

# A posteriori error estimates with inexact solvers and recovering mass balance in any situation

**Martin Vohralík**

*Inria Paris & Ecole des Ponts*

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European Research Council

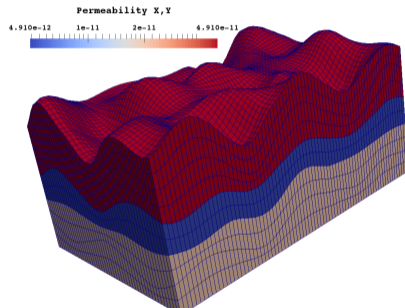
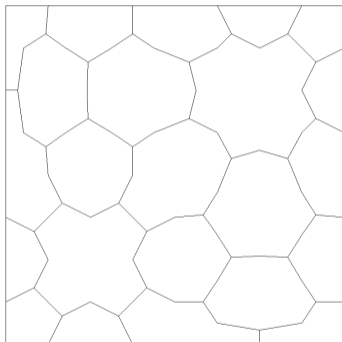


# Outline

- 1 Introduction: context, motivation, and goals
- 2 Steady linear Darcy flow
  - Discretization
  - A posteriori estimate
  - Numerical experiments
- 3 Steady nonlinear Darcy flow
  - Discretization, linearization, and algebraic resolution
  - A posteriori estimate
  - Recovering mass balance
- 4 Unsteady multi-phase multi-compositional Darcy flow
  - A posteriori estimate
  - Numerical experiments
  - Recovering mass balance
- 5 Conclusions

## Context

## General polygonal/polyhedral meshes, arbitrary locally conservative scheme

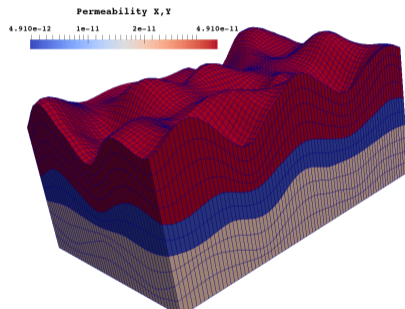
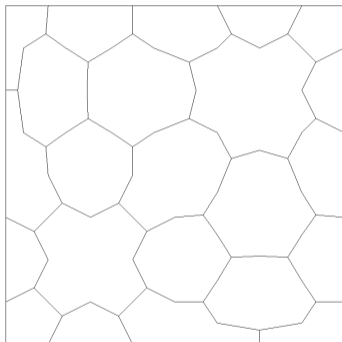


Multi-phase, multi-compositional porous media flows

- unsteady nonlinear degenerate systems of PDEs

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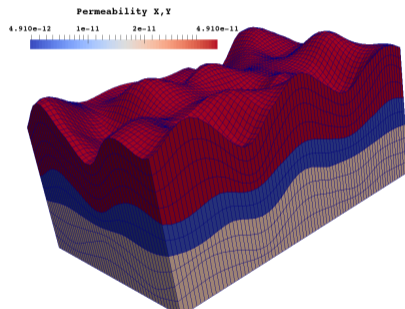
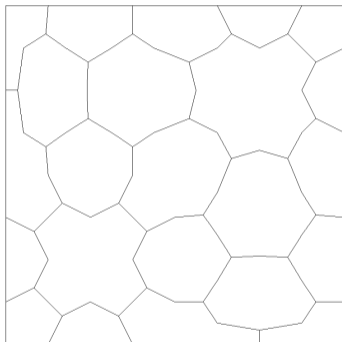


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- **unsteady nonlinear** degenerate **systems** of PDEs
- algebraic constraints

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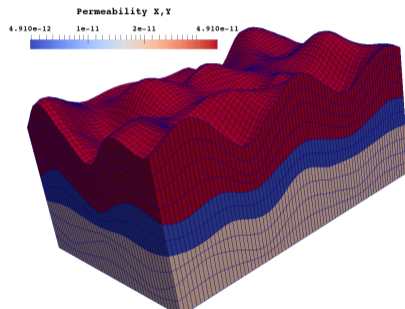
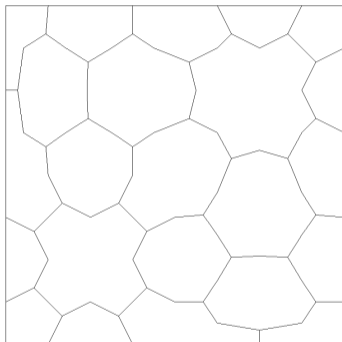


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- **unsteady nonlinear** degenerate **systems** of PDEs
- algebraic constraints phase appearance/disappearance

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## Multi-phase, multi-compositional porous media flows

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

# Example: steady nonlinear Darcy flow $\nabla \cdot (-\underline{\mathbf{K}}(\nabla p)\nabla p) = f$

## Discretization: system of nonlinear algebraic eqs

Find  $\mathbf{P} \in \mathbb{R}^N$  such that

$$\underbrace{\mathcal{U}}_{\text{nonlin. op.}}(\mathbf{P}) = \mathbf{F}$$

## Linearization: system of linear algebraic eqs

Find  $\mathbf{P}^k \in \mathbb{R}^N$  such that

$$\underbrace{\mathbf{U}^{k-1}}_{\text{matrix}} \mathbf{P}^k = \mathbf{F}^{k-1}$$

## Algebraic solver:

On step  $i$ , one has  $\mathbf{P}^{k,i} \in \mathbb{R}^N$  such that

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## Common situation

- *linearization stopping crit.:*  
 $\|\mathbf{P}^k - \mathbf{P}^{k-1}\|_{\infty}$  small

- *algebraic stopping crit.:*  
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- **comparing apples and oranges**, not comparing in the right norm

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- guaranteed **a posteriori** error **estimate**

$$\|\mathbf{u}|_{I_n} - \mathbf{u}_h^{n,k,i}\| \leq \eta_{\text{sp}}^{n,k,i} + \eta_{\text{tm}}^{n,k,i} + \eta_{\text{lin}}^{n,k,i} + \eta_{\text{alg}}^{n,k,i}$$

- valid at each step: time  $n$ , linearization  $k$ , linear solver  $i$
- distinguishing different error components, all estimators with the same (flux) physical units
- easy to code, fast to evaluate, cosy to use in practice
- full adaptivity (stopping criteria for linear and nonlinear solvers, mesh refinement, time step adjustment)

Construction of the estimates interconnected with recovering mass balance at each step  $n, k, i$ .



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# Linear Darcy flow

## Steady linear Darcy flow

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

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

## Unknowns

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

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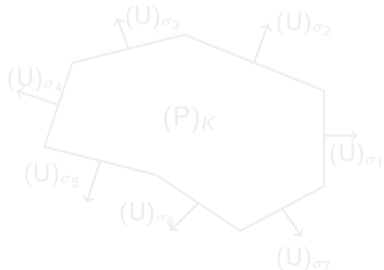
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# Locally conservative discretization

## Assumption A (Locally conservative discretization)

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

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



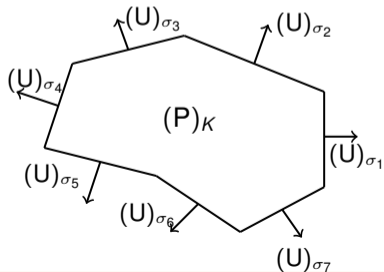
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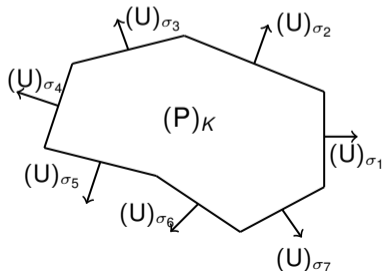
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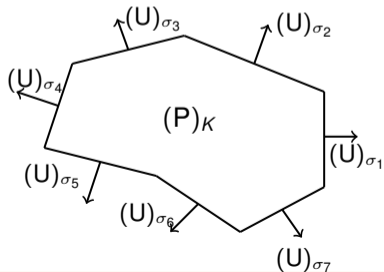
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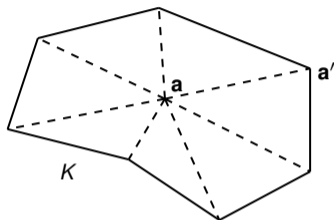
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# Three element **matrices** easily computable from the geometry of $K$



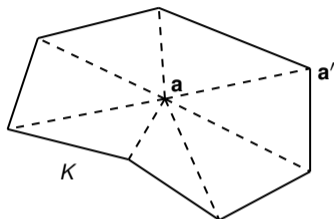
1 finite element stiffness matrix

$$(\mathbf{S}_K)_{\mathbf{a}, \mathbf{a}'} := (\underline{\mathbf{K}} \nabla \psi_{\mathbf{a}'}, \nabla \psi_{\mathbf{a}})_K \quad \mathbf{a}, \mathbf{a}' \in \mathcal{V}_{K,h}$$

2 finite element mass matrix

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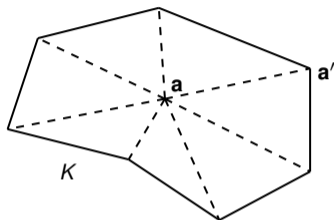
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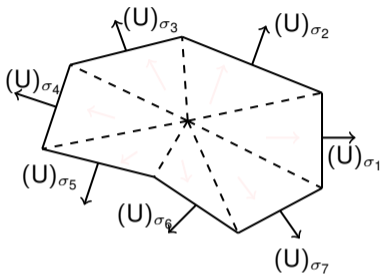
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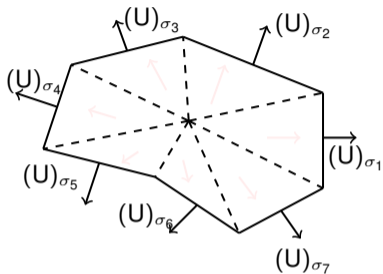


## 6 mixed finite element local static condensation matrix

$$\mathbf{v}_h; \langle \mathbf{v}_h \cdot \mathbf{n}, 1 \rangle_{\sigma} = (U)_{\sigma} \quad \min_{\nabla \cdot \mathbf{v}_h = \text{constant}} \|\underline{\mathbf{K}}^{-\frac{1}{2}} \mathbf{v}_h\|_K$$

• **element matrices** for secondary fluxes  $(U)_{\sigma}$  and the matrix  $\underline{\mathbf{K}}$

# Three **element matrices** easily computable from the geometry of $K$



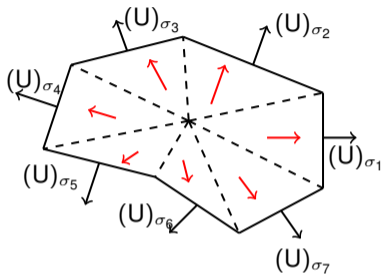
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$$\tilde{\Delta}_K \Leftrightarrow \mathbf{u}_h|_K := \arg \min_{\mathbf{v}_h: \langle \mathbf{v}_h \cdot \mathbf{n}, 1 \rangle_{\sigma} = (U)_{\sigma}, \nabla \cdot \mathbf{v}_h = \text{constant}} \left\| \underline{\mathbf{K}}^{-\frac{1}{2}} \mathbf{v}_h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

where  $\mathbf{u}_h|_K$  extends the boundary fluxes  $(U)_{\sigma}$  into the interior of  $K$

one can also use the scheme element matrix  $\tilde{\tilde{\Delta}}_K$

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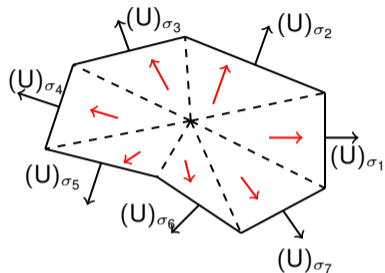
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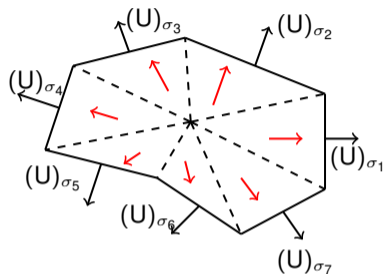
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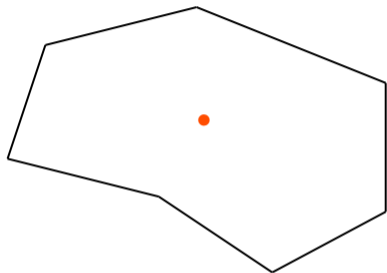
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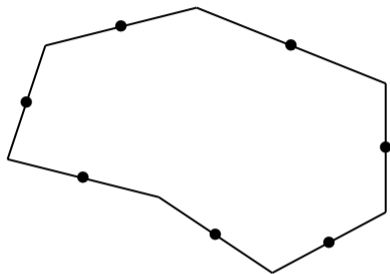


# Element pressure and flux vectors



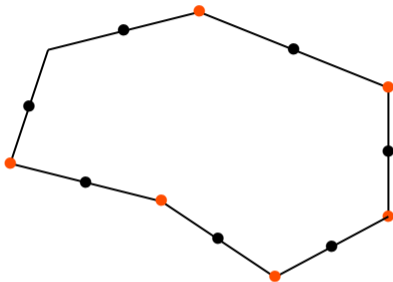
- cell pressure  $(P)_K$

# Element pressure and flux vectors

 $S_K^{\text{ext}}$ 

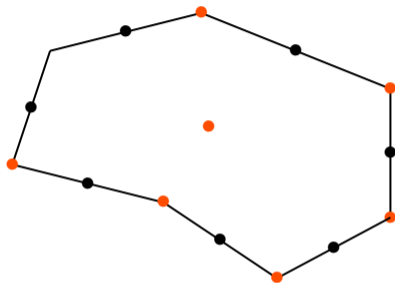
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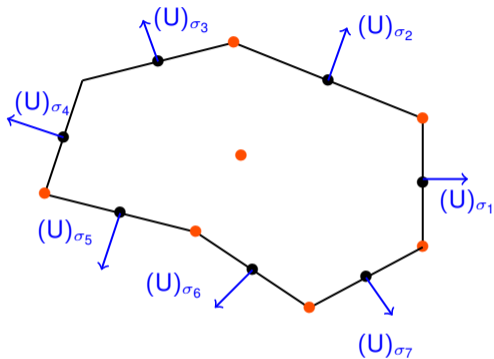
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- $U_K^{\text{ext}}$ : face fluxes

# A posteriori error estimate

## Theorem (Linear Darcy flow)

Under *Assumption A*, there holds

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

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## Comments

- **guaranteed upper bound** on the Darcy velocity error
- price: **matrix-vector multiplication** on each element (no (local) linear system, no (potential or flux) reconstruction)

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- Prager–Synge equality:

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

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

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

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- 1 Introduction: context, motivation, and goals
- 2 **Steady linear Darcy flow**
  - Discretization
  - A posteriori estimate
  - **Numerical experiments**
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  - Discretization, linearization, and algebraic resolution
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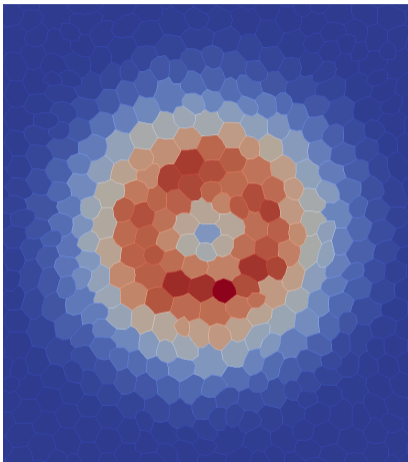


# Numerical experiment

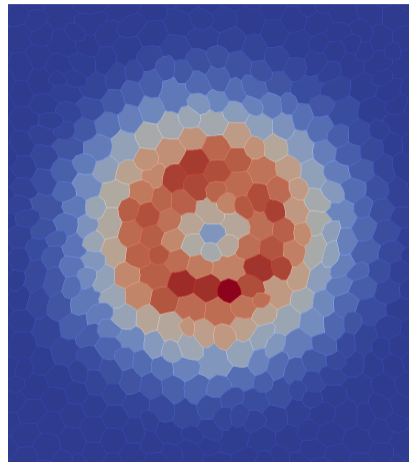
## Setting

- $-\Delta p = f$
- $\Omega = (0, 1)^2$
- 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 & reference estimate (triangular submesh)



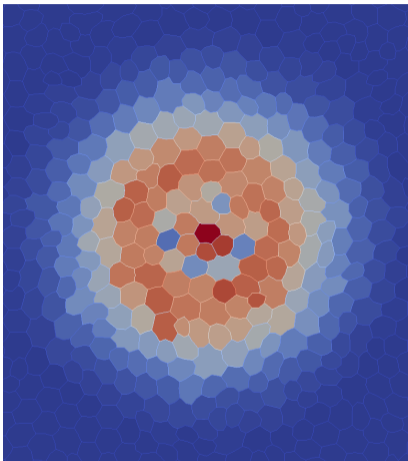
Energy error



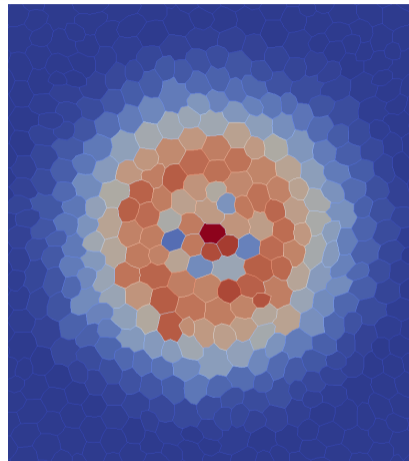
Reference estimate (Vohralík (2008))

M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering

# Simple polygonal estimates



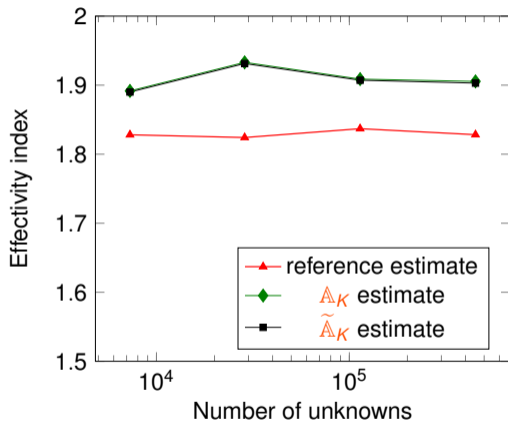
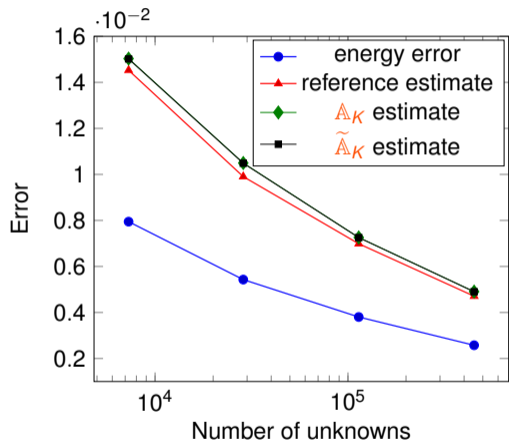
Using the MFE element matrix  $\mathbb{A}_K$



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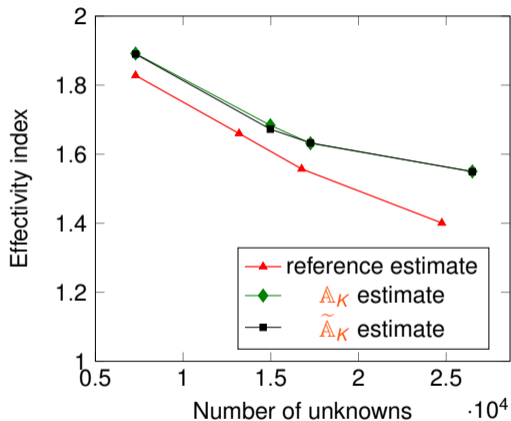
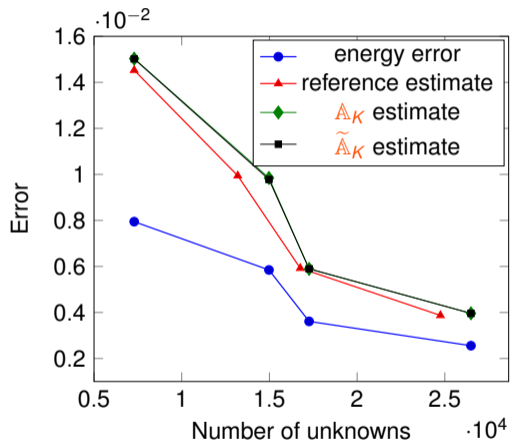
M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering

# Uniform mesh refinement



M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2020)

# Adaptive mesh refinement



M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2020)

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# Nonlinear Darcy flow

## Steady nonlinear Darcy flow

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

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## Assumptions

- invertible nonlinearity

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

- strong monotonicity

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

- Lipschitz-continuity

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

- for simple matrix-vector multiplication:

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



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## Weak solution

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

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

## Darcy velocity

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

## Inverse relation

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

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# Discretization, linearization, and algebraic resolution

## Discretization

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

$$\mathbf{U}(\mathbf{P}) = \mathbf{F}$$

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

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

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

$$\mathbf{U}^{k-1} \mathbf{P}^k = \mathbf{F}^{k-1}$$

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

## Algebraic resolution (step $i \geq 1$ )

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

$$\mathbf{U}^{k-1} \mathbf{P}^{k,i} = \mathbf{F}^{k-1} - \mathbf{R}^{k,i}$$

- $(\mathbf{R}^{k,i})_K$ : algebraic residual vector

# Discretization, linearization, and algebraic resolution

## Discretization

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

$$\mathbf{U}(\mathbf{P}) = \mathbf{F}$$

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

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# Discretization, linearization, and algebraic resolution

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# Estimating the algebraic error via additional solver steps

Perform  $j \geq 1$  additional algebraic solver steps

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

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# Face fluxes

## Discretization face normal flux

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

## Linearization error face normal flux

$$(\mathbf{U}_{\text{lin}}^{k,i})_\sigma := (\mathbf{U}^{k-1}(\mathbf{P}^{k,i}))_\sigma - (\mathbf{U}(\mathbf{P}^{k,i}))_\sigma$$

## Algebraic error face normal flux

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

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

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# A posteriori error estimate

## Theorem (Nonlinear Darcy flow)

Under *Assumption A*, there holds

$$c_{\underline{K}}^{\frac{1}{2}} \|\mathbf{u} - \mathbf{u}_h^{k,i}\| \leq \eta_{\text{sp}}^{k,i} + \eta_{\text{lin}}^{k,i} + \eta_{\text{alg}}^{k,i} + \eta_{\text{rem}}^{k,i}$$

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

$$\begin{aligned} \left( \eta_{\text{sp},K}^{k,i} \right)^2 &:= \left( \mathbf{U}_K^{k,i} \right)^t \mathbf{A}_K \mathbf{U}_K^{k,i} + \left( \mathbf{S}_K^{k,i} \right)^t \mathbf{S}_K \mathbf{S}_K^{k,i} \\ &\quad + 2c_{\underline{K}}^{-1} c_{\underline{K}} \left[ \left( \mathbf{U}_K^{k,i,\text{ext}} \right)^t \mathbf{S}_K^{k,i,\text{ext}} - \left( \mathbf{F} \right)_K |K|^{-1} \mathbf{1}^t \mathbf{M}_K \mathbf{S}_K^{k,i} \right], \end{aligned}$$

$$\left( \eta_{\text{lin},K}^{k,i} \right)^2 := \left( \mathbf{U}_{\text{lin},K}^{k,i} \right)^t \mathbf{A}_K \mathbf{U}_{\text{lin},K}^{k,i},$$

$$\left( \eta_{\text{alg},K}^{k,i} \right)^2 := \left( \mathbf{U}_{\text{alg},K}^{k,i} \right)^t \mathbf{A}_K \mathbf{U}_{\text{alg},K}^{k,i},$$

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

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# Nonlinear Darcy flow estimate

## Comments

- **guaranteed upper bound** on the Darcy velocity error
- same element matrices  $S_K$ ,  $M_K$ , and  $A_K$  or  $\tilde{A}_K$
- price: **matrix-vector multiplication** on each element
- **error components distinction**

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# Recovering mass balance: up to working precision

## Algebraic error (face normal) flux reconstruction

Backward problem: for a given residual vector  $\mathbf{R}^{k,i}$ , find a (face normal) flux s.t.

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

or

$$\nabla \cdot (\mathbf{u}_{h,\text{alg}}^{k,i}) = |K|^{-1} (\mathbf{R})_K^{k,i} \quad \forall K \in \mathcal{T}_H$$

$\Rightarrow$  Mass balance

On each mesh  $\mathcal{T}_H$ , linearization step  $k$ , and algebraic step  $i$ , there holds

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

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$$\nabla \cdot (\tilde{\mathbf{u}}_h^{k,i}) = f|_K \quad \forall K \in \mathcal{T}_H$$

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# Recovering mass balance: up to working precision

## Domain decomposition solver

- exact **coarse solve**
- backward residual problem on each **subdomain**
- S. Hassan, C. Japhet, M. Kern, M. Vohralík, Comput. Methods Appl. Math. (2018)

## Multilevel solver

- exact **coarse solve**
- backward residual problem on each **parent element** (patch) on each **level**
- J. Papež, U. Råde, M. Vohralík, B. Wohlmuth, HAL Preprint 01662944 (2020)

**Removes** the term  $\eta_{rem}^{k,j}$  from the a posteriori error estimate.

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# Recovering mass balance: up to working precision

## Domain decomposition solver

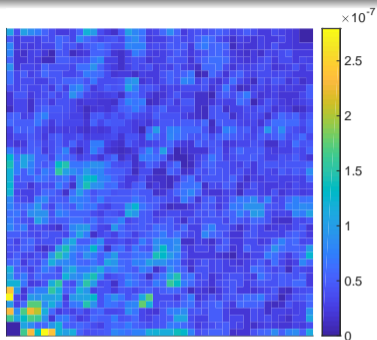
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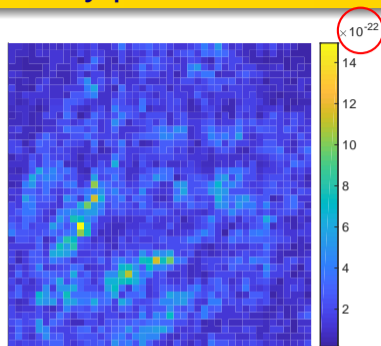
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# Recovering mass balance in a 2-phase Darcy porous media flow



original mass balance misfit ( $\text{m}^2\text{s}^{-1}$ )

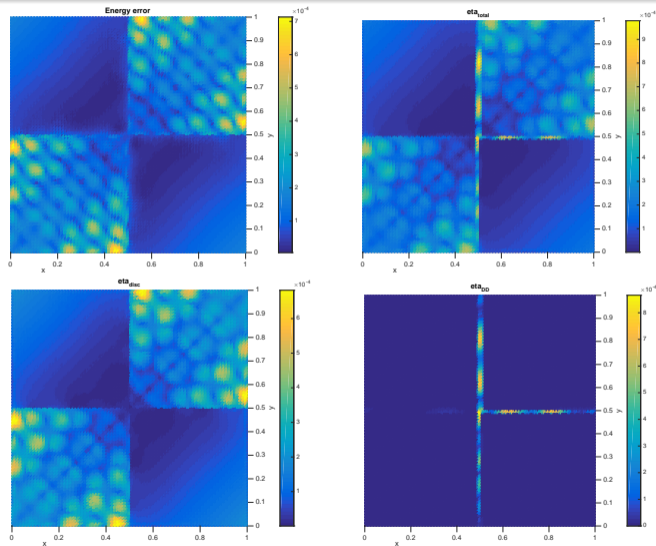


corrected mass balance misfit ( $\text{m}^2\text{s}^{-1}$ )

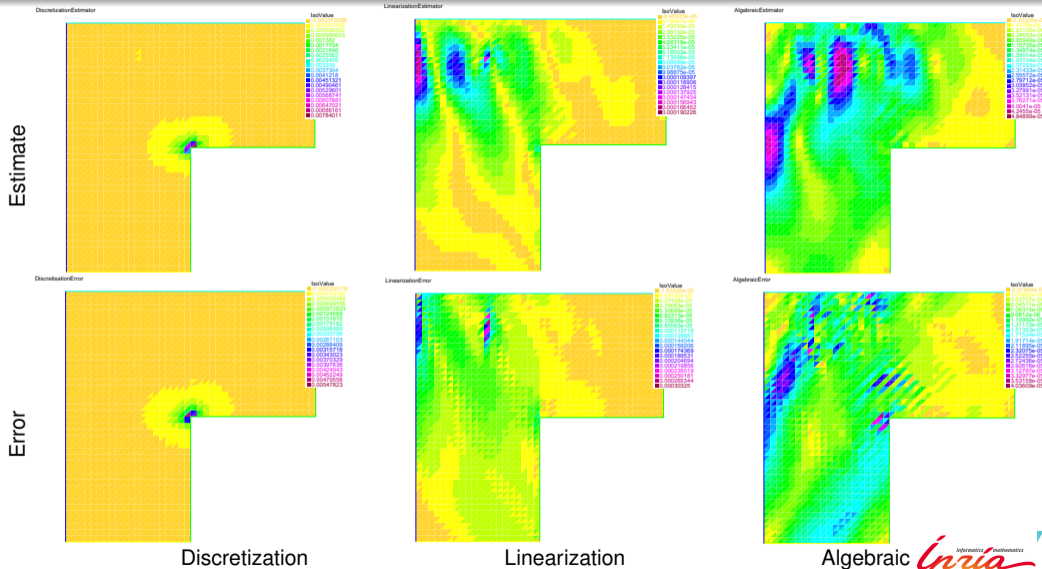
## Setting

- iterative coupling/IMPES discretization of a two-phase flow
- vertex-centered finite volumes on a square mesh
- time step 260, 1st iterative coupling linearization, CG iteration 171

# Domain decomposition for a 1-phase Darcy porous media flow



# Finite elements & 4-Laplacian (FreeFem++ implementation Z. Tang)



Discretization

Linearization

Algebraic

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# Multi-phase multi-compositional flows

## Unknowns

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

## Constitutive laws

- phase pressure = reference pressure + capillary pressure

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

- Darcy's law

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

- component fluxes

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

- amount of moles of component  $c$  per unit volume

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## Governing PDEs

- conservation of mass for **components**

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## Closure **algebraic** equations

- conservation of pore volume:  $\sum_{p \in \mathcal{P}} S_p = 1$
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### Mathematical issues

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

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# A posteriori error estimate

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

Under *Assumption A*, there holds

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

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### Comments

- immediate extension of the results of the steady case
- still matrix-vector multiplication on each element
- same element matrices  $S_K$ ,  $M_K$ , and  $A_K$  or  $\tilde{A}_K$
- input: available normal face fluxes, reference pressure, phase saturations, and component molar fractions
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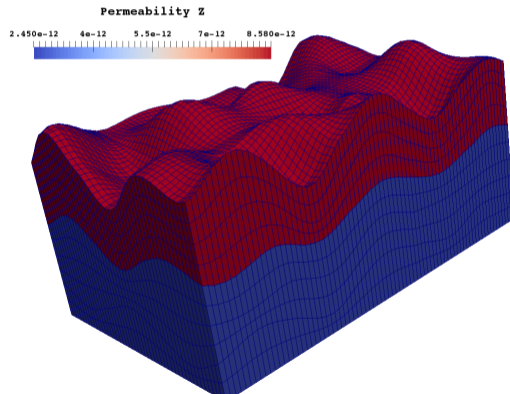
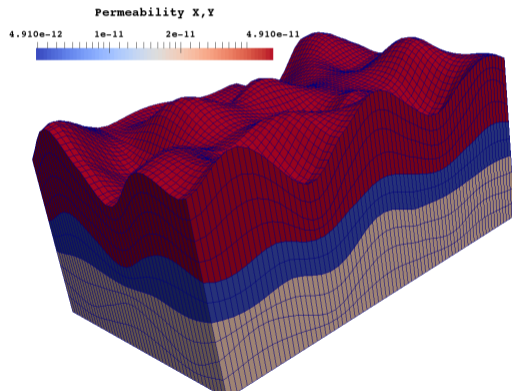
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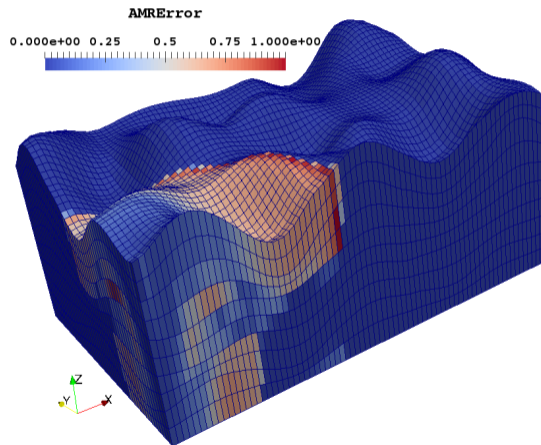
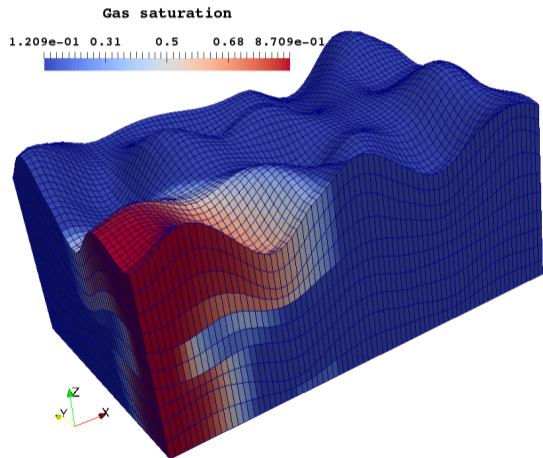
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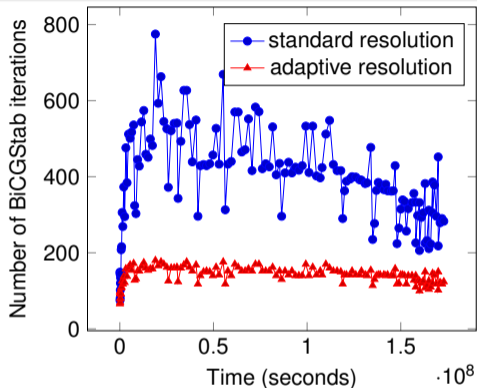
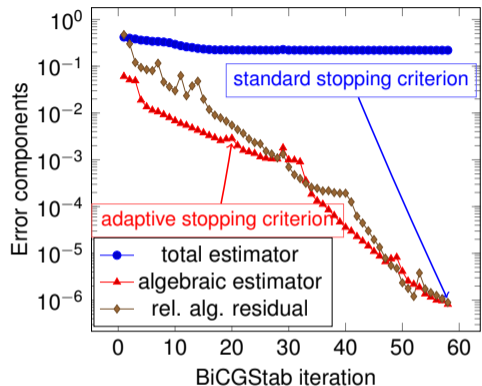
# 3 phases, 3 components (black-oil) problem: permeability



# 3 phases, 3 components (black-oil) problem: gas saturation and a posteriori estimate

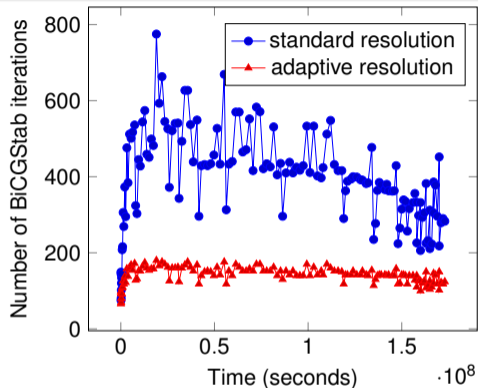
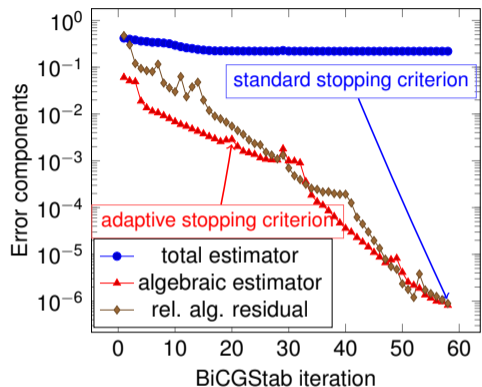


# 3 phases, 3 components (black-oil): alg. solver & mesh adaptivity



	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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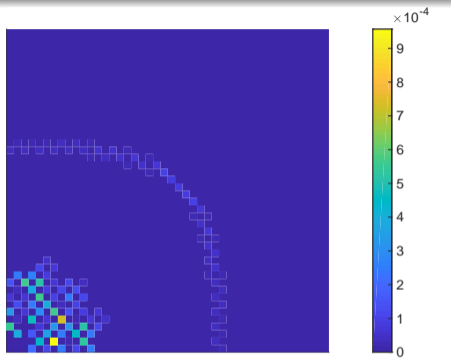


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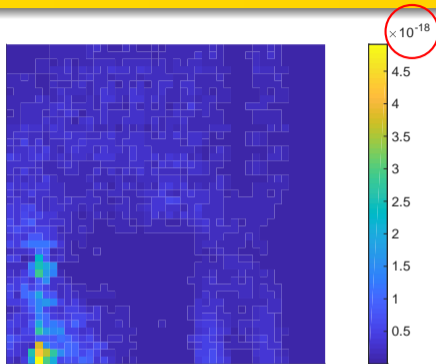
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## 2 phases: recovering water mass balance

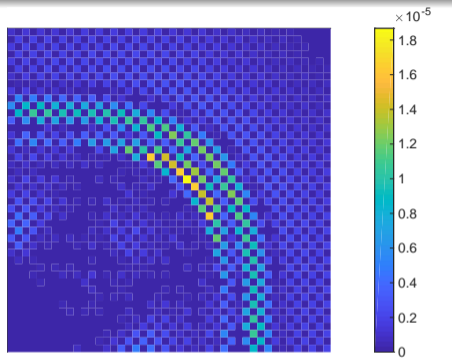


original mass balance misfit ( $\text{m}^2\text{s}^{-1}$ )

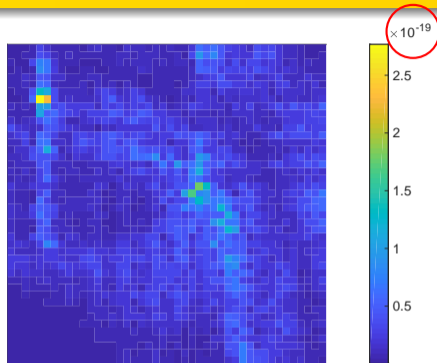


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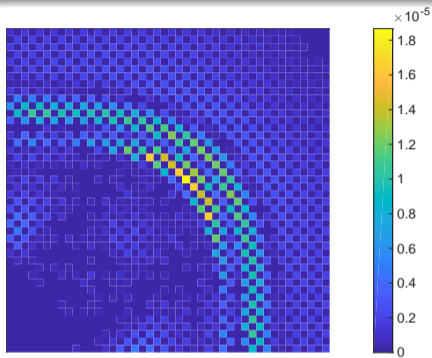
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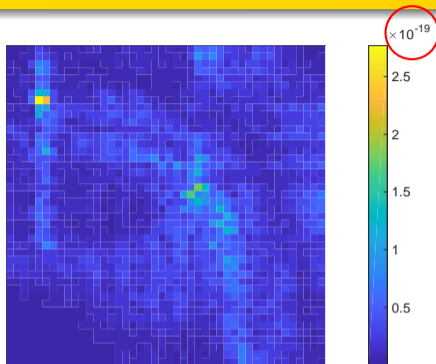
corrected mass balance misfit ( $\text{m}^2\text{s}^{-1}$ )



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### Setting

- fully implicit discretization
- cell-centered finite volumes on a square mesh
- time step 260 (60 days), 1st Newton linearization, GMRes iteration 195

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Thank you for your attention!

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