A posteriori error estimates and adaptive solvers for porous media flows

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informatics mathematics Inria

erc European Research Council

École des Ponts ParisTech

Outline

Context

Multi-phase, multi-compositional porous media flows

- **unsteady nonlinear** degenerate **systems** of PDEs
- possibly algebraic inequality constraints (phase appearance/disappearance)

General polygonal/polyhedral meshes, arbitrary scheme

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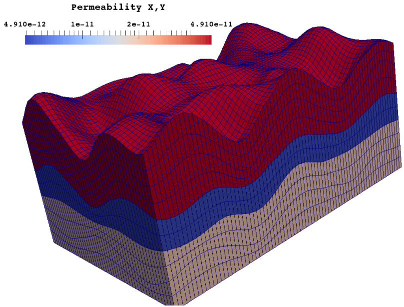

Example: steady nonlinear Darcy flow $\nabla\cdot(-\underline{\mathbf{K}}(\nabla p)\nabla p) = f$

Discretization: system of nonlinear algebraic eqs

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

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

Linearization: system of linear algebraic eqs

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

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

Algebraic solver:

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

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Common situation

- ***too costly*** *if* $i, k \to \infty$

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  mass balance lost

- *linearization stopping crit.* $\|\mathsf{P}^k - \mathsf{P}^{k-1}\|_\infty$ *small, algebraic stopping crit.* $\|\mathsf{R}^{k,i}\|_2/\|\mathsf{R}^{k,0}\|_2$ *small:* ***comparing apples*** *and* ***oranges***
- ***no control*** *of the* ***overall error*** *between the obtained numerical approximation* $\mathsf{P}^{k,i}$ *and the exact solution* p

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

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

- 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 hp refinement, time step adjustment)

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

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2. Steady linear Darcy flow
   - Discretization
   - A posteriori error estimate
   - Numerical experiments
3. Adaptivity: mesh, polynomial degree, linear solvers, nonlinear solvers
   - Mesh and polynomial degree
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   - Error in a quantity of interest
4. Unsteady multi-phase multi-compositional Darcy flow
5. Conclusions

Linear Darcy flow

Steady linear Darcy flow

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

- $\Omega \subset \mathbb{R}^d$, $d \geq 1$, 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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Locally conservative discretization

Assumption A (Locally conservative discretization)

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

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

- $(\mathsf{U})_\sigma \approx \langle \mathbf{u}\cdot\mathbf{n}, 1\rangle_\sigma = \int_\sigma \mathbf{u}\cdot\mathbf{n}$
- **any** (lowest-order) **locally conservative method**
- the link between $(\mathsf{U})_\sigma$ and $(\mathsf{P})_K$ is not important for the a posteriori error estimate upper bound

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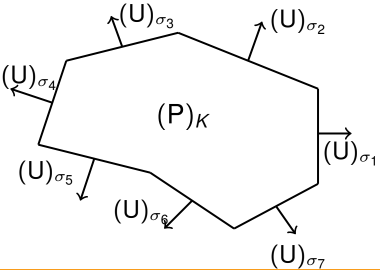

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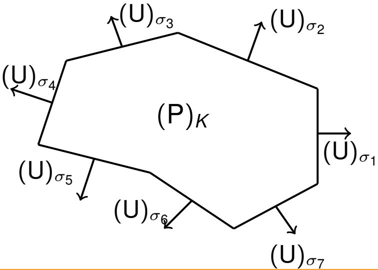

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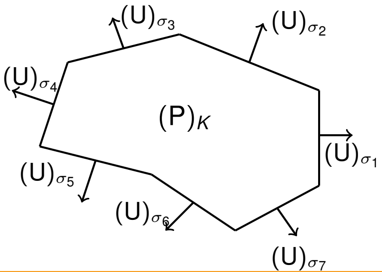

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A posteriori error estimate

Theorem (Linear Darcy flow)

Under Assumption A, there holds

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

where

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

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- $\mathsf{U}_K^{\mathrm{ext}}$, S_K, $\mathsf{S}_K^{\mathrm{ext}}$: flux and pressure vectors on element K
- $\mathbb{A}_K$, $\mathbb{S}_K$, $\mathbb{M}_K$: mass/stiffness matrices on element K
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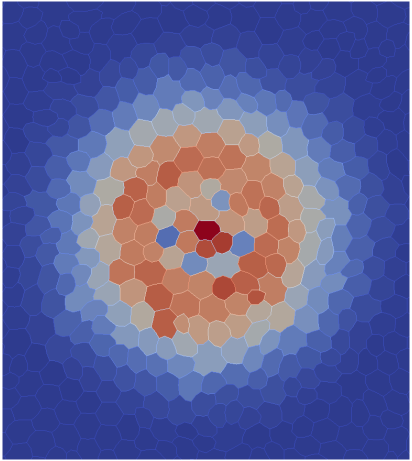
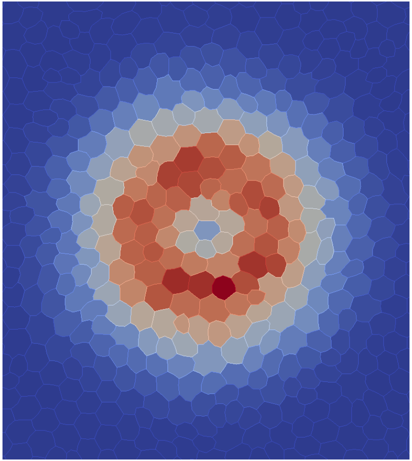
Energy error & simple polygonal estimate



Estimated error distribution



Exact error distribution

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

How large is the overall error?

h	m
h_0	1

How large is the overall error?

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

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

How large is the overall error? (model pb, known sol.)

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

How large is the overall error? (model pb, known sol.)

h	m	$\eta(p_h)$	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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$\approx h_0/4$		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
$\approx h_0/2$	2	4.23×10^{-2}	9.5×10^{-1}%	4.07×10^{-2}	9.2×10^{-1}%	1.04
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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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Outline

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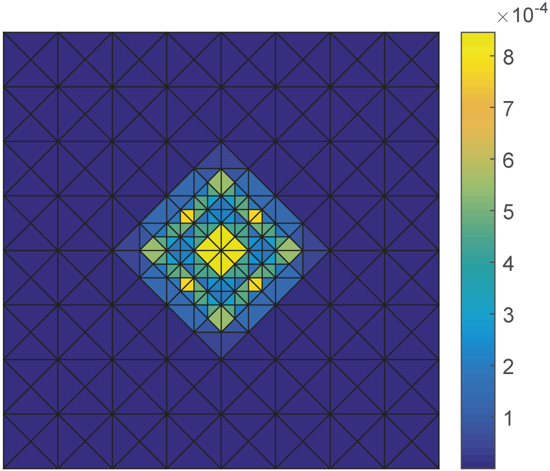
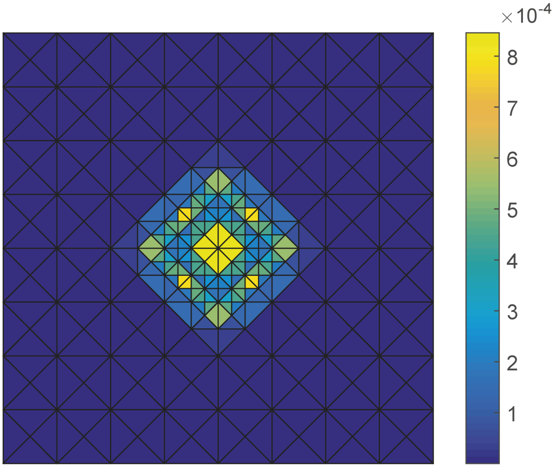
Where (in space) is the error localized?



Estimated error distribution $\eta_K(p_h)$



Exact error distribution $\|\nabla(p - p_h)\|_K$

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Adaptive mesh refinement (linear problem with exact solvers)

Adaptive mesh refinement

- Dörfler marking: subset $\mathcal{M}_\ell$ containing θ-fraction of the estimated error

$$\sum_{K\in\mathcal{M}_\ell} \eta_K(p_\ell)^2 \geq \theta^2 \sum_{K\in\mathcal{T}_\ell} \eta_K(p_\ell)^2$$

Convergence on a sequence of adaptively refined meshes

- $$\|\nabla(p-p_\ell)\| \to 0$$
- some mesh elements may not be refined at all: ~~$h \searrow 0$~~
- Babuška & Miller (1987), Dörfler (1996)

Optimal error decay rate wrt degrees of freedom

- $$\|\nabla(p-p_\ell)\| \lesssim |\mathrm{DoF}_\ell|^{-m/d} \qquad \text{(replaces } h^m\text{)}$$
- same for smooth & singular solutions: ~~higher-order only pay-off for sm. sol.~~
- decays to zero as fast as on a best-possible sequence of meshes
- Morin, Nochetto, Siebert (2000), Stevenson (2005, 2007), Cascón, Kreuzer, Nochetto, Siebert (2008), Canuto, Nochetto, Stevenson, Verani (2017)

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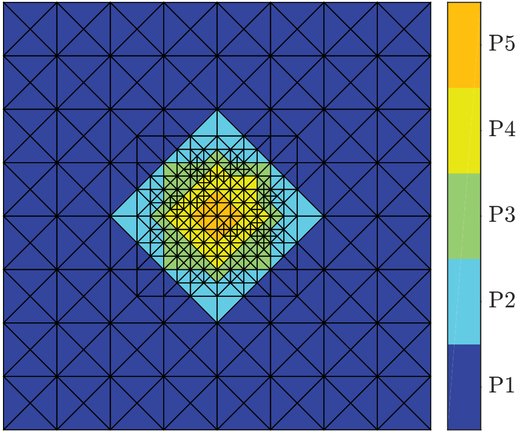
Can we decrease the error efficiently? *hp* adaptivity, (**smooth** solution)



Mesh $\mathcal{T}_\ell$ and pol. degrees m_K

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

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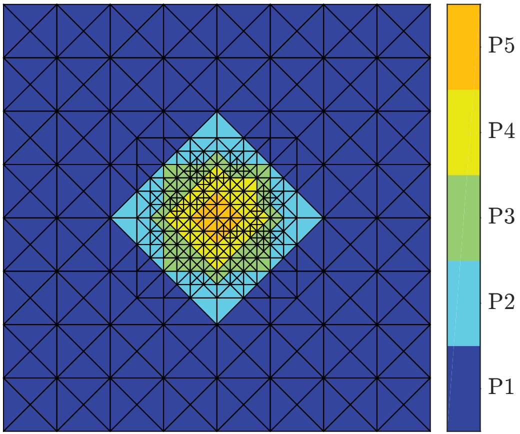

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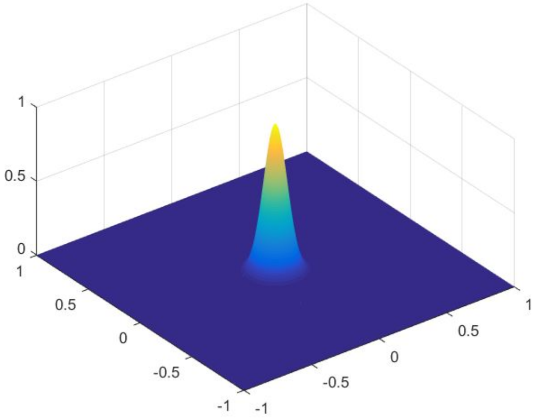

Exact solution

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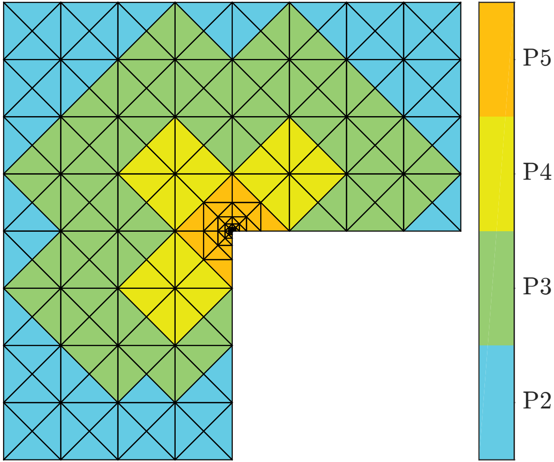
Can we decrease the error efficiently? *hp* adaptivity, (**singular** solution)



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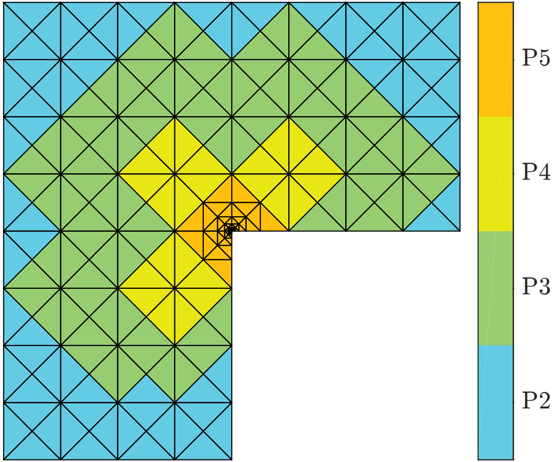

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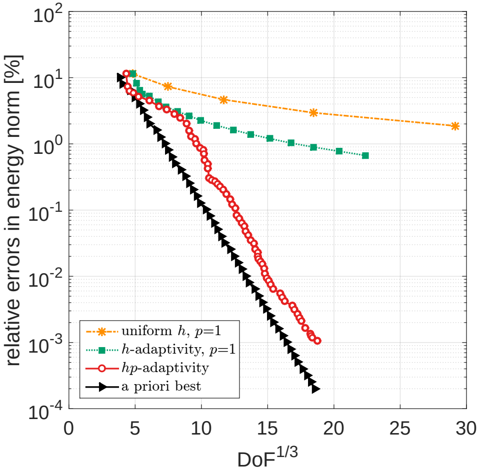

Relative error as a function of DoF

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

Outline

Balancing error components (nonlinear problem with inexact solvers)

Fully adaptive algorithm (adaptive inexact Newton method)

- **total error estimate** on mesh $\mathcal{T}_\ell$, linearization step k, algebraic solver step i

$$\underbrace{\|p - p_\ell^{k,i}\|_*}_{\text{total error}} \le \underbrace{\eta_{\ell,\mathrm{disc}}^{k,i}}_{\text{discretization estimate}} + \underbrace{\eta_{\ell,\mathrm{lin}}^{k,i}}_{\text{linearization estimate}} + \underbrace{\eta_{\ell,\mathrm{alg}}^{k,i}}_{\text{algebraic estimate}}$$

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- Gantner, Haberl, Praetorius, & Stiftner (2018), Heid & Wihler (2019)

Optimal error decay rate wrt overall computational cost

- Haberl, Praetorius, Schimanko, & Vohralík (preprint, 2020)

Balancing error components (nonlinear problem with inexact solvers)

Fully adaptive algorithm (**adaptive** inexact Newton method)

- **total error estimate** on mesh $\mathcal{T}_\ell$, linearization step k, algebraic solver step i

$$\underbrace{\|p - p_\ell^{k,i}\|_*}_{\text{total error}} \leq \underbrace{\eta_{\ell,\mathrm{disc}}^{k,i}}_{\text{discretization estimate}} + \underbrace{\eta_{\ell,\mathrm{lin}}^{k,i}}_{\text{linearization estimate}} + \underbrace{\eta_{\ell,\mathrm{alg}}^{k,i}}_{\text{algebraic estimate}}$$

- **balancing error components**: work where needed

$\eta_{\ell,\mathrm{alg}}^{k,i} \leq \gamma_{\mathrm{alg}} \max\{\eta_{\ell,\mathrm{disc}}^{k,i}, \eta_{\ell,\mathrm{lin}}^{k,i}\}$	stopping criterion linear solver,
$\eta_{\ell,\mathrm{lin}}^{k,i} \leq \gamma_{\mathrm{lin}} \eta_{\mathrm{disc}}^{k,i}$	stopping criterion nonlinear solver,
$\theta \eta_{\ell,\mathrm{disc}}^{k,i} \leq \eta_{\mathrm{disc},\mathcal{M}_\ell}^{k,i}$	adaptive mesh refinement

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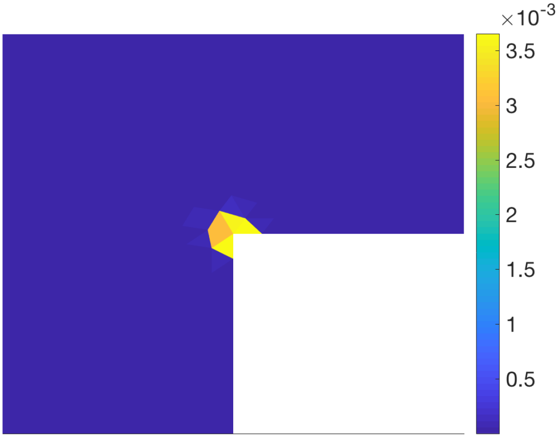
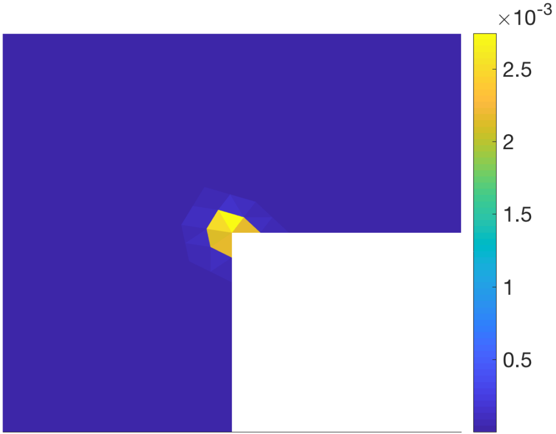


Estimated total errors $\eta_K(p_\ell^i)$



Exact total errors $\|\nabla(p - p_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth (2020)

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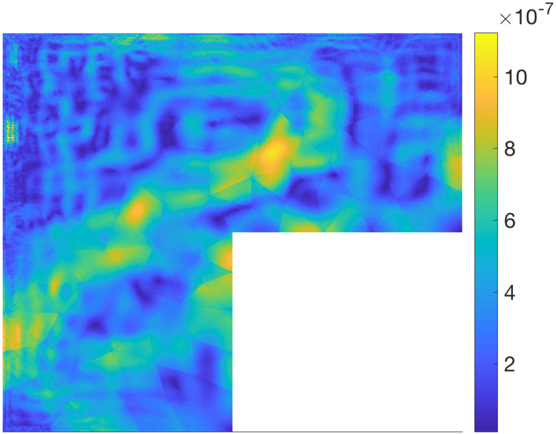
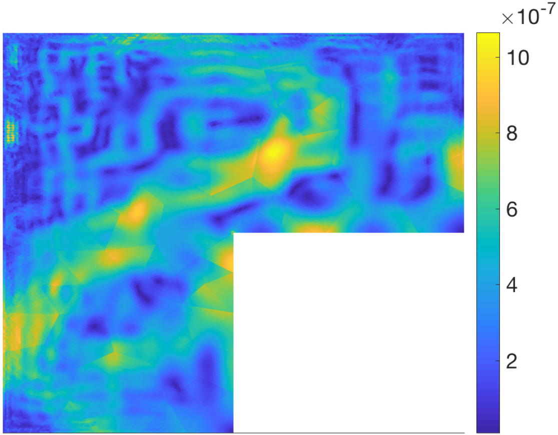


Estimated algebraic errors $\eta_{\mathrm{alg},K}(p_\ell^i)$



Exact algebraic errors $\|\nabla(p_\ell - p_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth (2020)

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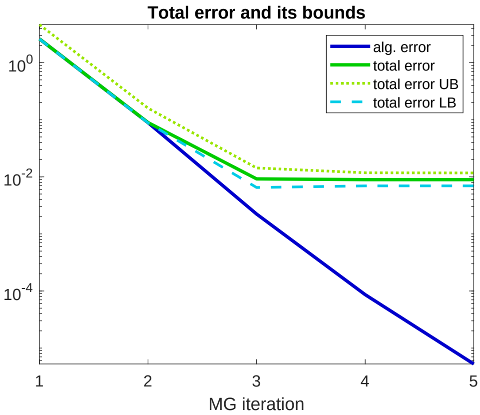
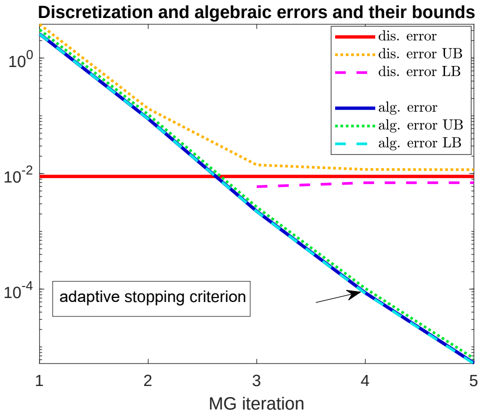


Total error



Error components and adaptive st. crit.

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth (2020)

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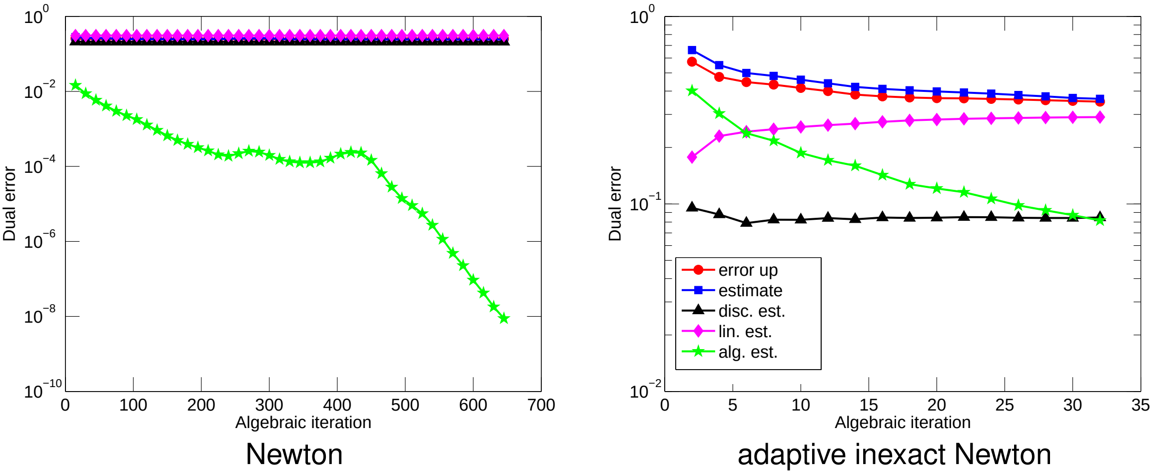

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

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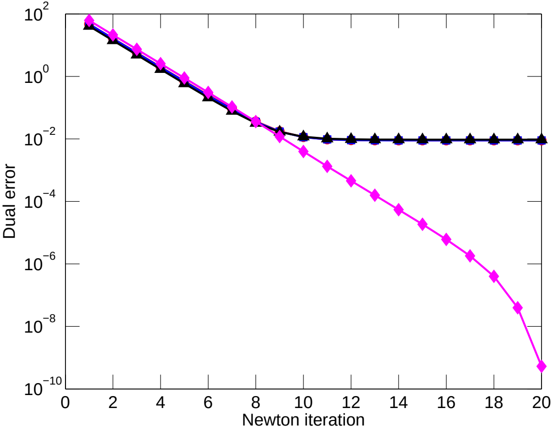
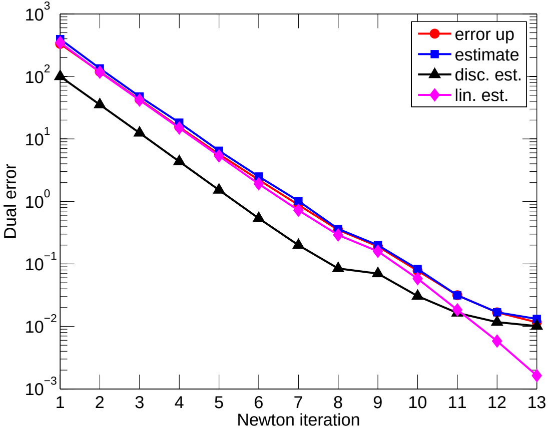


Newton



adaptive inexact Newton

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

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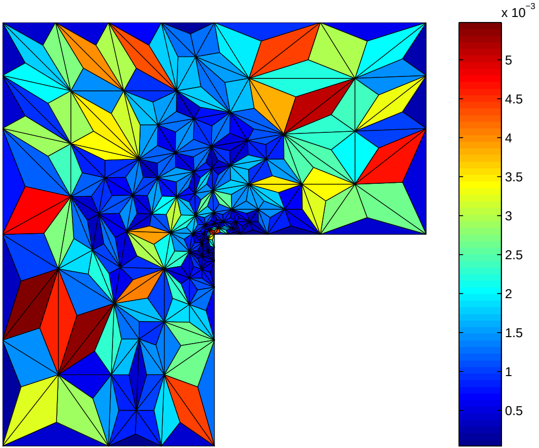

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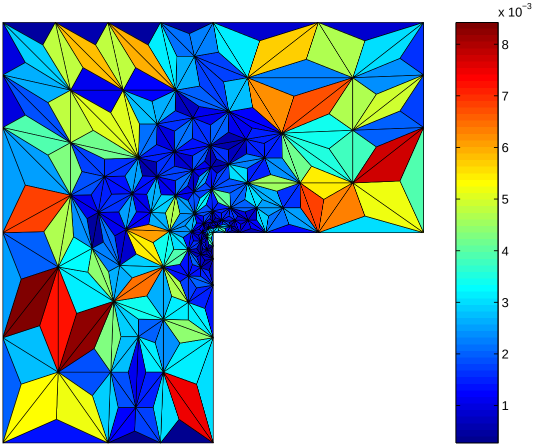
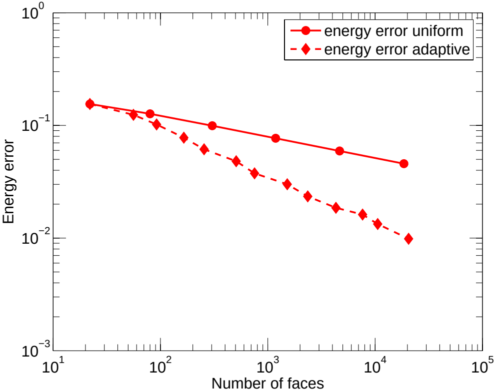


Exact errors $\|\boldsymbol{\sigma}(\nabla p) - \boldsymbol{\sigma}(\nabla p_\ell^{k,i})\|_{q,K}$

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

Convergence and optimal decay rate wrt DoFs & computational cost



Optimal decay rate wrt DoFs

classical	total alg. solver iterations	10890
	relative error estimate	4.6%

adaptive	total alg. solver iterations	242
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A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

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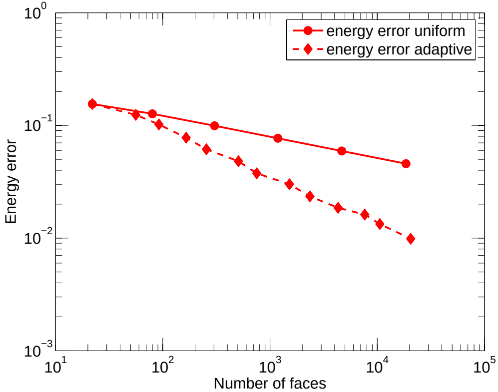

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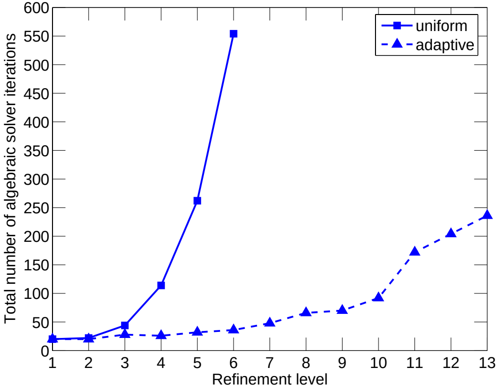

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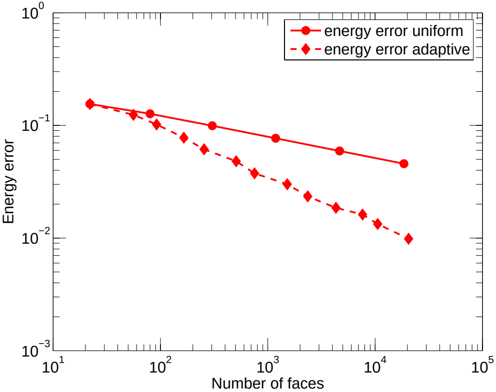

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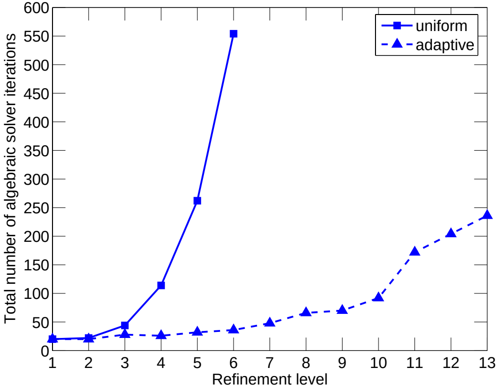

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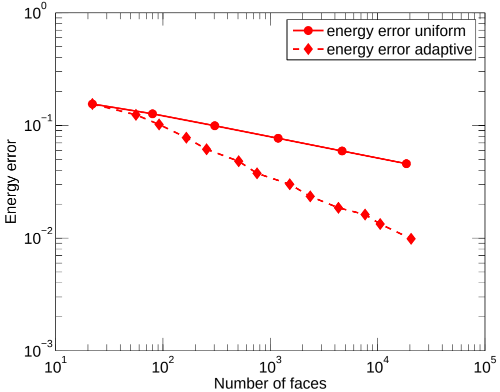

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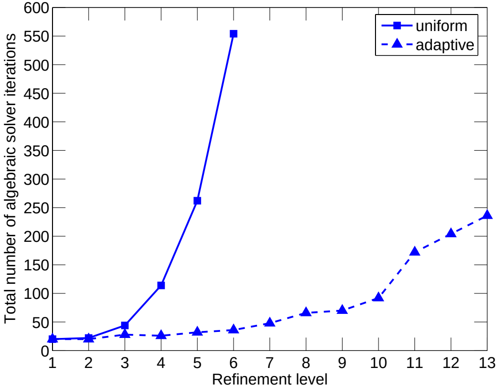

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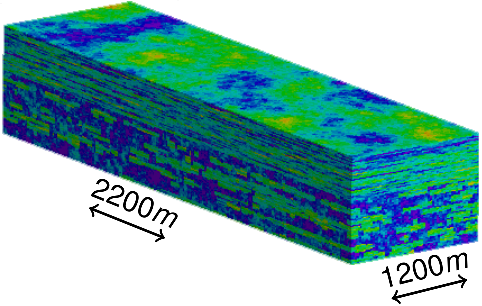
Outline

Can we certify error in a practical case $-\nabla\cdot(\mathbf{K}\nabla p) = f$: outflow error $\left|\int_{y=2200} \mathbf{K}\nabla(p - p_\ell)\cdot\mathbf{n}\right|$ (goal functional)

no of unknowns	825	3300	13200
rel. error est.	46%	34%	24%



Underground reservoir,
10th SPE test case

G. Mallik, M. Vohralík, S. Yousef, Journal of Computational and Applied Mathematics (2019)

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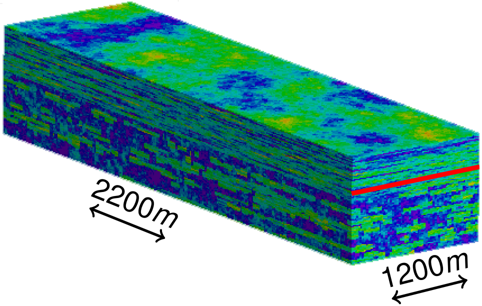

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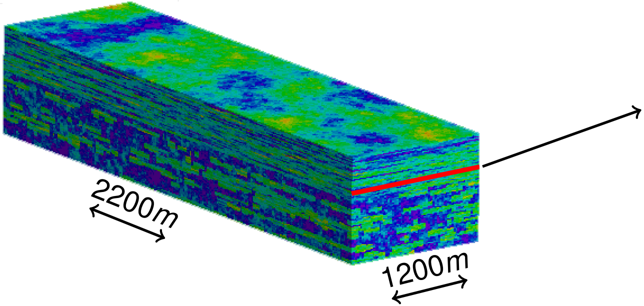

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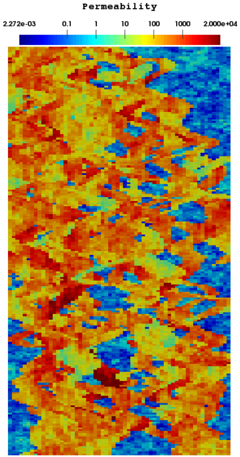

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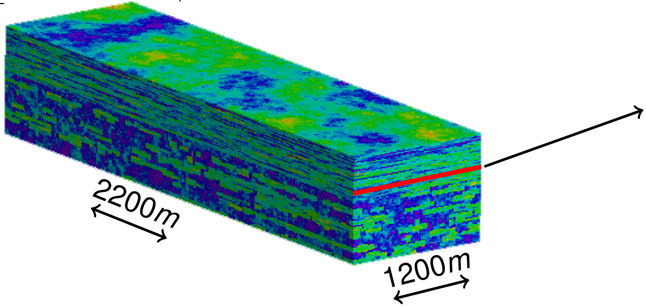

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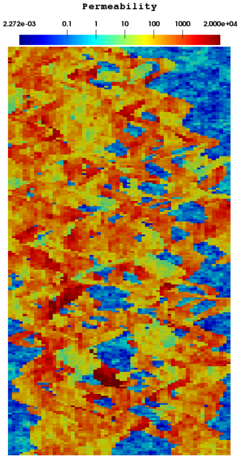

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Outline

Two-phase flow

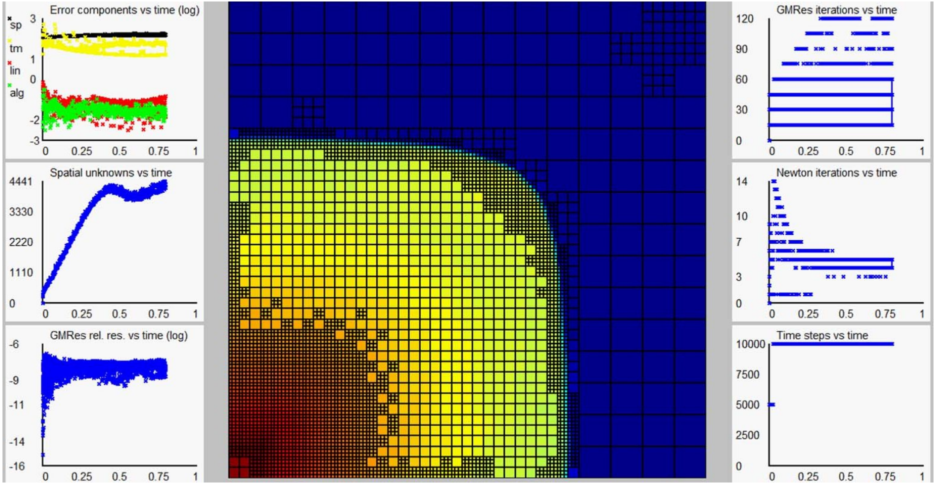
Incompressible two-phase flow in porous media

Find *saturations* s_α and *pressures* p_α, $\alpha \in \{\mathrm{g}, \mathrm{w}\}$, such that

$$\begin{aligned} \partial_t(\phi s_\alpha) - \nabla\cdot\left(\frac{k_{\mathrm{r},\alpha}(s_{\mathrm{w}})}{\mu_\alpha}\mathbf{K}(\nabla p_\alpha + \rho_\alpha g \nabla z)\right) &= q_\alpha, \qquad \alpha \in \{\mathrm{g}, \mathrm{w}\},\\ s_{\mathrm{g}} + s_{\mathrm{w}} &= 1,\\ p_{\mathrm{g}} - p_{\mathrm{w}} &= p_{\mathrm{c}}(s_{\mathrm{w}}) \end{aligned}$$

- unsteady, nonlinear, and degenerate problem
- coupled system of PDEs & algebraic constraints
- sharp evolving fronts

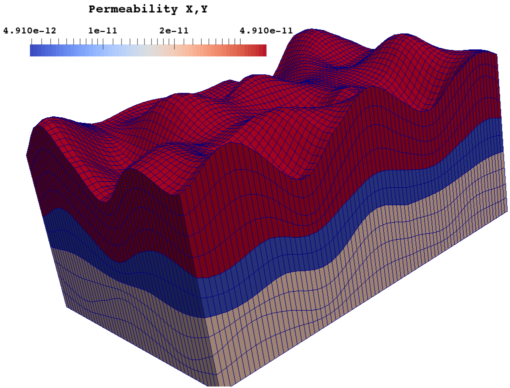
Space/time/nonlinear solver/linear solver adaptivity

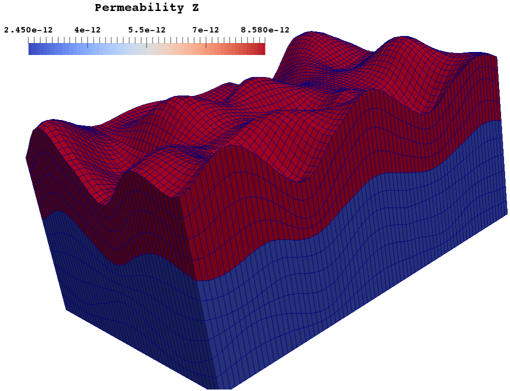


Fully adaptive computation

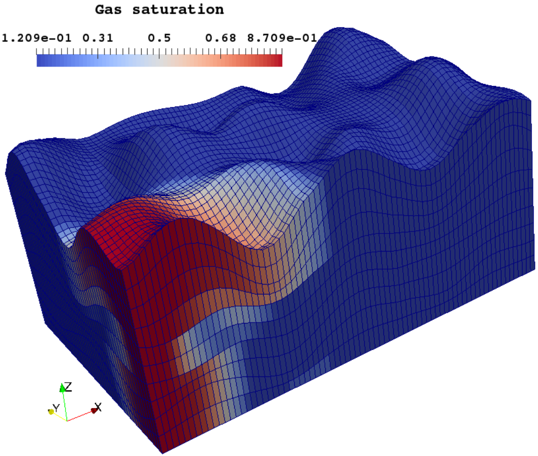
M. Vohralík, M.-F. Wheeler, Computational Geosciences (2013)

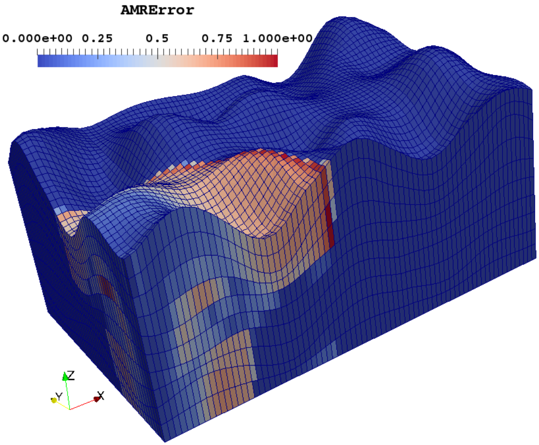
3 phases, 3 components (black-oil) problem: permeability



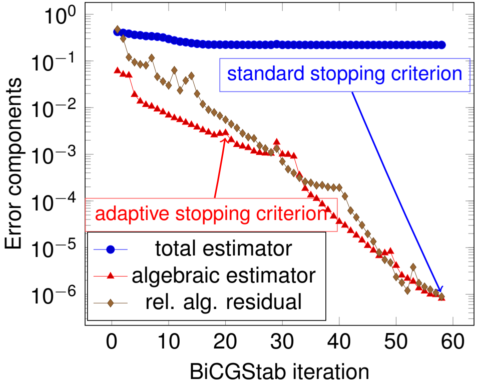


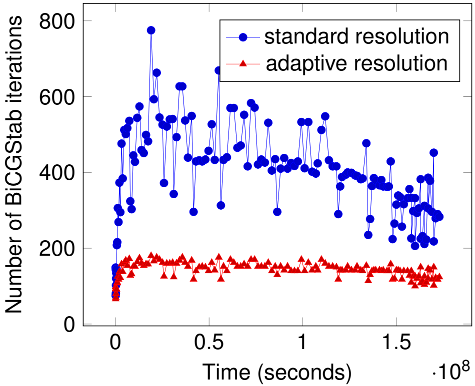
3 phases, 3 components (black-oil) problem: gas saturation and a posteriori estimate





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

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

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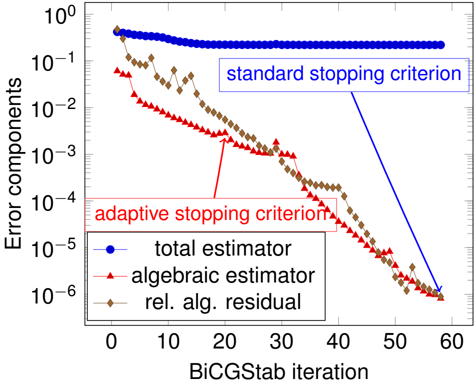

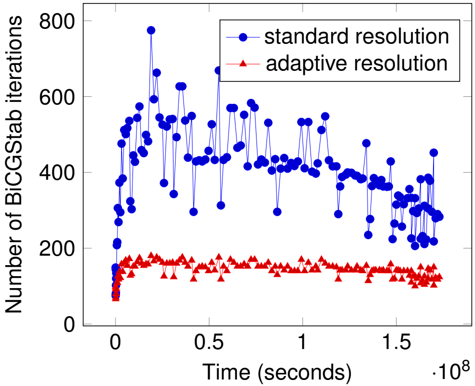

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- **full adaptivity**: linear solver, nonlinear solver, time step, space mesh (*hp*)
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Ongoing work

- convergence and optimality proofs
- application to challenging porous media problems

Thank you for your attention!

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