$$\eta_E^2 = \sum_{T \in \mathcal{T}_E} \eta_{\mathrm{P},T}^2 + \eta_{\mathrm{R},T}^2$$

The global error estimator

$$\eta_h^2 = \sum_{E \in \mathcal{T}_h} \eta_E^2$$

Numerical experiment

Initial condition

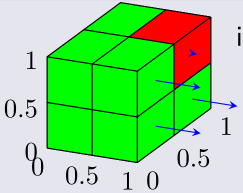
Dirichlet boundary condition

on $x = 0$	on $x = 1$
$p = 1$	$p = 0$

$$\mathbf{K} = \alpha \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad f = 0$$

No flow boundary elsewhere

Test definition



in the red corner

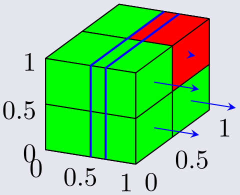
$$\alpha = \frac{1}{10}$$

elsewhere

$$\alpha = 1$$

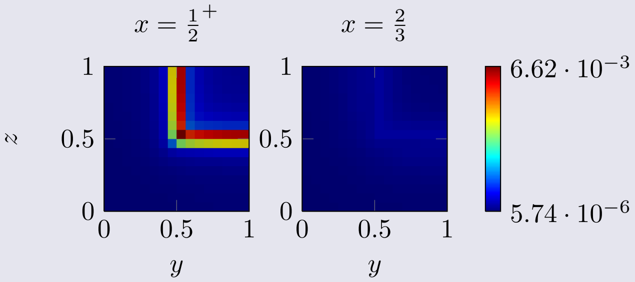
Numerical experiment

Test definition



Regular mesh
$16 \times 16 \times 16$

Local error estimator η_E

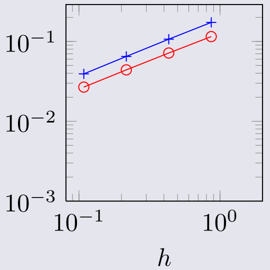


Another refinement criteria

- A simpler criteria is to adapt the mesh based on the variation of $\mathbf{K}$
- This does not give a good refinement level at $x = \frac{2}{3}$

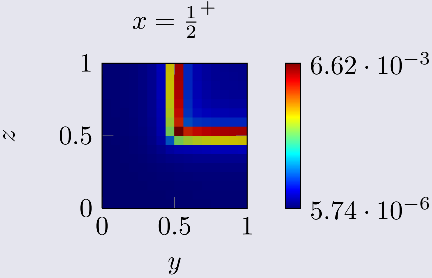
Numerical experiment

Global error estimators



rate
0.68
0.70
0.72

Local error estimator η_E



- a posteriori error estimator η_h
- error with a mesh 4 times finer $\|\!|\mathbf{u}_h - \mathbf{u}_{\frac{h}{4}}|\!\|_*$

Conclusion

Convergence errors for planar faces

- Convergence is optimal

Convergence errors for curved faces

- The method converges if the mesh is refined in a standard manner
- The velocity does not converge on meshes with fixed aspect ratio

A posteriori error

- A local and efficient estimator

Perspective

- Application in an industrial test case (ANDRA)

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