A simple a posteriori estimate on general polytopal meshes with applications to complex porous media flows

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Inria Paris & Ecole des Ponts

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Outline

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1. Introduction
   - Context and goals of the talk
   - Mixed finite elements on general polytopal meshes
2. Steady linear Darcy flow
   - Discretizations
   - A posteriori ingredients
   - A posteriori estimate
   - Numerical experiments
3. Steady nonlinear Darcy flow
   - Discretizations
   - A posteriori ingredients and estimate
4. Unsteady multi-phase multi-compositional Darcy flow
   - A posteriori ingredients and estimate
   - Numerical experiments
5. Conclusions

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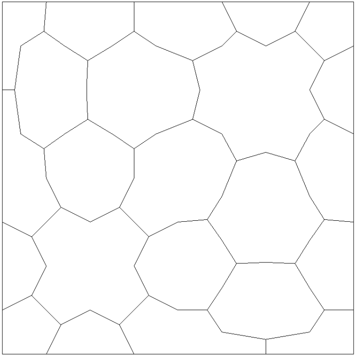
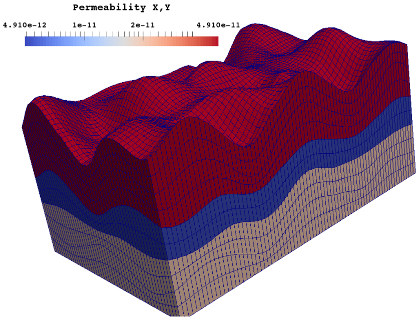
General polygonal/polyhedral meshes, arbitrary scheme





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Multi-phase, multi-compositional flows

- unsteady nonlinear degenerate coupled systems of PDEs
- algebraic constraints, phase appearance/disappearance

Goals

- **simple** estimates: **easy** coding, **fast** evaluation, **cosy** use in practical simulations
- guaranteed a posteriori error estimates on $\left\| \mathbf{u}|_{I_n} - \mathbf{u}_h^{n,k,i} \right\|$, valid at **each step**: time n, linearization k, linear solver i
- distinguishing different error components: **full adaptivity**

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Steady linear Darcy flow

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\begin{aligned}
-\nabla\cdot(\underline{\mathbf{K}}\nabla p) &= f && \text{in } \Omega,\\
p &= 0 && \text{on } \partial\Omega
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- $\Omega \subset \mathbb{R}^d$, $d \geq 1$, be an open interval/polygon/polyhedron or polytope in general
- $f \in L^2(\Omega)$ source term, pw polynomial for simplicity
- $\underline{\mathbf{K}} \in [L^\infty(\Omega)]^{d\times d}$ diffusion-dispersion tensor (pw constant)

Unknowns

- p pressure head
- $\mathbf{u} := -\underline{\mathbf{K}}\nabla p$ Darcy velocity (flux)

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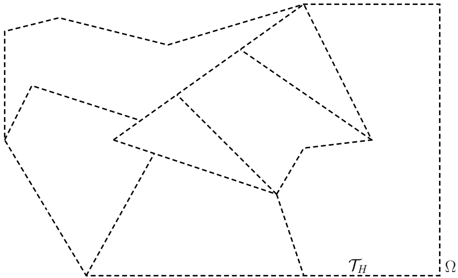

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- $\mathcal{T}_H$ can be nonmatching
- maximal number of faces of $K \in \mathcal{T}_H$ is not limited
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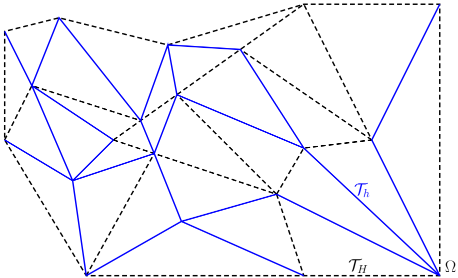

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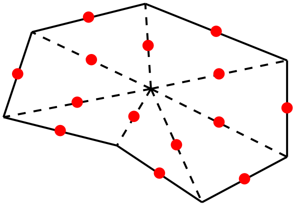

Static condensation

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- reconstruction from **Lagrange multipliers** Λ_σ on boundary of K
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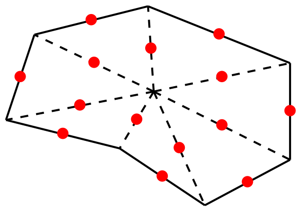

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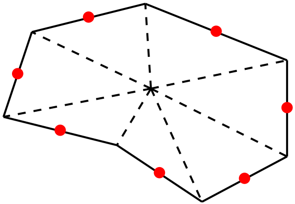

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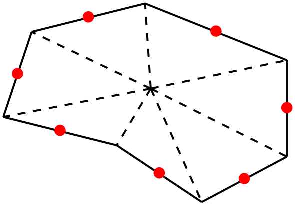

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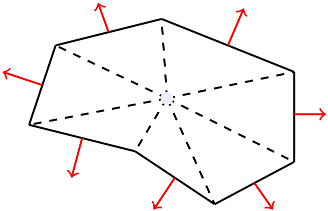

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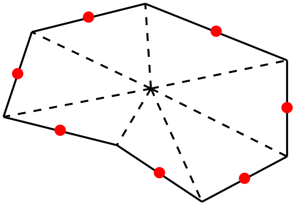

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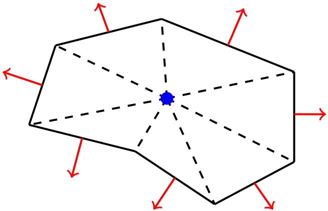

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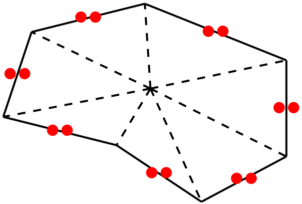

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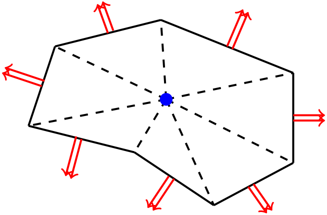

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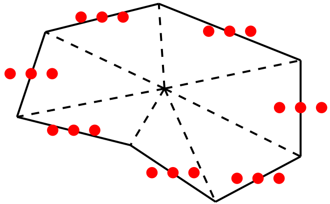

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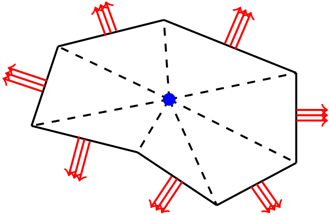

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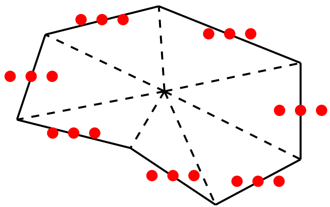

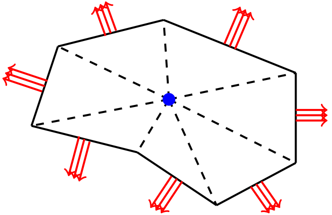

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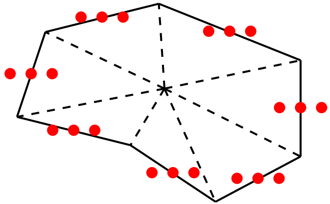

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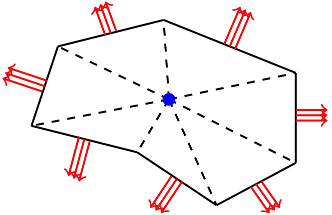

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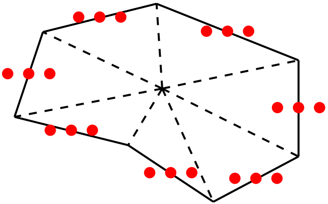

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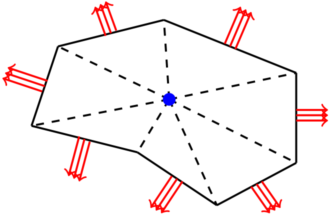

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Guaranteed and k-robust *a posteriori* error estimates

Guaranteed bound for any $\mathbf{u}_h \in \mathbf{V}_h \subset \mathbf{H}(\mathrm{div}, \Omega)$, $\nabla \cdot \mathbf{u}_h = f$

There holds for any $s_h \in V_h \subset H_0^1(\Omega)$

$$\underbrace{\left\| \underline{\mathbf{K}}^{-\frac{1}{2}}(\mathbf{u} - \mathbf{u}_h) \right\|}_{\text{unknown error}} = \min_{v \in H_0^1(\Omega)} \left\| \underline{\mathbf{K}}^{-\frac{1}{2}} \mathbf{u}_h + \underline{\mathbf{K}}^{\frac{1}{2}} \nabla v \right\| \leq \underbrace{\left\| \underline{\mathbf{K}}^{-\frac{1}{2}} \mathbf{u}_h + \underline{\mathbf{K}}^{\frac{1}{2}} \nabla s_h \right\|}_{\text{computable estimate}}$$

- Prager & Synge (1947), Dari, Durán, Padra, & Vampa (1996), Kim (2007), V. (2007), Ainsworth (2007)

Efficiency (& robustness wrt polynomial degree k for $d \leq 3$)

For polytopal MFE and suitable s_h, there holds (simplifying)

$$\left\| \underline{\mathbf{K}}^{-\frac{1}{2}} \mathbf{u}_h + \underline{\mathbf{K}}^{\frac{1}{2}} \nabla s_h \right\| \leq C(\kappa_{\mathcal{T}_h}, \underline{\mathbf{K}}, d) \left\| \underline{\mathbf{K}}^{-\frac{1}{2}}(\mathbf{u} - \mathbf{u}_h) \right\|$$

- $C(\kappa_{\mathcal{T}_h}, \underline{\mathbf{K}}, d)$ only depends on the shape-regularity of $\mathcal{T}_h$, the diffusion tensor $\underline{\mathbf{K}}$, and the space dimension d
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$$\left\|\underline{\mathbf{K}}^{-\frac{1}{2}}\mathbf{u}_h + \underline{\mathbf{K}}^{\frac{1}{2}}\nabla s_h\right\| \leq C(\kappa_{\mathcal{T}_h}, \underline{\mathbf{K}}, d) \left\|\underline{\mathbf{K}}^{-\frac{1}{2}}(\mathbf{u}-\mathbf{u}_h)\right\|$$

- $C(\kappa_{\mathcal{T}_h}, \underline{\mathbf{K}}, d)$ only depends on the shape-regularity of $\mathcal{T}_h$, the diffusion tensor $\underline{\mathbf{K}}$, and the space dimension d
- Braess, Pillwein, & Schöberl (2009) (conforming setting), Ern & V. (2015) (unified framework including MFEs)

Guaranteed and k-robust *a posteriori* error estimates

Guaranteed bound for any $\mathbf{u}_h \in \mathbf{V}_h \subset \mathbf{H}(\mathrm{div},\Omega)$, $\nabla\cdot\mathbf{u}_h = f$

There holds for any $s_h \in V_h \subset H_0^1(\Omega)$

$$\underbrace{\left\|\underline{\mathbf{K}}^{-\frac{1}{2}}(\mathbf{u}-\mathbf{u}_h)\right\|}_{\text{unknown error}} = \min_{v\in H_0^1(\Omega)} \left\|\underline{\mathbf{K}}^{-\frac{1}{2}}\mathbf{u}_h+\underline{\mathbf{K}}^{\frac{1}{2}}\nabla v\right\| \leq \underbrace{\left\|\underline{\mathbf{K}}^{-\frac{1}{2}}\mathbf{u}_h+\underline{\mathbf{K}}^{\frac{1}{2}}\nabla s_h\right\|}_{\text{computable estimate}}$$

- Prager & Synge (1947), Dari, Durán, Padra, & Vampa (1996), Kim (2007), V. (2007), Ainsworth (2007)

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Multi-phase, multi-compositional flows discussion

Mathematician

- all ingredients are ready to design an a posteriori error estimate, let us make it work in the given case

Engineer

- What is a Raviart–Thomas space?
- I do not have a simplicial mesh and cannot/do not want to build a simplicial submesh.
- I do not want to implement the Raviart–Thomas space.
- I do not want to implement (new) quadrature rules.
- I do not want to solve local problems.
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Outline

Linear Darcy flow

Steady linear Darcy flow

$$
\begin{aligned}
-\nabla\cdot(\underline{\mathbf{K}}\nabla p) &= f && \text{in } \Omega, \\
p &= 0 && \text{on } \partial\Omega
\end{aligned}
$$

- $\Omega \subset \mathbb{R}^d$, $d \geq 1$, polytope
- $f \in L^2(\Omega)$ source term, pw constant for simplicity
- $\underline{\mathbf{K}} \in [L^\infty(\Omega)]^{d\times d}$ diffusion-dispersion tensor (pw constant)

Unknowns

- p pressure head
- $\mathbf{u} := -\underline{\mathbf{K}}\nabla p$ Darcy velocity (flux)

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General discretizations

Assumption A (Locally conservative discretization)

1. *There is one **normal flux** $(\mathrm{U})_\sigma \in \mathbb{R}$ per face $\sigma \in \mathcal{E}_H$ and one **pressure** $(\mathrm{P})_K \in \mathbb{R}$ per element $K \in \mathcal{T}_H$.*
2. *The **flux balance** is satisfied, with $(\mathrm{F})_K := (f, 1)_K$:*

$$\sum_{\sigma \in \mathcal{E}_K} (\mathrm{U})_\sigma \mathbf{n}_{K,\sigma} \cdot \mathbf{n}_\sigma = (\mathrm{F})_K, \quad \forall K \in \mathcal{T}_H.$$

- **any** (lowest-order) **locally conservative method**
- how $(\mathrm{U})_\sigma$ obtained from $(\mathrm{P})_K$ is not important for the a posteriori error estimate upper bound

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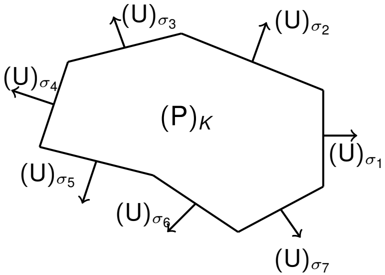

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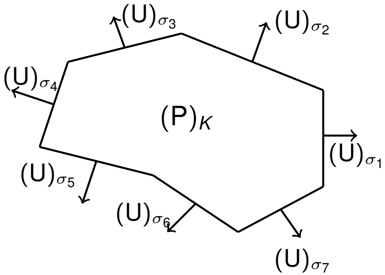

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Saddle-point discretizations

Assumption B (Saddle-point discretization)

The scheme writes: find $\mathsf{U} := \{(\mathsf{U})_\sigma\}_{\sigma\in\mathcal{E}_H} \in \mathbb{R}^{|\mathcal{E}_H|}$ *and* $\mathsf{P} := \{(\mathsf{P})_K\}_{K\in\mathcal{T}_H} \in \mathbb{R}^{|\mathcal{T}_H|}$ *such that*

$$\begin{pmatrix} \mathbb{A} & \mathbb{B}^{\mathrm{t}} \\ \mathbb{B} & 0 \end{pmatrix} \begin{pmatrix} \mathsf{U} \\ \mathsf{P} \end{pmatrix} = \begin{pmatrix} 0 \\ \mathsf{F} \end{pmatrix};$$

- $\mathbb{A}$ *defined by the element matrices* $\widehat{\mathbb{A}}_K \in \mathbb{R}^{|\mathcal{E}_K|\times|\mathcal{E}_K|}$ *of the given method;*
- $\mathbb{B}$*: entries* $1, -1, 0$*;*
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- satisfied by MFDs, HFVs, MVEs, HDGs, HHOs, MFEs ...

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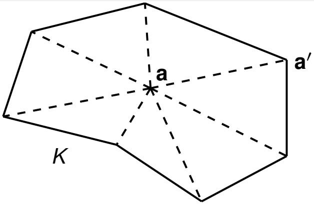
Outline

1. Introduction
   - Context and goals of the talk
   - Mixed finite elements on general polytopal meshes
2. Steady linear Darcy flow
   - Discretizations
   - A posteriori ingredients
   - A posteriori estimate
   - Numerical experiments
3. Steady nonlinear Darcy flow
   - Discretizations
   - A posteriori ingredients and estimate
4. Unsteady multi-phase multi-compositional Darcy flow
   - A posteriori ingredients and estimate
   - Numerical experiments
5. Conclusions

Ingredient 1: element matrices



- finite element stiffness matrix

$$(\widehat{\mathbb{S}}_{\mathrm{FE},K})_{\mathbf{a},\mathbf{a}'} := (\underline{\mathbf{K}}\nabla\psi_{\mathbf{a}'}, \nabla\psi_{\mathbf{a}})_K \qquad \mathbf{a}, \mathbf{a}' \in \mathcal{V}_{K,h}$$

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- mixed finite element local static condensation matrix

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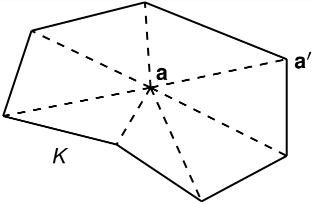

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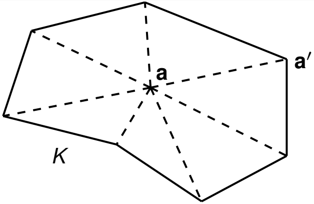

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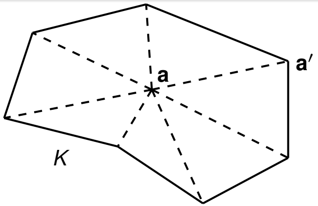

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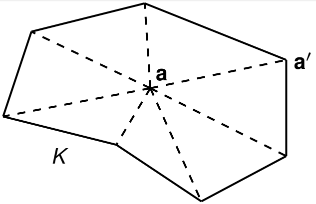

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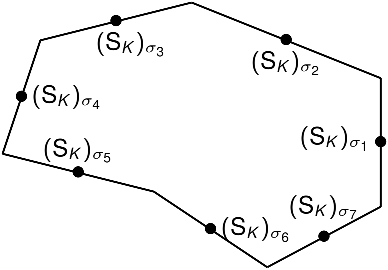

$$S_K^{\text{ext}} = \{(S_K)_{\sigma_i}\}_{i=1}^{7}$$

- Assumption A: $(S_K)_{\sigma_i}$ local averages of neighbor $(P)_{K'}$

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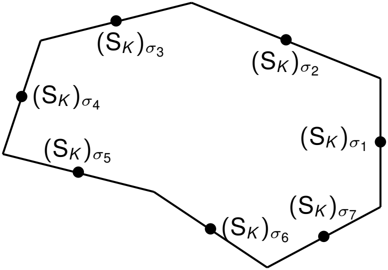

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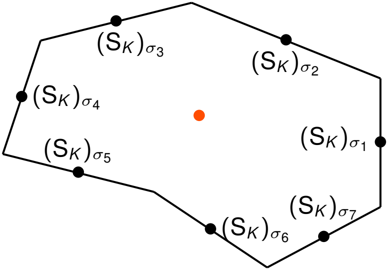

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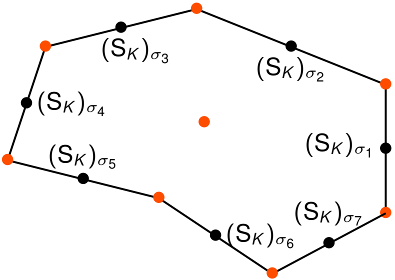

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- $(S_K)_{\mathbf{a}_8} := (P)_K$
- $S_K = \{(S_K)_{\mathbf{a}_i}\}_{i=1}^{7}$ constructed by local averaging

Outline

Linear Darcy flow estimate

Theorem (Linear Darcy flow)

Under Assumption A, there holds

$$\left\|\underline{\mathbf{K}}^{-\frac{1}{2}}(\mathbf{u}-\mathbf{u}_h)\right\| \leq \left\{\sum_{K\in\mathcal{T}_H} \eta_K^2\right\}^{\frac{1}{2}},$$

where

$$\eta_K^2 := (\mathsf{U}_K^{\mathrm{ext}})^{\mathrm{t}} \widehat{\mathbb{A}}_{\mathrm{MFE},K} \mathsf{U}_K^{\mathrm{ext}} + \mathsf{S}_K^{\mathrm{t}} \widehat{\mathbb{S}}_{\mathrm{FE},K} \mathsf{S}_K + 2(\mathsf{U}_K^{\mathrm{ext}})^{\mathrm{t}} \mathsf{S}_K^{\mathrm{ext}} - 2(\mathsf{F})_K |K|^{-1} 1^{\mathrm{t}} \widehat{\mathbb{M}}_{\mathrm{FE},K} \mathsf{S}_K.$$

Comments

- **guaranteed upper bound** on the Darcy velocity error
- price: **matrix-vector multiplication** on each element

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Comments

- **guaranteed upper bound** on the Darcy velocity error
- price: **matrix-vector multiplication** on each element
- $\mathbf{u}_h|_K$: discrete fictitious Darcy velocity on the submesh $\mathcal{T}_K$ by a MFE local Neumann problem with matrix $\widehat{\mathbb{A}}_{\mathrm{MFE},K}$

$$\mathbf{u}_h|_K := \arg \min_{\mathbf{v}_h;\ \langle \mathbf{v}_h\cdot\mathbf{n},1\rangle_\sigma = (\mathsf{U})_\sigma\ \nabla\cdot\mathbf{v}_h=\mathrm{constant}} \left\|\underline{\mathbf{K}}^{-\frac{1}{2}}\mathbf{v}_h\right\|_K;$$

not constructed in practice, unless in the test cases

Linear Darcy flow estimate

Corollary (Linear Darcy flow)

Under Assumption B, there holds

$$\left\|\underline{\mathbf{K}}^{-\frac{1}{2}}(\mathbf{u}-\tilde{\mathbf{u}}_h)\right\| \le \left\{\sum_{K\in\mathcal{T}_H} \tilde{\eta}_K^2\right\}^{\frac{1}{2}},$$

where

$$\tilde{\eta}_K{}^2 := (\mathsf{U}_K^{\mathrm{ext}})^{\mathrm{t}}\widehat{\mathbb{A}}_K\mathsf{U}_K^{\mathrm{ext}} + \mathsf{S}_K^{\mathrm{t}}\widehat{\mathbb{S}}_{\mathrm{FE},K}\mathsf{S}_K + 2(\mathsf{U}_K^{\mathrm{ext}})^{\mathrm{t}}\mathsf{S}_K^{\mathrm{ext}} - 2(\mathsf{F})_K|K|^{-1}\mathsf{1}^{\mathrm{t}}\widehat{\mathbb{M}}_{\mathrm{FE},K}\mathsf{S}_K.$$

Comments

- **guaranteed upper bound** on the Darcy velocity error
- price: **matrix-vector multiplication** on each element
- $\tilde{\mathbf{u}}_h$: continuous fictitious Darcy velocity (local Neumann problem on K) $\approx$ abstract MFD lifting operator of $\widehat{\mathbb{A}}_K$ (Brezzi, Lipnikov, & Shashkov (2005)); impossible to construct $\tilde{\mathbf{u}}_h$ in practice

Proof (1)

- Prager–Synge equality:

$$\left\|\underline{\mathbf{K}}^{-\frac{1}{2}}(\mathbf{u}-\mathbf{u}_h)\right\| = \inf_{v\in H_0^1(\Omega)} \left\|\underline{\mathbf{K}}^{-\frac{1}{2}}\mathbf{u}_h + \underline{\mathbf{K}}^{\frac{1}{2}}\nabla v\right\|$$

- consequently, for an arbitrary $s_h \in H_0^1(\Omega)$:

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- developing for each $K \in \mathcal{T}_H$

$$\left\|\underline{\mathbf{K}}^{-\frac{1}{2}}\mathbf{u}_h + \underline{\mathbf{K}}^{\frac{1}{2}}\nabla s_h\right\|_K^2 = \left\|\underline{\mathbf{K}}^{-\frac{1}{2}}\mathbf{u}_h\right\|_K^2 + 2(\mathbf{u}_h, \nabla s_h)_K + \left\|\underline{\mathbf{K}}^{\frac{1}{2}}\nabla s_h\right\|_K^2$$

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Proof (2)

- V. & Wohlmuth (2013): for the MFE element matrix $\widehat{\mathbb{A}}_{\mathrm{MFE},K}$, there holds, under Assumption A:

$$\left\|\underline{\mathbf{K}}^{-\frac{1}{2}}\mathbf{u}_h\right\|_K^2 = (\mathsf{U}_K^{\mathrm{ext}})^{\mathrm{t}}\widehat{\mathbb{A}}_{\mathrm{MFE},K}\mathsf{U}_K^{\mathrm{ext}}$$

- use the scheme element matrix $\widehat{\mathbb{A}}_K$ under Assumption B
- finite elements assembly:

$$\left\|\underline{\mathbf{K}}^{\frac{1}{2}}\nabla s_h\right\|_K^2 = \mathsf{S}_K{}^{\mathrm{t}}\widehat{\mathbb{S}}_{\mathrm{FE},K}\mathsf{S}_K;$$

- Green theorem:

$$\begin{aligned}(\mathbf{u}_h,\nabla s_h)_K &= \langle \mathbf{u}_h\cdot\mathbf{n}, s_h\rangle_{\partial K} - (\nabla\cdot\mathbf{u}_h, s_h)_K\\ &= (\mathsf{U}_K^{\mathrm{ext}})^{\mathrm{t}}\mathsf{S}_K^{\mathrm{ext}} - (\mathsf{F})_K|K|^{-1}\mathsf{1}^{\mathrm{t}}\widehat{\mathbb{M}}_{\mathrm{FE},K}\mathsf{S}_K\end{aligned}$$

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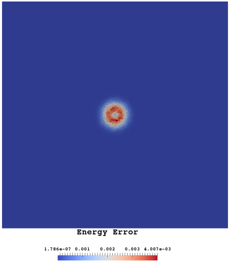
Outline

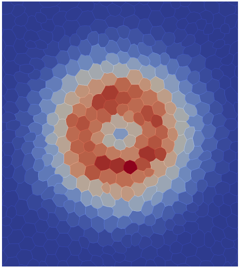
Numerical experiment

Setting

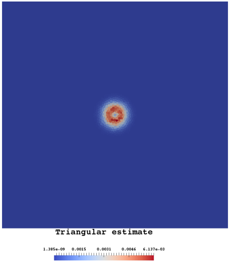
- $-\Delta p = f$
- $\Omega = (0, 1)^2$
- analytic solution $2^{4\alpha} x^\alpha (1 - x)^\alpha y^\alpha (1 - y)^\alpha$, $\alpha = 200$
- hybrid finite volume (HFV) discretization (Droniou, Eymard, Gallouët, Herbin (2010))

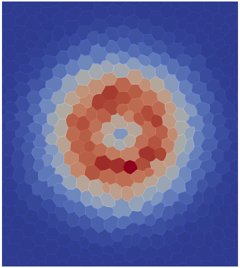
Energy error & reference estimate (triangular submesh)





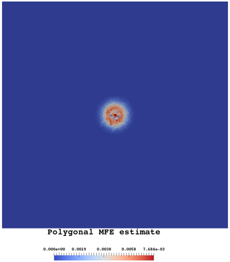
Energy error

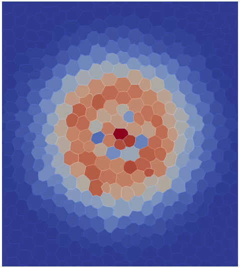




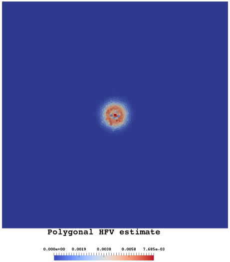
Estimate with s_h pw. quadratic over simplicial submesh (V. (2008))

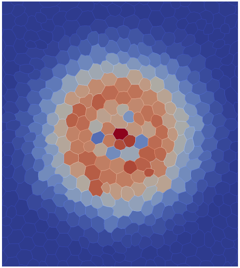
Simple polygonal estimates





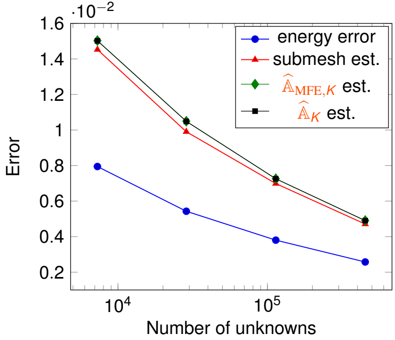
Using $\widehat{\mathbb{A}}_{\mathrm{MFE},K}$

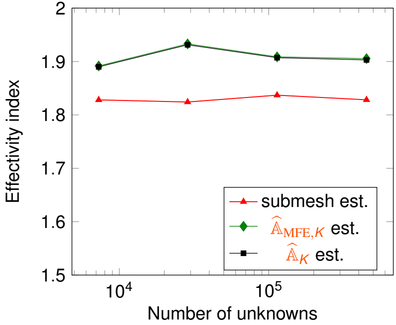




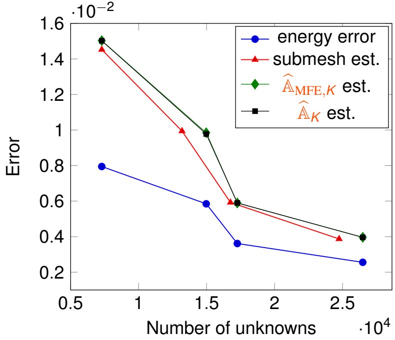
Using $\widehat{\mathbb{A}}_K$

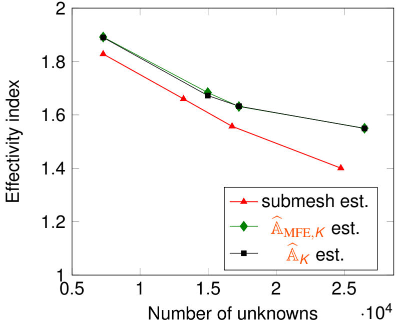
Uniform mesh refinement





Adaptive mesh refinement





Outline

Nonlinear Darcy flow

Steady nonlinear Darcy flow

$$-\nabla\cdot(\underline{\mathbf{K}}(\nabla p)\nabla p) = f \qquad \text{in } \Omega,$$

$$p = 0 \qquad \text{on } \partial\Omega.$$

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Assumptions

- invertible nonlinearity

$$\mathbf{v} = -\underline{\mathbf{K}}(\mathbf{w})\mathbf{w} \iff \mathbf{w} = -\underline{\tilde{\mathbf{K}}}(\mathbf{v})\mathbf{v}, \qquad \forall \mathbf{v}, \mathbf{w} \in \mathbb{R}^d$$

- strong monotonicity

$$c_{\underline{\tilde{\mathbf{K}}}}|\mathbf{v}-\mathbf{w}|^2 \leq (\mathbf{v}-\mathbf{w})\cdot(\underline{\tilde{\mathbf{K}}}(\mathbf{v})\mathbf{v} - \underline{\tilde{\mathbf{K}}}(\mathbf{w})\mathbf{w}), \qquad \forall \mathbf{v}, \mathbf{w} \in \mathbb{R}^d$$

- Lipschitz-continuity

$$|\underline{\tilde{\mathbf{K}}}(\mathbf{v})\mathbf{v} - \underline{\tilde{\mathbf{K}}}(\mathbf{w})\mathbf{w}| \leq C_{\underline{\tilde{\mathbf{K}}}}|\mathbf{v}-\mathbf{w}|, \qquad \forall \mathbf{v}, \mathbf{w} \in \mathbb{R}^d$$

- for simple matrix-vector multiplication:

$$c_{\underline{\tilde{\mathbf{K}}}}|\mathbf{v}|^2 \leq \mathbf{v}\cdot\underline{\tilde{\mathbf{K}}}(\mathbf{w})\mathbf{v}, \qquad |\underline{\tilde{\mathbf{K}}}(\mathbf{w})\mathbf{v}| \leq C_{\underline{\tilde{\mathbf{K}}}}|\mathbf{v}|, \qquad \forall \mathbf{v}, \mathbf{w} \in \mathbb{R}^d$$

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Steady nonlinear Darcy flow

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$$p = 0 \qquad \text{on } \partial\Omega.$$

Weak solution

$p \in H_0^1(\Omega)$ such that

$$(\underline{\mathbf{K}}(\nabla p)\nabla p, \nabla v) = (f, v) \qquad \forall v \in H_0^1(\Omega)$$

Darcy velocity

$$\mathbf{u} := -\underline{\mathbf{K}}(\nabla p)\nabla p \in \mathbf{H}(\mathrm{div}, \Omega)$$

Inverse relation

$$\nabla p = -\underline{\tilde{\mathbf{K}}}(\mathbf{u})\mathbf{u}$$

Outline

Discretization, linearization, and algebraic resolution

Discretization

$$\sum_{\sigma \in \mathcal{E}_K} (\mathrm{U}(\mathrm{P}))_\sigma \mathbf{n}_{K,\sigma} \cdot \mathbf{n}_\sigma = (\mathrm{F})_K \quad \forall K \in \mathcal{T}_H$$

- system of $|\mathcal{T}_H|$ **nonlinear** algebraic equations

Linearization (step $k \geq 1$)

$$\sum_{\sigma \in \mathcal{E}_K} (\mathrm{U}^{k-1}(\mathrm{P}^k))_\sigma \mathbf{n}_{K,\sigma} \cdot \mathbf{n}_\sigma = (\mathrm{F})_K \quad \forall K \in \mathcal{T}_H$$

- **linearized** face normal fluxes $\mathrm{U}^{k-1}(\mathrm{P}^k)$: affine fcts of P^k
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Algebraic resolution (step $i \geq 1$)

$$\sum_{\sigma \in \mathcal{E}_K} (\mathrm{U}^{k-1}(\mathrm{P}^{k,i}))_\sigma \mathbf{n}_{K,\sigma} \cdot \mathbf{n}_\sigma = (\mathrm{F})_K - (\mathrm{R})_K^{k,i} \quad \forall K \in \mathcal{T}_H$$

- $(\mathrm{R})^{k,i}$: **algebraic residual** vector
- $j \geq 1$ additional algebraic solver steps:

$$\sum_{\sigma \in \mathcal{E}_K} (\mathrm{U}^{k-1}(\mathrm{P}^{k,i+j}))_\sigma \mathbf{n}_{K,\sigma} \cdot \mathbf{n}_\sigma = (\mathrm{F})_K - (\mathrm{R})_K^{k,i+j} \quad \forall K \in \mathcal{T}_H$$

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Outline

Face fluxes

Discretization face normal flux

$$(\mathsf{U}_K^{k,i})_\sigma := (\mathsf{U}(\mathsf{P}^{k,i}))_\sigma$$

Linearization error face normal flux

$$(\mathsf{U}_{\mathrm{lin},K}^{k,i})_\sigma := (\mathsf{U}^{k-1}(\mathsf{P}^{k,i}))_\sigma - (\mathsf{U}(\mathsf{P}^{k,i}))_\sigma$$

Algebraic error face normal flux

$$(\mathsf{U}_{\mathrm{alg},K}^{k,i})_\sigma := (\mathsf{U}^{k-1}(\mathsf{P}^{k,i+j}))_\sigma - (\mathsf{U}^{k-1}(\mathsf{P}^{k,i}))_\sigma$$

One number per face **immediately available**
from the scheme on each step $k \geq 1$, $i \geq 1$.

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Nonlinear Darcy flow estimate

Theorem (Nonlinear Darcy flow)

Under Assumption A, there holds

$$c_{\underline{\tilde{\mathbf{K}}}}^{\frac{1}{2}} \left\| \mathbf{u} - \mathbf{u}_h^{k,i} \right\|_{L^2(\Omega)} \le \eta_{\mathrm{sp}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i} + \eta_{\mathrm{rem}}^{k,i}$$

with $\eta_{\bullet}^{k,i} = \left\{ \sum_{K \in \mathcal{T}_H} \left(\eta_{\bullet,K}^{k,i} \right)^2 \right\}^{\frac{1}{2}}$, $\bullet = \{\mathrm{sp}, \mathrm{lin}, \mathrm{alg}, \mathrm{rem}\}$, *and*

$$\left(\eta_{\mathrm{sp},K}^{k,i} \right)^2 := (\mathsf{U}_K^{k,i})^{\mathrm{t}} \widehat{\mathbb{A}}_{\mathrm{MFE},K} \mathsf{U}_K^{k,i} + (\mathsf{S}_K^{k,i})^{\mathrm{t}} \widehat{\mathbb{S}}_{\mathrm{FE},K} \mathsf{S}_K^{k,i} + 2 c_{\underline{\tilde{\mathbf{K}}}}^{-1} C_{\underline{\tilde{\mathbf{K}}}} \left[(\mathsf{U}_K^{k,i,\mathrm{ext}})^{\mathrm{t}} \mathsf{S}_K^{k,i,\mathrm{ext}} - (\mathsf{F})_K |K|^{-1} \mathsf{1}^{\mathrm{t}} \widehat{\mathbb{M}}_{\mathrm{FE},K} \mathsf{S}_K^{k,i} \right],$$

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Nonlinear Darcy flow estimate

Theorem (Nonlinear Darcy flow)

Under Assumption A, there holds

$$c_{\underline{\tilde{\mathbf{K}}}}^{\frac{1}{2}} \left\| \mathbf{u} - \mathbf{u}_h^{k,i} \right\|_{L^2(\Omega)} \le \eta_{\mathrm{sp}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i} + \eta_{\mathrm{rem}}^{k,i}$$

with $\eta_{\bullet}^{k,i} = \left\{ \sum_{K \in \mathcal{T}_H} \left(\eta_{\bullet,K}^{k,i} \right)^2 \right\}^{\frac{1}{2}}$, $\bullet = \{\mathrm{sp}, \mathrm{lin}, \mathrm{alg}, \mathrm{rem}\}$, *and*

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$$+ 2 c_{\underline{\tilde{\mathbf{K}}}}^{-1} C_{\underline{\tilde{\mathbf{K}}}} \left[(\mathsf{U}_K^{k,i,\mathrm{ext}})^{\mathrm{t}} \mathsf{S}_K^{k,i,\mathrm{ext}} - (\mathsf{F})_K |K|^{-1} \mathsf{1}^{\mathrm{t}} \widehat{\mathbb{M}}_{\mathrm{FE},K} \mathsf{S}_K^{k,i} \right],$$

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$$\left(\eta_{\mathrm{alg},K}^{k,i}\right)^2 := (\mathsf{U}_{\mathrm{alg},K}^{k,i})^{\mathrm{t}} \widehat{\mathbb{A}}_{\mathrm{MFE},K} \mathsf{U}_{\mathrm{alg},K}^{k,i},$$

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Nonlinear Darcy flow estimate

Comments

- **guaranteed upper bound** on the Darcy velocity error
- price: **matrix-vector multiplication** on each element
- $\mathbf{u}_h^{k,i}|_K$: discrete fictitious Darcy velocity on the submesh $\mathcal{T}_K$ (**linear** MFE local Neumann problem with matrix $\widehat{\mathbb{A}}_{\mathrm{MFE},K}$) (not constructed in practice)
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Some proof ingredients

- definition of $\mathbf{u}_h^{k,i}$: linear local Neumann problem

$$\mathbf{u}_h^{k,i}|_K := c_{\underline{\tilde{\mathbf{K}}}}^{-\frac{1}{2}} C_{\underline{\tilde{\mathbf{K}}}} \arg \min_{\mathbf{v}_h;\, \langle \mathbf{v}_h \cdot \mathbf{n}, 1\rangle_\sigma = (\mathrm{U}_K^{k,i})_\sigma,\ \nabla\cdot\mathbf{v}_h = \text{constant}} \|\mathbf{v}_h\|_K$$

- error structure: residual dual norm + distance to $H_0^1(\Omega)$

$$c_{\underline{\tilde{\mathbf{K}}}}^{\frac{1}{2}} \left\| \mathbf{u} - \mathbf{u}_h^{k,i} \right\|_{L^2(\Omega)} \leq c_{\underline{\tilde{\mathbf{K}}}}^{-\frac{1}{2}} \sup_{v \in H_0^1(\Omega),\ \|\underline{\mathbf{K}}(\nabla v)\nabla v\|_{L^2(\Omega)} = 1} (\mathbf{u} - \mathbf{u}_h^{k,i}, \nabla v)$$

$$+ c_{\underline{\tilde{\mathbf{K}}}}^{-\frac{1}{2}} \inf_{v \in H_0^1(\Omega)} \left\| \underline{\tilde{\mathbf{K}}}(\mathbf{u}_h^{k,i})\mathbf{u}_h^{k,i} + \nabla v \right\|_{L^2(\Omega)}$$

$$\leq 2 c_{\underline{\tilde{\mathbf{K}}}}^{-\frac{1}{2}} C_{\underline{\tilde{\mathbf{K}}}} \left\| \mathbf{u} - \mathbf{u}_h^{k,i} \right\|_{L^2(\Omega)}$$

- error components identification via fluxes:

$$\nabla\cdot\left(\mathbf{u}_h^{k,i} + \mathbf{u}_{\mathrm{lin},h}^{k,i} + \mathbf{u}_{\mathrm{alg},h}^{k,i}\right) = |K|^{-1} \sum_{\sigma \in \mathcal{E}_K} (\mathrm{U}^{k-1}(\mathrm{P}^{k,i+j}))_\sigma \mathbf{n}_{K,\sigma}\cdot\mathbf{n}_\sigma$$

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Outline

Multi-phase multi-compositional flows

Unknowns

- reference pressure P
- phase saturations $\mathbf{S} := (S_p)_{p\in\mathcal{P}}$
- component molar fractions $\mathbf{C}_p := (C_{p,c})_{c\in\mathcal{C}_p}$ of phase $p \in \mathcal{P}$

Constitutive laws

- phase pressure = reference pressure + capillary pressure

$$P_p := P + P_{c_p}(\mathbf{S})$$

- Darcy's law

$$\mathbf{v}_p(P_p) := -\underline{\mathbf{K}}(\nabla P_p + \rho_p g \nabla z)$$

- component fluxes

$$\theta_c := \sum_{p\in\mathcal{P}_c} \theta_{p,c}, \qquad \theta_{p,c} := \theta_{p,c}(\mathbf{X}) = \nu_p C_{p,c} \mathbf{v}_p(P_p)$$

- amount of moles of component c per unit volume

$$l_c = \phi \sum \zeta_p S_p C_{p,c}$$

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Multi-phase multi-compositional flows

Governing PDE

- conservation of mass for components

$$\partial_t l_c + \nabla\cdot\boldsymbol{\theta}_c = q_c, \qquad \forall c \in \mathcal{C}$$

- + boundary & initial conditions

Closure algebraic equations

- conservation of pore volume: $\sum_{p\in\mathcal{P}} S_p = 1$
- conservation of the quantity of the matter: $\sum_{c\in\mathcal{C}_p} C_{p,c} = 1$ for all $p \in \mathcal{P}$
- thermodynamic equilibrium (fugacity equations)

Mathematical issues

- coupled system PDE – algebraic constraints
- unsteady, nonlinear
- elliptic–degenerate parabolic type
- dominant advection

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Face fluxes

$$\mathbf{X}_{\mathcal{T}_H}^{n,k,i} := (\mathbf{X}_K^{n,k,i})_{K\in\mathcal{T}_H^n}, \mathbf{X}_K^{n,k,i} := \left(P_K^{n,k,i}, (S_{p,K}^{n,k,i})_{p\in\mathcal{P}}, (C_{p,c,K}^{n,k,i})_{p\in\mathcal{P},c\in\mathcal{C}_p}\right)$$

$$(\mathbf{U}_{K,p}^{n,k,i})_\sigma := \frac{t-t^{n-1}}{\tau^n} \sum_{K'\in\mathcal{S}_\sigma^L} \tau_{K'}^\sigma P_{p,K'}^{n,k,i} + \frac{t^n-t}{\tau^n} \sum_{K'\in\mathcal{S}_\sigma^L} \tau_{K'}^\sigma P_{p,K'}^{n-1},$$

$$(\Theta_{\mathrm{upw},K,c}^{n,k,i})_\sigma := \theta_{c,K,\sigma}(\mathbf{X}_{\mathcal{T}_H}^{n,k,i}) - \sum_{p\in\mathcal{P}_c} (\nu_{p,K}^{n,k,i} C_{p,c,K}^{n,k,i}) \theta_{p,K,\sigma}(\mathbf{X}_{\mathcal{T}_H}^{n,k,i}),$$

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One number per face **immediately available** from the scheme on each step $n \geq 1$, $k \geq 1$, $i \geq 1$.

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Estimators

spatial estimators

$$\eta^{n,k,i}_{\mathrm{sp},K,c} := \eta^{n,k,i}_{\mathrm{upw},K,c} + \left\{ \sum_{p\in\mathcal{P}_c} \left(\eta^{n,k,i}_{\mathrm{NC},K,c,p}\right)^2 \right\}^{\frac{1}{2}},$$

upwinding estimators

$$\left(\eta^{n,k,i}_{\mathrm{upw},K,c}\right)^2 := (\Theta^{n,k,i}_{\mathrm{upw},K,c})^{\mathrm{t}} \widehat{\mathbb{A}}_{\mathrm{MFE},K} (\Theta^{n,k,i}_{\mathrm{upw},K,c}),$$

nonconformity estimators

$$\left(\eta^{n,k,i}_{\mathrm{NC},K,c,p}\right)^2 := \left(\nu^{n,k,i}_{p,K} C^{n,k,i}_{p,c,K}\right)^2 \Big[(\mathsf{U}^{n,k,i}_{K,p})^{\mathrm{t}} \widehat{\mathbb{A}}_{\mathrm{MFE},K} \mathsf{U}^{n,k,i}_{K,p} + (\mathsf{S}^{n,k,i}_{K,p})^{\mathrm{t}} \widehat{\mathbb{S}}_{\mathrm{FE},K} \mathsf{S}^{n,k,i}_{K,p}$$

$$+2(\mathsf{U}^{n,k,i}_{K,p})^{\mathrm{t}} \mathsf{S}^{\mathrm{ext},n,k,i}_{K,p} - 2\textstyle\sum_{\sigma\in\mathcal{E}_K} (\mathsf{U}^{n,k,i}_{K,p})_\sigma |K|^{-1} 1^{\mathrm{t}} \widehat{\mathbb{M}}_{\mathrm{FE},K} \mathsf{S}^{n,k,i}_{K,p} \Big],$$

temporal estimators

$$\left(\eta^{n,k,i}_{\mathrm{tm},K,c}\right)^2 := (\Theta^{n,k,i}_{\mathrm{tm},K,c})^{\mathrm{t}} \widehat{\mathbb{A}}_{\mathrm{MFE},K} \Theta^{n,k,i}_{\mathrm{tm},K,c},$$

linearization estimators

$$\eta^{n,k,i}_{\mathrm{lin},K,c} := \{(\Theta^{n,k,i}_{\mathrm{lin},K,c})^{\mathrm{t}} \widehat{\mathbb{A}}_{\mathrm{MFE},K} \Theta^{n,k,i}_{\mathrm{lin},K,c}\}^{\frac{1}{2}} + h_K(\tau^n)^{-1} \left\| l_{c,K}(\mathbf{X}^{n,k,i}_K) - l^{n,k,i}_{c,K} \right\|_{L^2(K)},$$

algebraic estimators

$$\eta^{n,k,i}_{\mathrm{alg},K,c} := \{(\Theta^{n,k,i}_{\mathrm{alg},K,c})^{\mathrm{t}} \widehat{\mathbb{A}}_{\mathrm{MFE},K}\}^{\frac{1}{2}} \Theta^{n,k,i}_{\mathrm{alg},K,c} + h_K(\tau^n)^{-1} \left\| l^{n,k,i+j}_{c,K} - l^{n,k,i}_{c,K} \right\|_{L^2(K)},$$

algebraic remainder estimators

$$\eta^{n,k,i}_{\mathrm{rem},K,c} := \min\{C_{\mathrm{F}} h_\Omega c_{\underline{\mathbf{K}}}^{-\frac{1}{2}}, h_K\} |K|^{-\frac{1}{2}} |R^{n,k,i+j}_{c,K}|.$$

Multi-phase multi-compositional Darcy flow estimate

Theorem (Multi-phase multi-compositional Darcy flow)

Under Assumption A, there holds

$$\mathcal{N}^{n,k,i} \leq \left\{ \sum_{c\in\mathcal{C}} \left(\eta^{n,k,i}_{\mathrm{sp},c} + \eta^{n,k,i}_{\mathrm{tm},c} + \eta^{n,k,i}_{\mathrm{lin},c} + \eta^{n,k,i}_{\mathrm{alg},c} + \eta^{n,k,i}_{\mathrm{rem},c}\right)^2 \right\}^{\frac{1}{2}}$$

with $\eta^{n,k,i}_{\bullet,c} := \left\{ \delta_\bullet \int_{I_n} \sum_{K\in\mathcal{T}_H^n} \left(\eta^{n,k,i}_{\bullet,K,c}\right)^2 \mathrm{d}t \right\}^{\frac{1}{2}}$, $\bullet = \mathrm{sp}, \mathrm{tm}, \mathrm{lin}, \mathrm{alg}, \mathrm{rem}$, $\delta_\bullet = 2/4$.

Comments

- immediate extension of the results of the steady case
- still matrix-vector multiplication on each element
- same element matrices $\widehat{\mathbb{S}}_{\mathrm{FE},K}$, $\widehat{\mathbb{M}}_{\mathrm{FE},K}$, and $\widehat{\mathbb{A}}_{\mathrm{MFE},K}$ or $\widehat{\mathbb{A}}_K$
- input: normal face fluxes, reference pressure $P_K^{n,k,i}$, phase saturations $\boldsymbol{S}_K^{n,k,i}$, and component molar fractions $(\boldsymbol{C}_p)_K^{n,k,i}$
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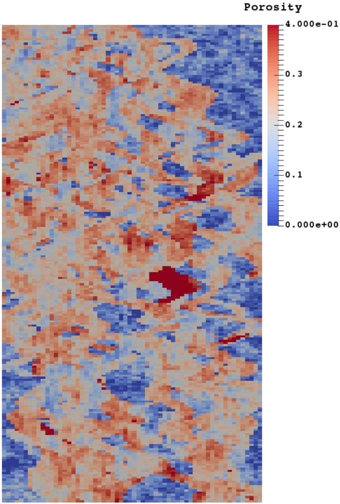
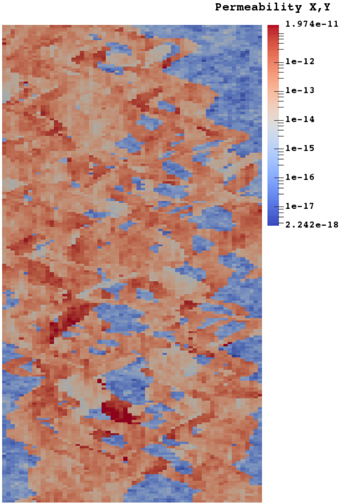
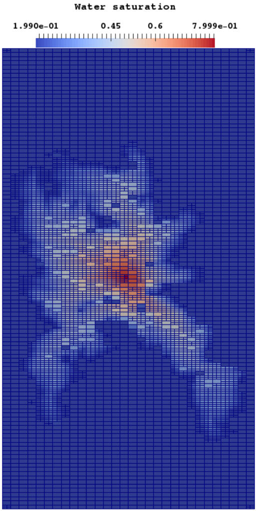
Outline

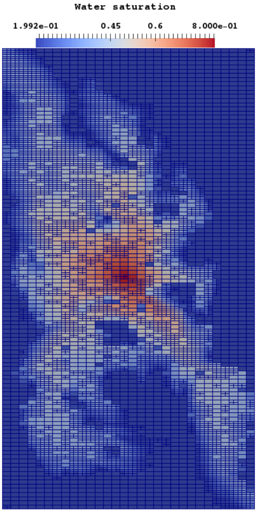
Two-phase flow: porosity & permeability (10th SPE)



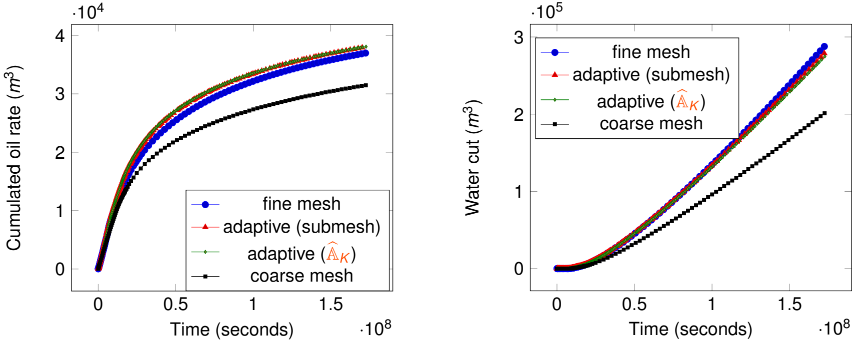


Two-phase flow: water saturation, adaptive mesh, 400 days and 1100 days



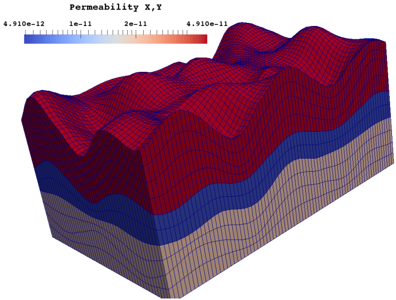


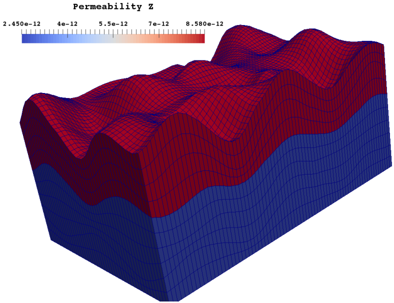
Two-phase flow: uniform vs adaptive mesh refinement



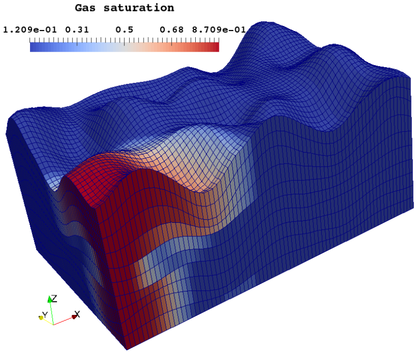
	Resolution	AMR	Estimators evaluation	Gain factor
Fine mesh	603s	-	-	-
Adaptive mesh	242s	46s	27s	1.9

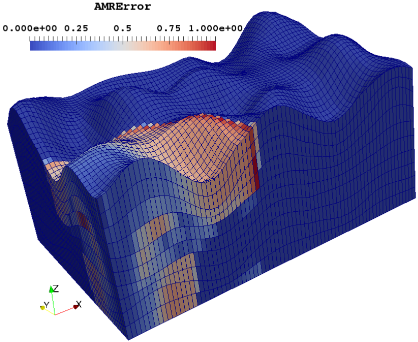
Three-phases, three-components (black-oil) problem: permeability



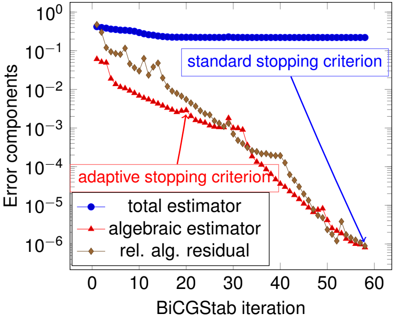


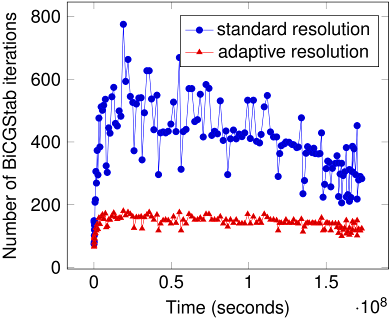
Three-phases, three-components (black-oil) problem: gas saturation and a posteriori estimate





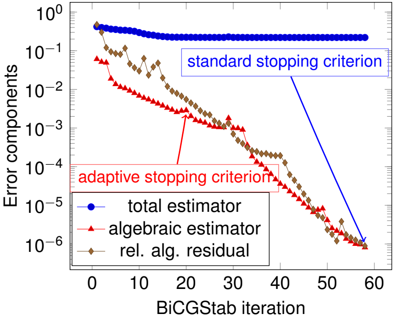
Three-phases, three-components (black-oil) problem: solver & mesh adaptivity

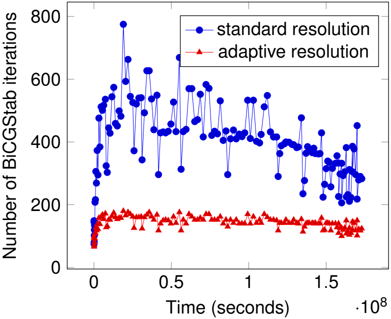




	Linear solver steps	Resolution time	AMR time	Estimators evaluation	Gain factor
Standard resolution	66386	1023s	-	-	-
Adaptive resolution	20184	201s	42s	26s	3.8

Three-phases, three-components (black-oil) problem: solver & mesh adaptivity





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- **simple** estimates on **polygonal/polyhedral meshes** (only matrix-vector multiplication in each element)
- a posteriori **error control**
- **full adaptivity**: linear solver, nonlinear solver, time step, space mesh

VOHRALÍK M., YOUSEF S., A simple a posteriori estimate on general polytopal meshes with applications to complex porous media flows, *Comput. Methods Appl. Mech. Engrg.* **331** (2018), 728–760.

Thank you for your attention!

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Two-phase flow in porous media

$$
\begin{aligned}
\partial_t(\phi s_\alpha) + \nabla\cdot\mathbf{u}_\alpha &= q_\alpha, & \alpha &\in \{\mathrm{o}, \mathrm{w}\},\\
-\lambda_\alpha(s_\mathrm{w})\underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha g \nabla z) &= \mathbf{u}_\alpha, & \alpha &\in \{\mathrm{o}, \mathrm{w}\},\\
s_\mathrm{o} + s_\mathrm{w} &= 1, & &\\
p_\mathrm{o} - p_\mathrm{w} &= p_\mathrm{c}(s_\mathrm{w}) & &
\end{aligned}
$$

+ boundary & initial conditions

Global pressure

$$\mathfrak{p}(s_{\rm w}, p_{\rm w}) := p_{\rm w} + \int_0^{s_{\rm w}} \frac{\lambda_{\rm o}(a)}{\lambda_{\rm w}(a) + \lambda_{\rm o}(a)} p_{\rm c}'(a) \mathrm{d}a$$

Complementary pressure

$$\mathfrak{q}(s_{\rm w}) := -\int_0^{s_{\rm w}} \frac{\lambda_{\rm w}(a)\lambda_{\rm o}(a)}{\lambda_{\rm w}(a) + \lambda_{\rm o}(a)} p_{\rm c}'(a) \mathrm{d}a$$

Comments

- necessary for the correct definition of the weak solution
- equivalent Darcy velocities expressions

$$\mathbf{u}_{\rm w}(s_{\rm w}, p_{\rm w}) := -\mathbf{K}(\lambda_{\rm w}(s_{\rm w})\nabla\mathfrak{p}(s_{\rm w}, p_{\rm w}) + \nabla\mathfrak{q}(s_{\rm w}) + \lambda_{\rm w}(s_{\rm w})\rho_{\rm w} g \nabla z),$$

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Two-phase flow: global and complementary pressures

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Energy space

$$X := L^2((0,T); H^1_{\mathrm{D}}(\Omega))$$

Definition (Weak solution (Arbogast 1992, Chen 2001))

Find $(s_{\mathrm{w}}, p_{\mathrm{w}})$ such that, with $s_{\mathrm{o}} := 1 - s_{\mathrm{w}}$,

$$s_{\mathrm{w}} \in C([0,T]; L^2(\Omega)), \; s_{\mathrm{w}}(\cdot, 0) = s^0_{\mathrm{w}},$$

$$\partial_t s_{\mathrm{w}} \in L^2((0,T); (H^1_{\mathrm{D}}(\Omega))'),$$

$$\mathfrak{p}(s_{\mathrm{w}}, p_{\mathrm{w}}) \in X,$$

$$\mathfrak{q}(s_{\mathrm{w}}) \in X,$$

$$\int_0^T \{\langle \partial_t(\phi s_\alpha), \varphi\rangle - (\mathbf{u}_\alpha(s_{\mathrm{w}}, p_{\mathrm{w}}), \nabla\varphi) - (q_\alpha, \varphi)\}\mathrm{d}t = 0$$

$$\forall \varphi \in X, \; \alpha \in \{\mathrm{o}, \mathrm{w}\}.$$

Two-phase flow: weak formulation

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$$\forall \varphi \in X, \; \alpha \in \{\mathrm{o}, \mathrm{w}\}.$$

Two-phase flow: error $\leftrightarrow$ dual norm of the residual

Dual norm of the residual on the time interval I_n

$$\mathcal{J}^n_{s_{\rm w},p_{\rm w}}(s_{{\rm w},h\tau},p_{{\rm w},h\tau}) := \left\{ \sum_{\alpha\in\{{\rm o},{\rm w}\}} \left\{ \sup_{\varphi\in X_n,\, \|\varphi\|_{X_n}=1} \int_{I_n} \{ \langle \partial_t(\phi s_\alpha) - \partial_t(\phi s_{\alpha,h\tau}), \varphi\rangle - (\mathbf{u}_\alpha(s_{\rm w},p_{\rm w}) - \mathbf{u}_\alpha(s_{{\rm w},h\tau},p_{{\rm w},h\tau}), \nabla\varphi)\} {\rm d}t \right\}^2 \right\}^{\frac{1}{2}}$$

Theorem (Link energy-type error – dual norm of the residual)

Let $(s_{\rm w},p_{\rm w})$ be the weak solution. Let $(s_{{\rm w},h\tau},p_{{\rm w},h\tau})$ be arbitrary such that $\mathfrak{p}(s_{{\rm w},h\tau},p_{{\rm w},h\tau}) \in X$ and $\mathfrak{q}(s_{{\rm w},h\tau}) \in X$ (and satisfying the initial and boundary conditions for simplicity). Then

$$\|s_{\rm w} - s_{{\rm w},h\tau}\|_{L^2((0,T);H^{-1}(\Omega))} + \|\mathfrak{q}(s_{\rm w}) - \mathfrak{q}(s_{{\rm w},h\tau})\|_{L^2(\Omega\times(0,T))} + \|\mathfrak{p}(s_{\rm w},p_{\rm w}) - \mathfrak{p}(s_{{\rm w},h\tau},p_{{\rm w},h\tau})\|_{L^2((0,T);H^1_0(\Omega))} \le C\left\{\sum_{n=1}^N \mathcal{J}^n_{s_{\rm w},p_{\rm w}}(s_{{\rm w},h\tau},p_{{\rm w},h\tau})^2\right\}^{\frac{1}{2}}$$

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Multi-phase multi-compositional flow: weak solution

Function spaces

$$X := L^2((0, t_{\mathrm{F}}); H^1(\Omega)),$$
$$Y := H^1((0, t_{\mathrm{F}}); L^2(\Omega))$$

Weak solution – we assume that

$l_c \in Y \qquad \forall c \in \mathcal{C},$

$P_p(P, \boldsymbol{S}) \in X \qquad \forall p \in \mathcal{P},$

$\boldsymbol{\theta}_c \in [L^2((0, t_{\mathrm{F}}); L^2(\Omega))]^d \qquad \forall c \in \mathcal{C},$

$$\int_0^{t_{\mathrm{F}}} \{(\partial_t l_c, \varphi) - (\boldsymbol{\theta}_c, \nabla\varphi)\}\,\mathrm{d}t = \int_0^{t_{\mathrm{F}}} (q_c, \varphi)\mathrm{d}t \qquad \forall \varphi \in X, \forall c \in \mathcal{C},$$

the initial condition holds,

the algebraic closure equations hold

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the initial condition holds,

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Multi-phase multi-compositional flow: error measure

Localized space

$X^n := L^2(I_n; H^1(\Omega))$ with

$$\|\varphi\|_{X^n}^2 := \int_{I_n} \sum_{K \in \mathcal{T}_H^n} \left\{ h_K^{-2} \|\varphi\|_{L^2(K)}^2 + \left\| \underline{\mathbf{K}}^{\frac{1}{2}} \nabla \varphi \right\|_{L^2(K)}^2 \right\} \mathrm{d}t$$

Localized error measure

$$\mathcal{N}^{n,k,i} := \left\{ \sum_{c \in \mathcal{C}} (\mathcal{N}_c^{n,k,i})^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{p \in \mathcal{P}} (\mathcal{N}_p^{n,k,i})^2 \right\}^{\frac{1}{2}},$$

where

$$\mathcal{N}_c^{n,k,i} := \sup_{\varphi \in X^n, \|\varphi\|_{X^n}=1} \int_{I_n} \left\{ (\partial_t l_c - \partial_t l_{c,h\tau}^{n,k,i}, \varphi) - \left(\boldsymbol{\theta}_c - \boldsymbol{\theta}_{c,h\tau}^{n,k,i}, \nabla \varphi \right) \right\} \mathrm{d}t$$

and

$$\mathcal{N}_p^{n,k,i} := \inf_{\delta_p \in X^n} \left\{ \sum_{c \in \mathcal{C}_p} \int_{I_n} \left\{ \sum_{K \in \mathcal{T}_H^n} \left(\nu_{p,K}^{n,k,i} C_{p,c,K}^{n,k,i} \right)^2 \left\| \mathbf{u}_{p,h\tau}^{n,k,i} + \underline{\mathbf{K}} \nabla \delta_p \right\|_{\underline{\mathbf{K}}^{-\frac{1}{2}};L^2(K)}^2 \right.\right.$$

Multi-phase multi-compositional flow: error measure

Localized space

$X^n := L^2(I_n; H^1(\Omega))$ with

$$\|\varphi\|_{X^n}^2 := \int_{I_n} \sum_{K\in\mathcal{T}_H^n} \left\{ h_K^{-2} \|\varphi\|_{L^2(K)}^2 + \left\| \underline{\mathbf{K}}^{\frac{1}{2}} \nabla\varphi \right\|_{L^2(K)}^2 \right\} \mathrm{d}t$$

Localized error measure

$$\mathcal{N}^{n,k,i} := \left\{ \sum_{c\in\mathcal{C}} (\mathcal{N}_c^{n,k,i})^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{p\in\mathcal{P}} (\mathcal{N}_p^{n,k,i})^2 \right\}^{\frac{1}{2}},$$

where

$$\mathcal{N}_c^{n,k,i} := \sup_{\varphi\in X^n, \|\varphi\|_{X^n}=1} \int_{I_n} \left\{ (\partial_t l_c - \partial_t l_{c,h\tau}^{n,k,i}, \varphi) - \left(\boldsymbol{\theta}_c - \boldsymbol{\theta}_{c,h\tau}^{n,k,i}, \nabla\varphi \right) \right\} \mathrm{d}t$$

and

$$\mathcal{N}_p^{n,k,i} := \inf_{\delta_p\in X^n} \left\{ \sum_{c\in\mathcal{C}_p} \int_{I_n} \left\{ \sum_{K\in\mathcal{T}_H^n} \left(\nu_{p,K}^{n,k,i} C_{p,c,K}^{n,k,i} \right)^2 \left\| \mathbf{u}_{p,h\tau}^{n,k,i} + \underline{\mathbf{K}}\nabla\delta_p \right\|_{\underline{\mathbf{K}}^{-\frac{1}{2}};L^2(K)}^2 \right.\right.$$

Fully adaptive algorithm

Set $n := 0$.
while $t^n \leq t_F$ **do** {Time}
  Set $n := n + 1$.
  loop {Spatial and temporal errors balancing}
    Set $k := 0$.
    loop {Newton linearization}
      Set $k := k + 1$; set up the linear system; set $i := 0$.
      loop {Algebraic solver}
        Perform an algebraic solver step; set $i := i + 1$; evaluate the estimators.
        Terminate (algebraic solver) if $\eta_{\mathrm{alg,t}}^{n,k,i} \leq \gamma_{\mathrm{alg}} \eta_{\mathrm{sp,t}}^{n,k,i}$.
      end loop
      Terminate (Newton linearization) if $\eta_{\mathrm{lin,t}}^{n,k,i} \leq \gamma_{\mathrm{lin}} \eta_{\mathrm{sp,t}}^{n,k,i}$.
    end loop
    Terminate (spatial & temporal errors balancing) if

$$\eta_{\mathrm{sp},K,\mathrm{t}}^{n,k,i} \geq \zeta_{\mathrm{ref}} \max_{K' \in \mathcal{T}_H^n} \left\{ \eta_{\mathrm{sp},K',\mathrm{t}}^{n,k,i} \right\} \qquad \forall K \in \mathcal{T}_H^n,$$

$$\gamma_{\mathrm{tm}} \left(\eta_{\mathrm{sp,t}}^{n,k,i} \right) \leq \eta_{\mathrm{tm,t}}^{n,k,i} \leq \Gamma_{\mathrm{tm}} \left(\eta_{\mathrm{sp,t}}^{n,k,i} \right);$$

    else refine the cells $K \in \mathcal{T}_H^n$ such that $\eta_{\mathrm{sp},K,\mathrm{t}}^{n,k,i} \geq \zeta_{\mathrm{ref}} \max_{K' \in \mathcal{T}_H^n} \left\{ \eta_{\mathrm{sp},K',\mathrm{t}}^{n,k,i} \right\}$.
    Derefine the cells $K \in \mathcal{T}_H^n$ such that $\eta_{\mathrm{sp},K,\mathrm{t}}^{n,k,i} \leq \zeta_{\mathrm{deref}} \max_{K' \in \mathcal{T}_H^n} \left\{ \eta_{\mathrm{sp},K',\mathrm{t}}^{n,k,i} \right\}$.
    Refine I_n if $\eta_{\mathrm{tm,t}}^{n,k,i} > \Gamma_{\mathrm{tm}} \eta_{\mathrm{sp,t}}^{n,k,i}$, derefine if $\gamma_{\mathrm{tm}} \eta_{\mathrm{sp,t}}^{n,k,i} > \eta_{\mathrm{tm,t}}^{n,k,i}$.
  end loop
end while