A posteriori error estimates robust with respect to nonlinearities and final time

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Outline

Modelling flow of water and air through soil

The Richards equation

Find $u : \Omega \times (0, T) \to \mathbb{R}$ such that

$$\begin{aligned} \partial_t S(u) - \nabla\cdot[\boldsymbol{K}\kappa(S(u))(\nabla u + \boldsymbol{g})] &= f \quad \text{in } \Omega \times (0, T), \\ u &= 0 \quad \text{on } \partial\Omega \times (0, T), \\ (S(u))(0) &= s_0 \quad \text{in } \Omega. \end{aligned}$$

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Setting

- u: pressure
- $s = S(u)$: saturation
- $\Omega \subset \mathbb{R}^d$, $1 \le d \le 3$, open polytope with Lipschitz boundary $\partial\Omega$
- T: final time
- diffusion tensor $\boldsymbol{K}$, source term f, gravity $\boldsymbol{g}$, initial saturation s_0
- **nonlinear (degenerate) functions** S and κ

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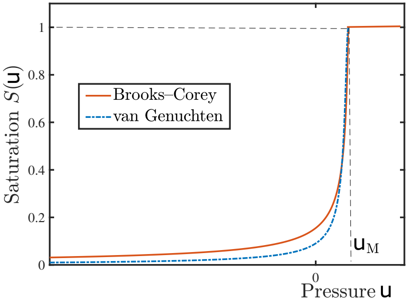

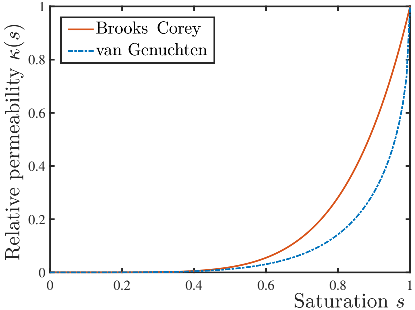

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- parabolic–hyperbolic: $\kappa(0) = 0$ leads to

$$\partial_t S(u) = f$$

- parabolic–elliptic: $S'(u) = 0$ for $u > u_{\mathrm{M}}$ leads to

$$-\nabla\cdot[\boldsymbol{K}\kappa(S(u))(\nabla u + \boldsymbol{g})] = f$$

A posteriori error estimates

Purpose

- provide sharp **computable bounds** on the unknown error between the unavailable exact solution and its numerical approximation
- predict the **error localization** (in space and in time)
- **adapt** the linear solver, the nonlinear solver, space mesh, time mesh ...

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Nonlinear problems

a posteriori error estimates

$$|||u - u_\ell||| \leq \eta(u_\ell)$$

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Guaranteed a posteriori error estimates **efficient**

$$|||u - u_\ell||| \le \eta(u_\ell) \le C_{\mathrm{eff}} |||u - u_\ell|||,$$

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Guaranteed a posteriori error estimates **efficient** and **robust** with respect to the **strength of nonlinearities**.

$$|||u - u_\ell||| \leq \eta(u_\ell) \leq C_{\mathrm{eff}} |||u - u_\ell|||, \quad C_{\mathrm{eff}} \text{ independent of nonlinearities}$$

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Guaranteed a posteriori error estimates **efficient** and **robust** with respect to the **strength of nonlinearities**.

$$|||u - u_\ell||| \leq \left\{ \sum_{K \in \mathcal{T}_\ell} \eta_K(u_\ell)^2 \right\}^{1/2} \leq C_{\mathrm{eff}} |||u - u_\ell|||,$$

Goals

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Guaranteed a posteriori error estimates **locally efficient** and **robust** with respect to the **strength of nonlinearities**.

$$\eta_K(u_\ell) \leq C_{\text{eff}} |||u - u_\ell|||_{\omega_K}, \qquad \text{for all } K \in \mathcal{T}_\ell$$

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Unsteady problems

Guaranteed a posteriori error estimates

$$\int_0^T |||u - u_\ell|||^2 \le \sum_{n=1}^{N} \sum_{K \in \mathcal{T}_\ell^n} \eta_K^n(u_\ell)^2$$

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Unsteady problems

Guaranteed a posteriori error estimates **locally space-time efficient** and **robust** with respect to the **final time**.

$$\eta_K^n(u_\ell)^2 \leq C_{\mathrm{eff}}^2 \int_{t^{n-1}}^{t^n} |||u - u_\ell|||_{\omega_K}^2, \quad \text{for all } n \text{ and } K \in \mathcal{T}_\ell^n$$

Outline

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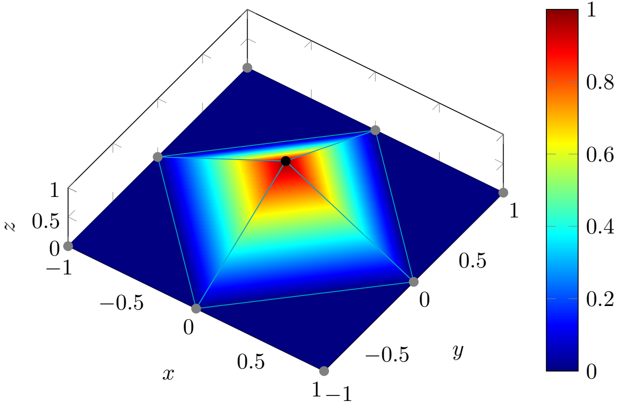
Partition of unity

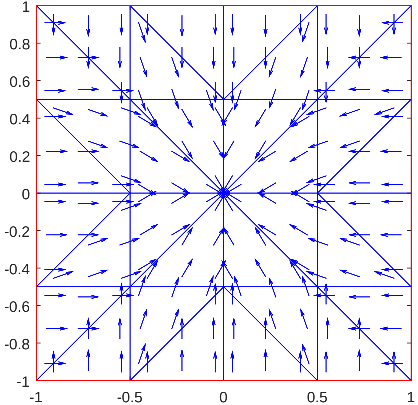
$$\sum_{\boldsymbol{a} \in \mathcal{V}_\ell} \psi^{\boldsymbol{a}} = 1$$



Hat basis function $\psi^{\boldsymbol{a}}$

Equilibrated flux reconstruction

Destuynder and Métivet (1998), Braess & Schöberl (2008), Ern & Vohralík (2013)



Flux $\boldsymbol{\iota}_\ell \notin \boldsymbol{H}(\mathrm{div})$ (e.g. FE flux $-\nabla u_\ell$)

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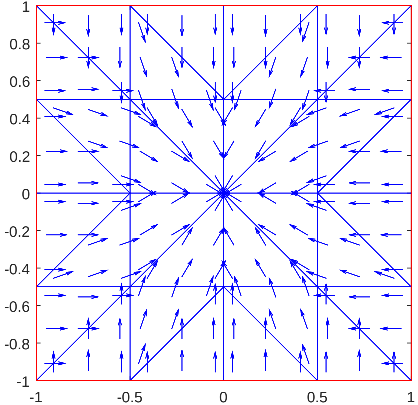

Flux $\boldsymbol{\iota}_\ell \notin \mathbf{H}(\mathrm{div})$, $\nabla\cdot\boldsymbol{\iota}_\ell \neq f$

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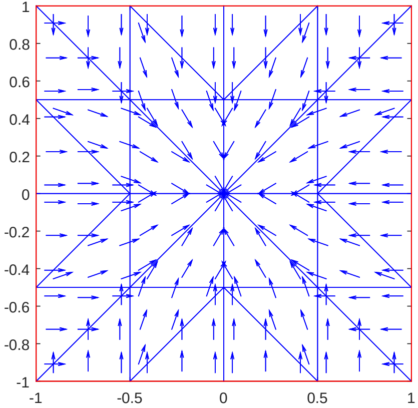

Flux $\boldsymbol{\iota}_\ell \notin \boldsymbol{H}(\mathrm{div})$, $\nabla\cdot\boldsymbol{\iota}_\ell \neq f$

$$\underbrace{\boldsymbol{\iota}_\ell \in \boldsymbol{\mathcal{RT}}_p(\mathcal{T}_\ell), f \in \mathcal{P}_p(\mathcal{T}_\ell)}$$

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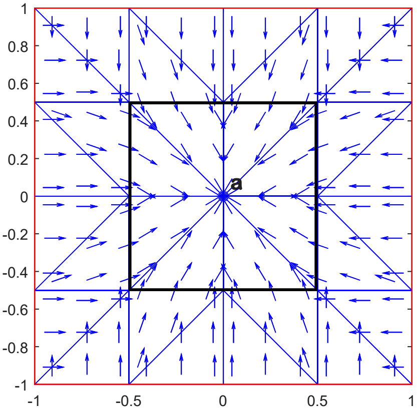

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$$\underbrace{\boldsymbol{\iota}_\ell \in \mathcal{RT}_p(\mathcal{T}_\ell),\, f \in \mathcal{P}_p(\mathcal{T}_\ell)}_{(f,\psi^{\mathbf{a}})_{\omega_{\mathbf{a}}}+(\boldsymbol{\iota}_\ell,\nabla\psi^{\mathbf{a}})_{\omega_{\mathbf{a}}}=0\ \forall \mathbf{a}\in\mathcal{V}_\ell^{\mathrm{int}}}$$

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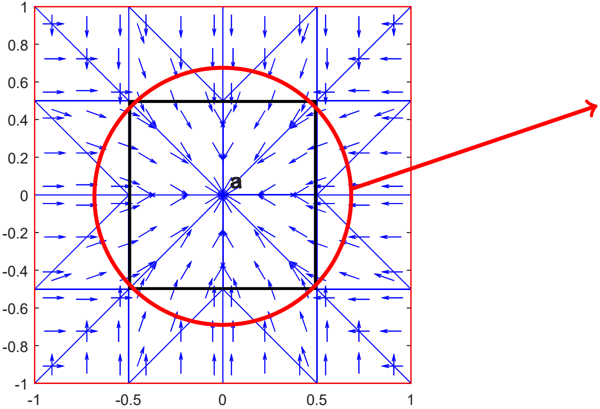

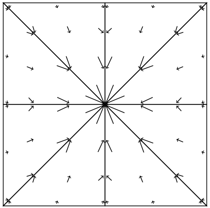

$\psi^{\boldsymbol{a}} \boldsymbol{\iota}_\ell$

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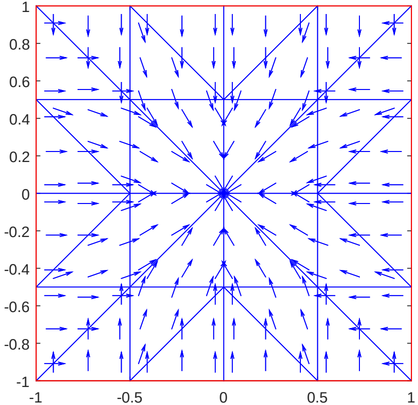

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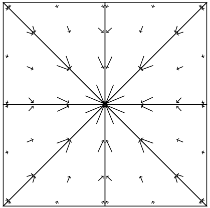

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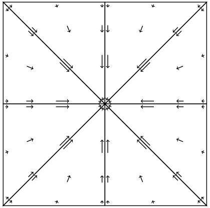

$\sigma_\ell^{\mathbf{a}}$

$$\underbrace{\iota_\ell \in \mathcal{RT}_p(\mathcal{T}_\ell),\, f \in \mathcal{P}_p(\mathcal{T}_\ell)} \qquad \sigma_\ell^{\mathbf{a}} := \arg \min_{\substack{\mathbf{v}_\ell \in \mathcal{RT}_{p+1}(\mathcal{T}_{\mathbf{a}}) \cap \mathbf{H}_0(\mathrm{div},\omega_{\mathbf{a}}) \\ \nabla\cdot\mathbf{v}_\ell = f\psi^{\mathbf{a}} + \iota_\ell\cdot\nabla\psi^{\mathbf{a}}}} \|\psi^{\mathbf{a}}\iota_\ell - \mathbf{v}_\ell\|^2_{\omega_{\mathbf{a}}}$$

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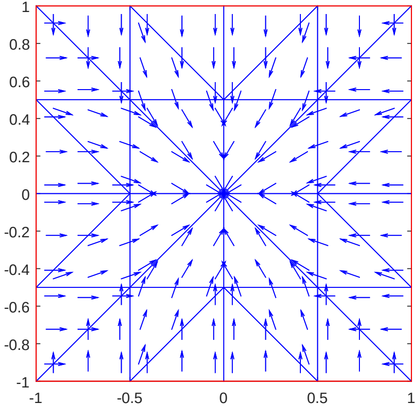

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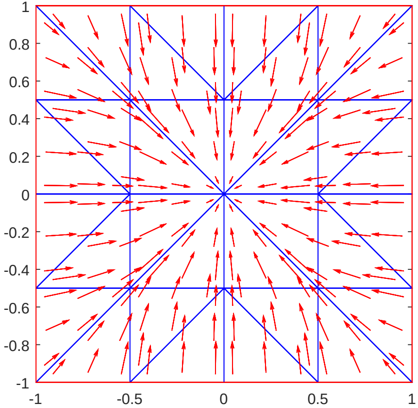

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$$\underbrace{\boldsymbol{\iota}_\ell \in \mathcal{RT}_p(\mathcal{T}_\ell), f \in \mathcal{P}_p(\mathcal{T}_\ell)} \to \boldsymbol{\sigma}_\ell := \sum_{\boldsymbol{a}\in\mathcal{V}_\ell} \boldsymbol{\sigma}_\ell^{\boldsymbol{a}} \in \mathcal{RT}_{p+1}(\mathcal{T}_\ell) \cap \boldsymbol{H}(\mathrm{div}), \nabla\cdot\boldsymbol{\sigma}_\ell = f$$

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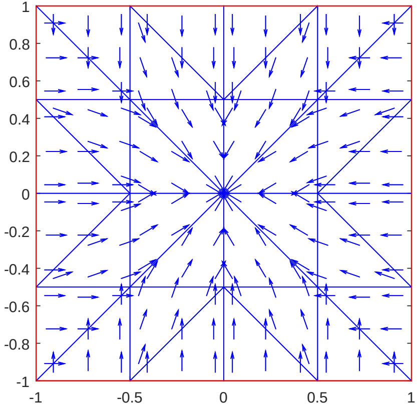

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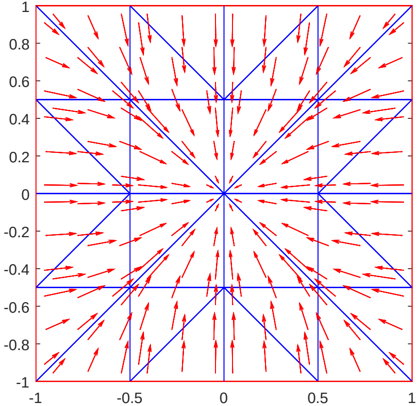

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Use

- **a posteriori error estimates**
  - comparison of the original & reconstructed flux $\|\nabla u_\ell + \sigma_\ell\|$: discretization error
  - error component fluxes: linearization and algebraic errors
- recovery of **mass conservative fluxes**
  - local on patches of mesh elements from FE-type approximations
  - local on elements from FV- & DG-type approximations
  - inexact nonlinear solvers (still local)
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How **large** is the error? (steady linear Darcy, known solution)

$h \approx 1/\lvert\mathcal{T}_\ell\rvert^{\frac{1}{2}}$	p	relative error estimate $\frac{\eta(u_\ell)}{\lVert\nabla u_\ell\rVert}$	relative error $\frac{\lVert\nabla(u-u_\ell)\rVert}{\lVert\nabla u_\ell\rVert}$	effectivity index $\frac{\eta(u_\ell)}{\lVert\nabla(u-u_\ell)\rVert}$
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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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How **large** is the error? (steady linear Darcy, known solution)

$h \approx 1/\lvert\mathcal{T}_\ell\rvert^{\frac{1}{2}}$	p	relative error estimate $\frac{\eta(u_\ell)}{\lVert\nabla u_\ell\rVert}$	relative error $\frac{\lVert\nabla(u-u_\ell)\rVert}{\lVert\nabla u_\ell\rVert}$	effectivity index $\frac{\eta(u_\ell)}{\lVert\nabla(u-u_\ell)\rVert}$
h_0	1	28%	24%	**1.17**
$\approx h_0/2$		14%	13%	**1.09**
$\approx h_0/4$		7.0%	6.6%	**1.06**
$\approx h_0/8$		3.3%	3.1%	**1.04**
$\approx h_0/2$	2	9.5×10^{-1}%	9.2×10^{-1}%	**1.04**
$\approx h_0/4$	3	5.9×10^{-3}%	5.9×10^{-3}%	**1.01**
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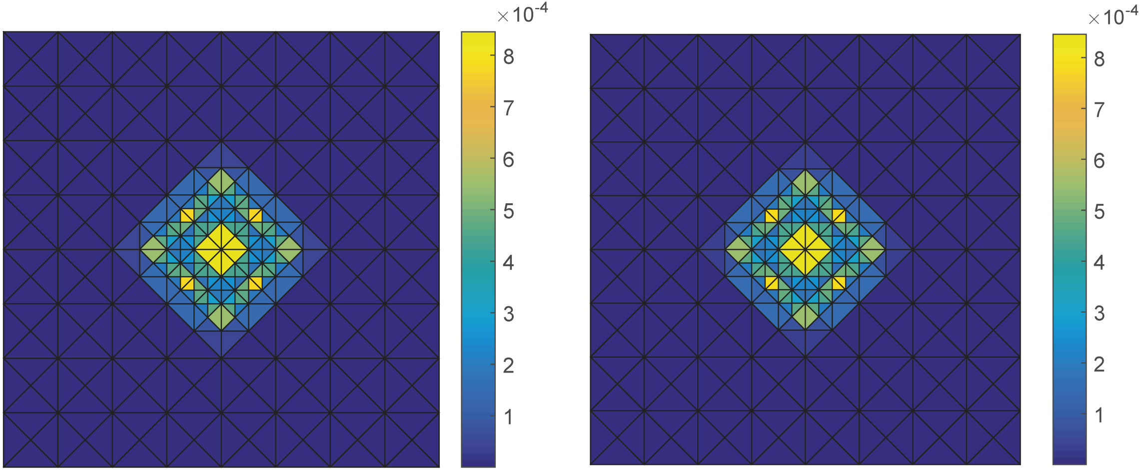
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

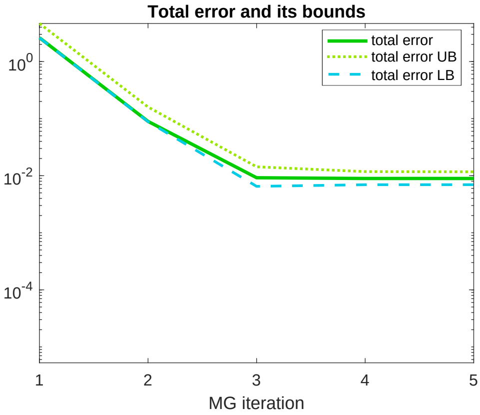
Where (in space) is the error **localized**? (steady linear Darcy)



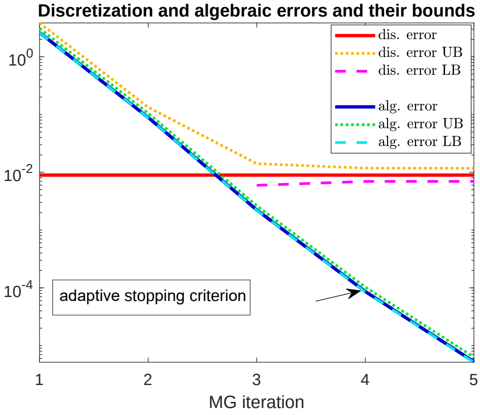
Estimated local error $\eta_K(u_\ell) = \|\nabla u_\ell + \boldsymbol{\sigma}_\ell\|_K$ Exact local error $\|\nabla(u - u_\ell)\|_K$

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

How **large** is the total error and its components? ($\mathbb{A}_\ell \mathsf{U}_\ell^i \neq \mathsf{F}_\ell$)



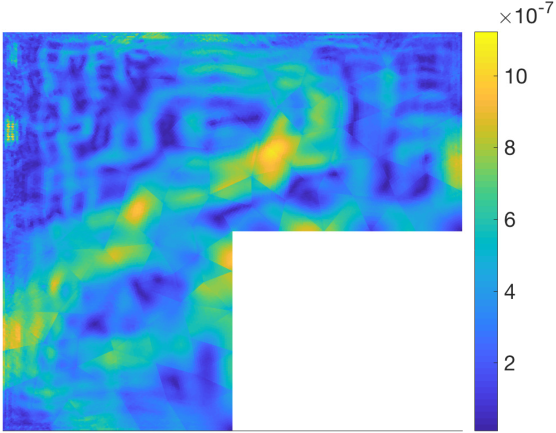
Total error



Error components and stopping criteria

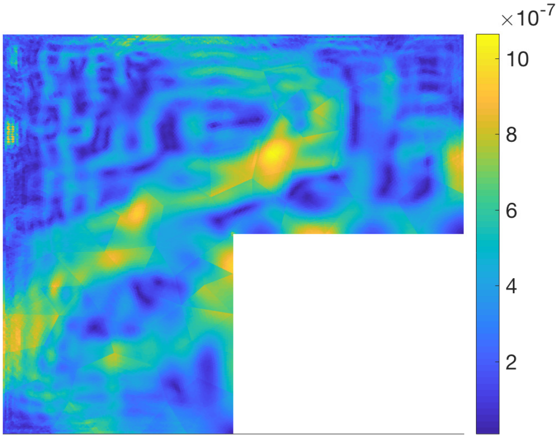
J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

Where (in space) is the algebraic error **localized**? ($\mathbb{A}_\ell U_\ell^i \neq F_\ell$)



Estimated local algebraic errors

$\eta_{\mathrm{alg},K}(u_\ell^i) = \|\boldsymbol{\sigma}_{\mathrm{alg},\ell}^i\|_K$



Exact local algebraic errors

$\|\nabla(u_\ell - u_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

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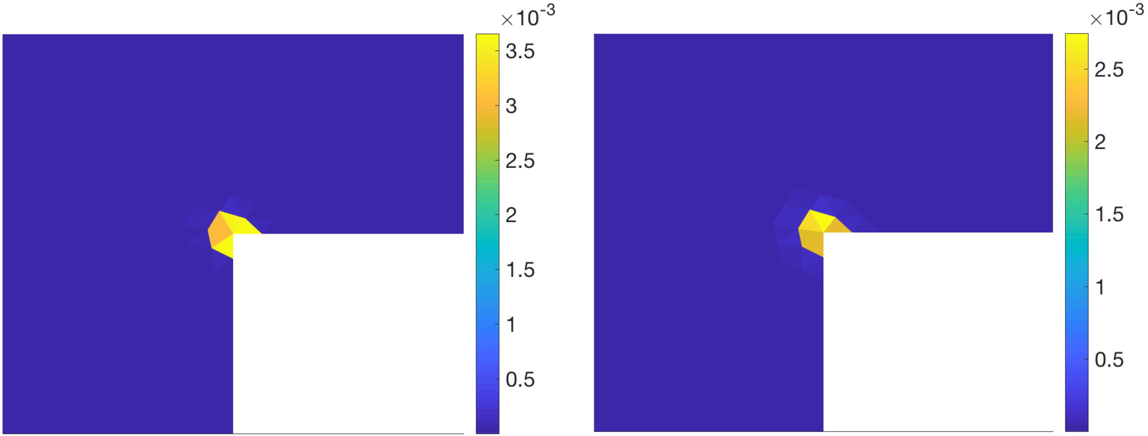


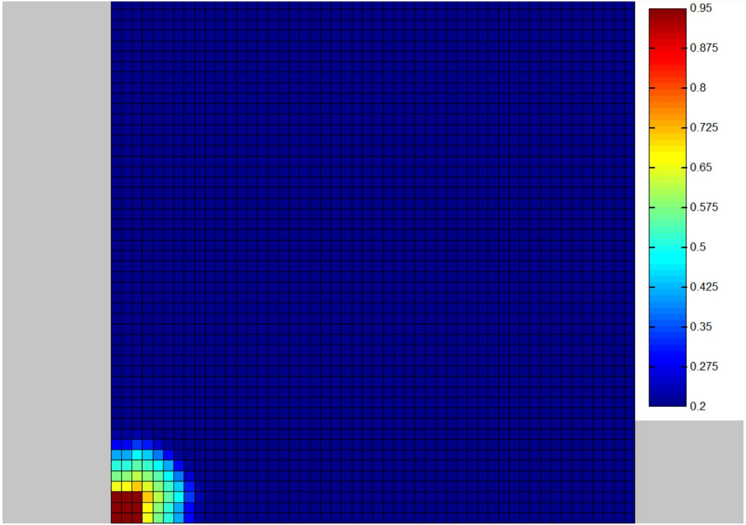
Estimated local total errors
$\eta_K(u_\ell^i) = \|\nabla u_\ell + \boldsymbol{\sigma}_\ell^i\|_K$

Exact local total errors
$\|\nabla(u - u_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

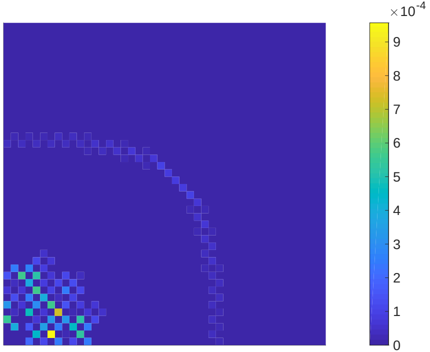
Outline

Two-phase flow, water saturation

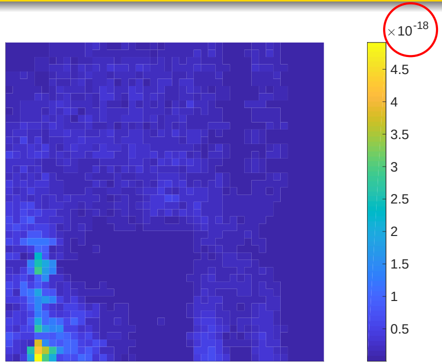


M. Vohralík, M. Wheeler, Computational Geosciences (2013)

Recovering mass balance: two-phase flow (inexact solver, water)



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



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Setting

- fully implicit discretization of a two-phase oil–water flow
- cell-centered finite volumes on a square mesh
- time step 260, 1st Newton linearization, GMRes iteration 195

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

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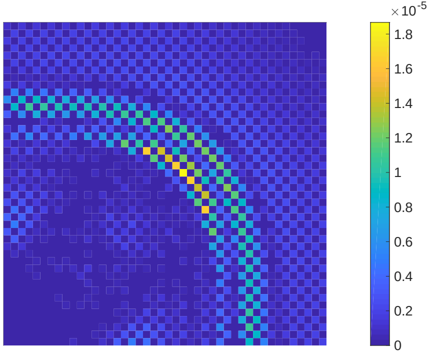

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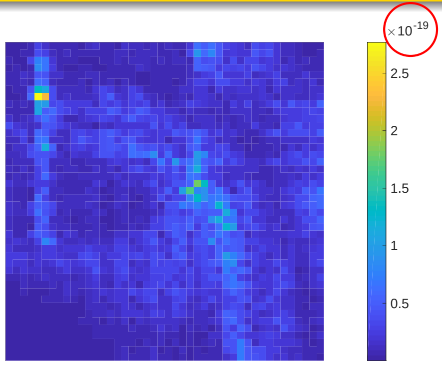

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J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

Outline

Outline

A model steady nonlinear problem

Nonlinear elliptic problem

Find $u : \Omega \to \mathbb{R}$ such that

$$\begin{aligned} -\nabla\cdot(a(|\nabla u|)\nabla u) &= f \quad \text{in} \quad \Omega, \\ u &= 0 \quad \text{on} \quad \partial\Omega. \end{aligned}$$

- $\Omega \subset \mathbb{R}^d$, $1 \leq d \leq 3$, open polytope with Lipschitz boundary $\partial\Omega$
- f piecewise polynomial for simplicity

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- f piecewise polynomial for simplicity

Assumption (Nonlinear function a)

Function $a : [0,\infty) \to (0,\infty)$, *for all* $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$,

$$
\begin{aligned}
|a(|\boldsymbol{x}|)\boldsymbol{x} - a(|\boldsymbol{y}|)\boldsymbol{y}| &\le a_{\mathrm{c}}|\boldsymbol{x} - \boldsymbol{y}| && \text{(Lipschitz continuity)},\\
(a(|\boldsymbol{x}|)\boldsymbol{x} - a(|\boldsymbol{y}|)\boldsymbol{y}) \cdot (\boldsymbol{x} - \boldsymbol{y}) &\ge a_{\mathrm{m}}|\boldsymbol{x} - \boldsymbol{y}|^2 && \text{(strong monotonicity)}.
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$$

- $a_{\rm m} \le a(r) \le a_{\rm c}$, $a_{\rm m} \le (a(r)r)' \le a_{\rm c}$

Example of the nonlinear function a

Example (Mean curvature nonlinearity)

$$a(r) := a_{\mathrm{m}} + \frac{a_{\mathrm{c}} - a_{\mathrm{m}}}{\sqrt{1 + r^2}}.$$

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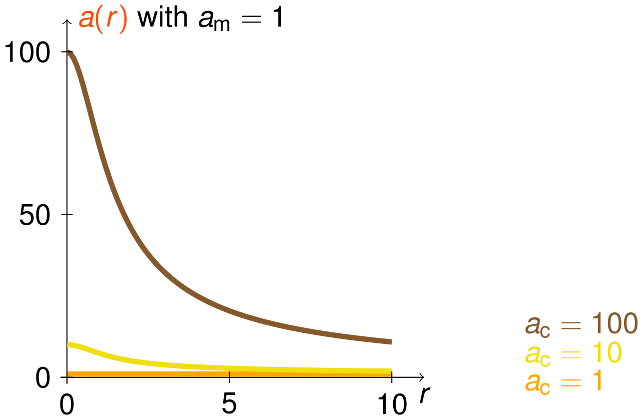

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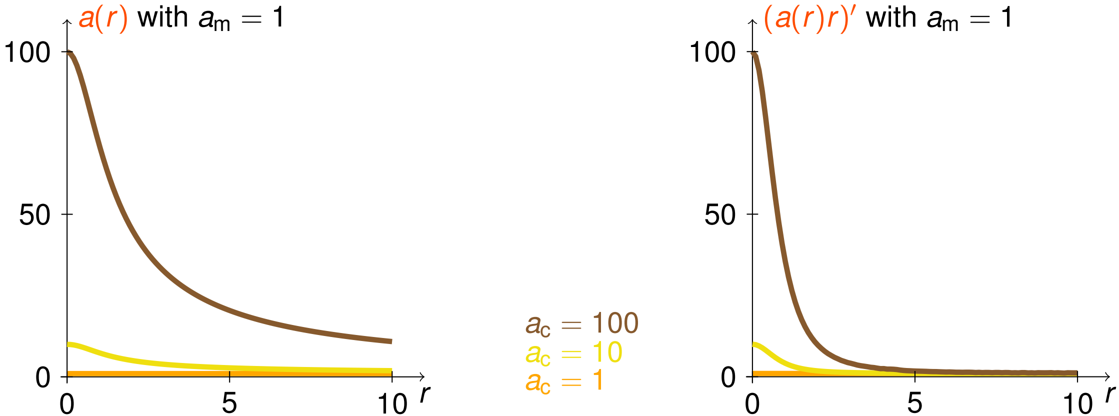

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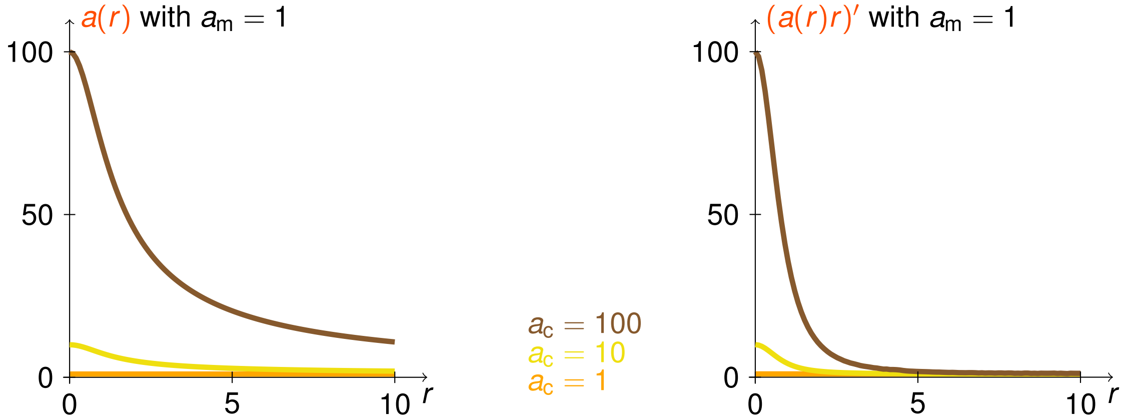
Strength of the nonlinearity

$$\frac{a_{\mathrm{c}}}{a_{\mathrm{m}}} = \frac{\text{Lipschitz continuity}}{\text{strong monotonicity}}$$



Weak solution

Definition (Weak solution)

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

$$(a(|\nabla u|)\nabla u, \nabla v) = (f, v) \qquad \forall v \in H_0^1(\Omega).$$

Energy

Definition (Energy functional)

$\mathcal{J} : H_0^1(\Omega) \to \mathbb{R}$

$$\mathcal{J}(v) := \int_\Omega \phi(|\nabla v|) - (f, v), \quad v \in H_0^1(\Omega),$$

with function $\phi : [0, \infty) \to [0, \infty)$ such that, for all $r \in [0, \infty)$,

$$\phi(r) := \int_0^r a(s) s \, \mathrm{d}s.$$

Equivalently

$$u = \arg \min_{v \in H_0^1(\Omega)} \mathcal{J}(v)$$

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Finite element approximation

Definition (Finite element approximation)

$u_\ell \in V_\ell^p$ such that

$$(a(|\nabla u_\ell|)\nabla u_\ell, \nabla v_\ell) = (f, v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

- $\mathcal{T}_\ell$ simplicial mesh of Ω
- $p \geq 1$ polynomial degree
- $V_\ell^p := \mathcal{P}_p(\mathcal{T}_\ell) \cap H_0^1(\Omega)$
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Energy difference

Energy difference

$$\boxed{\mathcal{J}(u_\ell) - \mathcal{J}(u)}$$

- $\mathcal{J}(u_\ell) - \mathcal{J}(u) \geq 0$, $\mathcal{J}(u_\ell) - \mathcal{J}(u) = 0$ if and only if $u_\ell = u$
- physically-based error measure

Previous results

Sobolev norm (not robust wrt $\frac{a_c}{a_m}$)

$$a_m \|\nabla(u_\ell - u)\| \le \eta(u_\ell) \le C_{\rm eff} a_c \|\nabla(u_\ell - u)\|$$

- Pousin & Rappaz (1994), Verfürth (1994), Kim (2007), Houston, Süli, & Wihler (2008), Garau, Morin, & Zuppa (2011), Gantner, Haberl, Praetorius, & Stiftner (2018), Heid & Wihler (2020), ...

Energy difference

$$\mathcal{J}(u_\ell) - \mathcal{J}(u) \le \eta(u_\ell)^2 \le C_{\rm eff}^2 \frac{a_c^2}{a_m^2} (\mathcal{J}(u_\ell) - \mathcal{J}(u))$$

Dual norm of the residual

$$|||\mathcal{R}(u_\ell)|||_{-1} \le \eta(u_\ell) \le C_{\rm eff} |||\mathcal{R}(u_\ell)|||_{-1}$$

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Energy difference (**not robust** wrt $\frac{a_{\mathrm{c}}}{a_{\mathrm{m}}}$)

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Dual norm of the residual (robust wrt $\frac{a_{\mathrm{c}}}{a_{\mathrm{m}}}$)

$$|||\mathcal{R}(u_\ell)|||_{-1} \le \eta(u_\ell) \le C_{\mathrm{eff}}|||\mathcal{R}(u_\ell)|||_{-1}$$

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Iterative linearization

Need to solve a nonlinear system

$$\mathcal{A}_\ell(\mathsf{U}_\ell) = \mathsf{F}_\ell$$

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Definition (Linearized finite element approximation)

$u_\ell^k \in V_\ell^p$ such that

$$(\boldsymbol{A}_\ell^{k-1} \nabla u_\ell^k, \nabla v_\ell) = (f, v_\ell) + (\boldsymbol{b}_\ell^{k-1}, \nabla v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

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- $u_\ell^0 \in V_\ell^p$ a given initial guess
- iterative linearization index $k \geq 1$
- **linearization**: $\boldsymbol{A}_\ell^{k-1}: \Omega \to \mathbb{R}^{d \times d}$ matrix, $\boldsymbol{b}_\ell^{k-1}: \Omega \to \mathbb{R}^d$ vector

Examples

Example (Picard (fixed-point))

$$\mathbf{A}_\ell^{k-1} = a(|\nabla u_\ell^{k-1}|)\mathbf{I}_d, \quad \mathbf{b}_\ell^{k-1} = \mathbf{0}.$$

Example (Zarantonello)

$$\mathbf{A}_\ell^{k-1} = \gamma \mathbf{I}_d, \quad \mathbf{b}_\ell^{k-1} = (\gamma - a(|\nabla u_\ell^{k-1}|))\nabla u_\ell^{k-1},$$

with $\gamma \geq \frac{a_c^2}{a_m}$ *a constant parameter.*

Example (Newton)

$$\mathbf{A}_\ell^{k-1} = a(|\nabla u_\ell^{k-1}|)\mathbf{I}_d + \frac{a'(|\nabla u_\ell^{k-1}|)}{|\nabla u_\ell^{k-1}|}\nabla u_\ell^{k-1} \otimes \nabla u_\ell^{k-1},$$

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None of the known approaches employs **in the analysis**, to define norms, the **iterative linearization**, i.e., **how** do we solve the nonlinear system $\mathcal{A}_\ell(\mathsf{U}_\ell) = \mathsf{F}_\ell$.

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Equivalently

$$u_\ell^k := \arg \min_{v_\ell \in V_\ell^p} \mathcal{J}_\ell^{k-1}(v_\ell)$$

Outline

A posteriori error estimates for an augmented energy difference

Theorem (A posteriori estimate of augmented energy)

For all linearization steps $k \geq 1$,
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- ✓ C_ℓ^k **computable**: we can affirm **robustness *a posteriori***, for the given case

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$$\mathcal{E}_\ell^k = \frac{1}{2}\text{energy difference} + \lambda_\ell^k \times \frac{1}{2}(\text{linearized energy difference})$$

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- λ_ℓ^k computable weight to make the two components comparable

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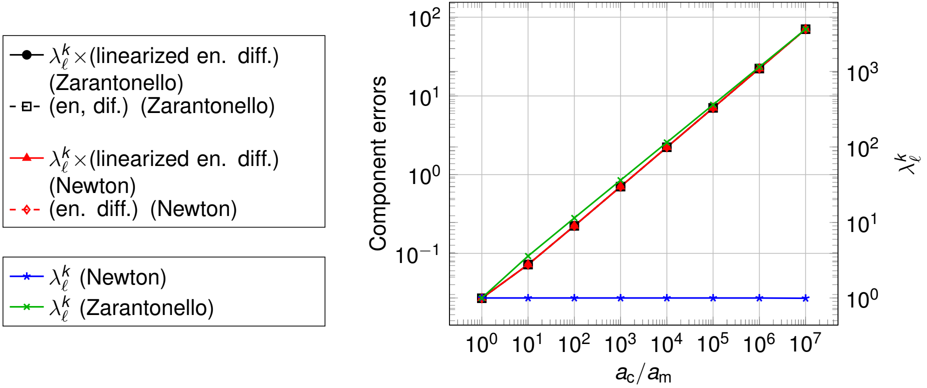

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Practically

$$\mathcal{E}_\ell^k = \mathcal{J}(u_\ell^k) - \mathcal{J}(u) \text{ at convergence}$$

Outline

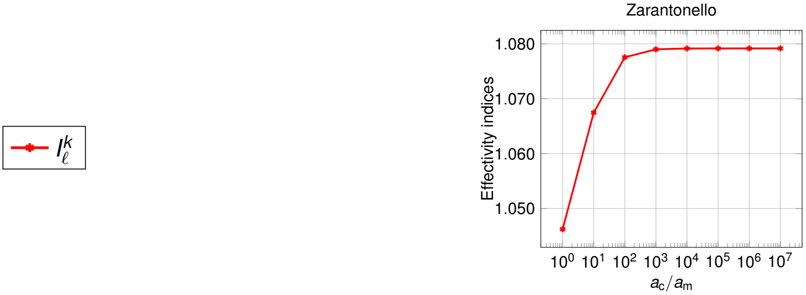
Smooth solution

Setting

- unit square $\Omega = (0,1)^2$
- known smooth solution $u(x,y) := 10\,x(x-1)y(y-1)$
- $p = 1$
- effectivity indices

$$\underbrace{I_\ell^k := \left(\frac{\eta_\ell^k}{\mathcal{E}_\ell^k}\right)^{\frac{1}{2}}}_{\text{total}}, \quad \underbrace{I_{\mathrm{N},\ell}^k := \left(\frac{\mathcal{J}(u_\ell^k) - \mathcal{J}^*(\boldsymbol{\sigma}_\ell^k)}{\mathcal{J}(u_\ell^k) - \mathcal{J}(u)}\right)^{\frac{1}{2}}}_{\text{energy difference}}$$

How **large** is the error? **Robustness** wrt the nonlinearities $\left(a(r) = a_{\mathrm{m}} + \frac{a_{\mathrm{c}} - a_{\mathrm{m}}}{\sqrt{1+r^2}}\right)$



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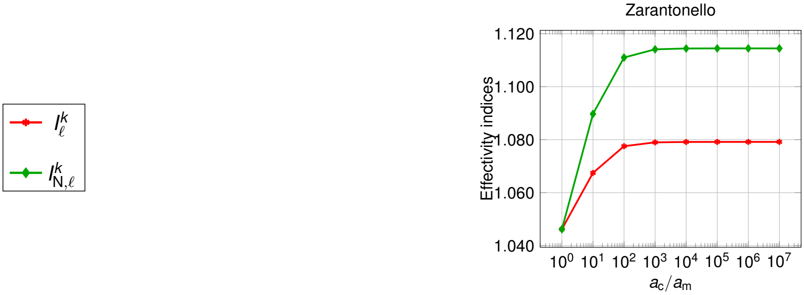

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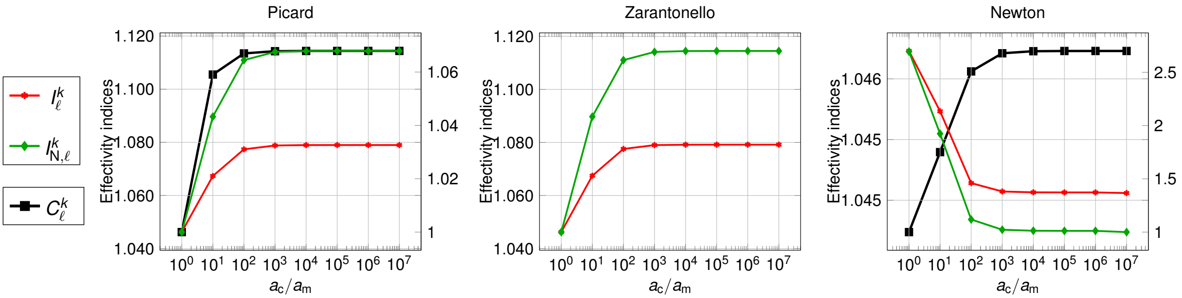
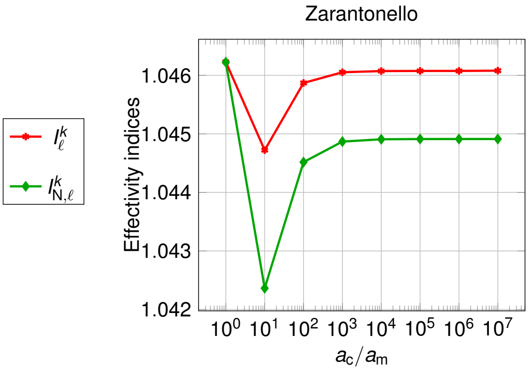


A. Harnist, K. Mitra, A. Rappaport, M. Vohralík, preprint (2023)

How **large** is the error? **Robustness** wrt the nonlinearities

$$\left(a(r) = a_{\mathrm{m}} + (a_{\mathrm{c}} - a_{\mathrm{m}})\frac{1-e^{-\frac{3}{2}r^2}}{1+2e^{-\frac{3}{2}}}\right)$$



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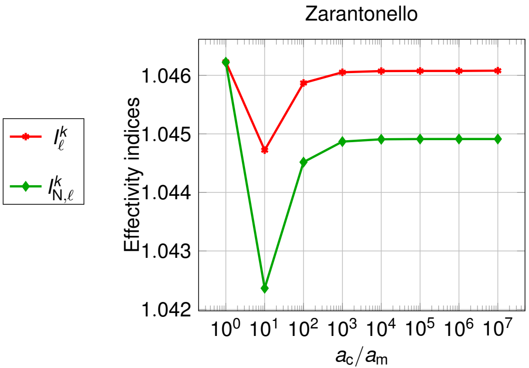
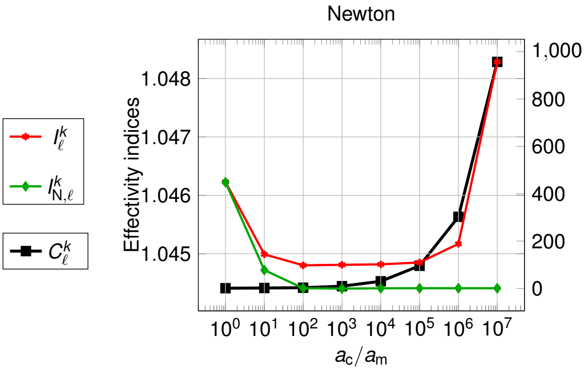
$(a(r) = a_{\mathrm{m}} + (a_{\mathrm{c}} - a_{\mathrm{m}})\frac{1-e^{-\frac{3}{2}r^2}}{1+2e^{-\frac{3}{2}}}$, robustness only for Zarantonello)





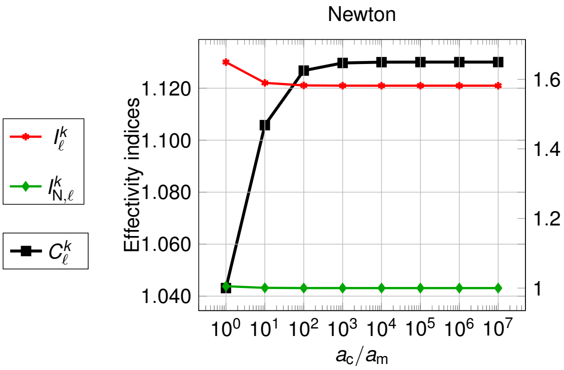
A. Harnist, K. Mitra, A. Rappaport, M. Vohralík, preprint (2023)

Singular solution

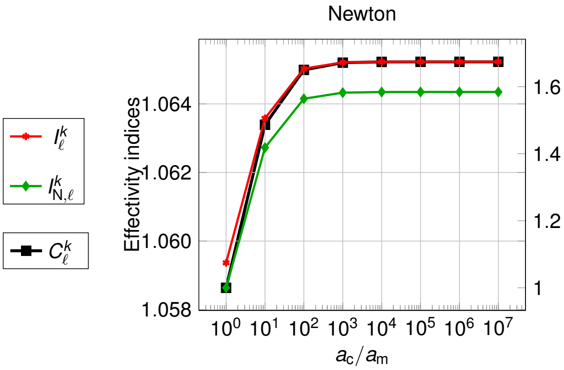
Setting

- L-shaped domain $\Omega = (-1,1)^2 \setminus ([0,1) \times (-1,0])$
- known singular solution $u(\rho,\theta) = \rho^{\frac{2}{3}} \sin(\frac{2}{3}\theta)$
- $a(r) = a_{\mathrm{m}} + (a_{\mathrm{c}} - a_{\mathrm{m}}) \frac{1-e^{-\frac{3}{2}r^2}}{1+2e^{-\frac{3}{2}}}$
- $p = 1$
- uniform or adaptive mesh refinement

How **large** is the error? **Robustness** wrt the nonlinearities



Uniform mesh refinement



Adaptive mesh refinement

A. Harnist, K. Mitra, A. Rappaport, M. Vohralík, preprint (2023)

Outline

Observation

Observation

Note all nonlinear problems admit an energy minimization structure.

A model steady nonlinear problem

Nonlinear elliptic problem

Find $u : \Omega \to \mathbb{R}$ such that

$$-\nabla\cdot\big(\tau \boldsymbol{K}(\boldsymbol{x})(\underbrace{\mathcal{D}(\boldsymbol{x},u)}_{\text{diffusion}}\nabla u + \underbrace{\boldsymbol{q}(\boldsymbol{x},u)}_{\text{advection}})\big) + \underbrace{f(\boldsymbol{x},u)}_{\text{reaction}} = 0 \quad \text{in} \quad \Omega,$$

$$u = 0 \quad \text{on} \quad \partial\Omega.$$

- $\tau > 0$ a parameter (time step size in transient problems: applies to Richards on each time step)

Assumption (Nonlinear functions $\mathcal{D}$, $\boldsymbol{q}$, and f)

$|\mathcal{D}(\boldsymbol{x}_1, u_1) - \mathcal{D}(\boldsymbol{x}_2, u_2)| \le \mathcal{D}_{\mathrm{M}}(|\boldsymbol{x}_1 - \boldsymbol{x}_2| + |u_1 - u_2|) \quad \forall \boldsymbol{x}_1, \boldsymbol{x}_2 \in \Omega$ *and* $u_1, u_2 \in \mathbb{R}$,

$0 \le f(\boldsymbol{x}, u_2) - f(\boldsymbol{x}, u_1) \le f_{\mathrm{M}}(u_2 - u_1) \quad \forall \boldsymbol{x} \in \Omega$ *and* $u_1, u_2 \in \mathbb{R}, u_2 \ge u_1$,

$\boldsymbol{q}$ *is "small" wrt* $\boldsymbol{K}\mathcal{D}$.

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Finite element discretization and iterative linearization

Definition (Linearized finite element approximation)

$u_\ell^k \in V_\ell^p$ such that

$$((u_\ell^k - u_\ell^{k-1}, v_\ell))_{u_\ell^{k-1}} = -\underbrace{\langle \mathcal{R}(u_\ell^{k-1}), v_\ell \rangle}_{\text{residual}} \qquad \forall v_\ell \in V_\ell^p.$$

- covers most linearization schemes: Picard (fixed-point), L & M-schemes, ...
- linearization: **reaction–diffusion scalar product**

$$((w, v))_{u_\ell^{k-1}} := (\underbrace{L_\ell^{k-1}}_{\text{reaction coef.}} w, v) + (\underbrace{\mathbf{A}_\ell^{k-1}}_{\text{diffusion coef.}} \nabla w, \nabla v), \quad w, v \in H_0^1(\Omega)$$

Iteration-dependent norm

- $$|||v|||^2_{1, u_\ell^{k-1}} := ((v, v))_{u_\ell^{k-1}} = \|(L_\ell^{k-1})^{1/2} v\|^2 + \|(\mathbf{A}_\ell^{k-1})^{1/2} \nabla v\|^2, \quad v \in H_0^1(\Omega)$$
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reaction coef. $=0$ if $f = f(\boldsymbol{x})$; diffusion coef. $= \tau \boldsymbol{K}(\boldsymbol{x}) \mathcal{D}(\boldsymbol{x}, u_\ell^{k-1})$

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An orthogonal decomposition of the total residual/error

Theorem (Orthogonal decomposition of the total error into linearization and discretization components)

For all linearization steps $k \geq 1$, there holds

$$\underbrace{|||\mathcal{R}(u_\ell^{k-1})|||^2_{-1,u_\ell^{k-1}}}_{\substack{\text{total residual/error} \\ |||u_\ell^{k-1} - u_{\langle\ell\rangle}^k|||_{1,u_\ell^{k-1}}}} = \underbrace{|||u_\ell^{k-1} - u_\ell^k|||^2_{1,u_\ell^{k-1}}}_{\substack{\text{linearization} \\ \text{error}}} + \underbrace{|||\mathcal{R}_{\text{disc}}^{u_\ell^{k-1}}(u_\ell^k)|||^2_{-1,u_\ell^{k-1}}}_{\substack{\text{discretization residual/error} \\ |||u_\ell^k - u_{\langle\ell\rangle}^k|||_{1,u_\ell^{k-1}}}}.$$

- **orthogonal decomposition**
- **error components**
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Outline

A posteriori error estimates for an iteration-dependent norm

Theorem (A posteriori estimate of iteration-dependent norm)

For all linearization steps $k \geq 1$,

$$|||\mathcal{R}(u_\ell^{k-1})|||_{-1,u_\ell^{k-1}} \leq \eta(u_\ell^k).$$

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For all linearization steps $k \geq 1$,

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Moreover, for all linearization steps $k \geq 1$, there holds

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✓ C_K^k given by **local conditioning** of the linearization matrix $\boldsymbol{A}_\ell^{k-1}$: typically **much better** than global conditioning (= worst-case scenario)

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- ✓ C_K^k given by **local conditioning** of the linearization matrix $\mathbf{A}_\ell^{k-1}$: typically **much better** than global conditioning (= worst-case scenario)
- ✓ C_K^k **computable**: we can affirm **robustness *a posteriori***, for the given case

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- ✓ C_K^k **computable**: we can affirm **robustness *a posteriori***, for the given case
- ✓ **local efficiency**

Outline

One time step of the Richards equation

Setting

- unit square $\Omega = (0,1)^2$
- realistic data

$$f(\boldsymbol{x},u) = S(u) - S(u_\ell^{n-1}(\boldsymbol{x})), \quad \mathcal{D}(\boldsymbol{x},u) = \kappa(S(u)), \quad \boldsymbol{q}(\boldsymbol{x},u) = -\kappa(S(u))\,\boldsymbol{g},$$

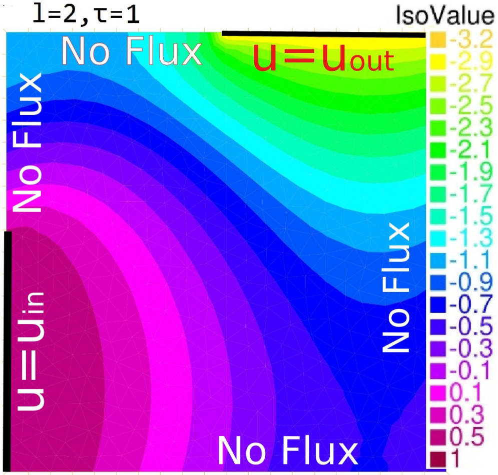
$$\boldsymbol{K} = \begin{bmatrix} 1 & 0.2 \\ 0.2 & 1 \end{bmatrix}, \quad \boldsymbol{g} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- **van Genuchten saturation** and **permeability** laws

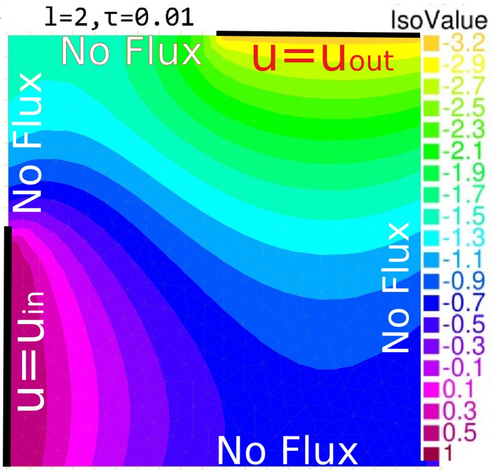
$$S(u) := \left(1 + (2-u)^{\frac{1}{1-\lambda}}\right)^{-\lambda}, \quad \kappa(s) := \sqrt{s}\left(1 - (1 - s^{\frac{1}{\lambda}})^{\lambda}\right)^2, \quad \lambda = 0.5$$

- time step length $\tau \in [10^{-3}, 1]$

One time step of the Richards equation: saturation u

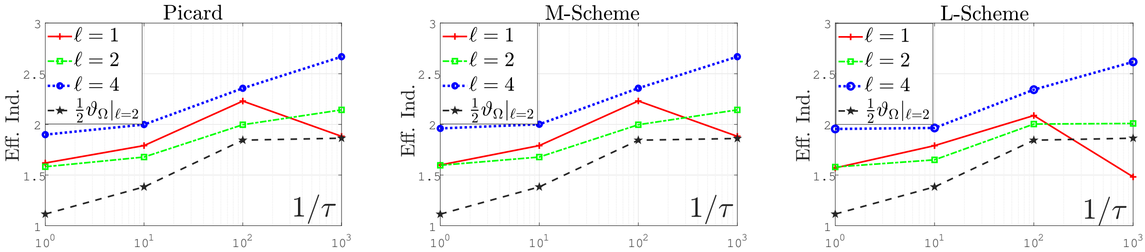


Time step length $\tau = 1$



Time step length $\tau = 0.01$

How **large** is the error? **Robustness** wrt the nonlinearities



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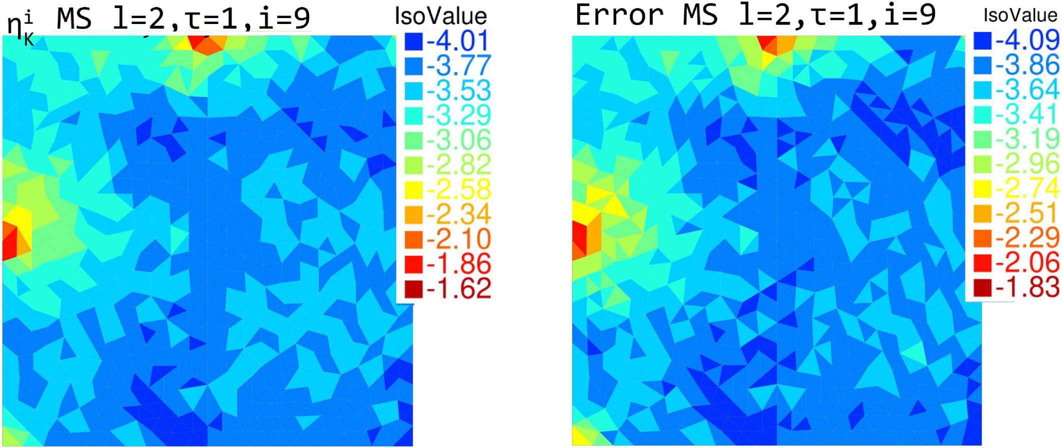
Where is the error **localized**?



Estimated local error, $\tau = 1$ Exact local error, $\tau = 1$

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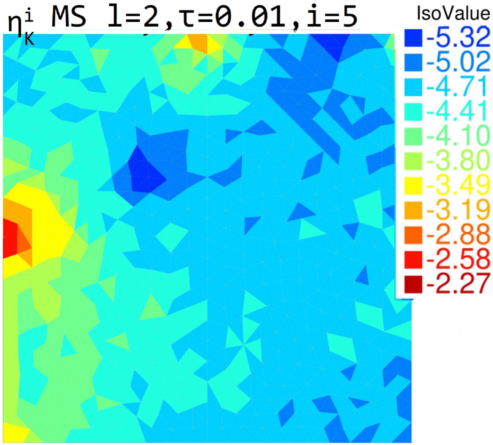
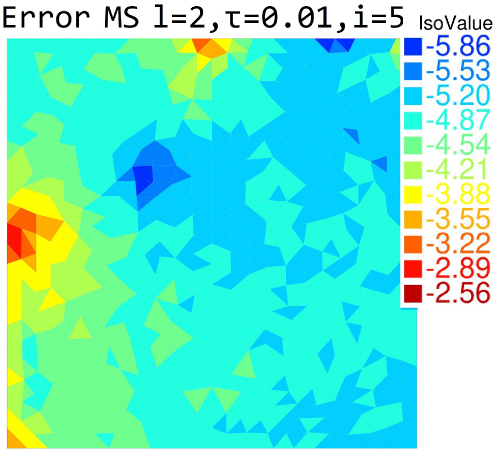


Estimated local error, $\tau = 0.01$



Exact local error, $\tau = 0.01$

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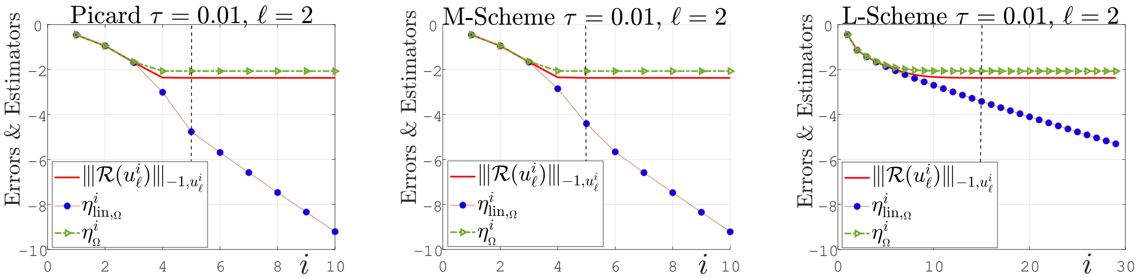
Error components and adaptivity via stopping criteria



Time step length $\tau = 0.01$

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Outline

A model unsteady linear problem

The unsteady linear Darcy (heat) equation

Find $u : \Omega \times (0, T) \to \mathbb{R}$ such that

$$\begin{aligned} \partial_t u - \Delta u &= f \quad \text{in } \Omega \times (0, T), \\ u &= 0 \quad \text{on } \partial\Omega \times (0, T), \\ u(0) &= u_0 \quad \text{in } \Omega. \end{aligned}$$

- T: final time
- f and u_0 piecewise polynomial for simplicity

Spaces and norms

$$\begin{aligned} X &:= L^2(0, T; H_0^1(\Omega)), \\ \|v\|_X^2 &:= \int_0^T \|\nabla v\|^2 \,\mathrm{d}t, \\ Y &:= L^2(0, T; H_0^1(\Omega)) \cap H^1(0, T; H^{-1}(\Omega)), \\ \|v\|_Y^2 &:= \int_0^T \|\partial_t v\|_{H^{-1}(\Omega)}^2 + \|\nabla v\|^2 \,\mathrm{d}t + \|v(T)\|^2 \end{aligned}$$

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Weak solution

Definition (Weak solution)

$u \in Y$ with $u(0) = u_0$ such that

$$\int_0^T \langle \partial_t u, v \rangle + (\nabla u, \nabla v) \, \mathrm{d}t = \int_0^T (f, v) \, \mathrm{d}t \qquad \forall v \in X.$$

Nonsymmetry

Trial space Y, test space X.

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Trial space Y, test space X.

Previous results

- Picasso / Verfürth (1998), work with the energy norm of X:
  - ✓ upper bound $\|u - u_\ell\|_X^2 \leq C^2 \sum_{n=1}^N \sum_{K \in \mathcal{T}_\ell^n} \eta_K^n(u_\ell)^2$
  - ✗ constrained lower bound (number of mesh elements $|\mathcal{T}_\ell^n|$ and time step τ strongly linked)
- Verfürth (2003) (cf. also Bergam, Bernardi, and Mghazli (2005)), work with the Y norm:
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  - ✓ efficiency $\sum_{K \in \mathcal{T}_\ell^n} \eta_K^n(u_\ell)^2 \leq C^2 \|u - \mathcal{I}u_\ell\|_{Y(I_n)}^2$
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Guaranteed upper bound

Augmented Y norm

$$\|u - u_\ell\|_{\mathcal{E}_Y}^2 := \|u - \mathcal{I}u_\ell\|_Y^2 + \underbrace{\|u_\ell - \mathcal{I}u_\ell\|_X^2}_{\text{known, computable, measures time jumps}}$$

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Outline

Modelling flow of water and air through soil

The Richards equation

Find $u : \Omega \times (0, T) \to \mathbb{R}$ such that

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- u: pressure
- $s = S(u)$: saturation
- $\Omega \subset \mathbb{R}^d$, $1 \le d \le 3$, open polytope with Lipschitz boundary $\partial\Omega$
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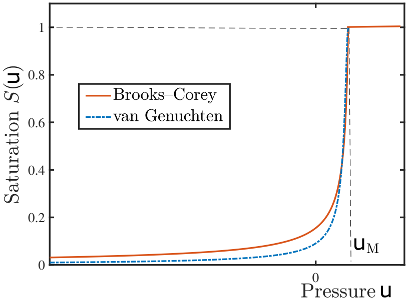

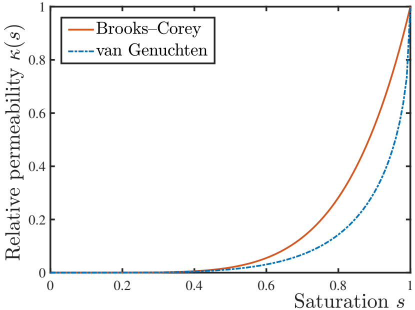

A posteriori error estimates

Nonsymmetry, nonlinearity, degeneracy

- Use all the tools from the above cases.
- Treatment of time-dependent nonlinearity: **sharp Gronwall lemma** not neglecting the integral terms.
- **Avoids** the appearance of the usual factor e^T, but gives rise to **integrated norms**.

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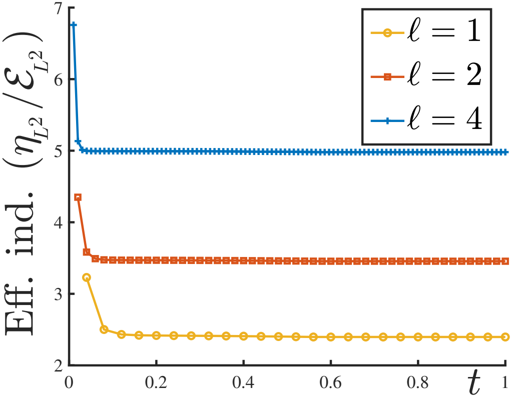
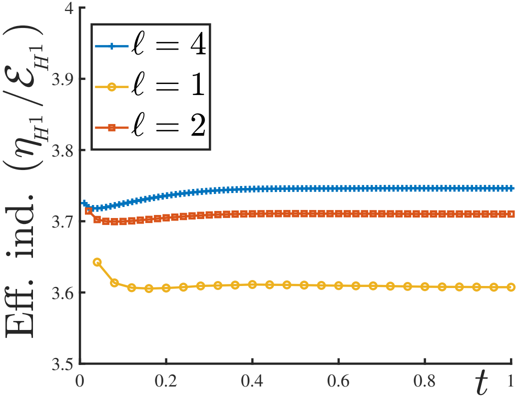
- Details in K. Mitra, M. Vohralík, preprint (2022)

How **large** is the error? **Robustness** wrt the final time (known sol.)



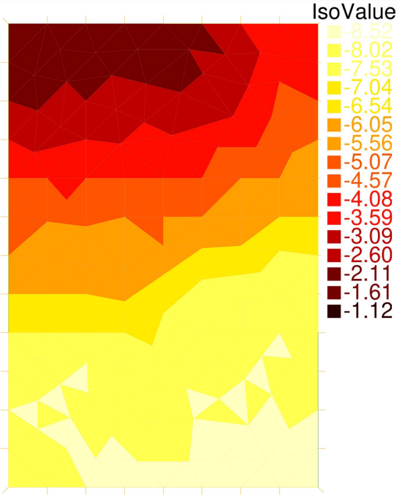
Integrated L^2 effectivity indices



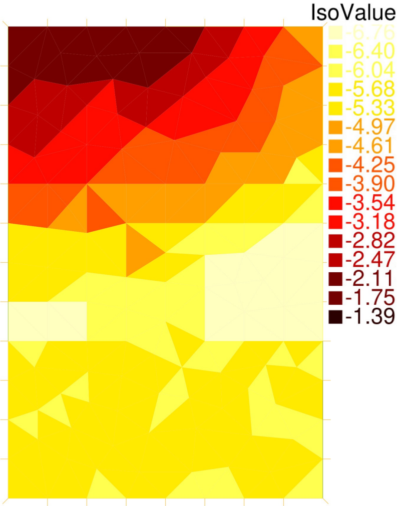
Integrated H^1 effectivity indices

K. Mitra, M. Vohralík, preprint (2022)

Where (in space and time) is the error **localized**? (benchmark case)



Estimated local error



Exact local error

K. Mitra, M. Vohralík, preprint (2022)

Realistic case

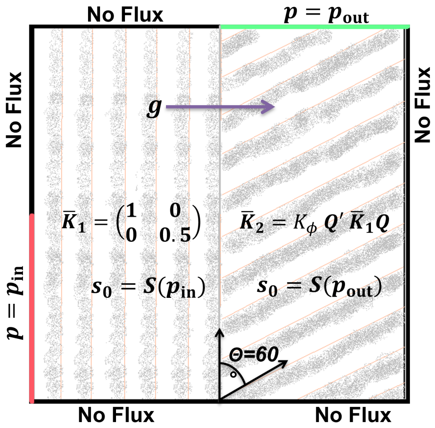
Setting

- unit square $\Omega = (0,1)^2$
- $T = 1$
- $f(\boldsymbol{x}, u) = 0$, heterogeneous and anisotropic $\boldsymbol{K}$, $\boldsymbol{g} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
- **Brooks–Corey**-type **saturation** and **permeability** laws

$$S(u) := \begin{cases} \frac{1}{(2-u)^{\frac{1}{3}}} & \text{if } u < 1, \\ 1 & \text{if } u \geq 1 \end{cases}, \quad \kappa(s) := s^3$$

- $(h, \tau) = (h_0, \tau_0)/\ell$ with $\ell \in \{1, 2, 4\}$, $h_0 = 0.2$, and $\tau_0 = 0.04$

Realistic case



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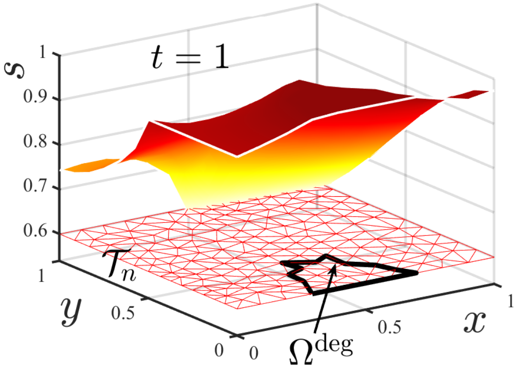
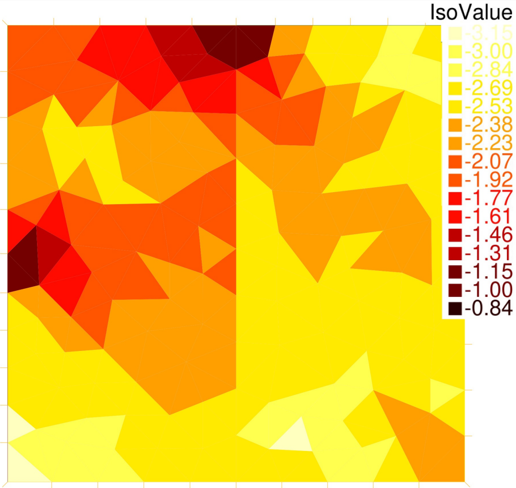


Numerical saturation for $\ell = 2$ at $t = 1$

Where (in space and time) is the error **localized**? (realistic test case)



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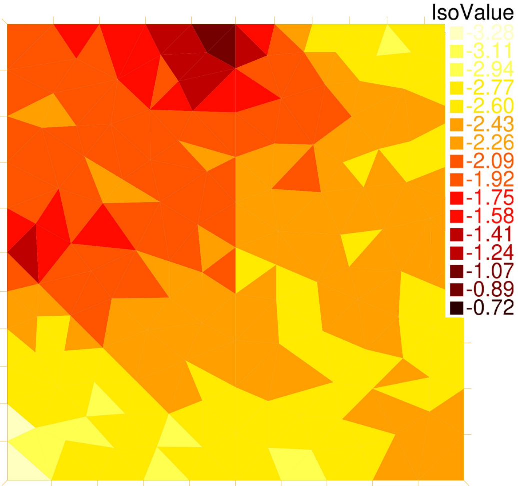

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Outline

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Thank you for your attention!

Outline

Sobolev space and error

Sobolev space

$$H_0^1(\Omega)$$

Sobolev norm error

$$\boxed{\|\nabla(u_\ell - u)\|}$$

Residual and its dual norm

Definition (Residual)

$\mathcal{R} : H_0^1(\Omega) \to H^{-1}(\Omega)$; for $w \in H_0^1(\Omega)$, $\mathcal{R}(w) \in H^{-1}(\Omega)$ is given by

$$\langle \mathcal{R}(w), v \rangle := (a(|\nabla w|)\nabla w, \nabla v) - (f, v), \quad v \in H_0^1(\Omega).$$

Definition (Dual norm of the finite element residual)

$$|||\mathcal{R}(u_\ell) - \mathcal{R}(u)|||_{-1} = \boxed{|||\mathcal{R}(u_\ell)|||_{-1}} := \sup_{v \in H_0^1(\Omega)} \frac{\langle \mathcal{R}(u_\ell), v \rangle}{|||v|||}.$$

- $|||\mathcal{R}(u_\ell)|||_{-1} \geq 0$, $|||\mathcal{R}(u_\ell)|||_{-1} = 0$ if and only if $u_\ell = u$
- subordinate to the choice of the norm $|||\cdot|||$ on the Sobolev space $H_0^1(\Omega)$
- the most straightforward choice: $|||v||| := \|\nabla v\|$
- mathematically-based error measure

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Outline

Fenchel conjugate, dual energy, flux equilibration

Definition (Fenchel conjugate)

$$\phi^*(\cdot, s) := \sup_{r \in [0,\infty)} (sr - \phi(\cdot, r)).$$

Definition (Dual energy)

$$\mathcal{J}^*(\boldsymbol{v}) := -\int_\Omega \phi^*(\cdot, |\boldsymbol{v}|), \qquad \boldsymbol{v} \in \boldsymbol{H}(\mathrm{div}, \Omega).$$

Definition (Flux equilibration)

$$\boldsymbol{\sigma}_\ell^{\boldsymbol{a},k} := \arg \min_{\substack{\boldsymbol{v}_\ell \in \mathcal{RT}_{p+1}(\mathcal{T}_{\boldsymbol{a}}) \cap \boldsymbol{H}_0(\mathrm{div},\omega_{\boldsymbol{a}}) \\ \nabla\cdot\boldsymbol{v}_\ell = \Pi_{\ell,p}(\psi^{\boldsymbol{a}} f - \nabla\psi^{\boldsymbol{a}}\cdot(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}))}} \|(\boldsymbol{A}_\ell^{k-1})^{-\frac{1}{2}}(\psi^{\boldsymbol{a}}\Pi^{RTN}_{\ell,p-1}(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}) + \boldsymbol{v}_\ell)\|^2_{\omega_{\boldsymbol{a}}}.$$

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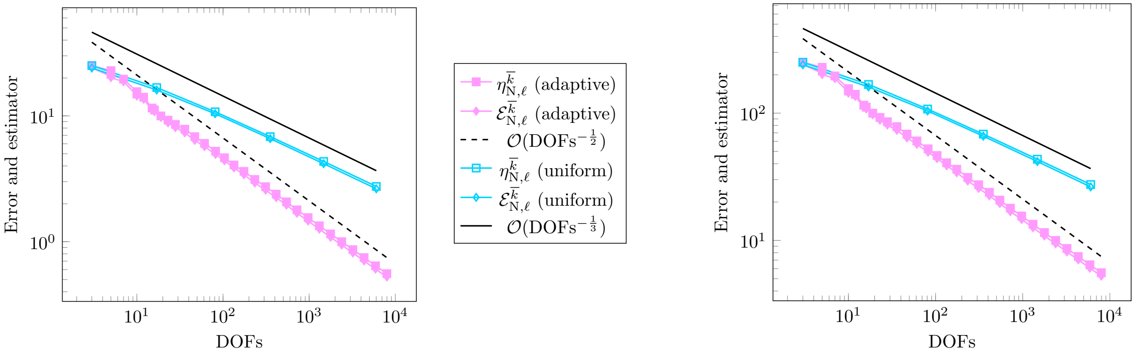
Outline

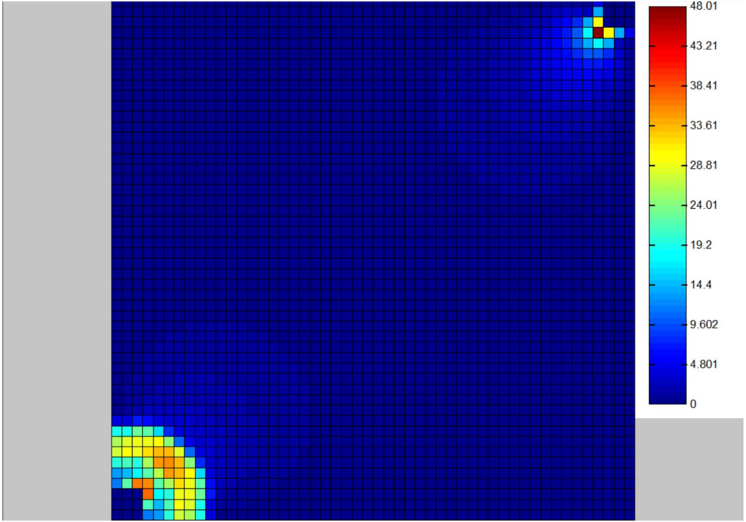
Decreasing the error efficiently: optimal decay rate wrt DoFs



$\frac{a_c}{a_m} = 10^3$ $\frac{a_c}{a_m} = 10^6$

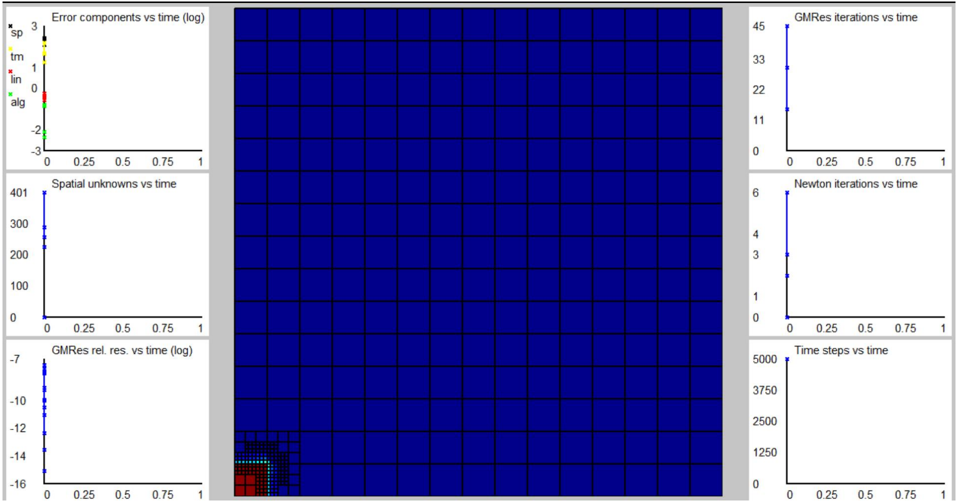
Outline

Where (in space and time) is the error **localized**? (two-phase flow)



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

All error components (two-phase flow)



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