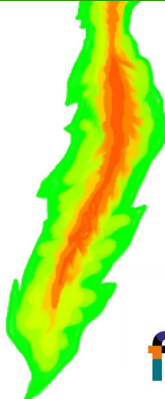
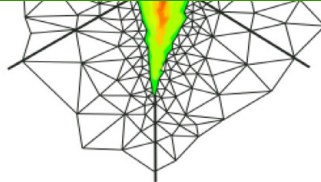
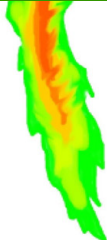




# Reliable, efficient, and robust a posteriori estimates for nonlinear elliptic & parabolic problems



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joint work with Martin Vohralík  
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- 1 Introduction: nonlinear elliptic problems
- 2 Main analytical results
- 3 Scope of the results
- 4 Numerical results
- 5 Nonlinear parabolic problems

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- ② Main analytical results
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## Nonlinear elliptic problems

For  $d \in \mathbb{N}$ , let  $\Omega \subset \mathbb{R}^d$  be an open and bounded polytope. Let  $u \in H_0^1(\Omega)$  solve the **nonlinear** elliptic operator equation: for  $\mathcal{R} : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$ ,

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Assumption 1  $\mathcal{R}$  is monotone & Lipschitz\*

For a numerical approximation  $u_\ell \in H_0^1(\Omega)$ , and constants  $\lambda_M > \lambda_m > 0$ ,

$$\lambda_m \operatorname{dist}(u_\ell, u) \leq \sup_{\varphi \in H_0^1(\Omega)} \frac{\langle \mathcal{R}(u_\ell) - \mathcal{R}(u), \varphi \rangle}{\|\nabla \varphi\|} \leq \lambda_M \operatorname{dist}(u_\ell, u).$$

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Then the estimate [Chaillou & Suri (2006), Kim (2007), Houston *et al* (2008), Garau *et al* (2011),...],

$$\lambda_m \operatorname{dist}(u_\ell, u) \leq \eta(u_\ell) \leq C \lambda_M \operatorname{dist}(u_\ell, u)$$

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## 1 Dual norm of the residual estimate

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**Reliable**, and **locally efficient** a posteriori error estimates **robust** with respect to the strength of the **nonlinearity**  $\lambda_M/\lambda_m$

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- ▶ The dual norm of the residual might be too weak an error measure



## 1 A linear example

Consider the diffusion eq:  $\langle \mathcal{R}(u), \varphi \rangle := (f, \varphi) - (\mathcal{D}\nabla u, \nabla \varphi) = 0$ .

Let  $\lambda_m |\mathbf{y}|^2 \leq \mathbf{y}^T \mathcal{D} \mathbf{y} \leq \lambda_M |\mathbf{y}|^2$ , for all  $\mathbf{y} \in \mathbb{R}^d$ .

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$$\|u - u_\ell\|_{1,\mathcal{D}} \leq \|u - \varphi_\ell\|_{1,\mathcal{D}}, \quad \forall \varphi_\ell \in V_\ell.$$

This motivates rather the error measure

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

which also results in robust estimates

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Example (nonlinear diffusion):  $\langle \mathcal{R}(u), \varphi \rangle := (f, \varphi) - (\mathcal{D}(u)\nabla u, \nabla \varphi) = 0.$

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Then  $\|\mathcal{R}(\cdot)\|_{-1, \mathcal{D}(u)}$  cannot be defined since  $u \in H_0^1(\Omega)$  is unknown.

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### Linearization iterations

We generally solve nonlinear equations by linearization iterations, i.e., by finding a sequence  $\{u_\ell^i\}_{i \in \mathbb{N}} \subset V_\ell \subset H_0^1(\Omega)$ .



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Then defining the **iteration-dependent energy norm**

$$\begin{cases} \|\varphi\|_{1, u_\ell^i} := \|\mathcal{D}(u_\ell^i)^{\frac{1}{2}} \nabla \varphi\| & \text{for } \varphi \in H_0^1(\Omega), \\ \|\varsigma\|_{-1, u_\ell^i} = \sup_{\varphi \in H_0^1(\Omega)} \langle \varsigma, \varphi \rangle / \|\varphi\|_{1, u_\ell^i} & \text{for } \varsigma \in H^{-1}(\Omega), \end{cases}$$

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we have (under conditions) robust estimates of

$$\left\| \mathcal{R}_{\text{lin}}^{u_\ell^i}(u_{\langle \ell \rangle}^{i+1}) \right\|_{-1, u_\ell^i} = \left\| u_{\langle \ell \rangle}^{i+1} - u_\ell^{i+1} \right\|_{1, u_\ell^i}$$

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Noting that

$$\langle \mathcal{R}_{\text{lin}}^{u_\ell^i}(u_\ell^{i+1}), \varphi \rangle := -(\mathcal{D}(u_\ell^i)\nabla(u_\ell^{i+1} - u_\ell^i), \nabla \varphi) + \langle \mathcal{R}(u_\ell^i), \varphi \rangle$$

can we provide a robust estimate for  $\|\mathcal{R}(u_\ell^i)\|_{-1, u_\ell^i}?$

- 1 Introduction: nonlinear elliptic problems
- 2 Main analytical results
  - Decomposition of error
  - A posteriori error estimates
- 3 Scope of the results
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## 2 An orthogonal decomposition result

### Theorem 1 Decomposition of the total error

Under Assumption 1, provided that the linearization iterations  $\{u_\ell^i\}_{i \in \mathbb{N}} \subset V_\ell$  are generated by FE approximations of  $u_{\langle \ell \rangle}^i \in H_0^1(\Omega)$  solving

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**Remark** We would consider  $\mathcal{L} : H_0^1(\Omega) \times H_0^1(\Omega) \mapsto \mathbb{R}$  corresponding to **linear reaction-diffusion** problems, i.e.,

$$\mathcal{L}(u_\ell^i; v, w) := \underbrace{(L(\mathbf{x}, u_\ell^i) v, w)}_{\text{known reaction coeff.}} + \underbrace{(\mathfrak{a}(\mathbf{x}, u_\ell^i) \nabla v, \nabla w)}_{\text{known diffusion coeff.}}$$



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we have

$$\underbrace{\|\mathcal{R}(u_{\ell}^i)\|_{-1, u_{\ell}^i}^2}_{\text{total error}} = \underbrace{\|\mathcal{R}_{\text{lin}}^{u_{\ell}^i}(u_{\ell}^{i+1})\|_{-1, u_{\ell}^i}^2}_{\text{discretization error of the linearization step}} + \underbrace{\|u_{\ell}^{i+1} - u_{\ell}^i\|_{1, u_{\ell}^i}^2}_{\text{linearization error}}.$$

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$$\|\varphi\|_{1, u_{\ell}^i} := \mathfrak{L}(u_{\ell}^i; \varphi, \varphi)^{\frac{1}{2}}, \quad \|\varsigma\|_{-1, u_{\ell}^i} := \sup_{\varphi \in H_0^1(\Omega)} \frac{\langle \varsigma, \varphi \rangle}{\|\varphi\|_{1, u_{\ell}^i}},$$

we have

$$\underbrace{\|\mathcal{R}(u_{\ell}^i)\|_{-1, u_{\ell}^i}^2}_{\text{total error}} = \underbrace{\|\mathcal{R}_{\text{lin}}^{u_{\ell}^i}(u_{\langle \ell \rangle}^{i+1})\|_{-1, u_{\ell}^i}^2}_{\text{discretization error of the linearization step}} + \underbrace{\|u_{\ell}^{i+1} - u_{\ell}^i\|_{1, u_{\ell}^i}^2}_{\text{linearization error}}.$$

$$\underbrace{\|u_{\ell}^i - u_{\langle \ell \rangle}^{i+1}\|_{1, u_{\ell}^i}^2}_{\text{total error}} \quad \underbrace{\|u_{\langle \ell \rangle}^{i+1} - u_{\ell}^{i+1}\|_{1, u_{\ell}^i}^2}_{\text{discretization error of the linearization step}}$$

## 2 An orthogonal decomposition result

**Proof:** Since  $u_\ell^{i+1} - u_\ell^i \in V_\ell$ ,

$$\begin{aligned} \left\| \mathcal{R}(u_\ell^i) \right\|_{-1, u_\ell^i}^2 &= \left\| u_\ell^i - u_{\langle \ell \rangle}^{i+1} \right\|_{1, u_\ell^i}^2 = \left\| (u_\ell^i - u_\ell^{i+1}) + (u_\ell^{i+1} - u_{\langle \ell \rangle}^{i+1}) \right\|_{1, u_\ell^i}^2 \\ &= \left\| u_{\langle \ell \rangle}^{i+1} - u_\ell^{i+1} \right\|_{1, u_\ell^i}^2 + \left\| u_\ell^{i+1} - u_\ell^i \right\|_{1, u_\ell^i}^2 + \underbrace{2 \mathfrak{L}(u_\ell^i; u_{\langle \ell \rangle}^{i+1} - u_\ell^{i+1}, u_\ell^{i+1} - u_\ell^i)}_{=0, \text{ due to Galerkin orthogonality}} \\ &= \left\| \mathcal{R}_{\text{lin}}^{u_\ell^i}(u_\ell^{i+1}) \right\|_{-1, u_\ell^i}^2 + \left\| u_\ell^{i+1} - u_\ell^i \right\|_{1, u_\ell^i}^2. \end{aligned}$$

## 2 An orthogonal decomposition result

| 7

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- The linearization error is computed directly, we define

$$\eta_{\text{lin}, \Omega}^i := \left\| u_\ell^{i+1} - u_\ell^i \right\|_{1, u_\ell^i}.$$

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- The linearization error is computed directly, we define

$$\eta_{\text{lin}, \Omega}^i := \left\| u_\ell^{i+1} - u_\ell^i \right\|_{1, u_\ell^i}.$$

- For estimating  $\left\| \mathcal{R}_{\text{lin}}^{u_\ell^i}(u_\ell^{i+1}) \right\|_{-1, u_\ell^i}$  we introduce  $\eta_{\text{disc}, \Omega}^i$ , following the analysis on robust estimates of **singularly perturbed reaction-diffusion problems** in [Verfürth (1998)], [Ainsworth & Vejchodský (2011, 2014)], [Smears & Vohralík (2020)]

Theorem 2 Reliable, efficient, and robust a posteriori estimates

Global reliability

$$\|\mathcal{R}(u_\ell^i)\|_{-1, u_\ell^i}^2 \leq [\eta_\Omega^i]^2 := \sum_{K \in \mathcal{T}_\ell} ([\eta_{\text{disc}, K}^i]^2 + [\eta_{\text{lin}, K}^i]^2).$$

Theorem 2 Reliable, efficient, and robust a posteriori estimates

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Global efficiency

$$[\eta_\Omega^i]^2 \lesssim \|\mathcal{R}(u_\ell^i)\|_{-1, u_\ell^i}^2 + (\text{data oscillation terms}).$$



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Global efficiency

$$[\eta_\Omega^i]^2 \lesssim \|\mathcal{R}(u_\ell^i)\|_{-1, u_\ell^i}^2 + (\text{data oscillation terms}).$$

Local efficiency

For  $\omega \subset \Omega$ , there exists a neighbourhood  $\mathfrak{T}_\omega \subseteq \Omega$  such that

$$[\eta_\omega^i]^2 \lesssim \|\mathcal{R}(u_\ell^{i+1})\|_{-1, u_\ell^i, \mathfrak{T}_\omega}^2 + [\eta_{\text{lin}, \mathfrak{T}_\omega}^i]^2 + (\text{data oscillation terms}).$$

- 1 Introduction: nonlinear elliptic problems
- 2 Main analytical results
- 3 Scope of the results**
  - Gradient-dependent diffusivity
  - Gradient-independent diffusivity
- 4 Numerical results
- 5 Nonlinear parabolic problems

### 3 Class of problems

#### Class 1: gradient-dependent diffusivity problems

For all  $\varphi \in H_0^1(\Omega)$ ,  $\mathcal{R} : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$  is defined as

$$\langle \mathcal{R}(u), \varphi \rangle := \langle f(\mathbf{x}, u), \varphi \rangle - (\boldsymbol{\sigma}(\mathbf{x}, \nabla u), \nabla \varphi)$$

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Assumption 1 is satisfied if  $f(\mathbf{x}, \cdot)$ ,  $\boldsymbol{\sigma}(\mathbf{x}, \cdot)$  are monotone and Lipschitz

$$(\boldsymbol{\sigma}(\mathbf{x}, \mathbf{y}) - \boldsymbol{\sigma}(\mathbf{x}, \mathbf{z})) \cdot (\mathbf{y} - \mathbf{z}) \geq \lambda_m |\mathbf{y} - \mathbf{z}|^2 \quad \text{for } \mathbf{x} \in \Omega \text{ and } \mathbf{y}, \mathbf{z} \in \mathbb{R}^d,$$

$$|\boldsymbol{\sigma}(\mathbf{x}, \mathbf{y}) - \boldsymbol{\sigma}(\mathbf{x}, \mathbf{z})| \leq \lambda_M |\mathbf{y} - \mathbf{z}| \quad \text{for } \mathbf{x} \in \Omega \text{ and } \mathbf{y}, \mathbf{z} \in \mathbb{R}^d.$$

with

$$\text{dist}(u, v) = \|\nabla(u - v)\|$$

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with

$$\text{dist}(u, v) = \|\nabla(u - v)\|$$

**Example** (Mean curvature flow) For  $a(\cdot)$  satisfying ellipticity condition

and  $b(\cdot) > 0$ :  $\boldsymbol{\sigma}(\mathbf{x}, \mathbf{y}) = a(\mathbf{x}) + \frac{b(\mathbf{x})\mathbf{y}}{(1+|\mathbf{y}|^2)^{\frac{1}{2}}}$

### 3 Linearization schemes: practical examples

#### Linearization operator

Considering the linearization operator

$$\mathfrak{L}(u_\ell^i; v, w) := (L(\mathbf{x}, u_\ell^i) v, w) + (\alpha(\mathbf{x}, u_\ell^i) \nabla v, \nabla w),$$

the coefficient functions for commonly used linearization schemes are

Scheme	$L(\mathbf{x}, v)$	$\alpha(\mathbf{x}, v)/\tau$
Kačanov (fixed point)	$\partial_\xi f(\mathbf{x}, v)$	$A(\mathbf{x},  \nabla v )$
Zarantonello	0	$\Lambda$ (constant) $> 0$

### 3 Class of problems

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#### Class 2: gradient-independent diffusivity problems

For all  $\varphi \in H_0^1(\Omega)$ ,  $\mathcal{R} : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$  is defined as

$$\langle \mathcal{R}(u), \varphi \rangle := \langle f(\mathbf{x}, u), \varphi \rangle - \tau(\bar{\mathbf{K}}(\mathbf{x})(\mathcal{D}(\mathbf{x}, u)\nabla u + \mathbf{q}(\mathbf{x}, u)), \nabla\varphi)$$

## Class 2: gradient-independent diffusivity problems

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Assumption 1 is satisfied if  $\tau > 0$  is small and

- ▶  $\mathcal{D} : \Omega \times \mathbb{R} \rightarrow \mathbb{R}^+$  is bounded and Lipschitz
- ▶  $\bar{\mathbf{K}} : \Omega \rightarrow \mathbb{R}^{d \times d}$  is symmetric positive definite
- ▶  $f : \Omega \times \mathbb{R} \rightarrow \mathbb{R}$  is monotone and Lipschitz upto the boundary
- ▶  $\mathbf{q} : \Omega \times \mathbb{R} \rightarrow \mathbb{R}^d$  is bounded and satisfies a Lipschitz condition\*

with

$$\text{dist}(u, v) = \left\| \bar{\mathbf{K}}^{\frac{1}{2}} \nabla \int_u^v \mathcal{D} \right\|$$



## Class 2: gradient-independent diffusivity problems

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Semilinear equations  $-\Delta u = f(\mathbf{x}, u)$ 

Such equations pop up in quantum mechanics (special solutions to nonlinear Klein–Gordon equations), gravitation influences on stars, membrane buckling problems...

## Time-discrete nonlinear advection-reaction-diffusion equations

with time-step  $\tau > 0$ , the following evolutions equations reduce to this case

poro-Fischer equations:  $\partial_t u = \Delta u^m + \lambda u(1 - u)$

the Richards equation:  $\partial_t S(u) = \nabla \cdot [\bar{\mathbf{K}}(\mathbf{x})\kappa(S(u))(\nabla u + \mathbf{g})] + f(\mathbf{x}, u)$

biofilm equations:  $\partial_t u_k = \mu_k \Delta \Phi_k(u_k) + f_k((u_k)_{k=1}^n)$

### 3 Linearization schemes: practical examples

#### Abstract linearization

Considering the linearization operator

$$\mathfrak{L}(u_\ell^i; v, w) := (L(\mathbf{x}, u_\ell^i) v, w) + (\alpha(\mathbf{x}, u_\ell^i) \nabla v, \nabla w),$$

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Scheme	$L(\mathbf{x}, v)$	$\alpha(\mathbf{x}, v)/\tau$
Picard (fixed point)	$\partial_\xi f(\mathbf{x}, v)$	$\bar{\mathbf{K}}(\mathbf{x}) \mathcal{D}(\mathbf{x}, v)$
Jäger–Kačur	$\max_{\xi \in \mathbb{R}} \left( \frac{f(\mathbf{x}, \xi) - f(\mathbf{x}, v)}{\xi - v} \right)$	$\bar{\mathbf{K}}(\mathbf{x}) \mathcal{D}(\mathbf{x}, v)$
$L$ -scheme	$L$ (constant) $\geq \frac{1}{2} \sup \partial_\xi f$	$\bar{\mathbf{K}}(\mathbf{x}) \mathcal{D}(\mathbf{x}, v)$
$M$ -scheme	$\partial_\xi f(\mathbf{x}, v) + M\tau$ (constant)	$\bar{\mathbf{K}}(\mathbf{x}) \mathcal{D}(\mathbf{x}, v)$

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- ▶ Newton scheme leads to a non-symmetric  $\mathfrak{L}$  and is treated separately

- 1 Introduction: nonlinear elliptic problems
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  - Gradient independent diffusivity case
  - The Newton scheme
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### Effectivity indices

Global effectivity index: Eff. Ind. :=  $\eta_{\Omega}^i / \|\mathcal{R}(u_{\ell}^i)\|_{-1, u_{\ell}^i}$

Local effectivity index: (Eff. Ind.) $_K := \eta_K^i / \|\mathcal{R}(u_{\ell}^i)\|_{-1, u_{\ell}^i, K}$ ,  $K \in \mathcal{T}_{\ell}$ ,

## 4 Gradient-independent diffusivity case: the Richards equation | 14

For  $\Omega = (0, 1) \times (0, 1)$  we study

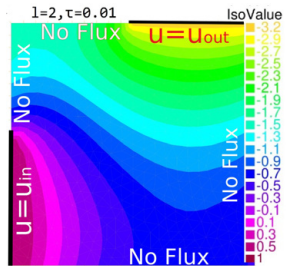
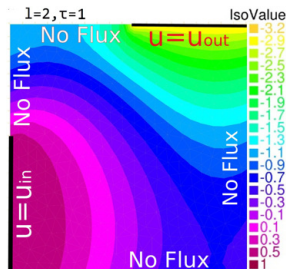
$$\langle \mathcal{R}(u_\ell), \varphi \rangle = (S(\bar{u}) - S(u_\ell), \varphi) - \tau(\bar{\mathbf{K}}\kappa(S(u_\ell))[\nabla u_\ell - \mathbf{g}], \nabla \varphi)$$

where the van Genuchten parametrization for  $S$ ,  $\kappa$  is used:

$$\begin{cases} S(\xi) := \left(1 + (2 - \xi)^{\frac{1}{1-\lambda}}\right)^{-\lambda}, \\ \kappa(s) := \sqrt{s} \left(1 - (1 - s^{\frac{1}{\lambda}})^{\lambda}\right)^2, \end{cases}$$

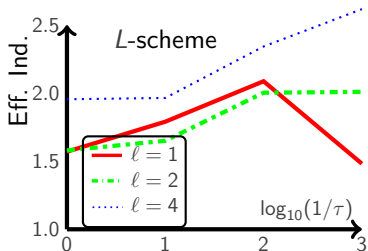
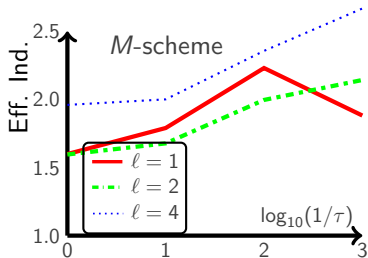
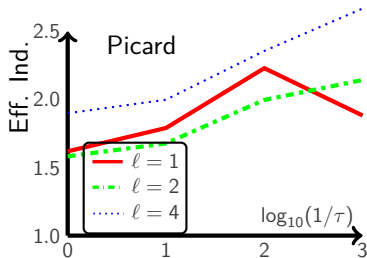
with  $\lambda = 0.5$ ,  $u_\ell^0 = 0$ ,

$$\bar{\mathbf{K}} = \begin{bmatrix} 1 & 0.2 \\ 0.2 & 1 \end{bmatrix}, \text{ and } \mathbf{g} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

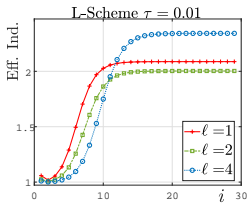
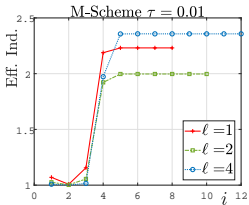
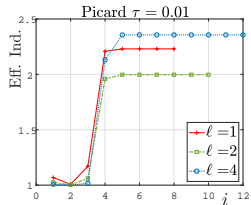
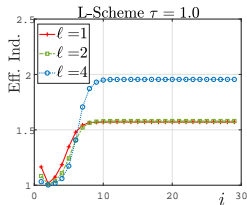
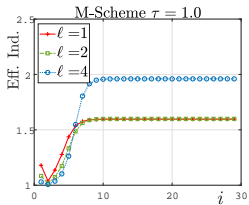
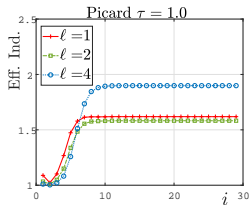


#### 4 Robustness with respect to $\lambda_M/\lambda_m$ represented by $1/\tau$

| 14



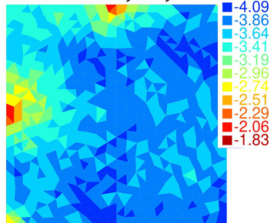
## 4 Global effectivity





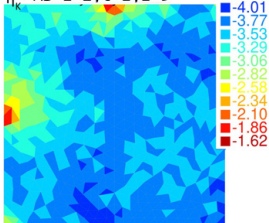
## 4 Distribution of error vs. estimates

Error MS  $l=2, \tau=1, i=9$



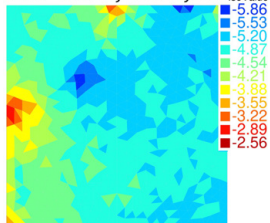
Error

$\eta_k^i$  MS  $l=2, \tau=1, i=9$

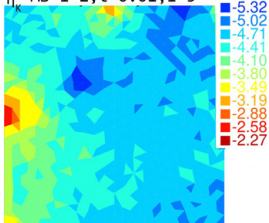


Estimate

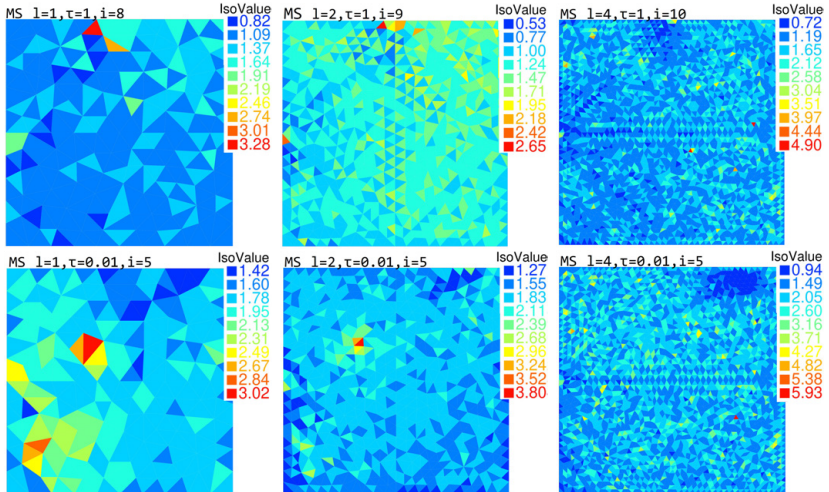
Error MS  $l=2, \tau=0.01, i=5$



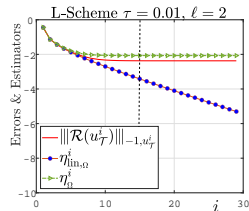
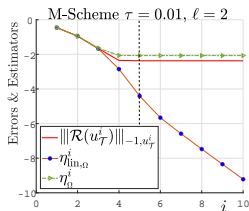
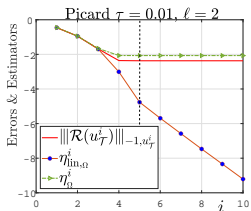
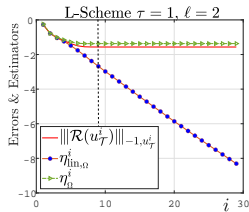
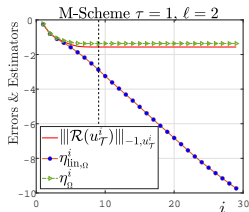
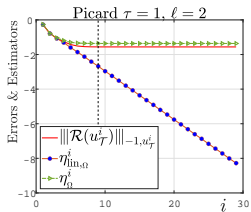
$\eta_k^i$  MS  $l=2, \tau=0.01, i=5$



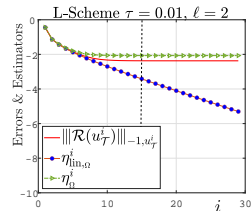
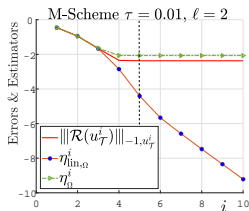
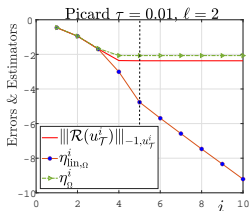
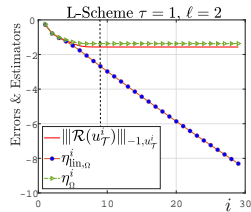
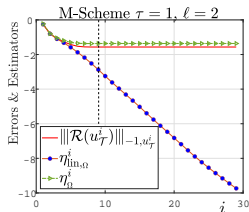
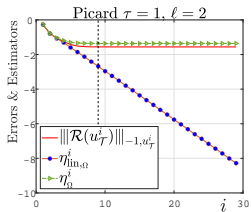
## 4 Local effectivity



## 4 Error with linearization iterations



## 4 Error with linearization iterations



Adaptive iteration stopping criteria:

$$\eta_{\text{lin}, \Omega}^i \leq 0.05 [\eta_\Omega^i].$$

## 4 Gradient independent diffusivity case

We consider in  $\Omega$  the equation

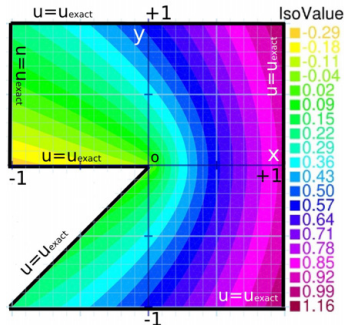
$$\varepsilon u - \nabla \cdot [A(|\nabla u|)\nabla u] = f$$

where

$$A(\mathbf{y}) = 2 + \frac{\mathbf{y}}{(1 + |\mathbf{y}|^2)},$$

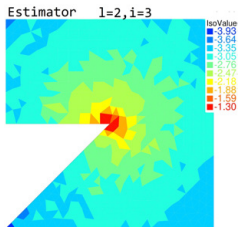
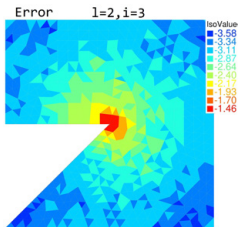
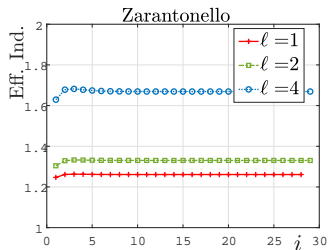
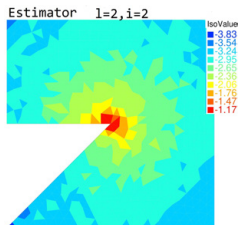
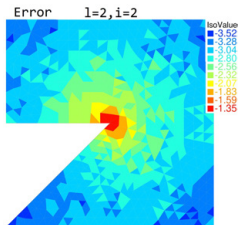
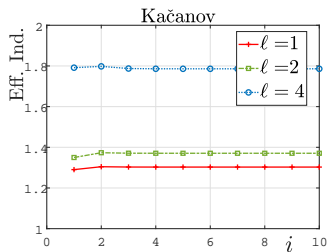
$\varepsilon = 10^{-2}$ , and a singular  $f \in H^{-1}(\Omega)$  is chosen such that the solution becomes

$$u_{\text{exact}} = r^{\frac{4}{7}} \cos\left(\frac{4}{7}\theta\right).$$

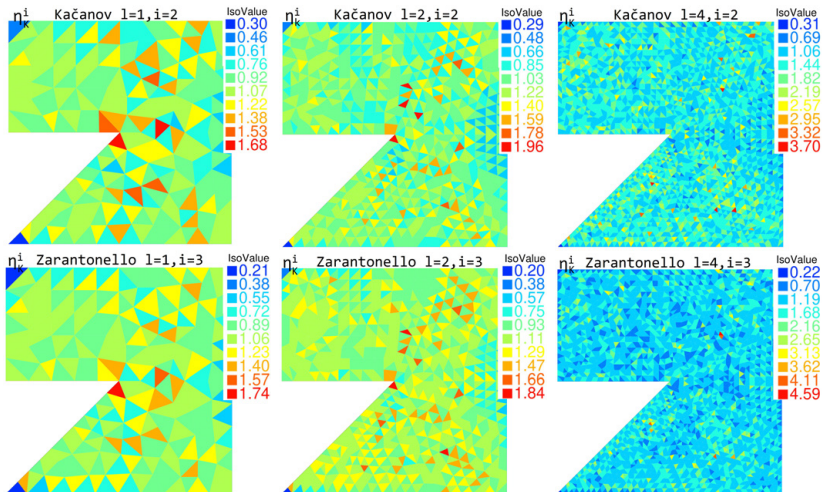


$\Omega$

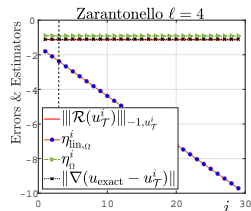
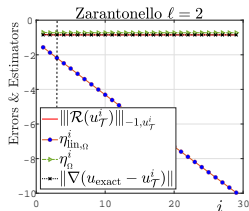
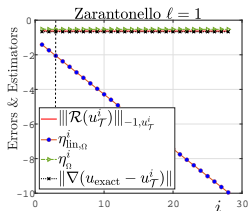
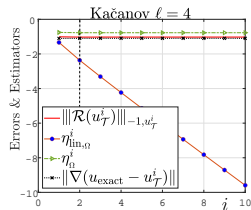
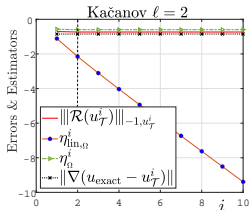
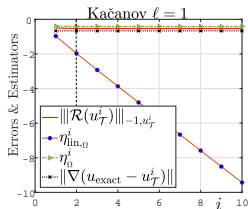
## 4 Global effectivity and distribution of error



## 4 Local effectivity



## 4 Error with linearization iterations





## 4 The Newton scheme

For the Newton scheme, the linearization operator

$$\mathfrak{L}(u_\ell^i; v, w) := (L(\mathbf{x}, u_\ell^i) v, w) + (\mathfrak{a}(\mathbf{x}, u_\ell^i) \nabla v, \nabla w) + (\mathbf{w}(\mathbf{x}, u_\ell^i) v, \nabla w),$$

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$$\mathbf{w}(\mathbf{x}, u_\ell^i) \mathfrak{a}^{-1}(\mathbf{x}, u_\ell^i) \mathbf{w}(\mathbf{x}, u_\ell^i) \leq C_N^2 L(\mathbf{x}, u_\ell^i), \quad \forall \mathbf{x} \in \Omega, \text{ and } i \in \mathbb{N},$$

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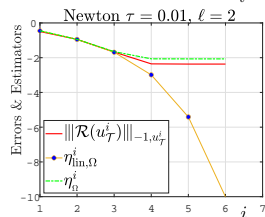
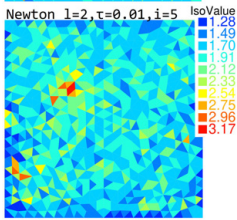
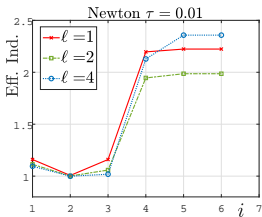
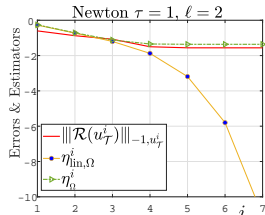
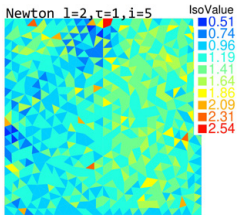
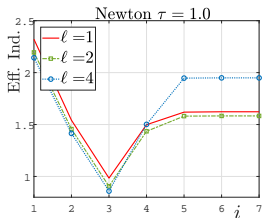
$$C_m(C_N) \left[ \left\| \mathcal{R}_{\text{lin}}^{u_\ell^i}(u_\ell^{i+1}) \right\|_{-1, u_\ell^i}^2 + \left\| u_\ell^{i+1} - u_\ell^i \right\|_{1, u_\ell^i}^2 \right] \leq \left\| \mathcal{R}(u_\ell^i) \right\|_{-1, u_\ell^i}^2$$

$$\leq C_M(C_N) \left[ \left\| \mathcal{R}_{\text{lin}}^{u_\ell^i}(u_\ell^{i+1}) \right\|_{-1, u_\ell^i}^2 + \left\| u_\ell^{i+1} - u_\ell^i \right\|_{1, u_\ell^i}^2 \right]$$

with  $C_m(C_N), C_M(C_N) \rightarrow 1$  if  $C_N \searrow 0$ .

## 4 The Newton scheme: numerical results

For gradient independent diffusivity case, we have



Global Effectivity

Local Effectivity

Error with iterations

① Introduction: nonlinear elliptic problems

② Main analytical results

③ Scope of the results

④ Numerical results

⑤ Nonlinear parabolic problems

Nonlinear advection-reaction-diffusion equation

Analytical properties

Error-residual relationship

A posteriori estimation

Numerical results

## 5 Nonlinear advection-reaction-diffusion equation

| 24

**Richards equation:** modelling flow of water through soil

$$\partial_t S(p) = \nabla \cdot [\bar{\mathbf{K}}_\kappa(S(p))(\nabla p + \mathbf{g})] + f(S(p), \mathbf{x}, t)$$

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- ▶ the *Darcy Law*

$$\boldsymbol{\sigma} = -\bar{\mathbf{K}}_\kappa(s)(\nabla p + \mathbf{g}),$$



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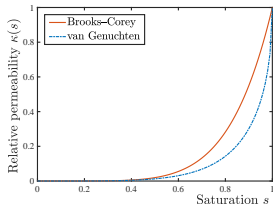
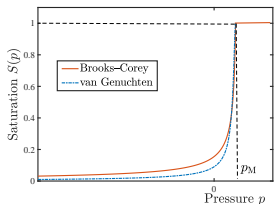
| 25

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$$\partial_t S(p) = \nabla \cdot [\bar{\mathbf{K}} \kappa(S(p)) (\nabla p + \mathbf{g})] + f(S(p), \mathbf{x}, t)$$

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- ▶  $S \in \text{Lip}(\mathbb{R})$  is increasing in  $(-\infty, p_M)$ ,  $S(-\infty) = 0$  and  $S'(p) = 0$ ,  $S(p) = 1$  for all  $p > p_M$ .
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- ▶  $\bar{\mathbf{K}} : \Omega \mapsto \mathbb{R}^{d \times d}$  is piece-wise constant in  $\Omega$ , bounded, symmetric positive definite, and satisfies the ellipticity condition,

$$K_m |\zeta|^2 \leq \zeta^T \bar{\mathbf{K}} \zeta \leq K_M |\zeta|^2, \quad \forall \zeta \in \mathbb{R}^d / \{0\}.$$

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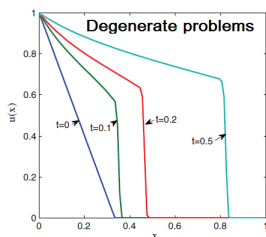
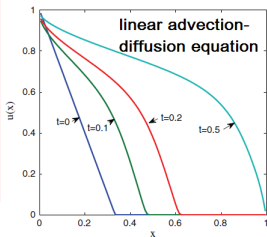
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**Literature:**  [Dolejší *et al* (2013)][Bernardi *et al* (2014)][Cancès *et al* (2014)] [Verfürth (2004)];  [Di Pietro *et al* (2015)];  [Ohlberger (2001)]



### Pressure formulation

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$$\mathcal{K}(p) = \int_0^p \kappa(S(\varrho)) \, d\varrho, \quad \theta = S \circ \mathcal{K}^{-1}$$

## 5 Alternative formulations

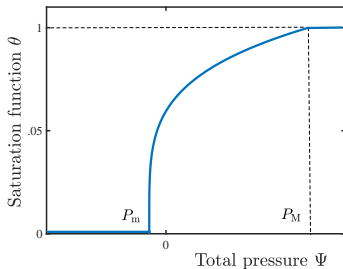
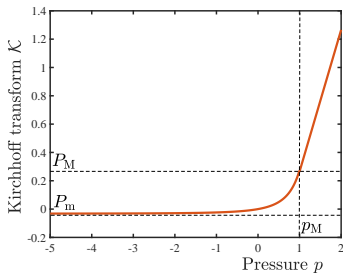
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### Total pressure formulation

For  $\Psi = \mathcal{K}(p)$ ,

$$\partial_t \theta(\Psi) = \nabla \cdot [\bar{\mathbf{K}} (\nabla \Psi + \mathcal{K}(\theta(\Psi)) \mathbf{g})] + f(\theta(\Psi), \mathbf{x}, t)$$

### Weak total pressure formulation

For the initial condition  $s_0$  bounded in  $(0, 1]$  a.e., find  $\Psi \in L^2(0, T; H_0^1(\Omega))$ ,  $s = \theta(\Psi) \in H^1(0, T; H^{-1}(\Omega))$ ,  $s(0) = s_0$  satisfying  $\forall \varphi \in L^2(0, T; H_0^1(\Omega))$ ,

$$\int_0^T [\langle \partial_t s, \varphi \rangle + (\bar{\mathbf{K}}[\nabla \Psi + \kappa(s)\mathbf{g}], \nabla \varphi)] = \int_0^T (f(s, \mathbf{x}, t), \varphi)$$

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Theorem [Alt & Luckhaus (1983)][Otto (1991)]

There exists a unique weak solution  $\Psi$  for the total pressure formulations.

## 5 Maximum principle

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To avoid the parabolic-hyperbolic degeneracy we need  $s \geq S_m > 0$

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### Proposition

If  $s_0$  is bounded in  $[\varepsilon, 1]$  for some  $\varepsilon > 0$ , then there exists *saturation lower-bound function*  $S_m : [0, T] \rightarrow (0, 1]$  such that for almost all  $(\mathbf{x}, t) \in \Omega \times [0, T]$ ,

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### Computing $S_m$

For example, under minor restrictions

$$S_m(t) = \min_{\mathbf{x} \in \Omega} \{s_0(\mathbf{x})\} + \int_0^t \min_{\mathbf{x} \in \Omega, \varrho > 0} \{f(S_m(\varrho), \mathbf{x}, \varrho)\} d\varrho$$

is a saturation lower-bound function.

## Residual

For  $\Psi_{h\tau} \in L^2(0, T; H_0^1(\Omega))$ ,  $s_{h\tau} = \theta(\Psi_{h\tau}) \in H^1(0, T; H^{-1}(\Omega))$  the residual  $\mathcal{R}(\Psi_{h\tau}) \in L^2(0, T; H^{-1}(\Omega))$  is

$$\int_0^T \langle \mathcal{R}(\Psi_{h\tau}), \varphi \rangle = \int_0^T [(f(s_{h\tau}, \mathbf{x}, t), \varphi) - \langle \partial_t s_{h\tau}, \varphi \rangle - (\bar{\mathbf{K}}[\nabla \Psi_{h\tau} + \kappa(s_{h\tau}) \mathbf{g}], \nabla \varphi)]$$

The  $H_{\bar{\mathbf{K}}}^{\pm 1}$  norm

For  $\omega \subseteq \Omega$ , the following equivalent norms of  $H^{\pm 1}(\omega)$  are defined

$$\begin{aligned}\|\varrho\|_{H_{\bar{\mathbf{K}}}^1(\omega)} &:= \|\bar{\mathbf{K}}^{\frac{1}{2}} \nabla \varrho\|_{L^2(\omega)}, \\ \|\varrho\|_{H_{\bar{\mathbf{K}}}^{-1}(\omega)} &:= \sup_{\varphi \in H_0^1(\omega)} \frac{\langle \varrho, \varphi \rangle_{H^{-1}(\omega), H_0^1(\omega)}}{\|\varphi\|_{H_{\bar{\mathbf{K}}}^1(\omega)}}.\end{aligned}$$

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The equivalent norm of  $L^2([0, T])$ 

For  $\alpha : \mathbb{R}^+ \rightarrow [0, \infty)$ , a time-smoothened equivalent of  $L^2([0, T])$ -norm is

$$\mathcal{J}_\alpha(\varrho) := \left[ \exp\left(-\int_0^T \alpha\right) \int_0^T \left( \varrho^2(t) + \alpha(t) \exp\left(\int_t^T \alpha\right) \int_0^t \varrho^2 \right) dt \right]^{\frac{1}{2}}.$$

## 5 Error measure

- ▶ The error measure  $\|\mathcal{R}(\Psi_{h\tau})\|_{L^2(0,T;H_{\bar{k}}^{-1}(\Omega))}$  might again be too weak

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### The error metric

For  $\omega \subseteq \Omega$ , interval  $I \subseteq [0, T]$ , and  $\alpha : \mathbb{R}^+ \rightarrow [0, \infty)$ , we choose

$$\begin{aligned} \text{dist}_{\omega,I}^{\alpha}(\Psi_1, \Psi_2) &:= \|\Psi_1 - \Psi_2\|_{L^2(I,H_K^1(\omega))} \\ &\quad + \|\alpha(\theta(\Psi_1) - \theta(\Psi_2))\|_{L^2(\omega \times I)} \\ &\quad + \|\partial_t(\theta(\Psi_1) - \theta(\Psi_2))\|_{L^2(I;H_K^{-1}(\omega))}. \end{aligned}$$

\*In the linear case,  $\alpha = 0$

## 5 Lower bound on error by residual

### Theorem 3 (a)

For a time-interval  $I \in [0, T]$ ,  $\omega \subseteq \Omega$ , and arbitrary  $\Psi_{h\tau} \in L^2(0, T; H_0^1(\Omega))$  with  $\theta(\Psi_{h\tau}) \in H^1(0, T; H^{-1}(\Omega))$  we have

$$\|\mathcal{R}(\Psi_{h\tau})\|_{L^2(I; H_{\bar{\kappa}}^{-1}(\omega))} \leq \text{dist}_{\omega, I}^{\alpha}(\Psi, \Psi_{h\tau}).$$

## 5 Lower bound on error by residual

### Theorem 3 (a)

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$$\|\mathcal{R}(\Psi_{hT})\|_{L^2(I; H_{\bar{\kappa}}^{-1}(\omega))} \leq \text{dist}_{\omega, I}^{\alpha}(\Psi, \Psi_{hT}).$$

**proof:** Use triangle inequality for the norm  $\|\cdot\|_{L^2(I; H_{\bar{\kappa}}^{-1}(\omega))}$



## 5 Upper bound on error by residual

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### Additional quantities

► For  $C_{h\tau}^\infty(t) := \|\bar{\mathbf{K}}^{\frac{1}{2}} \nabla s_{h\tau}(t)\|_{L^\infty(\Omega)}^2$ , assume that  $\int_0^T C_{h\tau}^\infty(t) dt < \infty$ .

## 5 Upper bound on error by residual

### Additional quantities

- ▶ For  $C_{h\tau}^\infty(t) := \|\bar{\mathbf{K}}^{\frac{1}{2}} \nabla s_{h\tau}(t)\|_{L^\infty(\Omega)}^2$ , assume that  $\int_0^T C_{h\tau}^\infty(t) dt < \infty$ .
- ▶ Parabolic–hyperbolic degeneracy  
Assume that  $s(t) \geq S_m(t) > 0$  a.e. in  $\Omega$  for  $t > 0$ .

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► Parabolic–hyperbolic degeneracy

Assume that  $s(t) \geq S_m(t) > 0$  a.e. in  $\Omega$  for  $t > 0$ .

► Parabolic–elliptic degeneracy

For  $\Omega^{\text{deg}} \supseteq \{s = 1\} \cup \{s_{h\tau} = 1\}$  we define

$$\eta^{\text{deg}}(t) := \sqrt{\frac{2}{D(1)}} \left[ \|\Psi_{h\tau}(t) - P_M\|_{H_{\bar{\mathbf{K}}}^1(\Omega)}^2 + \|[f(1, \mathbf{x}, t)]_+\|_{H_{\bar{\mathbf{K}}}^{-1}(\Omega^{\text{deg}}(t))} \right. \\ \left. + \left\| \left( \bar{\mathbf{K}}^{\frac{1}{2}} - \frac{\bar{\mathbf{K}}^{-\frac{1}{2}}}{|\Omega^{\text{deg}}(t)|} \int_{\Omega^{\text{deg}}(t)} \bar{\mathbf{K}} \mathbf{g} \right) \right\|_{\Omega^{\text{deg}}(t)}^2 \right]^{\frac{1}{2}}$$

## Theorem 3 (b)

Estimate in the  $L^2(\Omega \times [0, T])$  norm:

$$\begin{aligned} & \mathcal{J}_{\mathcal{E}_1}(\underline{\lambda}_1 \|s - s_{h\tau}\|)^2 \\ & \leq \|s_0 - s_{h\tau}(0)\|_{H_{\bar{k}}^{-1}(\Omega)}^2 + \mathcal{J}_{\mathcal{E}_1}(\bar{\lambda}_1 \|\mathcal{R}(\Psi_{h\tau})\|_{H_{\bar{k}}^{-1}(\Omega)})^2, \end{aligned}$$

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$$\begin{aligned} & \frac{1}{2} \mathcal{J}_{\mathcal{E}_2}(\underline{\lambda}_2 \|\Psi - \Psi_{h\tau}\|_{H_{\bar{k}}^1(\Omega)})^2 \\ & \leq \|s_0 - s_{h\tau}(0)\|^2 + \mathcal{J}_{\mathcal{E}_2}(\eta^{\text{deg}})^2 + 4 \mathcal{J}_{\mathcal{E}_2}(\bar{\lambda}_2 \|\mathcal{R}(\Psi_{h\tau})\|_{H_{\bar{k}}^{-1}(\Omega)})^2. \end{aligned}$$

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\*Similar expression holds for the  $\|\partial_t(\theta(\Psi_1) - \theta(\Psi_2))\|_{L^2(I; H_{\bar{k}}^{-1}(\Omega))}$  error component

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\*\*In the linear case  $\mathfrak{C}_1 = \mathfrak{C}_2 = 0$

## 5 Finite element solution

- ▶ Let  $\{t_0 := 0, t_1, \dots, t_N := T\}$  be the time-discretization, with  $\tau_n := t_n - t_{n-1}$ , and  $I_n := (t_{n-1}, t_n]$



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- ▶ Let  $\{p_{n,h} \in V_{n,h}\}_{n=1}^N$  be the sequence of finite elements solutions for backward Euler time discretization of the pressure formulation, i.e.,

$$\begin{aligned} & \left( \frac{1}{\tau_n} (S(p_{n,h}) - S(p_{n-1,h})), \nabla \varphi_h \right) + (\bar{\mathbf{K}} \kappa(S(p_{n,h})) [\nabla p_{n,h} + \mathbf{g}], \varphi_h) \\ & = (f(S(p_{n,h}), \mathbf{x}, t_n), \varphi_h), \quad \forall \varphi_h \in V_{n,h}. \end{aligned}$$

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- ▶ Define the time-discrete total pressure and saturation as

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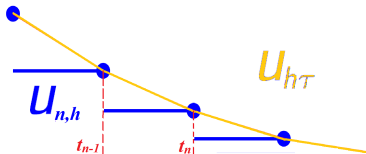
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- ▶ Let  $\Psi_{h\tau} \in C(0, T; H^1(\Omega))$  with  $s_{h\tau} \in W^{1,\infty}(0, T; L^2(\Omega))$  be their time-continuous interpolations, i.e., they satisfy

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$$\Psi_{h\tau}(t_n) = \Psi_{n,h}, \quad s_{h\tau}(t_n) = s_{n,h}.$$

- ▶ We introduce the a posteriori estimator  $\eta_\Omega : [0, T] \rightarrow [0, \infty)$ ,

$$\|\mathcal{R}(\Psi_{h\tau}(t))\|_{H_{\bar{\kappa}}^{-1}(\Omega)} \leq \eta_\Omega(t), \quad \forall t \in [0, T].$$

### Theorem 4 (a)

**Estimate in the  $L^2(\Omega \times [0, T])$  norm:**

$$\begin{aligned} [\mathcal{E}_{L^2}]^2 &:= \mathcal{J}_{\mathcal{C}_1}(\underline{\lambda}_1 \|s - s_{h\tau}\|)^2 \\ &\leq \|s_0 - s_{h\tau}(0)\|_{H_{\bar{\kappa}}^{-1}(\Omega)}^2 + \mathcal{J}_{\mathcal{C}_1}(\bar{\lambda}_1 \eta_\Omega)^2 =: [\eta_{L^2}]^2, \end{aligned}$$

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 [\mathcal{E}_{H^1}]^2 &:= \frac{1}{2} \mathcal{J}_{\mathcal{E}_2}(\lambda_2 \|\Psi - \Psi_{h\tau}\|_{H_{\bar{k}}^1(\Omega)})^2 \\
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## 5 Local space-time efficiency

### Theorem 4 (Local lower bounds)

For  $n \in \{1, \dots, N\}$ ,  $\omega \subseteq \Omega$  and some  $\mathfrak{I}_\omega \subset \Omega$  such that  $\omega \subseteq \Omega$ ,

$$\int_{I_n} \left( [\eta_\omega]^2 + \|\Psi_{h\tau} - \Psi_{n,h}\|_{H_K^1(\omega)}^2 \right)$$

$$\lesssim \text{dist}_{\mathfrak{I}_\omega, I_n}^\alpha(\Psi, \Psi_{h\tau})^2 + \left( \text{Data oscillation, quadrature, \& temporal discretization estimator} \right).$$

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$$\lesssim \text{dist}_{\mathfrak{T}_\omega, I_n}^\alpha(\Psi, \Psi_{h\tau})^2 + \left( \text{Data oscillation, quadrature, \& temporal discretization estimator} \right).$$

Similar estimate holds for the estimator

$$[\eta_{\text{LB}}^n]^2 := \int_{I_n} \left( [\eta_\Omega]^2 + \|\Psi_{h\tau} - \Psi_{n,h}\|_{H_K^1(\Omega)}^2 \right)$$

and the global-in-space error  $\text{dist}_{\Omega, I_n}^\alpha(\Psi_{h\tau}, \Psi)$ .

## 5 Numerical results: non-degenerate case

### Solution

$$p_{\text{exact}}(x, y, t) = 2 - e^{16(1+t^2)xy(1-x)(1-y)} \text{ in } (0, 1)^2$$

$$k(s) = s^3, S(p) = \frac{1}{(2-p)^{\frac{1}{3}}} \text{ (Brooks-Corey type)}$$

$$\bar{K} = \mathbb{I}, \mathbf{g} = -\mathbf{e}_x, f((x, y), t) \text{ set accordingly}$$

## 5 Reliability (upper bound) estimates

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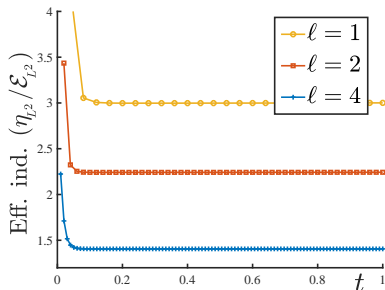
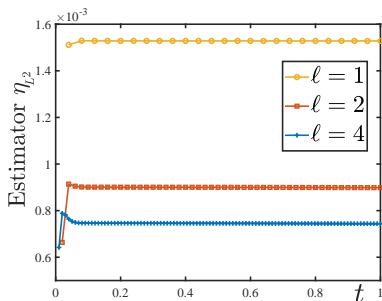
### Effectivity

Effectivity index := upper bound/error

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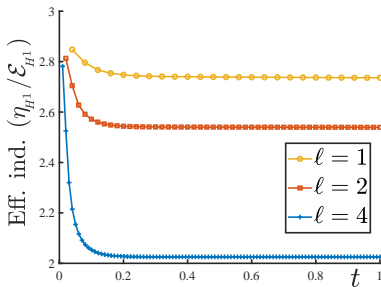
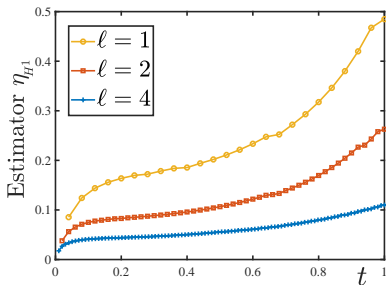


## 5 Reliability (upper bound) estimates

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### Effectivity

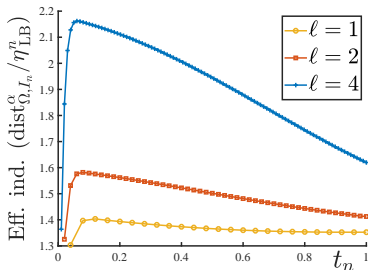
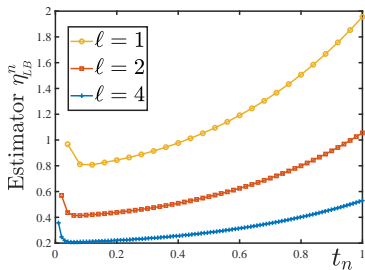
Effectivity index := upper bound/error =  $\eta_{H^1} / \mathcal{E}_{H^1}$



## 5 Global efficiency (lower bound)

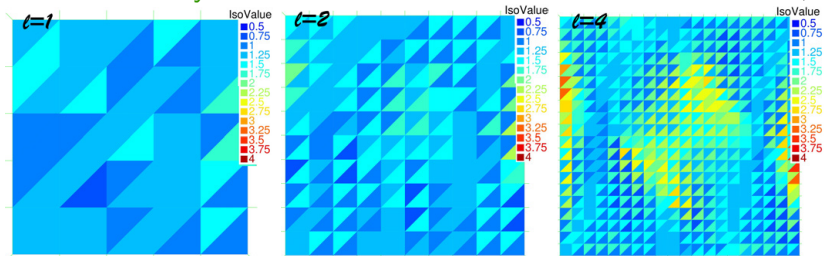
### Effectivity

Effectivity index := error/lower bound =  $\text{dist}_{\Omega, I_n}^{\alpha}(\Psi, \Psi_{h\tau}) / \eta_{\text{LB}}^n$ ,



## 5 Local efficiency

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## 5 Numerical results: degenerate case

### Solution

$$\Psi_{\text{exact}}(x, y, t) = 12(1 + t^2)xy(1 - x)(1 - y)$$

$$\theta(\Psi) = \begin{cases} \exp(\Psi - 1) & \text{if } \Psi < 1 \\ 1 & \text{if } \Psi \geq 1 \end{cases}$$

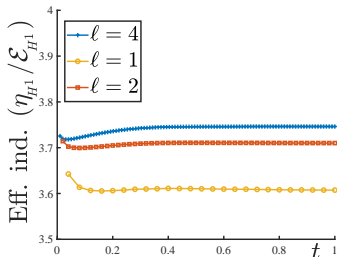
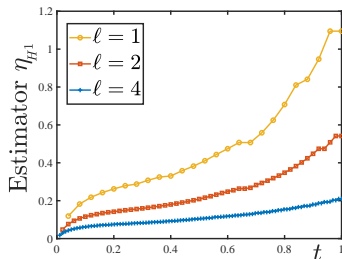
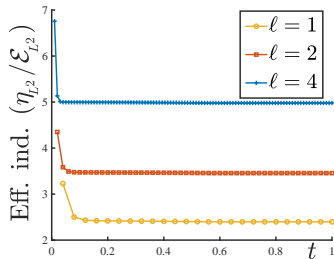
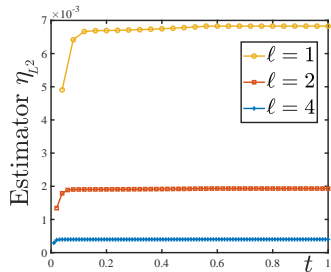
$$k(s) = \begin{cases} s & \text{if } s < 1 \\ 1 & \text{if } s \geq 1 \end{cases}$$

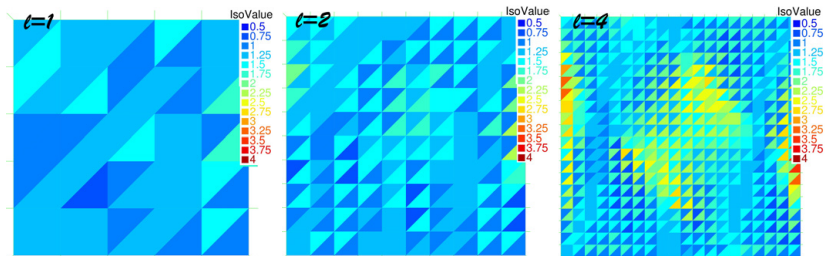
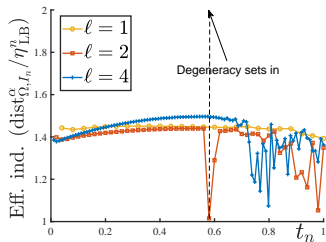
$$\bar{\mathbf{K}} = \mathbb{I}, \mathbf{g} = -\mathbf{e}_x$$

$f(x, y, t)$  set accordingly

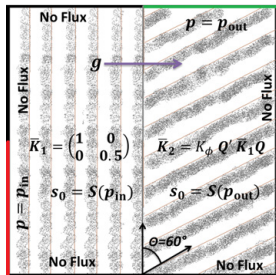
Degenerate domains

## 5 Reliability estimates

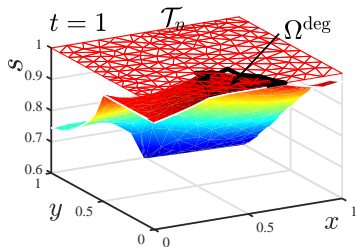
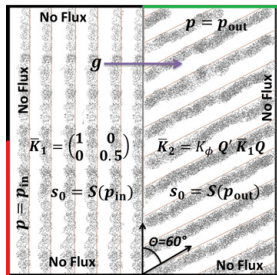




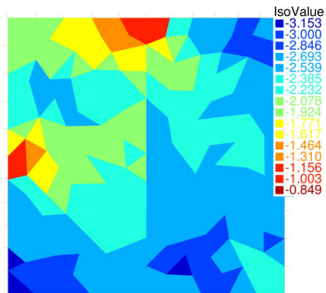
## 5 Numerical results: realistic case



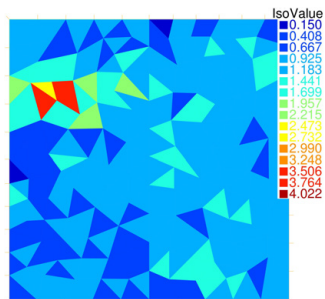
## 5 Numerical results: realistic case



## 5 Local efficiency



Estimate  $\log_{10}([\eta_n^F, h, K])$



Effectivity index

## 5 Nonlinear parabolic problems

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K. Mitra, & M. Vohralík. *A posteriori error estimates for the Richards equation*. arXiv preprint arXiv:2108.12507

## 5 Thank you for your time

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d'akujem Tak Dankie kiitos  
Спасибо תודה धन्यवाद terima kasih  
Asante Gracias شكرا mulțumesc hvala  
salamat 謝謝 Thank you Danke Hvala  
ありがとう Obrigado Merci Grazie 谢谢  
dank u ευχαριστώ Благодаря Děkuji  
ačiū Tack хвала Sağol تشکر از شما  
Дзякуй 감사합니다 dziękuję Спасибі  
paldies teşekkür ederim তোমাকে ধন্যবাদ