New approximation space configuration for the mixed finite element method for elliptic problems based on curved 3D meshes

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Model Problem

- Poisson problem written in the form:

\[ \nabla \cdot \sigma = f \quad \text{in} \quad \Omega, \]
\[ \sigma = -\nabla u \]
\[ u = u_D \quad \text{in} \quad \partial\Omega_D, \]
\[ \sigma \cdot \eta = q_N \quad \text{in} \quad \partial\Omega_N \]

- Required functional spaces
  - For the variable \( \sigma \)

\[ H(div, \Omega) = \left\{ q \in [L^2(\Omega)]^d \ ; \ \nabla \cdot q \in L^2(\Omega) \right\} \]
  - For the variable \( u \): \( L^2(\Omega) \)
Discrete variational mixed formulation

1. $\Gamma = \{K\}$ partition of the computational domain $\Omega$

2. Finite dimensional approximation subspaces
   - $V_\Gamma \subset H(\text{div}, \Omega)$ approximation space for $\sigma$
     - continuous normal components over element interfaces
   - $U_\Gamma \subset L^2(\Omega)$ approximation space for $u$
     - no continuity constraint
   - stability

3. To find $(\sigma, u) \in (V_\Gamma \times U_\Gamma)$ such that $\sigma \cdot \eta|_{\partial \Omega_N} = q_N$ and

\[
a(\sigma, q) - b(q, u) = -\int_{\partial \Omega} u_D q \cdot \eta \quad \forall q \in V_0^\Gamma
\]

\[
b(\sigma, \varphi) = \int_{\Omega} f \varphi \, d\Omega \quad \forall \varphi \in U^\Gamma
\]
Since Raviart and Thomas 1977

- a variety of $V^\Gamma \times U^\Gamma$ stable configurations have been proposed in the literature (Brezzi, Fortin 1991)

Most FE codes for real applications are based on $H^1$-conforming schemes

- Implementations of mixed formulations are much more complex

Complications increase for:

- higher order finite element schemes
- non-uniform order approximation on unstructured meshes
- curved elements
- variable topologies
Recent efforts on the development and/or implementation of convenient sets of basis functions for higher order $H(\text{div})$-conforming approximations in 3D

- **Fuentes, Keith, Demkowicz, Nagaraj**, Mathematics and Computers in Simulation 2015 (hierarchic, all geometries)

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Goals

- Systematic construction of hierarchic high order shape functions for approximation spaces
  \[ \mathbf{V}^\Gamma \subset H^{\text{div}}(\Omega) \]
  based on curved tetrahedra, hexahedra and prisms
- Different stable space configurations \( \mathbf{V}^\Gamma \times U^\Gamma \) with optimal \( h \)-convergence rates
  - configuration with enhanced accuracy in \( u \) without increasing DoF of the static condensed system
- Effect of condensation + parallelization on CPU time using an \( hp \)-adapted curved mesh
Construction of approximation spaces $\mathbf{V}^\Gamma \times U^\Gamma$: guidelines I

- $\hat{K}$: reference master element (tetrahedra, hexahedra or prism)
- $x : \hat{K} \to K$: geometric mapping (diffeomorphism)
- $F : \hat{\varphi} \to \varphi$, isomorphism mapping scalar functions $\hat{\varphi}$ of $H^1(\hat{K})$ to scalar functions $\varphi$ of $H^1(K)$ (induced by $x$)
  \[ \varphi(p) = \hat{\varphi}(x^{-1}(p)) \]

- $F^{\text{div}} : \hat{\mathbf{q}} \to \mathbf{q}$ contravariant Piola transformation: isomorphism mapping vector-valued functions $\hat{\mathbf{q}} \in H(\text{div}, \hat{K})$ to vector-valued functions $\mathbf{q} \in H(\text{div}, K)$
  \[ \mathbf{q} = F \left[ \frac{1}{\det J} J(\hat{\mathbf{q}}) \right] \]

where $J = \nabla x$ is the Jacobean of the geometric mapping.
Construction of approximation spaces $\mathbf{V}^\Gamma \times \mathbf{U}^\Gamma$: guidelines

- **Polynomial vector-valued approximation spaces**
  - $\mathbf{M}(\hat{K}) \subset H(\text{div}, \hat{K})$
    - **internal functions**: vanishing normal components on $\partial \hat{K}$
    - **face functions**: otherwise
  - $D(\hat{K}) \subset L^2(\hat{K})$
  - **Stability**: De Rham property
    $$\nabla \cdot \mathbf{M}(\hat{K}) = D(\hat{K})$$

- **Global approximation spaces**

\[
\begin{align*}
\mathbf{V}^\Gamma &= \left\{ \mathbf{q} \in H(\text{div}, \Omega); \ q|_K = \mathbb{F}^{\text{div}} \hat{\mathbf{q}}, \ \hat{\mathbf{q}} \in \mathbf{M}(\hat{K}) \right\} \\
\mathbf{U}^\Gamma &= \left\{ \varphi \in L^2(\Omega); \ \varphi|_K = \mathbb{F} \hat{\varphi}, \ \hat{\varphi} \in D(\hat{K}) \right\}
\end{align*}
\]
Different types of space configurations

\[ \mathbf{M}(\hat{K}) \times \mathbf{D}(\hat{K}) \subset H_{\text{div}}(\hat{K}) \times L^2(\hat{K}) \]

\[ \nabla \cdot \mathbf{M}(\hat{K}) = \mathbf{D}(\hat{K}) \]

| \( P_k \) \( P_{k-1} \) \((BDM_k)\) | \( D(\hat{K}) = \mathcal{P}_{k-1} \) \\
| only for tetrahedra | \( \mathbf{M}(\hat{K}) = [\mathcal{P}_k]^3 \), |

| \( P_k^* \) \( P_k \) \((BDMF_{k+1}, RT_k)\) | \( D(\hat{K}) = \mathcal{P}_k \) \\
| all geometries | \([\mathcal{P}_k]^3 \subsetneq \mathbf{M}(\hat{K}) \subsetneq [\mathcal{P}_{k+1}]^3\): \\
| & face functions in \([\mathcal{P}_k]^3\) \\
| & internal functions in \([\mathcal{P}_{k+1}]^3\) with divergence in \(\mathcal{P}_k\) |

| \( P_k^{**} \) \( P_{k+1} \)(new) | \( D(\hat{K}) = \mathcal{P}_{k+1} \) \\
| all geometries | \([\mathcal{P}_k]^3 \subsetneq \mathbf{M}(\hat{K}) \subsetneq [\mathcal{P}_{k+2}]^3\): \\
| & face functions in \([\mathcal{P}_k]^3\) \\
| & internal functions in \([\mathcal{P}_{k+2}]^3\) with divergence in \(\mathcal{P}_{k+1}\) |

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Castro; Devloo; Farias; Gomes; de Siqueira; Durán. Three dimensional hierarchical mixed finite element approximations with enhanced primal variable accuracy. Computer Methods in Applied Mechanics and Engineering, 306: 479-502, 2016. (3D affine uniform meshes)
## Accuracy

### $L^2$ - Error estimations

<table>
<thead>
<tr>
<th></th>
<th>$P_k P_{k-1}$</th>
<th>$P_k^* P_k$</th>
<th>$P_k^{**} P_{k+1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>tetrahedra</td>
<td>all</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$|\sigma - \sigma_h|$</td>
<td>$k + 1$</td>
<td>$k + 1$</td>
<td>$k + 1$</td>
</tr>
<tr>
<td>$|u - u_h|$</td>
<td>$k$</td>
<td>$k + 1$</td>
<td>$k + 2$</td>
</tr>
</tbody>
</table>

![Graphs showing error vs number of equations for different approximation spaces.](image)

New approximation space configuration for the mixed finite element method based on curved 3D meshes.
NeoPZ (object oriented platform for FE)

Geometric map:
- H-refinement
- Curvilinear maps
- Refinement patterns

Approximation spaces:
- H1
- Hdiv - HCurl
- Discontinuous
- Reduced approximations
- Multiphysics

Variational statement:
- System of differential equations
- Linear and nonlinear

NeoPZ

Linear algebra:
- Matrix storage patterns
- Decomposition methods
- Substructuring
- Preconditioning

Finite element tools:
- hp-adaptivity
- Unit tests
- Performance assessment

In development:
- Electromagnetics (HCurl)
- Parallel computing
- Cloud computing

http://github.com/labmec/neopz

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New approximation space configuration for the mixed finite element method.
Hierarchic scalar shape functions in NeoPZ

- **Polynomial space** $\mathcal{P}_k$ restricted to $\hat{K}$:
  
  Tetrahedron: total degree $k$
  
  Cube: maximum degree $k$ in each coordinate
  
  Prism: total degree $k$ in $(\xi_0, \xi_1)$, and maximum degree $k$ in $\xi_2$

- **Hierarchic scalar bases** $\mathcal{B}_k^{\hat{K}}$ for $\mathcal{P}_k$:
  
<table>
<thead>
<tr>
<th>vertex</th>
<th>edge</th>
<th>face</th>
<th>volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varphi^{\hat{a}}$</td>
<td>$\varphi^{\ell,n}$</td>
<td>$\varphi^{\hat{F},n_1,n_2}$</td>
<td>$\varphi^{\hat{K},n_1,n_2,n_3}$</td>
</tr>
</tbody>
</table>

Hierarchic vector-valued bases $B_{k}^{\hat{K}}$ for $P_{k} = [P_{k}]^{3}$

- Shape functions of type

$$\hat{\Phi} = \hat{\varphi}\hat{\mathbf{v}},$$

- $\hat{\mathbf{v}} \rightarrow$ constant vector fields (connected to faces or volume of $\hat{K}$)
- $\hat{\varphi} \rightarrow$ scalar shape functions in $B_{k}^{\hat{K}}$

- **internal shape functions:**
  - vanishing normal components over all the faces of $\hat{K}$.

- **face shape functions:** otherwise

$$B_{k}^{\hat{K}} = \left\{ \Phi^{\hat{K},i,n}, \Phi^{\hat{K},l,n}, \Phi^{\hat{K},n_{1},n_{2}}, \Phi_{(1)}^{\hat{K},n_{1},n_{2},n_{3}}, \Phi_{(2)}^{\hat{K},n_{1},n_{2},n_{3}}, \Phi_{(3)}^{\hat{K},n_{1},n_{2},n_{3}} \right\}.$$
Hierarchic shape functions in $\mathbf{B}_{k}^{\hat{K}}$: main properties

<table>
<thead>
<tr>
<th>Face functions</th>
<th>Normal components</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Phi^{\hat{F},\hat{\alpha}} = \varphi^{\hat{\alpha}} v^{\hat{F},\hat{\alpha}}$</td>
<td>$= \varphi^{\hat{\alpha}}$ in $\hat{F}$, vanish in faces $\neq \hat{F}$</td>
</tr>
<tr>
<td>$\Phi^{\hat{F},\hat{\ell},n} = \varphi^{\hat{\ell},n} v^{\hat{F},\hat{\ell}}$</td>
<td>$= \varphi^{\hat{\ell},n}$ in $\hat{F}$, vanish in faces $\neq \hat{F}$</td>
</tr>
<tr>
<td>$\Phi^{\hat{F},n_{1},n_{2}} = \varphi^{\hat{F},n_{1},n_{2}} v^{\hat{F},\perp}$</td>
<td>$= \varphi^{\hat{F},n_{1},n_{2}}$ in $\hat{F}$, vanish in faces $\neq \hat{F}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Internal functions</th>
<th>Normal components</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Phi^{\hat{K},\hat{\ell},n} = \varphi^{\hat{\ell},n} v^{\hat{F},\top}$</td>
<td>vanish in all faces</td>
</tr>
<tr>
<td>$\Phi^{\hat{K},\hat{F},n_{1},n_{2}}^{(i)} = \varphi^{\hat{F},n_{1},n_{2}} v^{\hat{F},\top}_{(i)}$</td>
<td>vanish in all faces</td>
</tr>
<tr>
<td>$\Phi^{\hat{F},n_{1},n_{2},n_{3}}^{(j)} = \varphi^{\hat{F},n_{1},n_{2},n_{3}} v^{\hat{K}}_{(j)}$</td>
<td>vanish in all faces</td>
</tr>
</tbody>
</table>
Assembly of conforming spaces $V^\Gamma \subset H(div, \Omega)$

- $B^K_k$ hierarchic basis in $H(div, K)$ mapped from $B^\hat{K}_k$

  $$\Phi = F^{\text{div}} \hat{\Phi} = F\left[\frac{1}{\det J} J \hat{\Phi}\right] = F[\hat{\varphi} \frac{1}{\det J} J \hat{v}] = \varphi b$$

  $$b = F\left[\frac{1}{\det J} J \hat{v}\right] = F^{\text{div}} v$$

- $V^\Gamma$ space of piecewise functions: $q|_K := q^K \in \text{span } B^K_k$

- Normal components on interfaces: only contributions of face functions

  $$q^K \cdot n^K|_F = \left[ \sum_{a \in V_F} \alpha_{F,a} \varphi^{F,a} b^{F,a} \cdot n^K + \sum_{\ell \in E_F} \sum_n \beta_{F,\ell,n} \varphi^{F,\ell,n} b^{F,\ell,n} \cdot n^K + \sum_{n_1,n_2} \gamma_{F,n_1,n_2} \varphi^{F,n_1,n_2} b^{F,n_1,n_2} \cdot n^K \right]|_F$$

- Goal: continuity of normal components: is a consequence of
  - continuity of scalar shape functions
  - continuity of normal components of $b$
  - multiplying coefficients on each side of $F$ sum zero

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Application to the mixed formulation: static condensation

- **Primary variables**
  - \( \sigma_e \rightarrow \) face bases;
  - \( u_0 \rightarrow \) one scalar value for \( u \) in each element;

- **Secondary variables**
  - \( \sigma_i \rightarrow \) internal bases;
  - \( u_i \rightarrow \) the remaining DoF of \( u \)

\[
\begin{pmatrix}
A_{ii} & B_{ii}^T & B_{ie}^T & A_{ie} \\
B_{ii} & 0 & 0 & B_{ie} \\
B_{ie} & 0 & 0 & B_{ee} \\
A_{ei} & B_{ie}^T & B_{ee}^T & A_{ee}
\end{pmatrix}
\begin{pmatrix}
\sigma_i \\
u_i \\
u_0 \\
\sigma_e
\end{pmatrix}
= 
\begin{pmatrix}
0 \\
-f_{ih} \\
-f_{0h} \\
0
\end{pmatrix}
\]

- Secondary DoF (\( \sigma_i \) and \( u_i \)) are condensed, to get a condensed system in terms of primary DoF (\( \sigma_e \) and \( u_0 \))

For a given geometry, condensed systems have the same dimension for all space configurations
Test problem: using uniform 3D curved elements

- **Computational domain:** \( \Omega = \{ \mathbf{x} \in \mathbb{R}^3; \frac{1}{4} \leq ||\mathbf{x}|| \leq 1 \} \)
- **Exact solution:**
  \[
  u = \frac{\pi}{2} - \tan^{-1} \left( 5 \left( \sqrt{\left( x - \frac{5}{4} \right)^2 + \left( y + \frac{1}{4} \right)^2 + \left( z + \frac{1}{4} \right)^2 - \frac{\pi}{3}} \right) \right)
  \]

- **Initial hexahedral mesh**
  - The faces of a cube are projected onto the internal and external spherical boundaries.
  - These curved quadrilaterals are *blended by transfinite interpolation* (Coons, 1967) to form 6 hexahedra

- **Initial tetrahedral mesh**
  - Prismatic elements with triangular faces over the internal and external spherical boundaries (by quadratic interpolation).
  - Each curved prism is subdivided into 3 curved tetrahedra.

- **Direct frontal linear solver.**
Curved hexahedral elements)

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New approximation space configuration for the mixed finite elem
Error versus $h$ (hexahedral elements)

$MF^* = P_k^* P_k$ (continuous) $MF^{**} = P_{k+1}^*$ (dashed)
Error versus $h$ (tetrahedral elements)

\[ MF^* = P_k^* P_k \text{ (continuous)} \quad MF^{**} = P_k^{**} P_{k+1} \text{ (dashed)} \]

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New approximation space configuration for the mixed finite element method.
Effect of static condensation

Tetrahedral elements

Hexahedral elements

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New approximation space configuration for the mixed finite element
Application: flow around a horizontal well

- **BC:** $u = 1$ on the outer elliptical belt, $u = 0$ on the well, no flow on the top and bottom flat faces
- $P_k^*P_k$ space configuration
- MacBook: 4 processors and 8GB of memory.
- Matrix computation and assembly: Pthreads + direct skyline linear solver.
Initial mesh (thanks to Simworx)

- 19 curved elements: 11 hexahedra + 8 prisms.
- Trasfinite hexahedra matching the cylindrical well.

Figure 3: Problem 2: initial mesh (left side) and its details (right side).

Figure 4: Problem 2: trasfinite hexahedron matching the circular well.
Refinement procedure

- Directional mesh refinement towards the well, and transversal refinement along the well.
- A basic $k_{min}$ is applied all over the mesh.
- Fix $k_{max} > k$ for the elements touching the toe and heel circular ring; for the neighboring elements assign one degree lower.
- Repeat the procedure until reaching $k_{min}$. 
Amount of flux per unit well length

Due to spherical flux close to heel and toe

Quantidade de fluido/unidade de comprimento do poço

p = 1 / 8 elementos  p = 2 / 8 elementos
p = 1 / 12 elementos  p = 2 / 12 elementos
Effects of static condensation and parallelization on the CPU time

- 75% of dof are condensed
- 97988 dof
- 24850 dof

$k = 2$ and 12 elements on the well

- 8% of CPU time
- 90
- 1017
Current research on related topics

- Mixed finite element-finite volume method for two-phase flows in heterogeneous media (O. Durán PhD Thesis)
- Approximation spaces in $H(\text{div}, \Omega)$ for pyramids
- Multi scale hybrid dual methods combined with high order $H(\text{div})$-conforming approximations on the macro-elements for preconditioning.

Acknowledgments

Minisymposium

RECENTS RESULTS ON HYBRID DISCONTINUOUS GALERKIN
FINITE ELEMENT METHODS
Congress on Numerical Methods in Engineering, CMN 2017
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DEADLINES

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