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:

$$\begin{aligned} \nabla.\boldsymbol{\sigma} &= f \quad \text{in} \quad \Omega, \\ \boldsymbol{\sigma} &= -\nabla u \\ u &= u_D \quad \text{in} \quad \partial\Omega_D, \\ \boldsymbol{\sigma}\cdot\boldsymbol{\eta} &= \mathbf{q}_N \quad \text{in} \quad \partial\Omega_N \end{aligned}$$

- Required functional spaces
  - For the variable $\boldsymbol{\sigma}$

$$H(div,\Omega) = \left\{ \mathbf{q} \in \left[L^2(\Omega)\right]^d ; \nabla.\mathbf{q} \in L^2(\Omega) \right\}$$

  - For the variable u: $L^2(\Omega)$

Discrete variational mixed formulation

1. $\Gamma = \{K\}$ **partition of the computational domain** Ω
2. **Finite dimensional approximation subspaces**
   - $\mathbf{V}^{\Gamma} \subset H(div, \Omega)$ approximation space for $\boldsymbol{\sigma}$
     continuous normal components over element interfaces
   - $U^{\Gamma} \subset L^2(\Omega)$ approximation space for u
     no continuity constraint
   - stability
3. To find $(\boldsymbol{\sigma}, u) \in \left(\mathbf{V}^{\Gamma} \times U^{\Gamma}\right)$ such that $\boldsymbol{\sigma} \cdot \boldsymbol{\eta}|_{\partial\Omega_N} = \mathbf{q}_N$ and

$$\boxed{\begin{aligned} a(\boldsymbol{\sigma},\ \mathbf{q}) - b(\mathbf{q}, u) &= -\int_{\partial\Omega} u_D \mathbf{q} \cdot \boldsymbol{\eta} \ \ \forall \mathbf{q} \in \mathbf{V}_0^{\Gamma} \\ b(\boldsymbol{\sigma}, \varphi) &= \int_{\Omega} f\ \varphi\ d\Omega\ \ \forall \varphi \in U^{\Gamma} \end{aligned}}$$

Motivation

- Since Raviart and Thomas 1977
  - a variety of $\mathbf{V}^{\Gamma} \times U^{\Gamma}$ 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

Motivation

- Recent efforts on the development and/or implementation of convenient sets of basis functions for higher order H(div)-conforming approximations in 3D
  - **Arnold, Falk, Winther**, Comput. Methods Appl. Mech. Engrg., 2009 (Berstein-Bézier,simplices)
  - **Ainsworth, Andriamaro, Davydov**, SIAM J. Sci. Comput. 2011 (Berstein-Bézier,simplices)
  - **Fuentes, Keith, Demkowicz,** Nagaraj, Mathematics and Computers in Simulation 2015 (hierarchic, all geometries)
  - **Castro, Devloo, Farias, G, Siqueira, Durán**, Comput. Meth. Appl. Mech. 2016 (hierachic, affine, all geometries excepting pyramides)
  - **Castro, Devloo, Farias, G, Durán**, Jr. Comp. Appl. Math 2016. (hierachic, curved 2D + surfaces)

Goals

- Systematic construction of hierarchic high order shape functions for approximation spaces

$$\mathbf{V}^{\Gamma} \subset Hdiv(\Omega)$$

  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)
- $\mathbf{x} : \hat{K} \to K$: geometric mapping (diffeomorphism)
- $\mathbb{F} : \hat{\varphi} \to \varphi$, isomorphism mapping scalar functions $\hat{\varphi}$ of $H^1(\hat{K})$ to scalar functions φ of $H^1(K)$ (induced by $\mathbf{x}$)

$$\varphi(\mathbf{p}) = \hat{\varphi}(\mathbf{x}^{-1}(\mathbf{p}))$$

- $\mathbb{F}^{div} : \hat{\mathbf{q}} \to \mathbf{q}$ contravariant Piola transformation: isomorphism mapping vector-valued functions $\hat{\mathbf{q}} \in H(div, \hat{K})$ to vector-valued functions $\mathbf{q} \in H(div, K)$

$$\mathbf{q} = \mathbb{F}\left[\frac{1}{det\mathbf{J}}\mathbf{J}(\hat{\mathbf{q}})\right]$$

where $\mathbf{J} = \nabla\mathbf{x}$ is the Jacobean of the geometric mapping.

Construction of approximation spaces $\mathbf{V}^\Gamma \times U^\Gamma$: guidelines II

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

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

- Global approximation spaces

$$\boxed{\begin{aligned} \mathbf{V}^\Gamma &= \left\{ \mathbf{q} \in \mathbf{H}(div, \Omega);\ \mathbf{q}|_K = \mathbb{F}^{div}\hat{\mathbf{q}},\ \hat{\mathbf{q}} \in \mathbf{M}(\hat{K}) \right\} \\ U^\Gamma &= \left\{ \varphi \in L^2(\Omega);\ \varphi|_K = \mathbb{F}\hat{\varphi},\ \hat{\varphi} \in D(\hat{K}) \right\} \end{aligned}}$$

Different types of space configurations

$$\mathbf{M}(\hat{K}) \times D(\hat{K}) \subset Hdiv(\hat{K}) \times L^2(\hat{K})$$

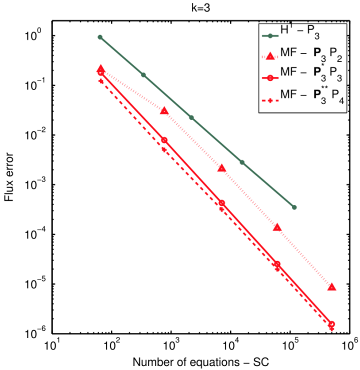
$$\nabla.\mathbf{M}(\hat{K}) = D(\hat{K})$$

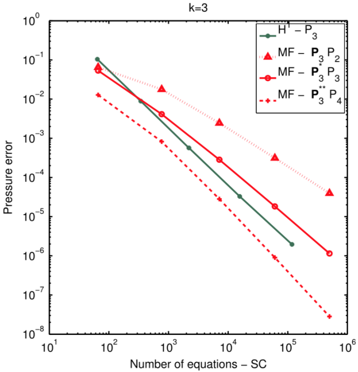
$\mathbf{P}_k$ P_{k-1} (BDM_k) only for tetrahedra	$D(\hat{K}) = \mathcal{P}_{k-1}$ $\mathbf{M}(\hat{K}) = [\mathcal{P}_k]^3$,
$\mathbf{P}_k^*$ P_k $(BDMF_{k+1},\ RT_k)$ all geometries	$D(\hat{K}) = \mathcal{P}_k$ $[\mathcal{P}_k]^3 \subsetneq \mathbf{M}(\hat{K}) \subsetneq [\mathcal{P}_{k+1}]^3$: **face functions** in $[\mathcal{P}_k]^3$ **internal functions** in $[\mathcal{P}_{k+1}]^3$ with divergence in $\mathcal{P}_k$
$\mathbf{P}_k^{**}$ P_{k+1} (new) all geometries	$D(\hat{K}) = \mathcal{P}_{k+1}$ $[\mathcal{P}_k]^3 \subsetneq \mathbf{M}(\hat{K}) \subsetneq [\mathcal{P}_{k+2}]^3$: **face functions** in $[\mathcal{P}_k]^3$ **internal functions** in $[\mathcal{P}_{k+2}]^3$with divergence in $\mathcal{P}_{k+1}$

- **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)**

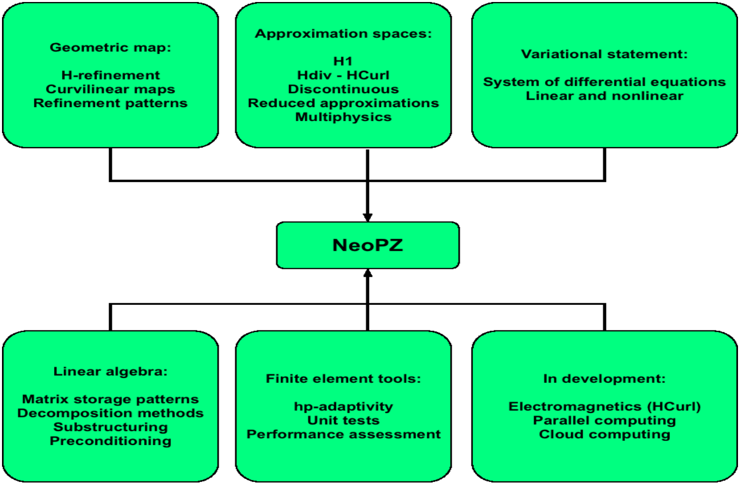
L^2 - **Error estimations**

	$\mathbf{P}_k P_{k-1}$	$\mathbf{P}_k^* P_k$	$\mathbf{P}_k^{**} P_{k+1}$
	tetrahedra	all	
$\|\|\boldsymbol{\sigma} - \boldsymbol{\sigma}_h\|\|$	$k+1$	$k+1$	$k+1$
$\|\|u - u_h\|\|$	k	$k+1$	$k+2$





NeoPZ (object oriented platform for FE)



http://github.com/labmec/neopz

Hierarchic scalar shape functions in NeoPZ

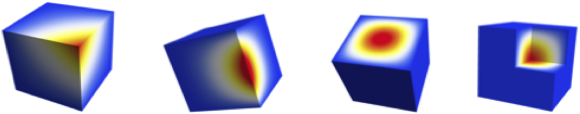
- Polynomial space $\mathcal{P}_k$ restricted to $\hat{K}$:

  Tetrahedron: total degree k

  Cube: maximum degree k in each coordinate
  Prism: total degree k in (ξ_0, ξ_1), and maximum degree k in ξ_2

- Hierarchic scalar bases $\mathcal{B}_k^{\hat{K}}$ for $\mathcal{P}_k$:

vertex	edge	face	volume
$\varphi^{\hat{a}}$	$\varphi^{\ell,n}$	$\varphi^{\hat{F},n_1,n_2}$	$\varphi^{\hat{K},n_1,n_2,n_3}$



- P. Devloo, C. Bravo, and E. Rylo. Systematic and generic construction of shape functions for p-adaptive meshes of multidimensional finite elements. Comput. Methods Appl. Mech. Engrg., 198:1716 – 1725, 2009.

Hierarchic vector-valued bases $\mathbf{B}_k^{\hat{K}}$ for $\mathbf{P}_k = [\mathcal{P}_k]^3$

- Shape functions of type

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

  - $\hat{\mathbf{v}} \to$ constant vector fields (connected to faces or volume of $\hat{K}$)
  - $\hat{\varphi} \to$ scalar shape functions in $\mathcal{B}_k^{\hat{K}}$
- internal shape functions:
  - vanishing normal components over all the faces of $\hat{K}$.
- face shape functions: otherwise

$$\begin{aligned}\mathbf{B}_k^{\hat{K}} &= \underbrace{\left\{\mathbf{\Phi}^{\hat{F},\hat{a}},\ \mathbf{\Phi}^{\hat{F},\hat{l},n},\ \mathbf{\Phi}^{\hat{F},n_1,n_2}\right\}}_{\text{face functions}} \\ &\cup \underbrace{\left\{\mathbf{\Phi}^{\hat{K},\hat{l},n}, \mathbf{\Phi}_{(1)}^{\hat{K},\hat{F},n_1,n_2}, \mathbf{\Phi}_{(2)}^{\hat{K},\hat{F},n_1,n_2}, \mathbf{\Phi}_{(1)}^{\hat{K},n_1,n_2,n_3}, \mathbf{\Phi}_{(2)}^{\hat{K},n_1,n_2,n_3}, \mathbf{\Phi}_{(3)}^{\hat{K},n_1,n_2,n_3}\right\}}_{\text{internal functions}}.\end{aligned}$$

Hierarchic shape functions in $\mathbf{B}_k^{\hat{K}}$: main properties

Face functions	Normal components
$\mathbf{\Phi}^{\hat{F},\hat{a}} = \varphi^{\hat{a}}\mathbf{v}^{\hat{F},\hat{a}}$	$= \varphi^{\hat{a}}$ in $\hat{F}$, vanish in faces $\neq \hat{F}$
$\mathbf{\Phi}^{\hat{F},\hat{\ell},n} = \varphi^{\hat{\ell},n}\mathbf{v}^{\hat{F},\hat{l}}$	$= \varphi^{\hat{\ell},n}$ in $\hat{F}$, vanish in faces $\neq \hat{F}$
$\mathbf{\Phi}^{\hat{F},n_1,n_2} = \varphi^{\hat{F},n_1,n_2}\mathbf{v}^{\hat{F},\perp}$	$= \varphi^{\hat{F},n_1,n_2}$ in $\hat{F}$, vanish in faces $\neq \hat{F}$
Internal functions	Normal components
$\mathbf{\Phi}^{\hat{K},\hat{\ell},n} = \varphi^{\hat{\ell},n}\mathbf{v}^{\hat{F},\top}$	vanish in all faces
$\mathbf{\Phi}_{(i)}^{\hat{K},\hat{F},n_1,n_2} = \varphi^{\hat{F},n_1,n_2}\mathbf{v}_{(i)}^{\hat{F},\top}$	vanish in all faces
$\mathbf{\Phi}_{(j)}^{\hat{F},n_1,n_2,n_3} = \varphi^{\hat{F},n_1,n_2,n_3}\mathbf{v}_{(j)}^{\hat{K}}$	vanish in all faces

Assembly of conforming spaces $\mathbf{V}^\Gamma \subset \mathbf{H}(div, \Omega)$

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

$$\mathbf{\Phi} = \mathbb{F}^{div}\hat{\mathbf{\Phi}} = \mathbb{F}[\frac{1}{det\ \mathbf{J}}\mathbf{J}\hat{\mathbf{\Phi}}] = \mathbb{F}[\hat{\varphi}\frac{1}{det\ \mathbf{J}}\mathbf{J}\mathbf{v}] = \varphi\mathbf{b}$$

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

- $\mathbf{V}^\Gamma$ space of piecewise functions: $\mathbf{q}|_K := \mathbf{q}^K \in span\ \mathbf{B}_k^K$
- Normal components on interfaces: only contributions of face functions

$$\begin{aligned} \mathbf{q}^K \cdot \mathbf{n}^K|_F &= \Bigg[\sum_{a \in \mathcal{V}_F} \alpha_{F,a}\varphi^a\mathbf{b}^{F,a} \cdot \mathbf{n}^K + \sum_{\ell \in \mathcal{E}_F}\sum_n \beta_{F,\ell,n}\varphi^{\ell,n}\mathbf{b}^{F,\ell,n} \cdot \mathbf{n}^K \\ &+ \sum_{n_1,n_2} \gamma_{F,n_1,n_2}\varphi^{F,n_1,n_2}\mathbf{b}^{F,n_1,n_2} \cdot \mathbf{n}^K\Bigg]\Bigg|_F . \end{aligned}$$

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

Application to the mixed formulation: static condensation

- **Primary variables**
  - $\boldsymbol{\sigma}_e \rightarrow$ face bases;
  - $u_0 \rightarrow$ one scalar value for u in each element;
- **Secondary variables**
  - $\boldsymbol{\sigma}_i \rightarrow$ internal bases;
  - $u_i \rightarrow$ the remaining DoF of u

$$\left(\begin{array}{cc|cc} A_{ii} & B_{ii}^T & B_{ie}^T & A_{ie} \\ B_{ii} & 0 & 0 & B_{ie} \\ \hline B_{ie} & 0 & 0 & B_{ee} \\ A_{ei} & B_{ie}^T & B_{ee}^T & A_{ee} \end{array}\right) \left(\begin{array}{c} \boldsymbol{\sigma}_i \\ u_i \\ \hline u_0 \\ \boldsymbol{\sigma}_e \end{array}\right) = \left(\begin{array}{c} 0 \\ -f_{ih} \\ \hline -f_{0h} \\ 0 \end{array}\right)$$

- Secondary DoF ($\boldsymbol{\sigma}_i$ and u_i) are condensed, to get a condensed system in terms of primary DoF ($\boldsymbol{\sigma}_e$ and u_0)

For a given geometry, condensed systems have the same dimension for all space configurations

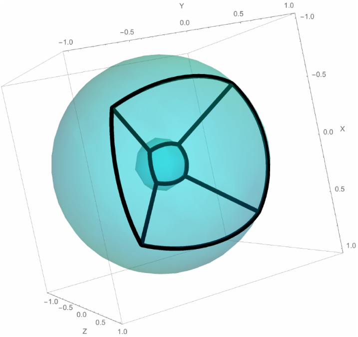
Test problem: using uniform 3D curved elements

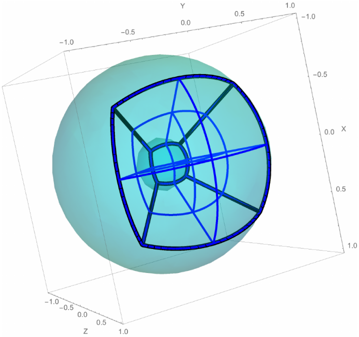
- Computational domain: $\Omega = \{\mathbf{x} \in \mathbb{R}^3; \frac{1}{4} \leq ||\mathbf{x}|| \leq 1\}$
- Exact solution:

$$u = \frac{\pi}{2} - \tan^{-1}\left(5\left(\sqrt{(x-\frac{5}{4})^2 + (y+\frac{1}{4})^2 + (z+\frac{1}{4})^2} - \frac{\pi}{3}\right)\right)$$

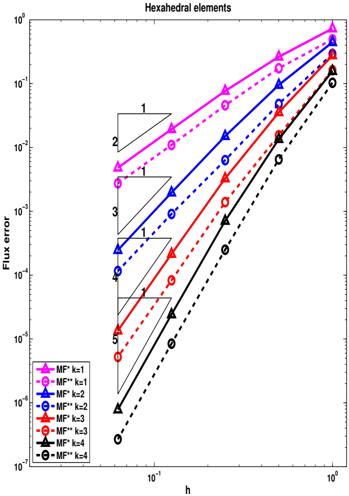
- Initial hexahedral mesh
    - The faces of a cube are projected onto the internal and external spherical boundaries.
    - These curved quadrilaterals are *blended* by *transfinite interpolation (Coons, 1967) to form 6 hexahedra*
- Initial tetrahedral mesh
    - Prismatic elements with triangular faces over the internal and external spherical boundaries (by quadratic interpolation).
    - Each curved prism is subdivided into 3 curved tetrahedra.
- Direct frontal linear solver.

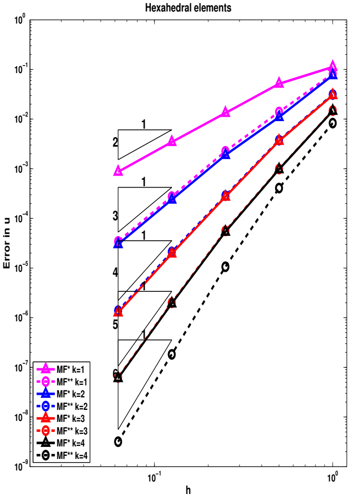
Curved hexahedral elements)





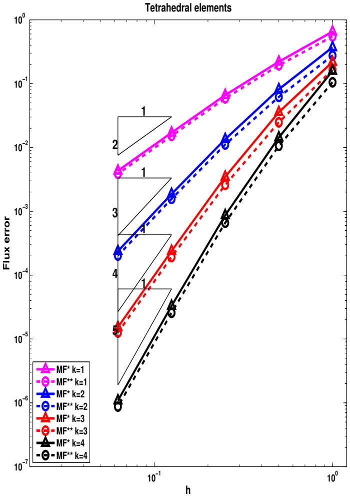
Error versus h (hexahedral elements)

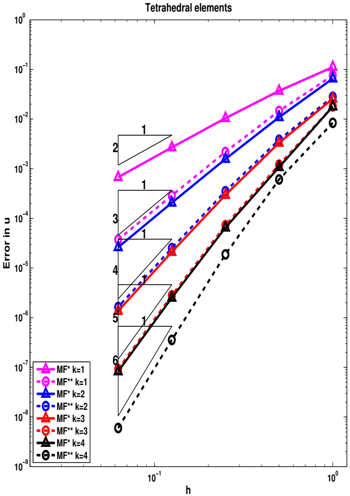




$MF^* = \mathbf{P}_k^* P_k$ (continuous) $MF^{**} = \mathbf{P}_k^{**} P_{k+1}$ (dashed)

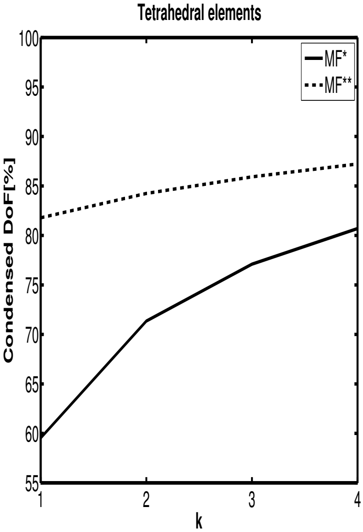
Error versus h (tetrahedral elements)

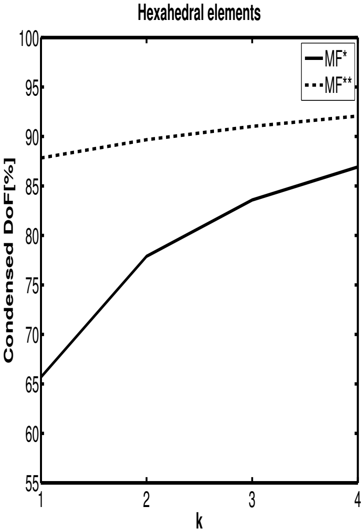




$MF^* = \mathbf{P}_k^* P_k$ (continuous) $MF^{**} = \mathbf{P}_k^{**} P_{k+1}$ (dashed)

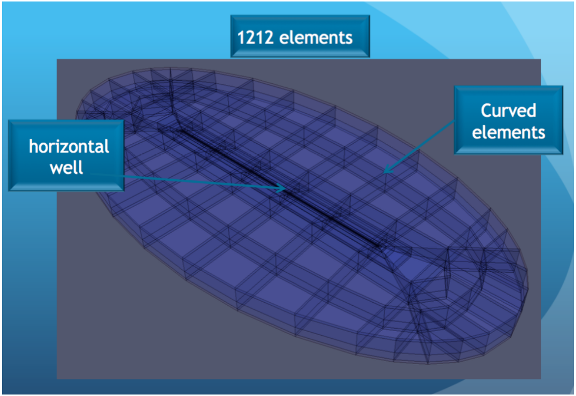
Effect of static condensation





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
- $\mathbf{P}_k^* P_k$ 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 cilindrical well.

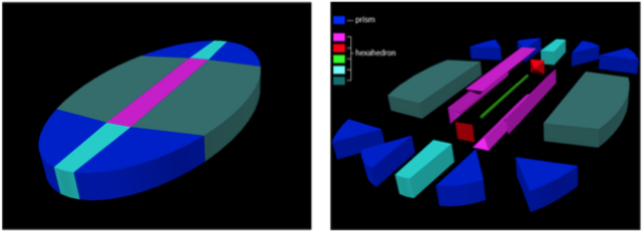


Figure 3: Problem 2: initial mesh (left side) and its details (right side).

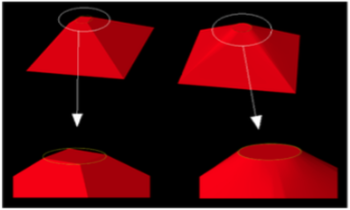
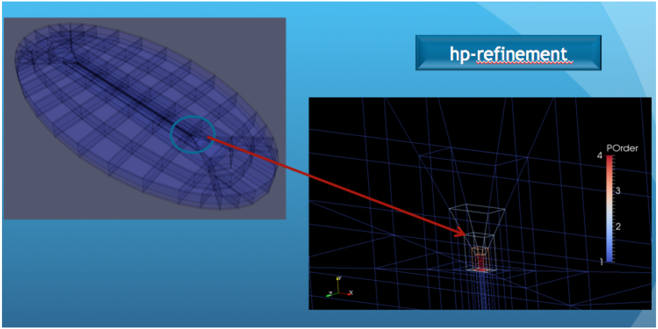


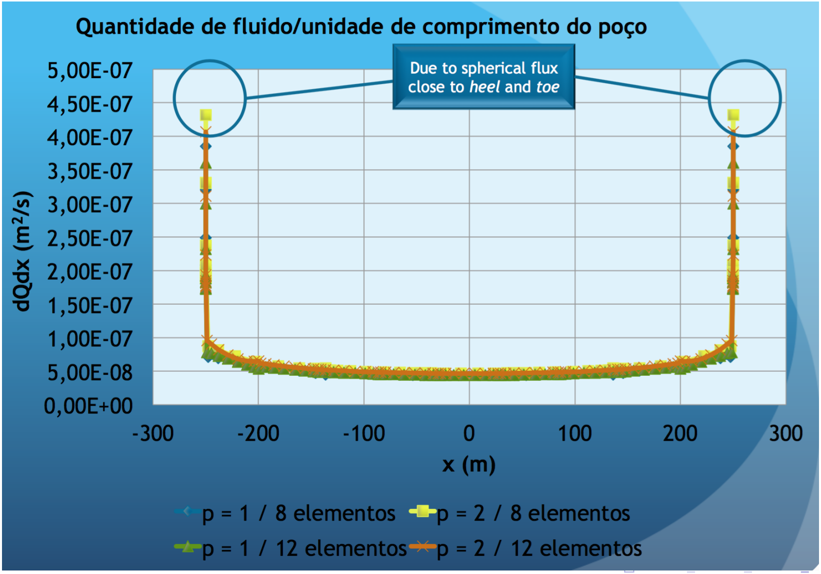
Figure 4: Problem 2: transfinite hexahedron matching the circular well.

Refinement procedure

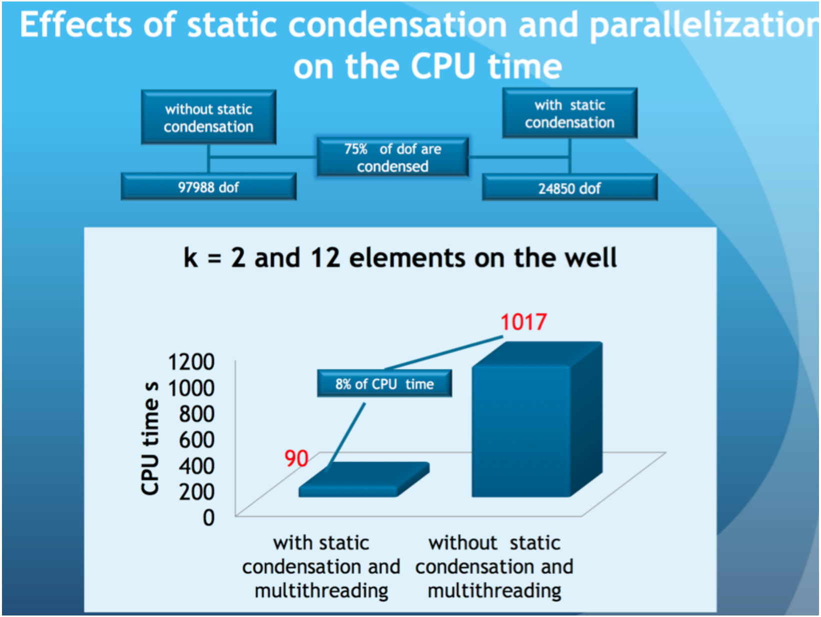
- Directional mesh refinement towards the well, and transversal refinement along the well.
- A basic k_{min} is applied all over the mesh.
- Fix $k_{max} > k$ for the elements touching the toe and heel circular ring; for the neighboring elements assign one degree lower.
- Repeat the procedure until reaching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



Amount of flux per unit well length



Effects of static condensation and parallelization



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 $\mathbf{H}(div, \Omega)$ for pyramids
- Multi scale hybrid dual methods combined with high order $\mathbf{H}(div)$-conforming approximations on the macro-elements for preconditioning.

Acknowledgments

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