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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1. Introduction
   - Energy a posteriori error estimates – quick state of the art
   - Context and goals of the talk
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

Laplace equation $-\Delta p = f$ in Ω, $p = 0$ on $\partial\Omega$, f pw pol.

Guaranteed bounds for $p_h \in \mathbb{P}_m(\mathcal{T}_h) \cap H_0^1(\Omega)$

Equilibrated flux rec. $p_h \to \boldsymbol{\sigma}_h \in \mathbf{RTN}_m(\mathcal{T}_h) \cap \mathbf{H}(\mathrm{div}, \Omega)$, $\nabla \cdot \boldsymbol{\sigma}_h = f$

$$\|\nabla(p - p_h)\| \leq \|\nabla p_h + \boldsymbol{\sigma}_h\|$$

- Prager & Synge (1947), Ladevèze (1975), Destuynder & Métivet (1999), Luce & Wohlmuth (2004), Braess & Schöberl (2008); Ainsworth & Oden (2000), Verfürth (2013)

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$$\|\nabla(p - p_h)\|^2 \leq \|\nabla p_h + \boldsymbol{\sigma}_h\|^2 + \|\nabla(p_h - s_h)\|^2$$

- Dari, Durán, Padra, & Vampa (1996), Ainsworth (2005), Kim (2007), V. (2007) ...

Robustness wrt pol. degree m: $\eta_K(p_h) \leq C(\mathcal{T}_h) \|\nabla(p - p_h)\|_{\omega_K}$

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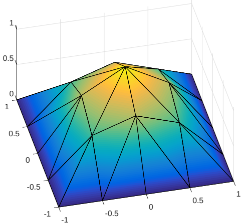
Equilibrated flux reconstruction $\boldsymbol{\sigma}_h$



Pressure $p_h \in \mathbb{P}_1(\mathcal{T}_h) \cap H_0^1(\Omega)$

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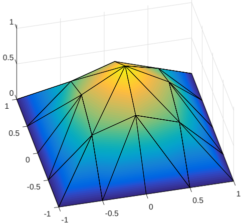

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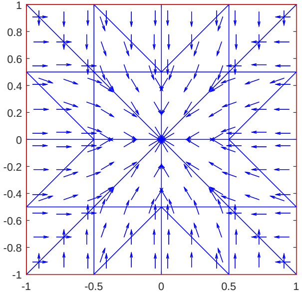

Flux $-\nabla p_h \notin \mathbf{H}(\mathrm{div}, \Omega)$

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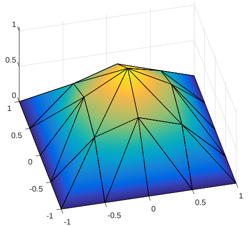

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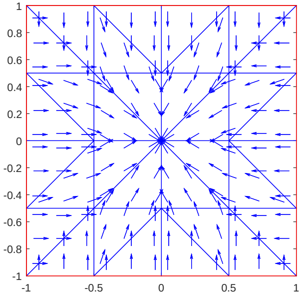

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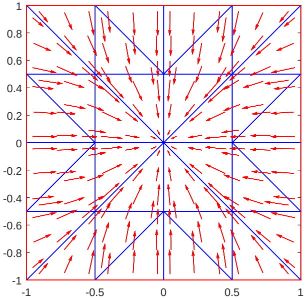
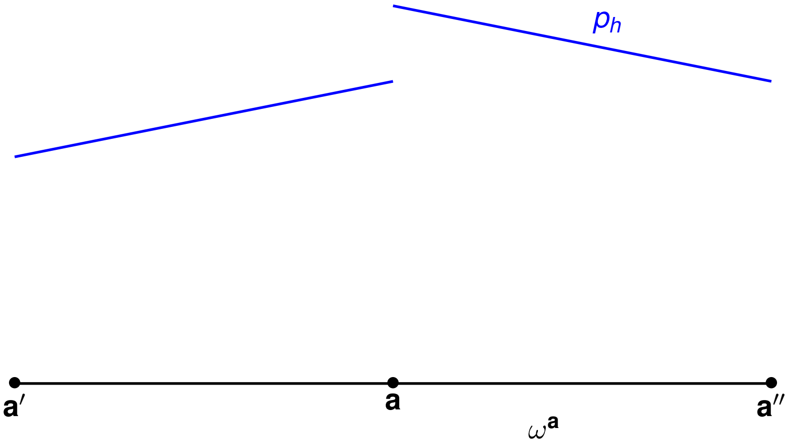


Flux rec. $\boldsymbol{\sigma}_h \in \mathbf{RTN}_1(\mathcal{T}_h) \cap \mathbf{H}(\mathrm{div}, \Omega)$

Pressure reconstruction s_h in 1D



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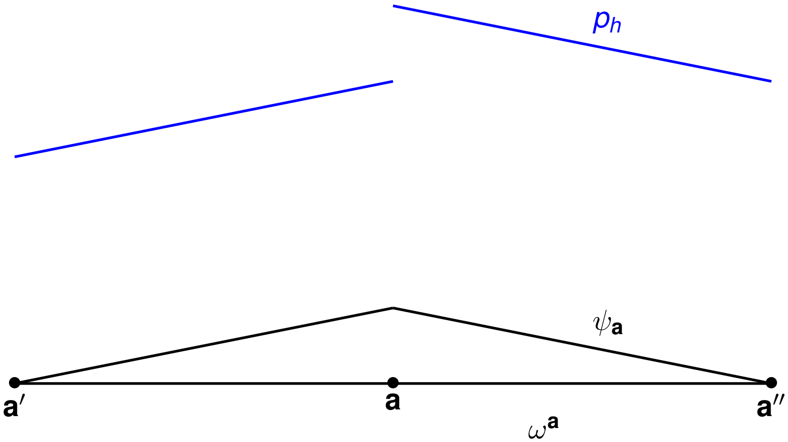

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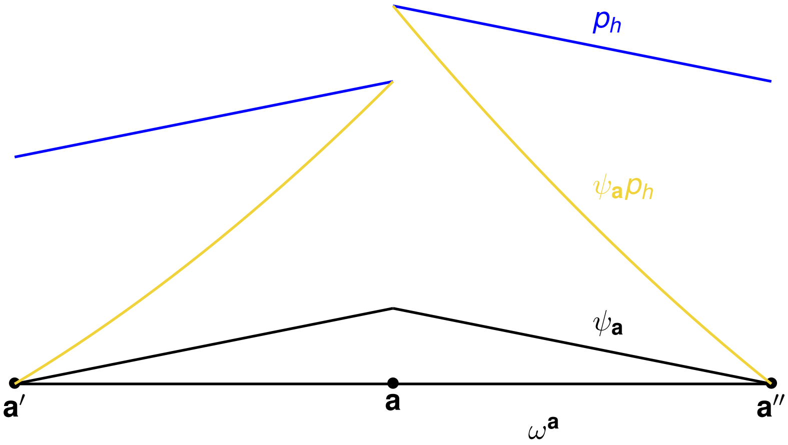

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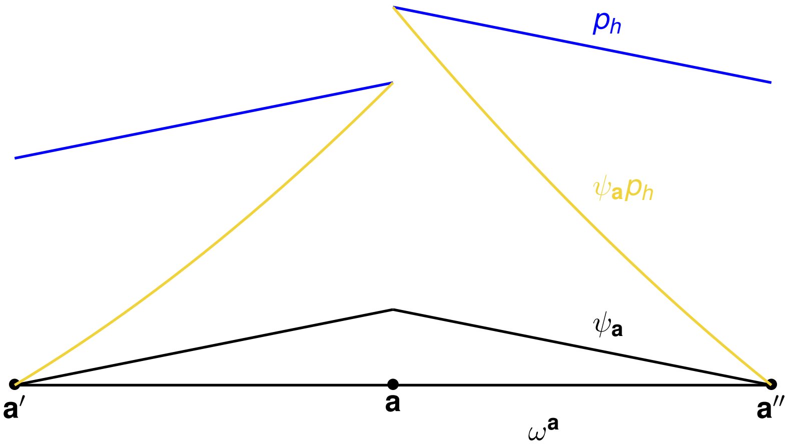
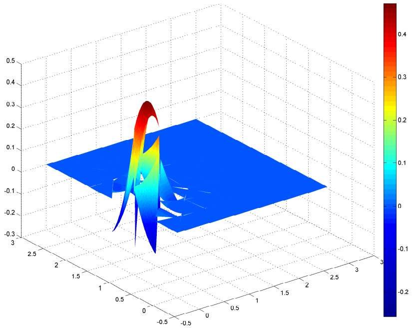


Pressure reconstruction

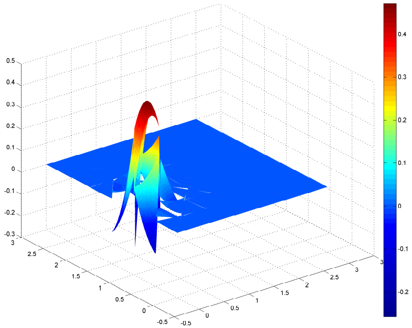
$$s_h^{\mathbf{a}} := \arg\min_{v_h \in \mathbb{P}_{m+1}(\mathcal{T}_{\mathbf{a}}) \cap H_0^1(\omega^{\mathbf{a}})} \|\nabla(\psi_{\mathbf{a}} p_h - v_h)\|_{\omega^{\mathbf{a}}}, \quad s_h := \sum_{\mathbf{a} \in \mathcal{V}_h} s_h^{\mathbf{a}}$$

Pressure reconstruction s_h in 2D



Pressure p_h

Pressure reconstruction s_h in 2D



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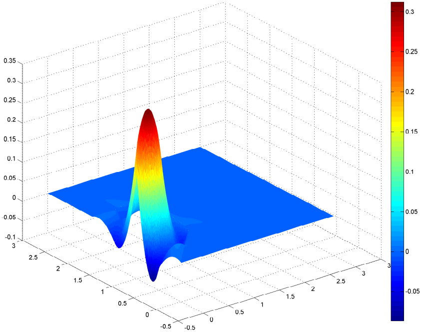

Pressure reconstruction s_h

Symmetric IPDG, smooth solution

h	p
h_0	1

Symmetric IPDG, smooth solution

h	p	$\eta(p_h)$
h_0	1	1.25

Symmetric IPDG, smooth solution

h	p	$\eta(p_h)$	rel. error estimate $\frac{\eta(p_h)}{\|\nabla p_h\|}$
h_0	1	1.25	28%

Symmetric IPDG, smooth solution

h	p	$\eta(p_h)$	rel. error estimate $\frac{\eta(p_h)}{\|\nabla p_h\|}$	$\|\nabla(p-p_h)\|$
h_0	1	1.25	28%	1.07

Symmetric IPDG, smooth solution

h	p	$\eta(p_h)$	rel. error estimate $\frac{\eta(p_h)}{\|\nabla p_h\|}$	$\|\nabla(p-p_h)\|$	rel. error $\frac{\|\nabla(p-p_h)\|}{\|\nabla p_h\|}$
h_0	1	1.25	28%	1.07	24%

Symmetric IPDG, smooth solution

h	p	$\eta(p_h)$	rel. error estimate $\frac{\eta(p_h)}{\|\nabla p_h\|}$	$\|\nabla(p-p_h)\|$	rel. error $\frac{\|\nabla(p-p_h)\|}{\|\nabla p_h\|}$	$I^{\mathrm{eff}} = \frac{\eta(p_h)}{\|\nabla(p-p_h)\|}$
h_0	1	1.25	28%	1.07	24%	**1.17**
$\approx h_0/2$		6.07×10^{-1}	14%	5.56×10^{-1}	13%	**1.09**
$\approx h_0/4$		3.10×10^{-1}	7.0%	2.92×10^{-1}	6.6%	**1.06**
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	**1.04**
h_0	2	1.63×10^{-1}	3.7%	1.54×10^{-1}	3.5%	**1.06**
$\approx h_0/2$	2	4.23×10^{-2}	9.5×10^{-1}%	4.07×10^{-2}	9.2×10^{-1}%	**1.04**
h_0	3	1.41×10^{-2}	3.2×10^{-1}%	1.37×10^{-2}	3.1×10^{-1}%	**1.03**
$\approx h_0/4$	3	2.62×10^{-4}	5.9×10^{-3}%	2.60×10^{-4}	5.9×10^{-3}%	**1.01**
h_0	4	1.01×10^{-3}	2.3×10^{-2}%	9.87×10^{-4}	2.2×10^{-2}%	**1.02**
$\approx h_0/8$	4	2.60×10^{-7}	5.9×10^{-6}%	2.58×10^{-7}	5.8×10^{-6}%	**1.01**

A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

Symmetric IPDG, smooth solution

h	p	$\eta(p_h)$	rel. error estimate $\frac{\eta(p_h)}{\|\nabla p_h\|}$	$\|\nabla(p-p_h)\|$	rel. error $\frac{\|\nabla(p-p_h)\|}{\|\nabla p_h\|}$	$I^{\mathrm{eff}} = \frac{\eta(p_h)}{\|\nabla(p-p_h)\|}$
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Symmetric IPDG, smooth solution

h	p	$\eta(p_h)$	rel. error estimate $\frac{\eta(p_h)}{\lVert\nabla p_h\rVert}$	$\lVert\nabla(p-p_h)\rVert$	rel. error $\frac{\lVert\nabla(p-p_h)\rVert}{\lVert\nabla p_h\rVert}$	$I^{\text{eff}} = \frac{\eta(p_h)}{\lVert\nabla(p-p_h)\rVert}$
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Symmetric IPDG, smooth solution

h	p	$\eta(p_h)$	rel. error estimate $\frac{\eta(p_h)}{\lVert\nabla p_h\rVert}$	$\lVert\nabla(p-p_h)\rVert$	rel. error $\frac{\lVert\nabla(p-p_h)\rVert}{\lVert\nabla p_h\rVert}$	$I^{\mathrm{eff}} = \frac{\eta(p_h)}{\lVert\nabla(p-p_h)\rVert}$
h_0	1	1.25	28%	1.07	24%	**1.17**
$\approx h_0/2$		6.07×10^{-1}	14%	5.56×10^{-1}	13%	**1.09**
$\approx h_0/4$		3.10×10^{-1}	7.0%	2.92×10^{-1}	6.6%	**1.06**
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	**1.04**
h_0	2	1.63×10^{-1}	3.7%	1.54×10^{-1}	3.5%	**1.06**
$\approx h_0/2$	2	4.23×10^{-2}	9.5×10^{-1}%	4.07×10^{-2}	9.2×10^{-1}%	**1.04**
h_0	3	1.41×10^{-2}	3.2×10^{-1}%	1.37×10^{-2}	3.1×10^{-1}%	**1.03**
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A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

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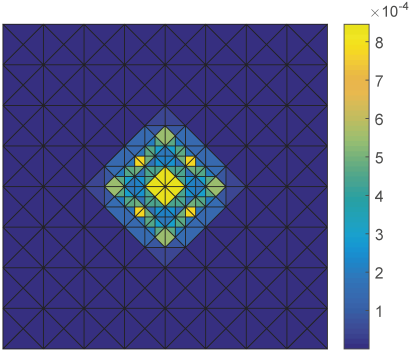
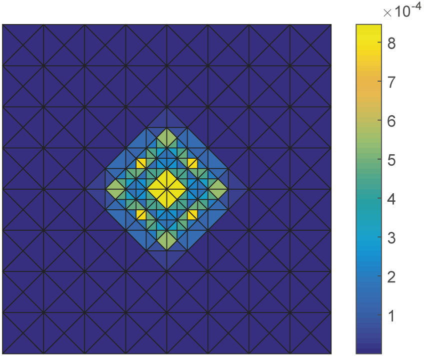
A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

Conforming FEs, smooth solution



Estimated error distribution

$\eta_K(p_h)$

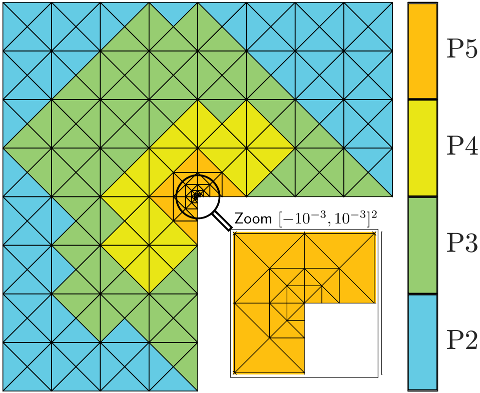


Exact error distribution

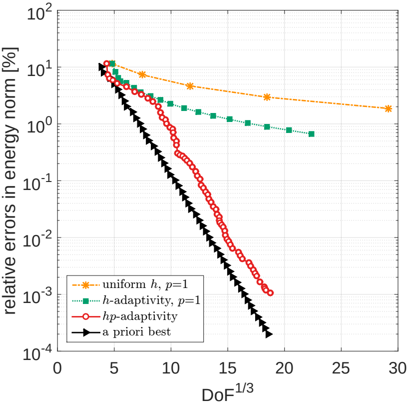
$\|\nabla(p - p_h)\|_K$

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

Incomplete IPDG, singular solution



Mesh $\mathcal{T}_h$ and polynomial degrees m_K



Relative error as a function of no. of unknowns

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

Model problems

Reaction-diffusion

- $-\Delta p + rp = f$ in Ω, $p = 0$ on $\partial\Omega$, $r \gg 1$
- robustness wrt r: Verfürth (1998), Ainsworth & Babuška (1998)
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Heat equation

- $\partial_t p - \Delta p = f$ in $\Omega \times (0, t_F)$, $p = 0$ on $\partial\Omega \times (0, t_F)$, $p = p_0$ in Ω
- robustness wrt t_F and mutual sizes of h and τ: Verfürth (2003)
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Multi-phase, multi-compositional flows discussion

Mathematician

- all ingredients are ready to design an 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.
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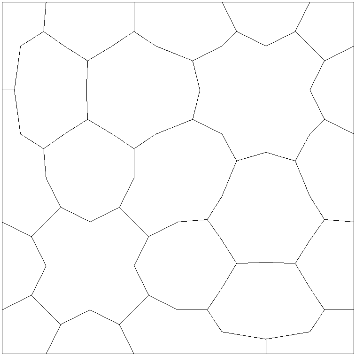
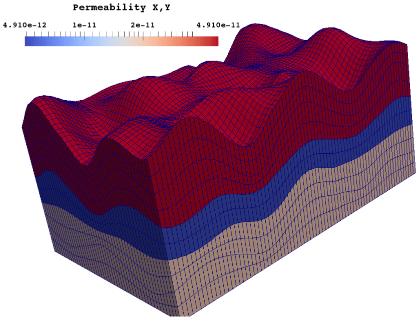
Outline

1. Introduction
   - Energy a posteriori error estimates – quick state of the art
   - Context and goals of the talk
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

Context and goals

General polygonal/polyhedral meshes, arbitrary scheme





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- finite volumes / gradient schemes (Droniou, Eymard, Gallouët, Herbin . . .)
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Context and goals

General polygonal/polyhedral meshes, arbitrary scheme

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Multi-phase, multi-compositional flows

- described in physical variables
- no global pressure, no Kirchhoff transform . . .

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- **simple** estimates: **easy** coding, **fast** evaluation, **cosy** use in practical simulations
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Outline

1. Introduction
   - Energy a posteriori error estimates – quick state of the art
   - Context and goals of the talk
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

Linear Darcy flow

Steady linear Darcy flow

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

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ 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 (flux)

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Outline

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
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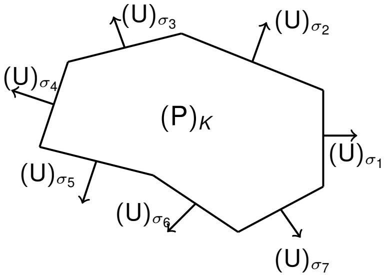

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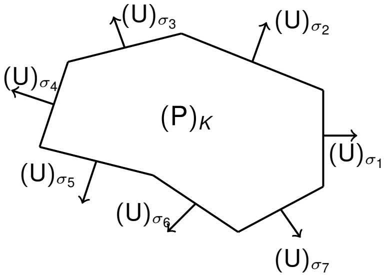

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Saddle-point discretizations

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;*
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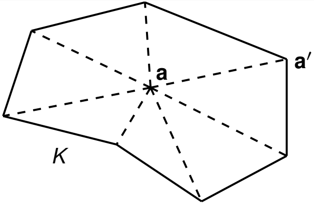

- finite element stiffness matrix

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

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- mixed finite element local static condensation matrix

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  - obtained by local Neumann MFE problem in the polytope K
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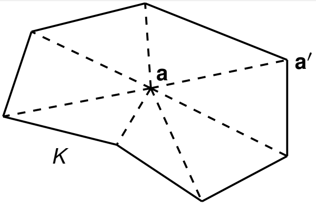

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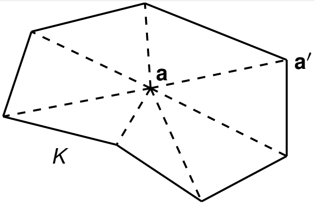

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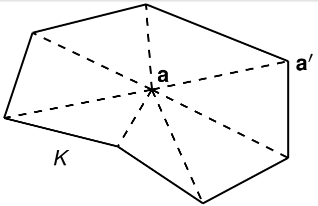

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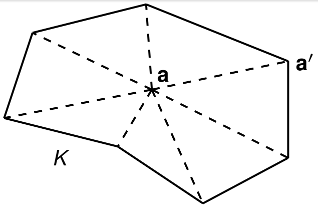

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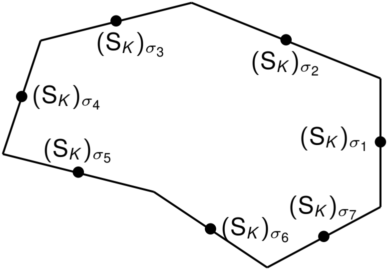

$$S_K^{\rm ext} = \{(S_K)_{\sigma_i}\}_{i=1}^7$$

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

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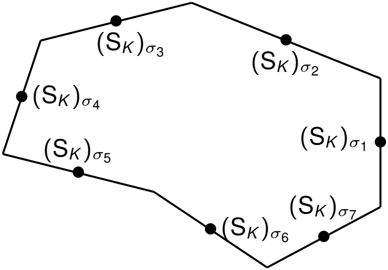

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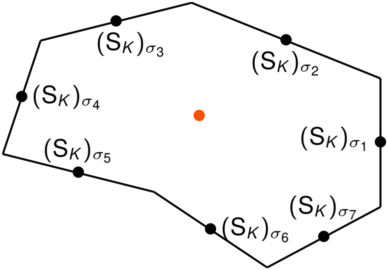

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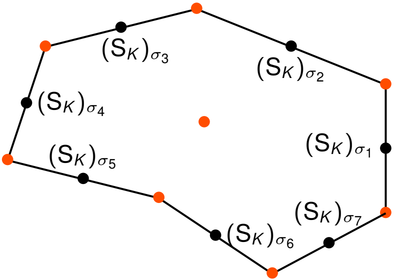

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- Assumption A: $(S_K)_{\sigma_i}$ local averages of neighbor $(P)_{K'}$
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- $(S_K)_{\mathbf{a}_8} := (P)_K$
- $S_K = \{(S_K)_{\mathbf{a}_i}\}_{i=1}^{7}$ constructed by local averaging

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

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

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

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

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) $\approx$ 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-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 simplicial submesh $\mathcal{T}_h$, 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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- choose s_h continuous and piecewise affine wrt simplicial submesh $\mathcal{T}_h$, given by the nodal values of the vector S
- developing for each $K \in \mathcal{T}_H$

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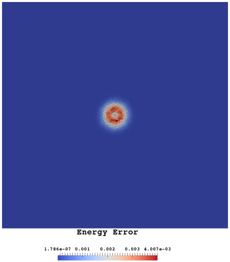
Outline

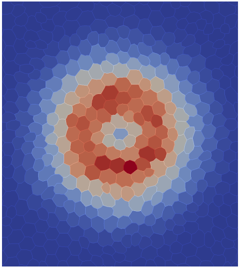
Numerical experiment

Setting

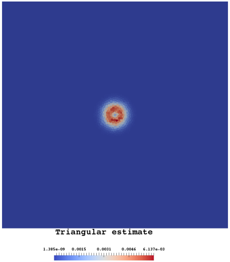
- $-\Delta p = f$
- $\Omega = (0,1)^2$
- analytic solution $2^{4\alpha} x^\alpha (1-x)^\alpha y^\alpha (1-y)^\alpha$, $\alpha = 200$
- hybrid finite volume (HFV) discretization (Droniou, Eymard, Gallouët, Herbin (2010))

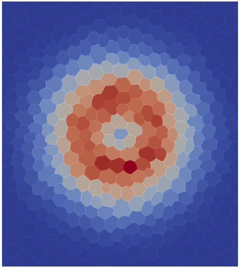
Energy error & reference estimate (triangular submesh)





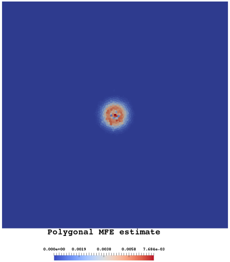
Energy error

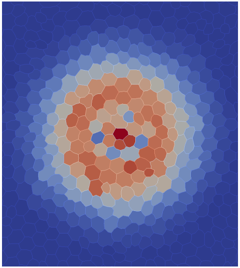




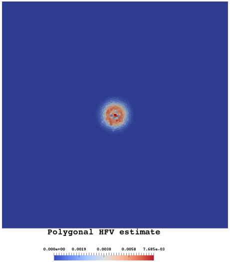
Estimate with s_h pw. quadratic over submesh (V. (2008))

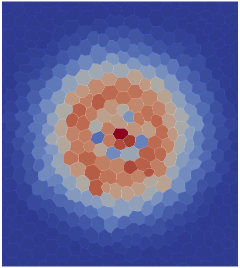
Simple polygonal estimates





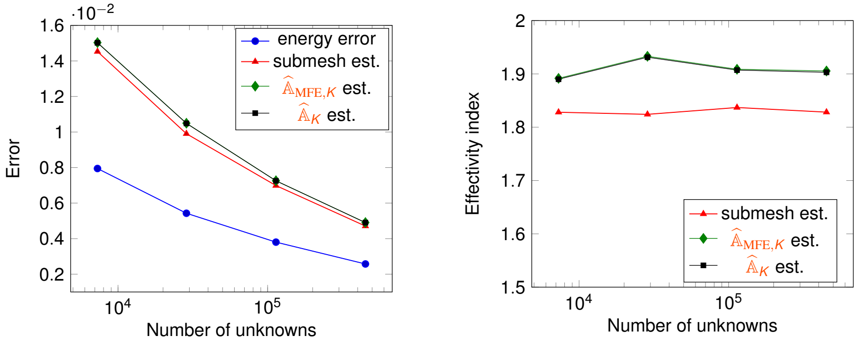
Using $\widehat{\mathbb{A}}_{\mathrm{MFE},K}$



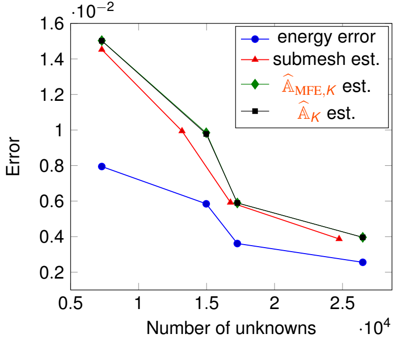


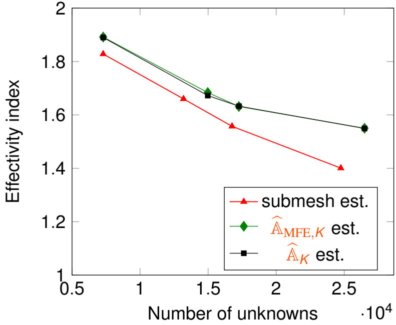
Using $\widehat{\mathbb{A}}_K$

Uniform mesh refinement



Adaptive mesh refinement





Outline

Nonlinear Darcy flow

Steady nonlinear Darcy flow

$$
\begin{aligned}
-\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

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

- 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:

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

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Steady nonlinear Darcy flow

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

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

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

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*

$$\left(\eta_{\mathrm{sp},K}^{k,i} \right)^2 := (\mathsf{U}_K^{k,i})^{\mathrm{t}} \widehat{\mathbb{A}}_{\mathrm{MFE},K} \mathsf{U}_K^{k,i} + (\mathsf{S}_K^{k,i})^{\mathrm{t}} \widehat{\mathbb{S}}_{\mathrm{FE},K} \mathsf{S}_K^{k,i}$$
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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
- $\mathbf{u}_h^{k,i}|_K$: 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)
- **error components distinction**

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- **error components distinction**

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 $H_0^1(\Omega)$

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

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

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

- error components identification via fluxes:

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

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

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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

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

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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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Outline

Face fluxes

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

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

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

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

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

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

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

Face fluxes

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

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

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

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

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

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

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

Estimators

spatial estimators

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

upwinding estimators

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

nonconformity estimators

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

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

temporal estimators

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

linearization estimators

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

algebraic estimators

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

algebraic remainder estimators

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

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 $(\boldsymbol{C}_p)_K^{n,k,i}$
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- naturally relative stopping criteria

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

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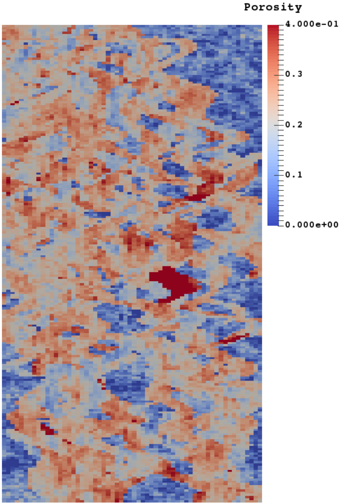
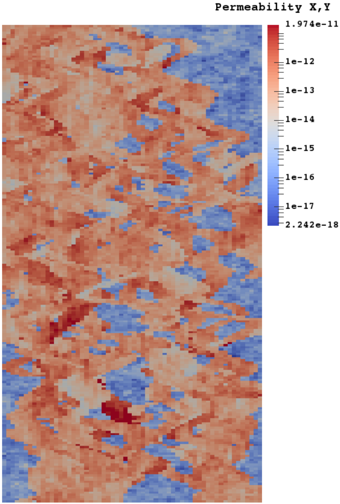
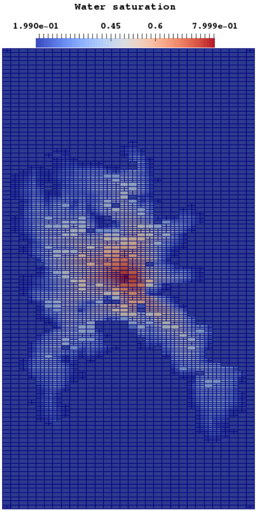
Outline

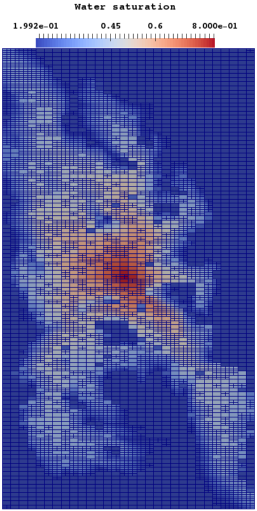
Two-phase flow: porosity & permeability (10th SPE)



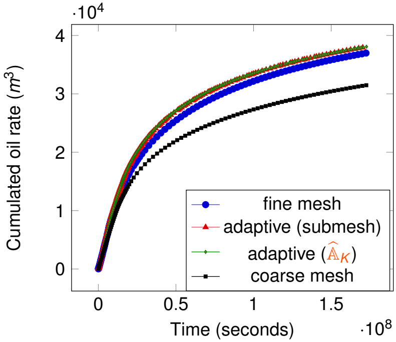


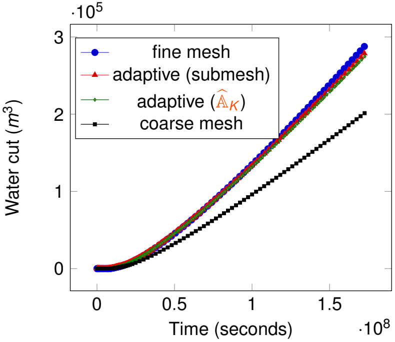
Two-phase flow: water saturation, adaptive mesh, 400 days and 1100 days





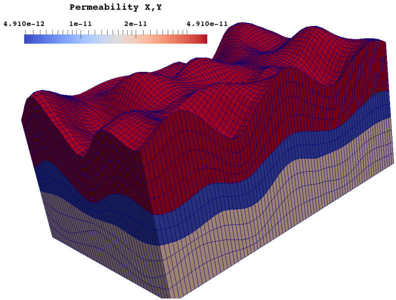
Two-phase flow: uniform vs adaptive mesh refinement

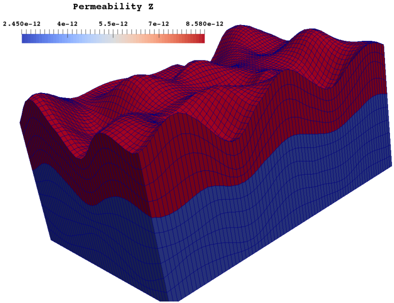




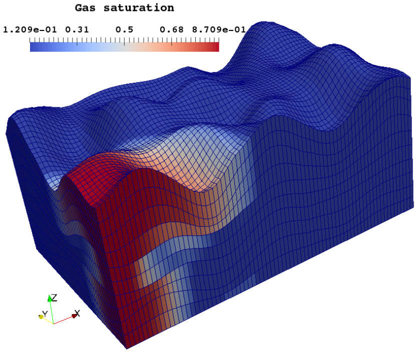
	Resolution	AMR	Estimators evaluation	Gain factor
Fine mesh	603s	-	-	-
Adaptive mesh	242s	46s	27s	1.9

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

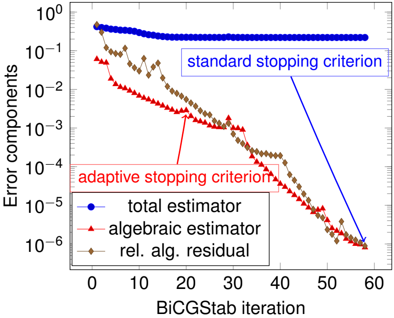


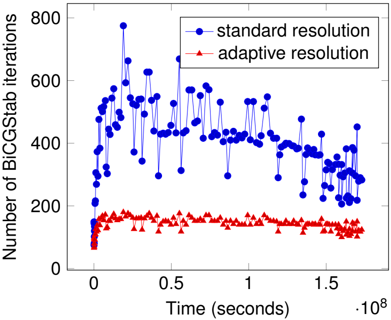


Three-phases, three-components (black-oil) problem: gas saturation and a posteriori estimate



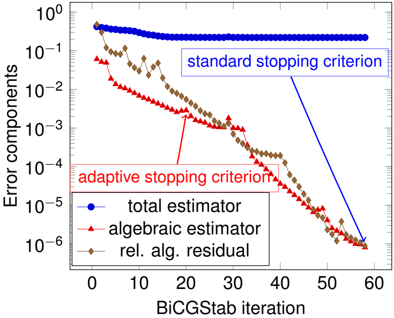
Three-phases, three-components (black-oil) problem: solver & mesh adaptivity

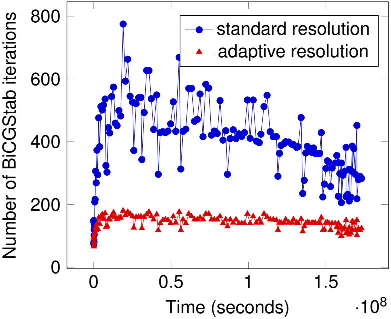




	Linear solver steps	Resolution time	AMR time	Estimators evaluation	Gain factor
Standard resolution	66386	1023s	-	-	-
Adaptive resolution	20184	201s	42s	26s	3.8

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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Thank you for your attention!

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

Two-phase flow: global and complementary pressures

Global pressure

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

Complementary pressure

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

Comments

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

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

Global pressure

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

Complementary pressure

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

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

Global pressure

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

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Two-phase flow: weak formulation

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 $s_{\mathrm{o}} := 1 - s_{\mathrm{w}}$,

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

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

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

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

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

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

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$$\mathfrak{p}(s_{\mathrm{w}}, p_{\mathrm{w}}) \in X,$$
$$\mathfrak{q}(s_{\mathrm{w}}) \in X,$$
$$\int_0^T \left\{ \langle \partial_t(\phi s_\alpha), \varphi \rangle - (\mathbf{u}_\alpha(s_{\mathrm{w}}, p_{\mathrm{w}}), \nabla \varphi) - (q_\alpha, \varphi) \right\} \mathrm{d}t = 0$$
$$\forall \varphi \in X,\ \alpha \in \{\mathrm{o}, \mathrm{w}\}.$$

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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$$\left.\left. - (\mathbf{u}_\alpha(s_{\rm w},p_{\rm w}) - \mathbf{u}_\alpha(s_{{\rm w},h\tau},p_{{\rm w},h\tau}), \nabla\varphi)\}{\rm d}t \right\}^2 \right\}^{\frac{1}{2}}$$

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

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Multi-phase multi-compositional flow: weak solution

Function spaces

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

Weak solution – we assume that

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

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

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

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

the initial condition holds,

the algebraic closure equations hold

Multi-phase multi-compositional flow: weak solution

Function spaces

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

the initial condition holds,

the algebraic closure equations hold

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

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

Localized space

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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 $t^n \le t_F$ **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 $\eta_{\mathrm{alg,t}}^{n,k,i} \le \gamma_{\mathrm{alg}} \eta_{\mathrm{sp,t}}^{n,k,i}$.
      end loop
      Terminate (Newton linearization) if $\eta_{\mathrm{lin,t}}^{n,k,i} \le \gamma_{\mathrm{lin}} \eta_{\mathrm{sp,t}}^{n,k,i}$.
    end loop
    Terminate (spatial & temporal errors balancing) if

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

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

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