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

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# Outline

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# Context and goals

**General polygonal/polyhedral meshes**

- appealing in practice, growing mathematical background
  - mimetic finite differences (Brezzi, Lipnikov, Shashkov, Beirão da Veiga, Manzini . . . )
  - finite volumes (Droniou, Eymard, Gallouët, Herbin, . . . )
  - MPFAs (Aavatsmark, Eigestad, Klausen, Wheeler, Yotov)
  - virtual elements (B. da Veiga, Brezzi, Marini, Russo . . . )
  - HHO/HDG discretizations (Cockburn, Di Pietro, Ern . . . )
  - mixed finite elements (Kuznetsov, Repin, Jaffré, Roberts, Vohralík, Wohlmuth . . . )

**A posteriori error control and adaptivity**

- computable a posteriori error estimates on $\left\| \mathbf{u}|_{I_n} - \mathbf{u}_h^{n,k,i} \right\|$
- valid on each step: time $n$, linearization $k$, linear solver $i$
- distinguishing different error components: full adaptivity

**Goals**

- **simple** estimates on **polygonal/polyhedral meshes**: easy coding, fast evaluation, use in practical simulations

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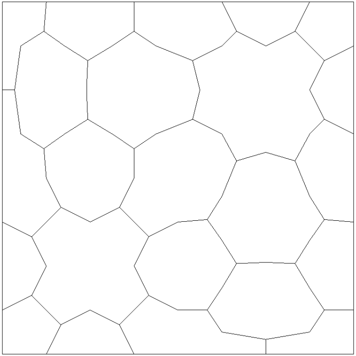
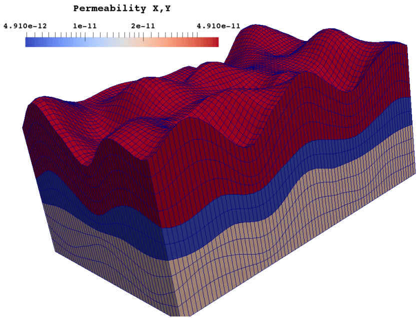
# General polygonal/polyhedral meshes

## A general polygonal/polyhedral mesh $\mathcal{T}_H$






- nonconvex and possibly non star-shaped elements in $\mathcal{T}_H$
- $\mathcal{T}_H$ can be nonmatching
- maximal number of sides of $K \in \mathcal{T}_H$ in principle not limited
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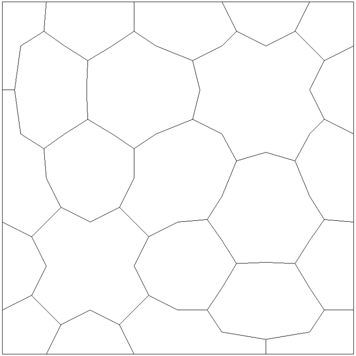

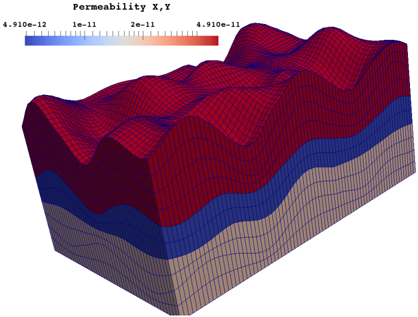


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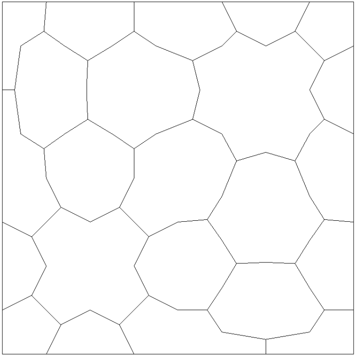

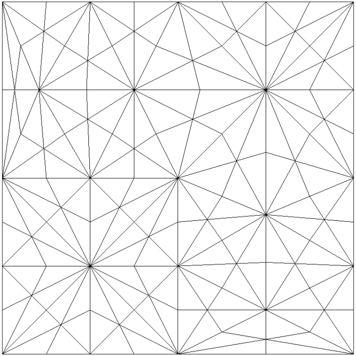

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# Linear Darcy flow

**Steady linear Darcy flow**

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

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ polygon/polyhedron
- $f \in L^2(\Omega)$ 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

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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

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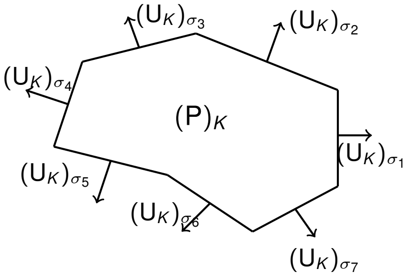


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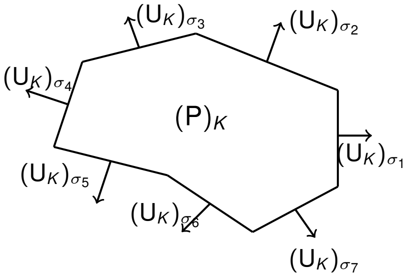


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# Saddle-point discretizations

## 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, MFEs ...

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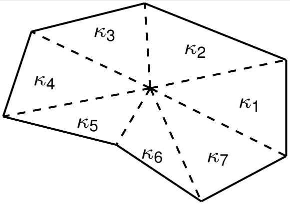


- finite element stiffness matrix

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

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- mixed finite element local static condensation matrix

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

  - obtained by local Neumann MFE problem in the polytope $K$
  - MFEs on general polytopal meshes (Vohralík & Wohlmuth (2013))
- under Assumption B, $\widehat{\mathbb{A}}_K$ can be used in place of $\widehat{\mathbb{A}}_{\mathrm{MFE},K}$

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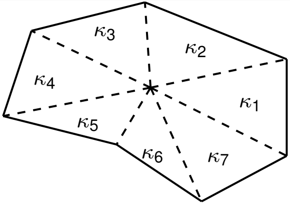


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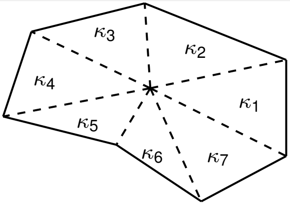


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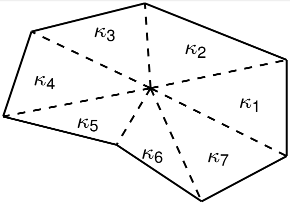


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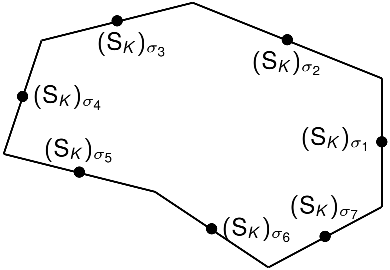


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- Assumption A: $(S_K)_{\sigma_i}$ local averages of neighbor $(P)_{K'}$

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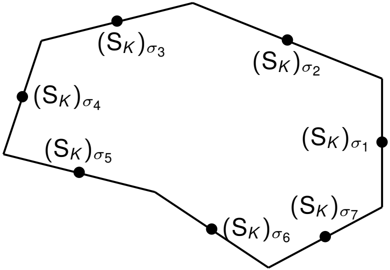


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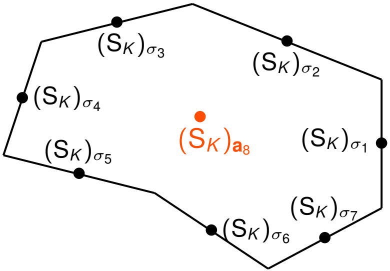


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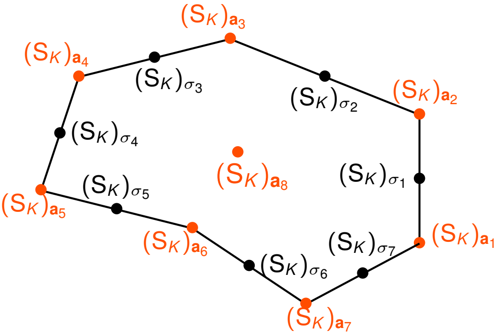


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- $(S_K)_{a_8} := (P)_K$
- $S_K = \{(S_K)_{a_i}\}_{i=1}^{7}$ constructed by local averaging

# 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*

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

**Comments**

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

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

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

- $\mathbf{u}_h|_K$ not constructed in practice, unless in the test cases

# Linear Darcy flow estimate

## Corollary (Linear Darcy flow)

*Under Assumption B, there holds*

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

*where*

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

**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 $K$)
- 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-type argument:

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

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

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

- choose $s_h$ continuous and piecewise affine wrt $\mathcal{T}_h$, given by the nodal values of the vector $S$
- 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)

- Vohralík & 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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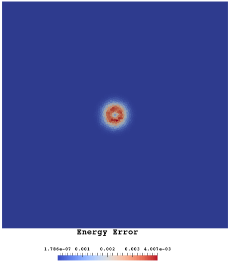
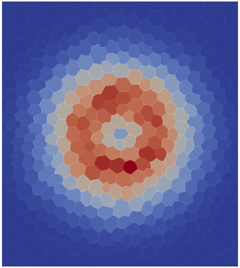
# Numerical experiment

**Setting**

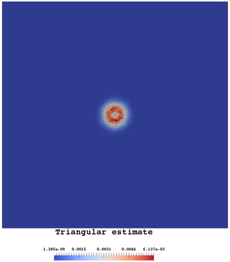
- $-\Delta p = f$
- $\Omega = (0, 1)^2$
- analytic solution $2^{4\alpha} x^\alpha (1-x)^\alpha y^\alpha (1-y)^\alpha$, $\alpha = 200$
- hybrid finite volume (HFV) discretization (Droniou, Eymard, Gallouët, Herbin (2010))

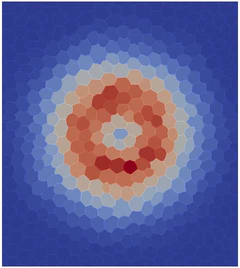
# Energy error and optimal estimate on triangles



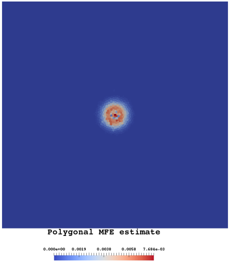
Energy error

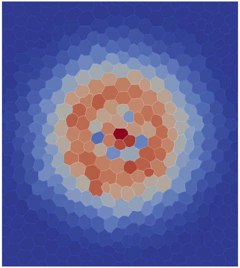


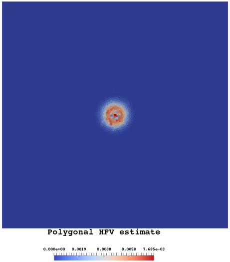
Estimate with $s_h$ pw. quadratic over $\mathcal{T}_h$ (Vohralík (2008))

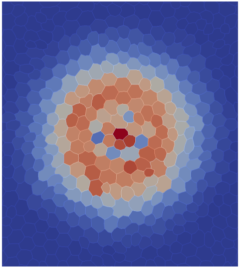
# Simple polygonal estimates



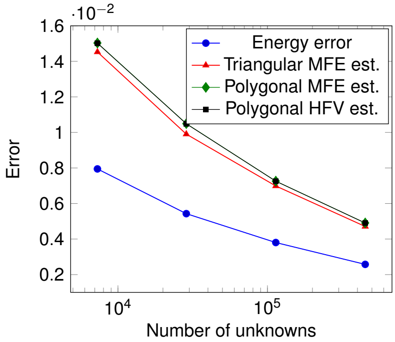
Using $\widehat{\mathbb{A}}_{\mathrm{MFE},K}$



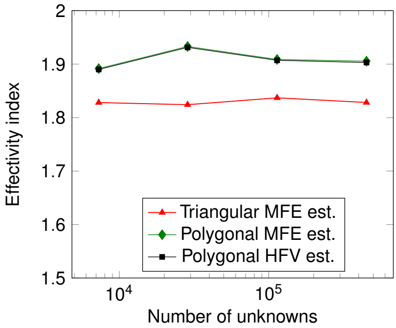



Using $\widehat{\mathbb{A}}_{K}$

# Uniform mesh refinement

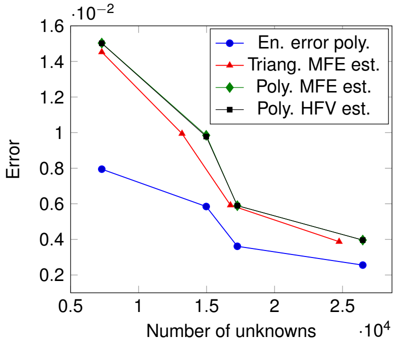



Error and estimators




Effectivity indices

# Adaptive mesh refinement

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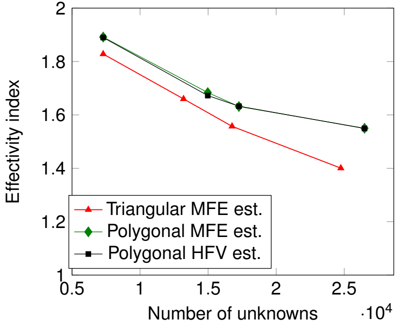


Effectivity indices

# Outline

# Nonlinear Darcy flow

**Steady nonlinear Darcy flow**

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

# Nonlinear Darcy flow

**Steady nonlinear Darcy flow**

$$-\nabla\cdot(\underline{\mathbf{K}}(\nabla p)\nabla p) = f \qquad \text{in } \Omega,$$
$$p = 0 \qquad \text{on } \partial\Omega.$$

**Assumptions**

- invertible nonlinearity

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

- strong monotonicity

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

- Lipschitz-continuity

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

- for simple matrix-vector multiplication:

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

# Nonlinear Darcy flow

**Steady nonlinear Darcy flow**

$$-\nabla\cdot(\underline{\mathbf{K}}(\nabla p)\nabla p) = f \quad \text{in } \Omega,$$
$$p = 0 \quad \text{on } \partial\Omega.$$

**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**

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

# Discretization, linearization, and algebraic resolution

**Discretization**

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

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

**Linearization** (step $k\geq 1$)

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

- linearized face normal fluxes $\mathsf{U}^{k-1}(\mathsf{P}^k)$: affine fcts of $\mathsf{P}^k$
- system of $|\mathcal{T}_H|$ linear algebraic equations

**Algebraic resolution**

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

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

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

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# Face fluxes

**Discretization face normal flux**

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

**Linearization error face normal flux**

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

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

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

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# Nonlinear Darcy flow estimate

## Theorem (Nonlinear Darcy flow)

*Under Assumption A, there holds*

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

*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*

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

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

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

$$\eta_{\mathrm{rem},K}^{k,i} := c_{\underline{\tilde{\mathbf{K}}}}^{-\frac{1}{2}} C_{\underline{\tilde{\mathbf{K}}}} C_{\mathrm{F}} h_\Omega |K|^{-\frac{1}{2}} |(\mathsf{R})_K^{k,i+j}|.$$

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

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

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

$$\eta_{\mathrm{rem},K}^{k,i} := c_{\underline{\tilde{\mathbf{K}}}}^{-\frac{1}{2}} C_{\underline{\tilde{\mathbf{K}}}} C_{\mathrm{F}} h_\Omega |K|^{-\frac{1}{2}} |(\mathsf{R})_K^{k,i+j}|.$$

# Nonlinear Darcy flow estimate

## Theorem (Nonlinear Darcy flow)

*Under Assumption A, there holds*

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

*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*

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

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

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

$$\eta_{\mathrm{rem},K}^{k,i} := c_{\underline{\tilde{\mathbf{K}}}}^{-\frac{1}{2}} C_{\underline{\tilde{\mathbf{K}}}} C_{\mathrm{F}} h_{\Omega} |K|^{-\frac{1}{2}} |(\mathsf{R})_K^{k,i+j}|.$$

# Nonlinear Darcy flow estimate

**Comments**

- guaranteed upper bound on the Darcy velocity error
- price: matrix-vector multiplication on each element
- **error components distinction**
- $\mathbf{u}_h^{k,i}|_K$: 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)

# Some proof ingredients

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

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

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

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

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

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

- error components identification via fluxes:

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

$$= f|_K - |K|^{-1} (\mathrm{R})_K^{k,i+j} \quad \forall K \in \mathcal{T}_H$$

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# Outline

# Multi-phase multi-compositional flows

## Unknowns

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

## Constitutive laws

- phase pressure = reference pressure + capillary pressure

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

- 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

$$l_c = \phi \sum_{p\in\mathcal{P}_c} \zeta_p S_p C_{p,c}$$

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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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# 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

$$l_c \in Y \qquad \forall c \in \mathcal{C},$$
$$P_p(P,\mathbf{S}) \in X \qquad \forall p \in \mathcal{P},$$
$$\boldsymbol{\theta}_c \in [L^2((0,t_{\mathrm{F}});L^2(\Omega))]^d \qquad \forall c \in \mathcal{C},$$
$$\int_0^{t_{\mathrm{F}}} \{(\partial_t l_c,\varphi) - (\boldsymbol{\theta}_c,\nabla\varphi)\}\,\mathrm{d}t = \int_0^{t_{\mathrm{F}}} (q_c,\varphi)\mathrm{d}t \qquad \forall \varphi \in X,\ \forall c \in \mathcal{C},$$

the initial condition holds,

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the initial condition holds,

the algebraic closure equations hold

# 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

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

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**Localized error measure**

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# Face fluxes

$$(\mathrm{U}^{n,k,i}_{K,p})_\sigma := \frac{t-t^{n-1}}{\tau^n}\sum_{K'\in\mathcal{S}^L_\sigma}\tau^\sigma_{K'}P^{n,k,i}_{p,K'} + \frac{t^n-t}{\tau^n}\sum_{K'\in\mathcal{S}^L_\sigma}\tau^\sigma_{K'}P^{n-1}_{p,K'},$$

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

$$(\Theta^{n,k,i}_{\mathrm{tm},K,c})_\sigma := \frac{t^n-t}{\tau^n}\sum_{p\in\mathcal{P}_c}\left[\nu^{n,k,i}_{p,K}C^{n,k,i}_{p,c,K}\theta_{p,K,\sigma}(\mathbf{X}^{n,k,i}_{\mathcal{T}_H}) - \nu^{n-1}_{p,K}C^{n-1}_{p,c,K}\theta_{p,K,\sigma}(\mathbf{X}^{n-1}_{\mathcal{T}_H})\right],$$

$$(\Theta^{n,k,i}_{\mathrm{lin},K,c})_\sigma := \theta^{n,k,i}_{c,K,\sigma} - \theta_{c,K,\sigma}(\mathbf{X}^{n,k,i}_{\mathcal{T}_H}),$$

$$(\Theta^{n,k,i}_{\mathrm{alg},K,c})_\sigma := \theta^{n,k,i+j}_{c,K,\sigma} - \theta^{n,k,i}_{c,K,\sigma}$$

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

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

$$(\Theta^{n,k,i}_{\mathrm{tm},K,c})_\sigma := \frac{t^n - t}{\tau^n} \sum_{p\in\mathcal{P}_c} \left[\nu^{n,k,i}_{p,K} C^{n,k,i}_{p,c,K}\theta_{p,K,\sigma}(\mathbf{X}^{n,k,i}_{\mathcal{T}_H}) - \nu^{n-1}_{p,K} C^{n-1}_{p,c,K}\theta_{p,K,\sigma}(\mathbf{X}^{n-1}_{\mathcal{T}_H})\right],$$

$$(\Theta^{n,k,i}_{\mathrm{lin},K,c})_\sigma := \theta^{n,k,i}_{c,K,\sigma} - \theta_{c,K,\sigma}(\mathbf{X}^{n,k,i}_{\mathcal{T}_H}),$$

$$(\Theta^{n,k,i}_{\mathrm{alg},K,c})_\sigma := \theta^{n,k,i+j}_{c,K,\sigma} - \theta^{n,k,i}_{c,K,\sigma}$$

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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

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

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

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*

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

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

## 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 $(\boldsymbol{C}_p)_K^{n,k,i}$
- same physical units of estimators of all error components
- naturally relative stopping criteria

# Multi-phase multi-compositional Darcy flow estimate

## Theorem (Multi-phase multi-compositional Darcy flow)

*Under Assumption A, there holds*

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

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

**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 $(\boldsymbol{C}_p)_K^{n,k,i}$
- same physical units of estimators of all error components
- naturally relative stopping criteria

# Fully adaptive algorithm

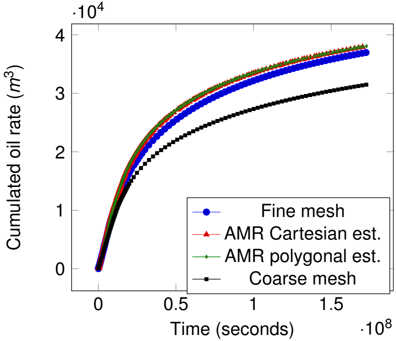
Set $n := 0$.
**while** $t^n \leq t_{\mathrm{F}}$ **do** {Time}
  Set $n := n + 1$.
  **loop** {Spatial and temporal errors balancing}
    Set $k := 0$.
    **loop** {Newton linearization}
      Set $k := k + 1$; set up the linear system; set $i := 0$.
      **loop** {Algebraic solver}
        Perform 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**

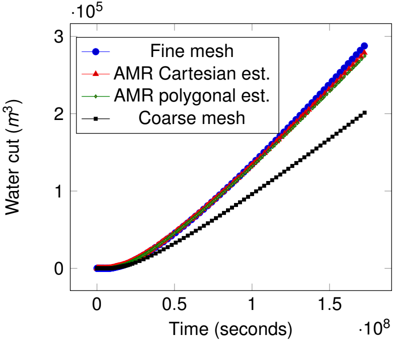
$$\eta_{\mathrm{sp},K,\mathrm{t}}^{n,k,i} \geq \zeta_{\mathrm{ref}} \max_{K' \in \mathcal{T}_H^n} \left\{ \eta_{\mathrm{sp},K',\mathrm{t}}^{n,k,i} \right\} \qquad \forall K \in \mathcal{T}_H^n,$$

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

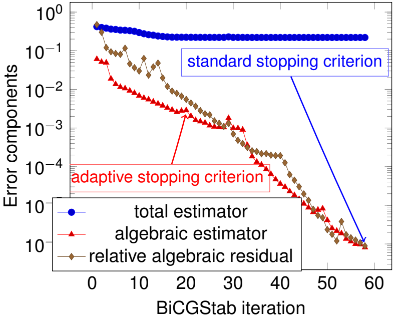
    **else** refine the cells $K \in \mathcal{T}_H^n$ such that $\eta_{\mathrm{sp},K,\mathrm{t}}^{n,k,i} \geq \zeta_{\mathrm{ref}} \max_{K' \in \mathcal{T}_H^n} \left\{ \eta_{\mathrm{sp},K',\mathrm{t}}^{n,k,i} \right\}$.
    Derefine the cells $K \in \mathcal{T}_H^n$ such that $\eta_{\mathrm{sp},K,\mathrm{t}}^{n,k,i} \leq \zeta_{\mathrm{deref}} \max_{K' \in \mathcal{T}_H^n} \left\{ \eta_{\mathrm{sp},K',\mathrm{t}}^{n,k,i} \right\}$.
    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**

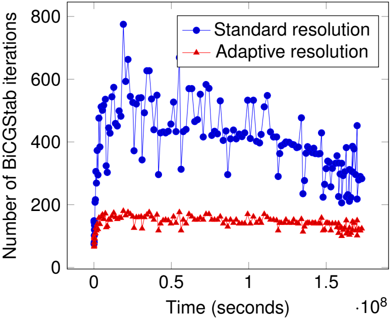
# Two-phase flow: uniform vs adaptive mesh refinement



# 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 |

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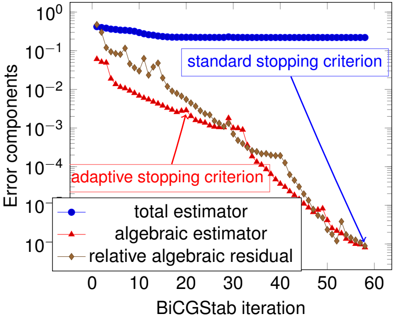


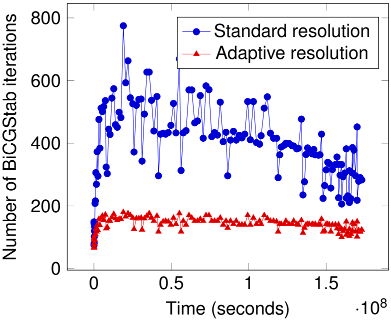


| | Linear solver steps | Resolution time | AMR time | Estimators evaluation | Gain factor |
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# Three-phases, three-components (black-oil) problem

movie

# Outline

# Conclusions

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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, HAL Preprint 01532195, submitted for publication.

**Merci de votre attention !**

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