

A posteriori error estimates robust with respect to nonlinearities and orthogonal decomposition based on iterative linearization

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- 1 Introduction
- 2 Iteration-dependent norms
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 - Discretization and iterative linearization
 - Iteration-dependent norm and orthogonal decomposition
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- 3 Augmented energy difference
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 - Fenchel conjugate, dual energy, estimator, flux equilibration
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- 4 Conclusions

Goals

Error control

a posteriori error estimates

$$\underbrace{\|u - u_\ell\|}_{\text{unknown error}} \leq \underbrace{\eta(u_\ell)}_{\text{computable estimator}}$$

Goals

Error control

Guaranteed a posteriori error estimates

$$\underbrace{\|u - u_\ell\|}_{\text{unknown error}} \leq \underbrace{\eta(u_\ell)}_{\text{computable estimator}}$$

Goals

Error control

Guaranteed a posteriori error estimates **efficient**

$$\underbrace{\|u - u_\ell\|}_{\text{unknown error}} \leq \underbrace{\eta(u_\ell)}_{\text{computable estimator}} \leq C_{\text{eff}} \|u - u_\ell\|,$$

Goals

Error control

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

$$\underbrace{\|u - u_\ell\|}_{\text{unknown error}} \leq \underbrace{\eta(u_\ell)}_{\text{computable estimator}} \leq C_{\text{eff}} \|u - u_\ell\|, \quad C_{\text{eff}} \text{ independent of } \text{data}$$

Goals

Error control

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

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

Goals

Error control

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

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

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Question

- what to choose for $\|\cdot\|$?

Previous results

Model nonlinear elliptic problem

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

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

Previous results

Model nonlinear elliptic problem

Find $\textcolor{orange}{u} : \Omega \rightarrow \mathbb{R}$ such that

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

- $\Omega \subset \mathbb{R}^d$, $1 \leq d \leq 3$, open bounded polytope with Lipschitz boundary $\partial\Omega$
- a strongly monotone ($\textcolor{orange}{a}_m$) and Lipschitz continuous ($\textcolor{orange}{a}_c$)
- f piecewise polynomial for simplicity
- numerical approximation $\textcolor{orange}{u}_\ell$

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- f piecewise polynomial for simplicity
- numerical approximation $\textcolor{orange}{u}_\ell$
- strength of the nonlinearity (“nonlinear condition number”): $\textcolor{orange}{a}_c / \textcolor{orange}{a}_m$

Previous results

Sobolev norm

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

Previous results

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

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Energy difference

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

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Dual norm of the residual

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Dual norm of the residual (robust wrt $\frac{a_c}{a_m}$), “bypasses” the nonlinearity, “weak”

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- El Alaoui, Ern, & Vohralík (2011), Blechta, Málek, & Vohralík (2020), ...

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A model nonlinear problem I

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

$$(\mathbf{a}(|\nabla u|)\nabla u, \nabla v) + (f, v) = 0 \quad \forall v \in H_0^1(\Omega).$$

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Assumption (Gradient-dependent diffusivity)

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

$$|a(|\mathbf{x}|)\mathbf{x} - a(|\mathbf{y}|)\mathbf{y}| \leq a_c |\mathbf{x} - \mathbf{y}| \quad (\text{Lipschitz continuity}),$$

$$(a(|\mathbf{x}|)\mathbf{x} - a(|\mathbf{y}|)\mathbf{y}) \cdot (\mathbf{x} - \mathbf{y}) \geq a_m |\mathbf{x} - \mathbf{y}|^2 \quad (\text{strong monotonicity}).$$

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- $a_m \leq a(r) \leq a_c$, $a_m \leq (a(r)r)' \leq a_c$

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

$$\langle \mathcal{R}(u), v \rangle := (\mathbf{a}(|\nabla u|) \nabla u, \nabla v) + (f, v) = 0 \quad \forall v \in H_0^1(\Omega).$$

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Example of the nonlinear function a

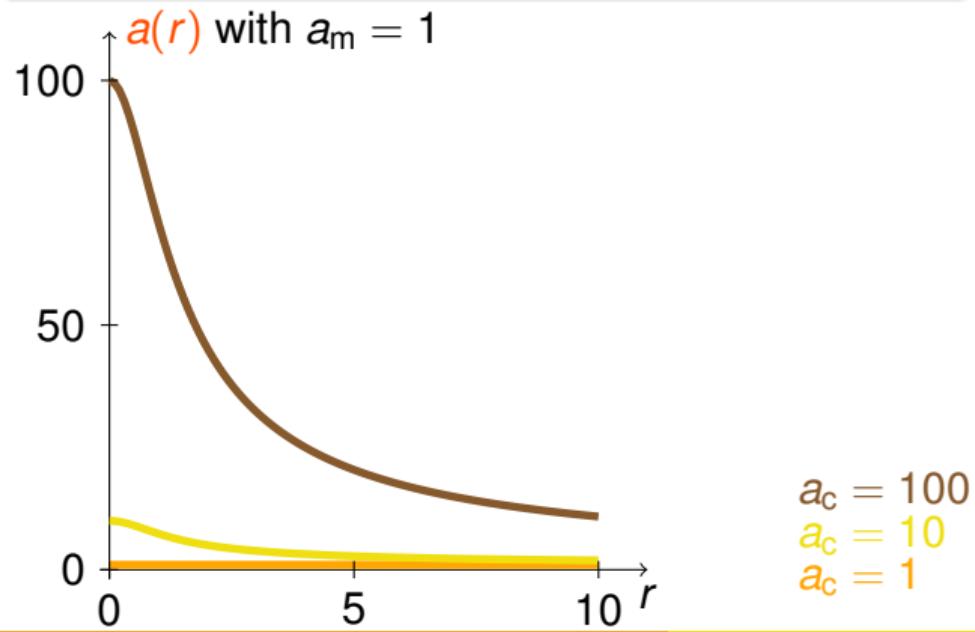
Example (Mean curvature nonlinearity)

$$a(r) := a_m + \frac{a_c - a_m}{\sqrt{1 + r^2}}.$$

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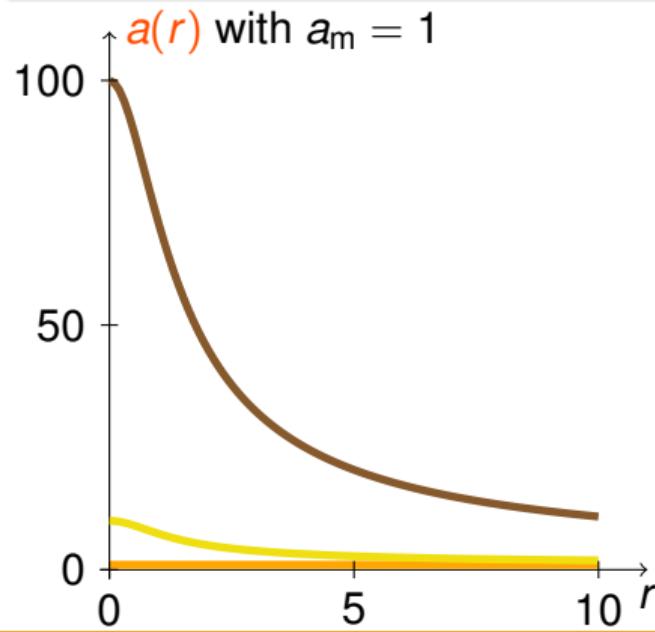
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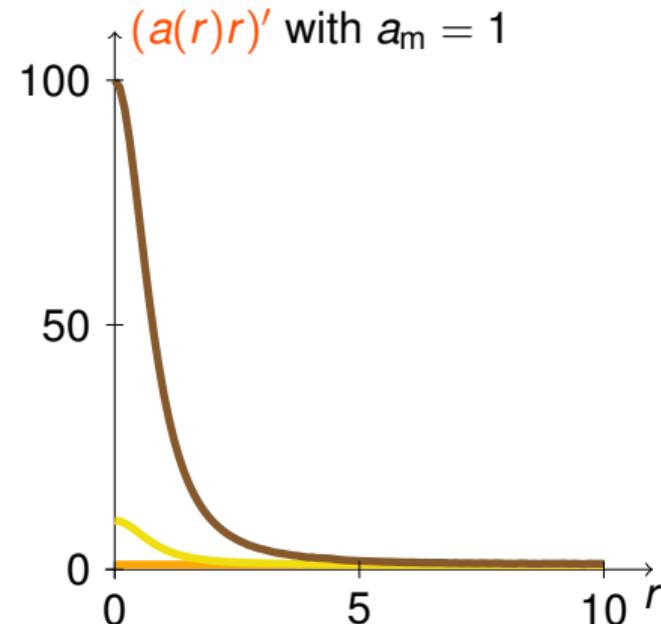
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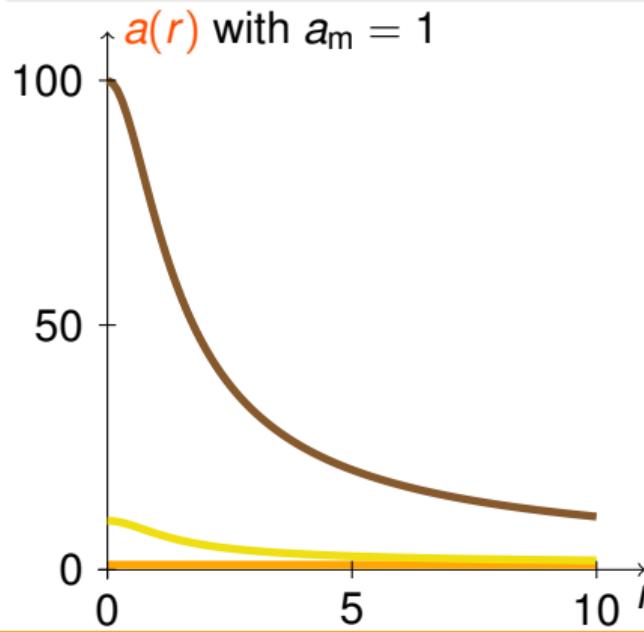
$$\begin{aligned}a_c &= 100 \\a_c &= 10 \\a_c &= 1\end{aligned}$$



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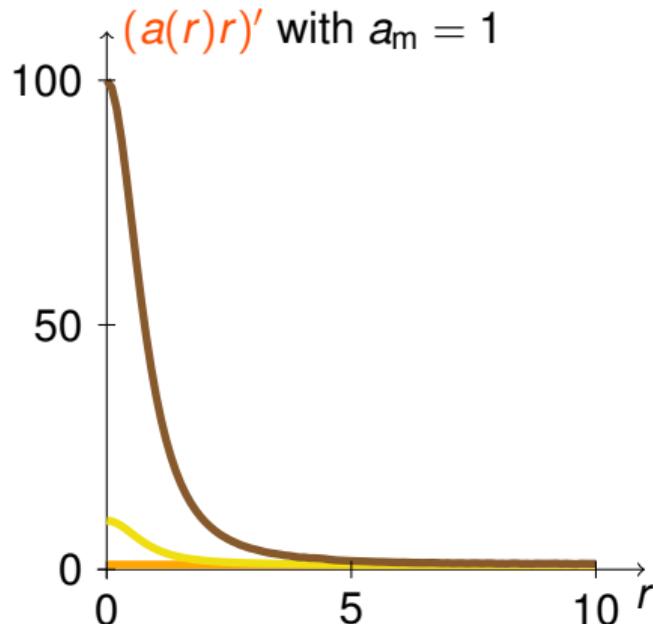
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$a_c = 100$
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Strength of the nonlinearity

$$\frac{a_c}{a_m} = \frac{\text{Lipschitz continuity}}{\text{strong monotonicity}}$$



A model nonlinear problem II

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

$$\langle \mathcal{R}(u), v \rangle := (\tau \mathbf{K}(\underbrace{\mathbf{a}(u)}_{\text{diffusion}} \nabla u + \underbrace{\mathbf{q}(u)}_{\text{advection}}, \nabla v) + (\underbrace{\mathbf{f}(u)}_{\text{reaction}}, v) = 0 \quad \forall v \in H_0^1(\Omega).$$

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- semilinear equations with $a = 1$, $\mathbf{K} = \mathbf{I}_d$, $\tau = 1$, $\mathbf{q} = \mathbf{0}$: ignition of gases, gravitational influences on stars, quantum field theory ...
- implicit time-discretization of nonlinear (degenerate) parabolic equations ($\tau > 0$ a time step size): Fischer–KPP, porous medium, Richards, biofilms ...

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diffusion advection reaction

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Assumption (Gradient-independent diffusivity)

- $|a(\mathbf{x}_1, u_1) - a(\mathbf{x}_2, u_2)| \leq L_a(|\mathbf{x}_1 - \mathbf{x}_2| + |u_1 - u_2|) \quad \forall \mathbf{x}_1, \mathbf{x}_2 \in \Omega \text{ and } u_1, u_2 \in \mathbb{R}$
- $0 \leq f(\mathbf{x}, u_2) - f(\mathbf{x}, u_1) \leq L_f(u_2 - u_1) \quad \forall \mathbf{x} \in \Omega \text{ and } u_1, u_2 \in \mathbb{R}, u_2 \geq u_1$
- \mathbf{K} is uniformly symmetric positive definite and bounded with eigenvalues a_m, a_c
- \mathbf{q} is “small” wrt a

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Linear case

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Classical choices discussed above

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$$\|\mathcal{R}(u_\ell)\|_{-1} \leq \bar{\eta}(u_\ell) \leq C_{\text{eff}} \|\mathcal{R}(u_\ell)\|_{-1}$$

Trivial nonlinear case

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

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Ideal but impossible choice

$$\| \cdot \| := \|\mathbf{K}^{1/2} \mathbf{a}^{1/2}(u) \nabla(\cdot)\|$$

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Discretization and fixed-point iterative linearization

- **discretization:** finite element subspace $V_\ell \subset H_0^1(\Omega)$, find $u_\ell \in V_\ell$ s.t.

$$(\mathbf{K} \mathbf{a}(u_\ell) \nabla u_\ell, \nabla v_\ell) + (f, v_\ell) = 0 \quad \forall v_\ell \in V_\ell.$$

Trivial nonlinear case

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

$$\langle \mathcal{R}(u), v \rangle := (\mathbf{K} \mathbf{a}(u) \nabla u, \nabla v) + (f, v) = 0 \quad \forall v \in H_0^1(\Omega).$$

Ideal but impossible choice

$$\| \cdot \| := \| \mathbf{K}^{1/2} \mathbf{a}^{1/2}(\mathbf{u}) \nabla (\cdot) \|$$

Discretization and fixed-point iterative linearization

- **discretization:** finite element subspace $V_\ell \subset H_0^1(\Omega)$, find $u_\ell \in V_\ell$ s.t.

$$(\mathbf{K} \mathbf{a}(u_\ell) \nabla u_\ell, \nabla v_\ell) + (f, v_\ell) = 0 \quad \forall v_\ell \in V_\ell.$$

- fixed-point **iterative linearization:** from $u_\ell^{k-1} \in V_\ell$, find $u_\ell^k \in V_\ell$ such that

$$(\mathbf{K} \mathbf{a}(u_\ell^{k-1}) \nabla u_\ell^k, \nabla v_\ell) + (f, v_\ell) = 0 \quad \forall v_\ell \in V_\ell.$$

Trivial nonlinear case: main idea

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Discretization and fixed-point iterative linearization

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Iteration-dependent discrete energy norm

$$||| \cdot |||_{u_\ell^{k-1}} := \| \mathbf{K}^{1/2} \mathbf{a}^{1/2}(u_\ell^{k-1}) \nabla (\cdot) \|$$

Trivial nonlinear case: main idea

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Iteration-dependent discrete energy and dual norms

$$\|\cdot\|_{u_\ell^{k-1}} := \|\mathbf{K}^{1/2} \mathbf{a}^{1/2}(u_\ell^{k-1}) \nabla(\cdot)\|, \quad \|\mathcal{R}(u_\ell)\|_{-1, u_\ell^{k-1}} := \sup_{v \in H_0^1(\Omega)} \frac{\langle \mathcal{R}(u_\ell), v \rangle}{\|\cdot\|_{u_\ell^{k-1}}}$$

Main idea

Main idea

Apply in the **a posteriori analysis** and in **adaptivity**, to define norms, the **iterative linearization** on the **discrete level**.

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Weak solution

Definition (Weak solution)

Find $\textcolor{red}{u} \in H_0^1(\Omega)$ s.t.

$$\langle \mathcal{R}(u), v \rangle = 0 \quad \forall v \in H_0^1(\Omega).$$

Finite element discretization

Definition (Finite element discretization)

Find $u_\ell \in V_\ell$ s.t.

$$\langle \mathcal{R}(u_\ell), v_\ell \rangle = 0 \quad \forall v_\ell \in V_\ell.$$

Finite element discretization

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Find $u_\ell \in V_\ell$ s.t.

$$\langle \mathcal{R}(u_\ell), v_\ell \rangle = 0 \quad \forall v_\ell \in V_\ell.$$

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

Iterative linearization

Definition (Iterative linearization)

Find $u_\ell^k \in V_\ell$ s.t.

$$\left(\underbrace{(\underline{u_\ell^k - u_\ell^{k-1}}, v_\ell)}_{\text{increment}}, v_\ell \right)_{u_\ell^{k-1}} = - \underbrace{\langle \mathcal{R}(u_\ell^{k-1}), v_\ell \rangle}_{\text{residual}} \quad \forall v_\ell \in V_\ell.$$

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- iterative linearization index $k \geq 1$

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- iterative linearization index $k \geq 1$
- $u_\ell^0 \in V_\ell$ a given initial guess

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- iterative linearization index $k \geq 1$
- $u_\ell^0 \in V_\ell$ a given initial guess
- **iteration-dependent** reaction–diffusion **scalar product**

$$\left((w, v) \right)_{u_\ell^{k-1}} := (\mathcal{L}_\ell^{k-1} w, v) + (\mathcal{A}_\ell^{k-1} \nabla w, \nabla v), \quad w, v \in H_0^1(\Omega)$$

Iterative linearization

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Find $u_\ell^k \in V_\ell$ s.t.

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- iteration-dependent** reaction–diffusion **scalar product**

$$\left((w, v) \right)_{u_\ell^{k-1}} := (L_\ell^{k-1} w, v) + (\mathbf{A}_\ell^{k-1} \nabla w, \nabla v), \quad w, v \in H_0^1(\Omega)$$

- $\mathbf{A}_\ell^{k-1}: \Omega \rightarrow \mathbb{R}^{d \times d}$ **matrix**-valued function constructed from u_ℓ^{k-1} , $L_\ell^{k-1}: \Omega \rightarrow \mathbb{R}$ **scalar**-valued function constructed from u_ℓ^{k-1}

Iterative linearization

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- $\mathbf{A}_\ell^{k-1}: \Omega \rightarrow \mathbb{R}^{d \times d}$ **matrix**-valued function constructed from u_ℓ^{k-1} , $L_\ell^{k-1}: \Omega \rightarrow \mathbb{R}$ **scalar**-valued function constructed from u_ℓ^{k-1}
- $L_\ell^{k-1} = 0$ if $f = f(\mathbf{x})$ (linear, source term)

Iterative linearization

Definition (Iterative linearization)

Find $u_\ell^k \in V_\ell$ s.t.

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

- examples for the gradient-dependent diffusivity:
 - $\mathbf{A}_\ell^{k-1} = a(|\nabla u_\ell^{k-1}|) \mathbf{I}_d$, $L_\ell^{k-1} = \partial_u f(u_\ell^{k-1})$ (Kačanov)
 - $\mathbf{A}_\ell^{k-1} = a(|\nabla u_\ell^{k-1}|) \mathbf{I}_d + \frac{a'(|\nabla u_\ell^{k-1}|)}{|\nabla u_\ell^{k-1}|} \nabla u_\ell^{k-1} \otimes \nabla u_\ell^{k-1}$, $L_\ell^{k-1} = \partial_u f(u_\ell^{k-1})$ (Newton)
 - $\mathbf{A}_\ell^{k-1} = \gamma \mathbf{I}_d$ with $\gamma \geq \frac{a_c^2}{a_m}$ a **constant parameter**, $L_\ell^{k-1} = 0$ (Zarantonello)

Iterative linearization

Definition (Iterative linearization)

Find $\mathbf{u}_\ell^k \in V_\ell$ s.t.

$$\left(\underbrace{(\mathbf{u}_\ell^k - \mathbf{u}_\ell^{k-1}, \mathbf{v}_\ell)}_{\text{increment}}, \mathbf{v}_\ell \right)_{\mathbf{u}_\ell^{k-1}} = - \underbrace{\langle \mathcal{R}(\mathbf{u}_\ell^{k-1}), \mathbf{v}_\ell \rangle}_{\text{residual}} \quad \forall \mathbf{v}_\ell \in V_\ell.$$

- examples for the gradient-independent diffusivity:
 - $\mathbf{A}_\ell^{k-1} = \tau \mathbf{K} \mathbf{a}(\mathbf{u}_\ell^{k-1})$ (fixed point)

Iterative linearization

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Find $\mathbf{u}_\ell^k \in V_\ell$ s.t.

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- examples for the gradient-independent diffusivity:

- $\mathbf{A}_\ell^{k-1} = \tau \mathbf{K} \mathbf{a}(\mathbf{u}_\ell^{k-1})$ (fixed point)
- Picard: $L_\ell^{k-1} = \partial_u f(u_\ell^{k-1})$
- Jäger–Kačur: $L_\ell^{k-1} = \max_{u \in \mathbb{R}} \left(\frac{f(u) - f(u_\ell^{k-1})}{u - u_\ell^{k-1}} \right)$
- L -scheme: $L_\ell^{k-1} = \text{cnst} \geq \frac{1}{2} \sup \partial_u f$
- M -scheme: $L_\ell^{k-1} = \partial_u f(u_\ell^{k-1}) + \tau \times \text{cnst}$

Iterative linearization

Definition (Iterative linearization)

Find $u_\ell^k \in V_\ell$ s.t.

$$\langle \mathcal{R}_{\text{disc}}^{u_\ell^{k-1}}(u_\ell^k), v_\ell \rangle := ((u_\ell^k - u_\ell^{k-1}, v_\ell))_{u_\ell^{k-1}} + \langle \mathcal{R}(u_\ell^{k-1}), v_\ell \rangle = 0 \quad \forall v_\ell \in V_\ell.$$

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Iteration-dependent norm

Definition (Iteration-dependent norm)

$$\|v\|_{u_\ell^{k-1}}^2 := ((v, v))_{u_\ell^{k-1}} = \|(L_\ell^{k-1})^{1/2} v\|^2 + \|(A_\ell^{k-1})^{1/2} \nabla v\|^2, \quad v \in H_0^1(\Omega)$$

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- induced by the linearization scalar product

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

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

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- orthogonal decomposition into error components
- linearization error is computable

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- **orthogonal decomposition** into **error components**
- **linearization error** is **computable**
- $\langle \mathcal{R}_{\text{disc}}^{u_\ell^{k-1}}(u_\ell^k), v \rangle = ((u_\ell^k - u_\ell^{k-1}, v))_{u_\ell^{k-1}} + \langle \mathcal{R}(u_\ell^{k-1}), v \rangle, v \in H_0^1(\Omega) \text{ (0 if } v \in V_\ell)$

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- **orthogonal decomposition** into **error components**
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- $u_{\langle \ell \rangle}^k \in H_0^1(\Omega)$ such that $\langle \mathcal{R}_{\text{disc}}^{u_\ell^{k-1}}(u_{\langle \ell \rangle}^k), v \rangle = 0 \forall v \in H_0^1(\Omega)$

An orthogonal decomposition of the total residual/error

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$$\|u_\ell^{k-1} - u_{\langle \ell \rangle}^k\|_{u_\ell^{k-1}}$$

$$\|u_\ell^k - u_{\langle \ell \rangle}^k\|_{u_\ell^{k-1}}$$

- **orthogonal decomposition** into **error components**
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- $\langle \mathcal{R}_{\text{disc}}^{u_\ell^{k-1}}(u_\ell^k), v \rangle = ((u_\ell^k - u_\ell^{k-1}, v))_{u_\ell^{k-1}} + \langle \mathcal{R}(u_\ell^{k-1}), v \rangle, v \in H_0^1(\Omega) \text{ (0 if } v \in V_\ell)$
- $u_{\langle \ell \rangle}^k \in H_0^1(\Omega)$ such that $\langle \mathcal{R}_{\text{disc}}^{u_\ell^{k-1}}(u_{\langle \ell \rangle}^k), v \rangle = 0 \forall v \in H_0^1(\Omega)$
- **discretization error** is given by a **linear** reaction-diffusion problem

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A posteriori error estimates in an iteration-dependent norm

Theorem (A posteriori estimate in iteration-dependent norm)

For all linearization steps $k \geq 1$,

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

A posteriori error estimates in an iteration-dependent norm

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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

$$\eta(u_\ell^k) \leq C_{\text{eff}}(d, \kappa\tau, p) C_\ell^k \|\mathcal{R}(u_\ell^{k-1})\|_{-1, u_\ell^{k-1}} + \text{quadrature error terms},$$

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$$\eta_K(u_\ell^k) \leq C_{\text{eff}}(d, \kappa_T, p) C_K^k \| \mathcal{R}(u_\ell^{k-1}) \|_{-1, u_\ell^{k-1}, \omega_K} + \text{quadrature error terms},$$

A posteriori error estimates in an iteration-dependent norm

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where

$$C_K^k := \left(\frac{\max. \text{ eig. } \mathbf{A}_\ell^{k-1}|_{\omega_K}}{\min. \text{ eig. } \mathbf{A}_\ell^{k-1}|_{\omega_K}} \right)^{1/2} + \left(\frac{\max. L_\ell^{k-1}|_{\omega_K}}{\min. L_\ell^{k-1}|_{\omega_K}} \right)^{1/2} \quad \text{if react. dom.}$$

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✓ $C_\ell^k = 1$ for Zarantonello \Rightarrow robustness wrt the strength of nonlinearities

A posteriori error estimates in an iteration-dependent norm

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- ✓ $C_\ell^k = 1$ for Zarantonello \Rightarrow robustness wrt the strength of nonlinearities
- ✓ C_K^k given by local conditioning of the linearization matrix \mathbf{A}_ℓ^{k-1} (and scalar L_ℓ^{k-1}):

A posteriori error estimates in an iteration-dependent norm

Theorem (A posteriori estimate in iteration-dependent norm)

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- ✓ $C_\ell^k = 1$ for Zarantonello \Rightarrow robustness wrt the strength of nonlinearities
- ✓ C_K^k given by local conditioning of the linearization matrix \mathbf{A}_ℓ^{k-1} (and scalar L_ℓ^{k-1}): typically much better than global conditioning (= worst-case scenario)

A posteriori error estimates in an iteration-dependent norm

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

Moreover, for all linearization steps $k \geq 1$ and for each element $K \in \mathcal{T}_\ell$, there holds

$$\eta_K(u_\ell^k) \leq C_{\text{eff}}(d, \kappa_T, p) C_K^k \|\mathcal{R}(u_\ell^{k-1})\|_{-1, u_\ell^{k-1}, \omega_K} + \text{quadrature error terms},$$

where

$$C_K^k := \left(\frac{\max. \text{ eig. } \mathbf{A}_\ell^{k-1}|_{\omega_K}}{\min. \text{ eig. } \mathbf{A}_\ell^{k-1}|_{\omega_K}} \right)^{1/2} + \left(\frac{\max. L_\ell^{k-1}|_{\omega_K}}{\min. L_\ell^{k-1}|_{\omega_K}} \right)^{1/2} \quad \text{if react. dom.}$$

- ✓ $C_\ell^k = 1$ for Zarantonello \Rightarrow robustness wrt the strength of nonlinearities
- ✓ C_K^k given by local conditioning of the linearization matrix \mathbf{A}_ℓ^{k-1} (and scalar L_ℓ^{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

A posteriori error estimates in an iteration-dependent norm

Theorem (A posteriori estimate in iteration-dependent norm)

For all linearization steps $k \geq 1$,

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

Moreover, for all linearization steps $k \geq 1$ and for each element $K \in \mathcal{T}_\ell$, there holds

$$\eta_K(u_\ell^k) \leq C_{\text{eff}}(d, \kappa_T, p) C_K^k \|\mathcal{R}(u_\ell^{k-1})\|_{-1, u_\ell^{k-1}, \omega_K} + \text{quadrature error terms},$$

where

$$C_K^k := \left(\frac{\max. \text{ eig. } \mathbf{A}_\ell^{k-1}|_{\omega_K}}{\min. \text{ eig. } \mathbf{A}_\ell^{k-1}|_{\omega_K}} \right)^{1/2} + \left(\frac{\max. L_\ell^{k-1}|_{\omega_K}}{\min. L_\ell^{k-1}|_{\omega_K}} \right)^{1/2} \quad \text{if react. dom.}$$

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

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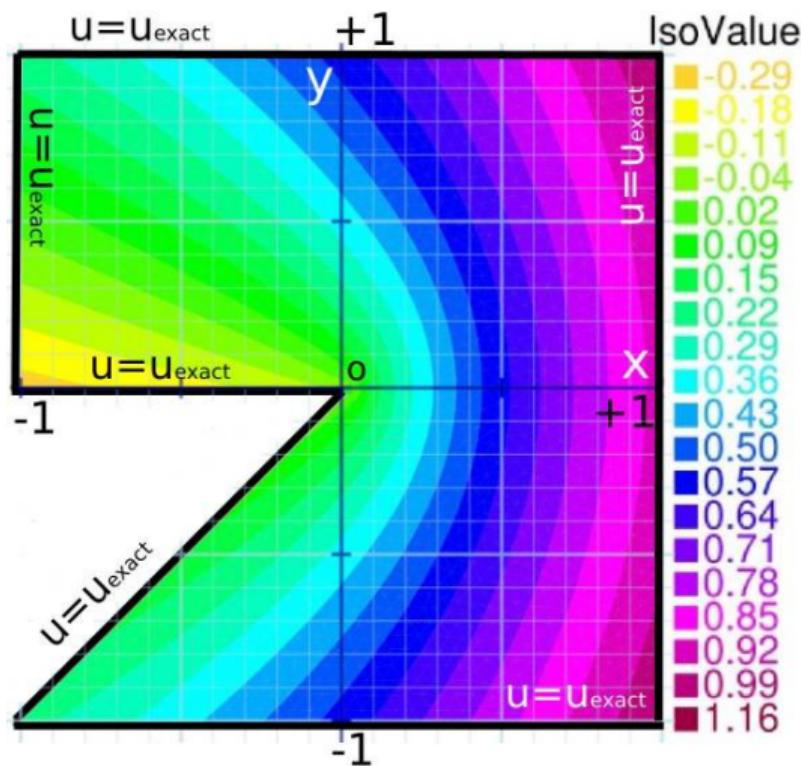
4 Conclusions

Gradient-dependent diffusivity

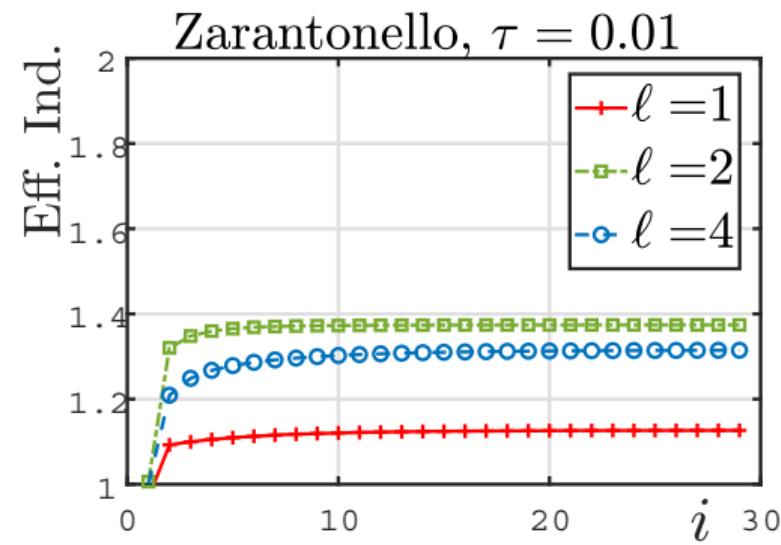
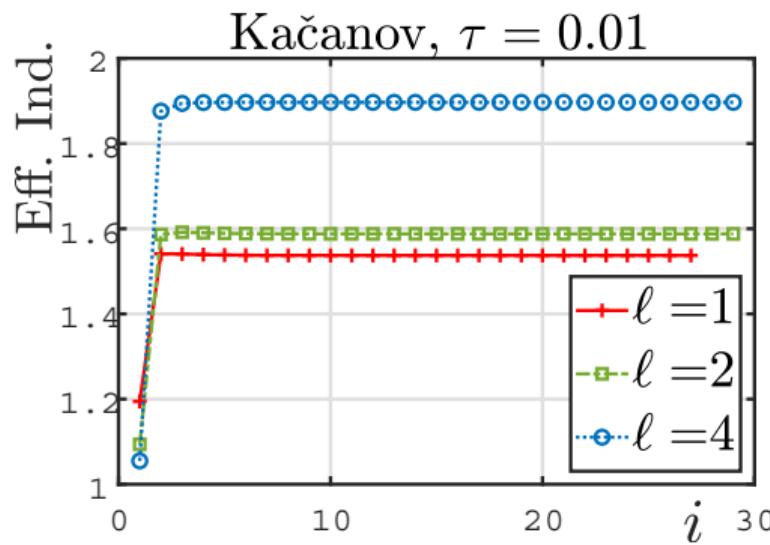
Setting

- mean curvature with $a(r) := a_m + \frac{a_c - a_m}{\sqrt{1+r^2}}$
- $a_c := a_m + 1$, $a_m := 2\tau$, $\frac{a_c}{a_m} = 1 + 0.5\frac{1}{\tau}$, $\frac{1}{\tau} \in [1, 10^3]$
- $f(\mathbf{x}, \xi) := \nu \xi - g(\mathbf{x})$, $\nu = 10^{-2}$
- $g(\mathbf{x}) := \left[r^{-1} \frac{(1-\lambda)(\lambda r^{\lambda-1})^3}{(1+(\lambda r^{\lambda-1})^2)^{\frac{3}{2}}} + \nu r^\lambda \right] \cos(\lambda\theta)$, $\lambda := 4/7$
- weak solution $u(\mathbf{x}) := r^\lambda \cos(\lambda\theta)$

Solution u

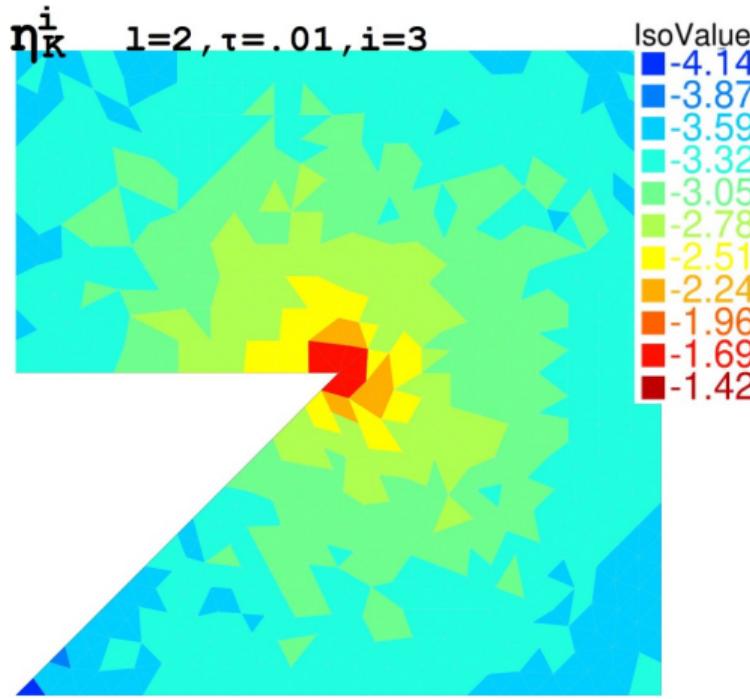


How large is the error?

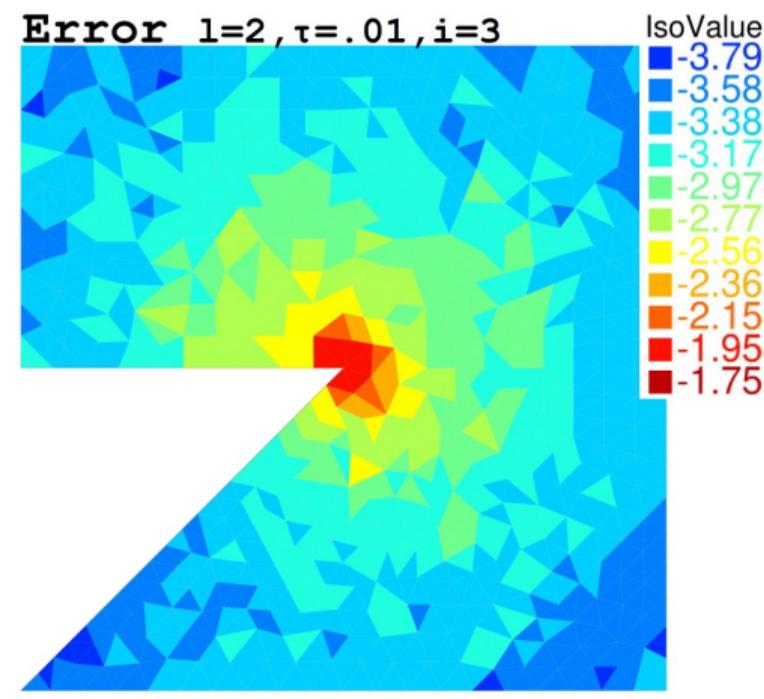


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Where is the error **localized**?

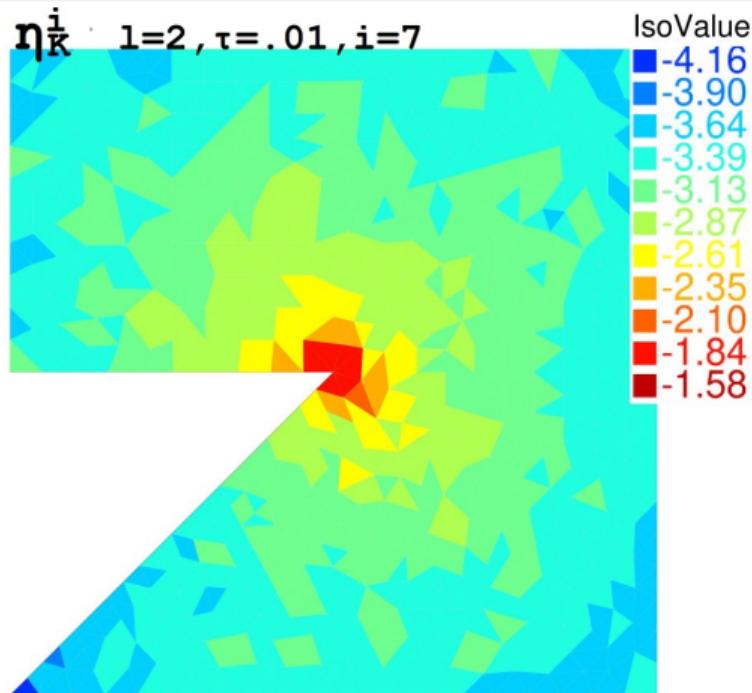


Estimated error, $\tau = 0.01$, Kačanov

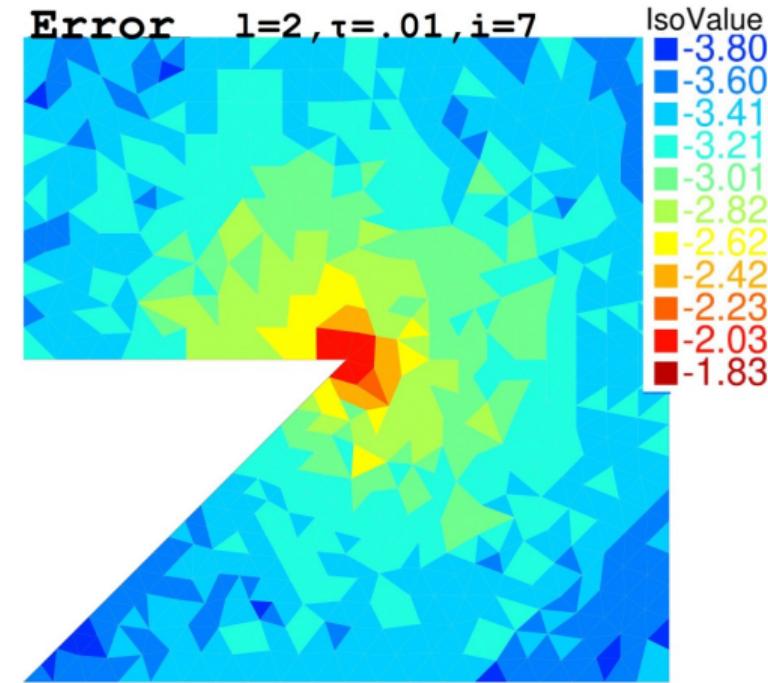


Exact error, $\tau = 1, \tau = 0.01$, Kačanov

Where is the error **localized**?

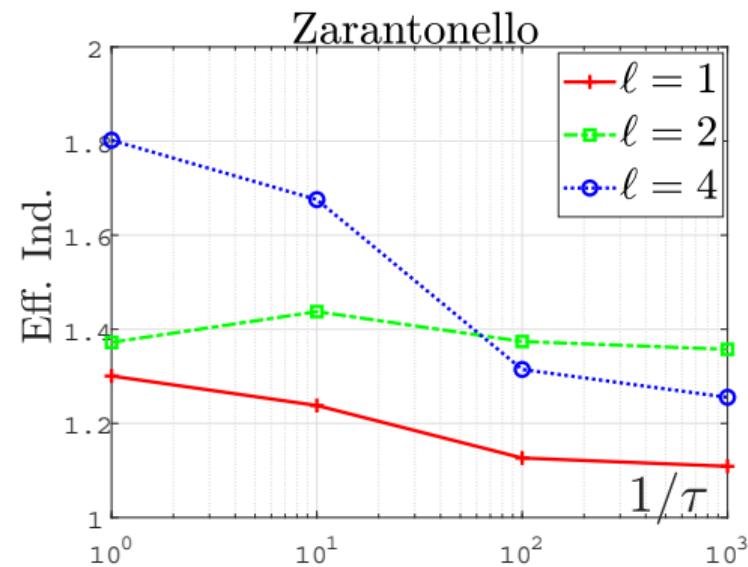
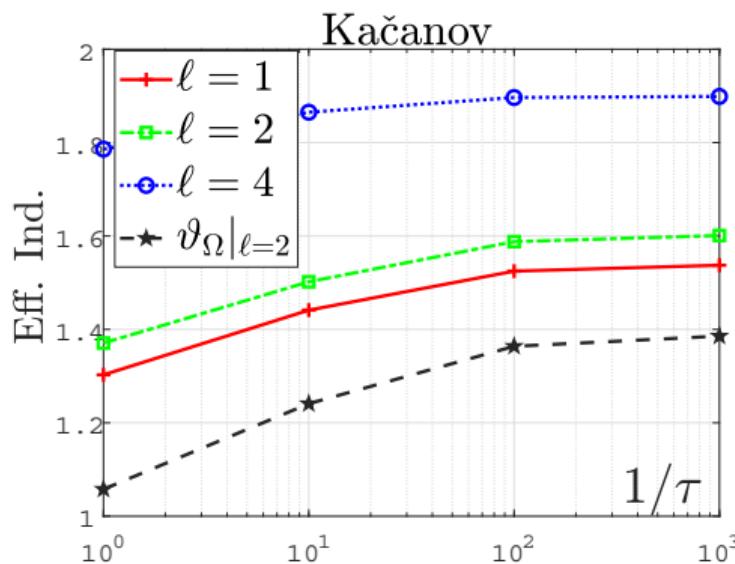


Estimated error, $\tau = 0.01$, Zarantonello



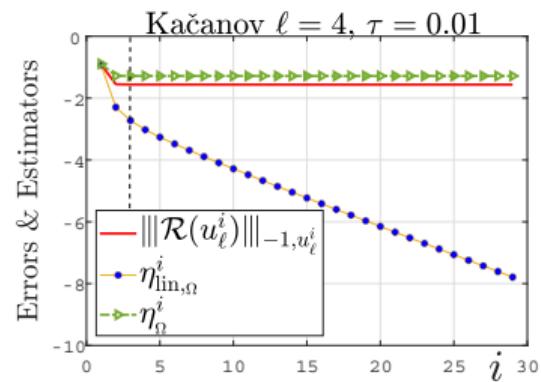
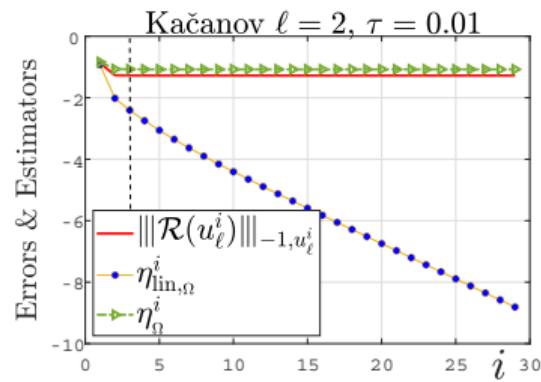
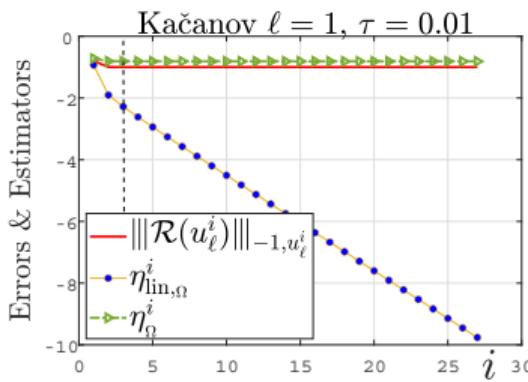
Exact error, $\tau = 1, \tau = 0.01$, Zarantonello

Robustness wrt the nonlinearities



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Error components and adaptivity via stopping criteria



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Gradient-independent diffusivity

Setting

- one time step of the Richards equation
- unit square $\Omega = (0, 1)^2$
- realistic data

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

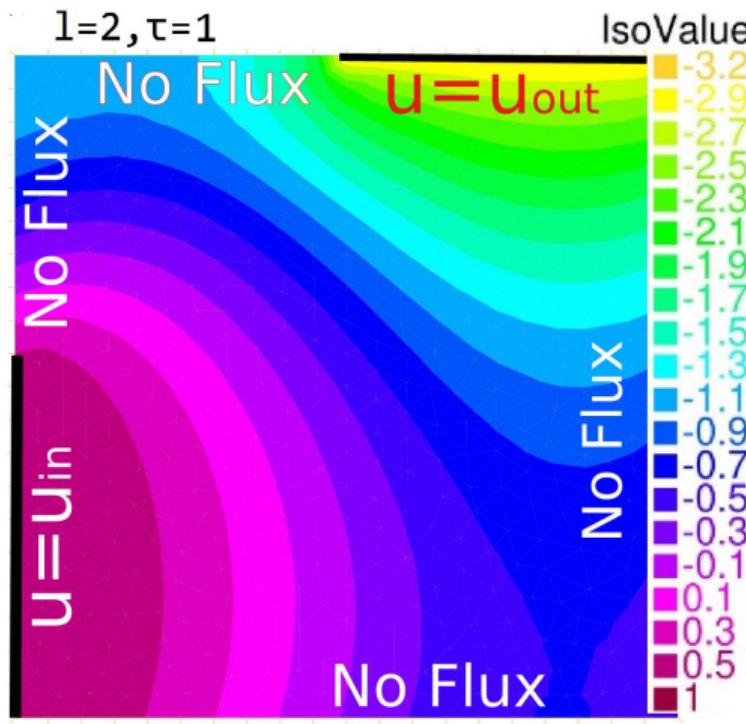
$$\mathbf{K} = \begin{bmatrix} 1 & 0.2 \\ 0.2 & 1 \end{bmatrix}, \quad \mathbf{g} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

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

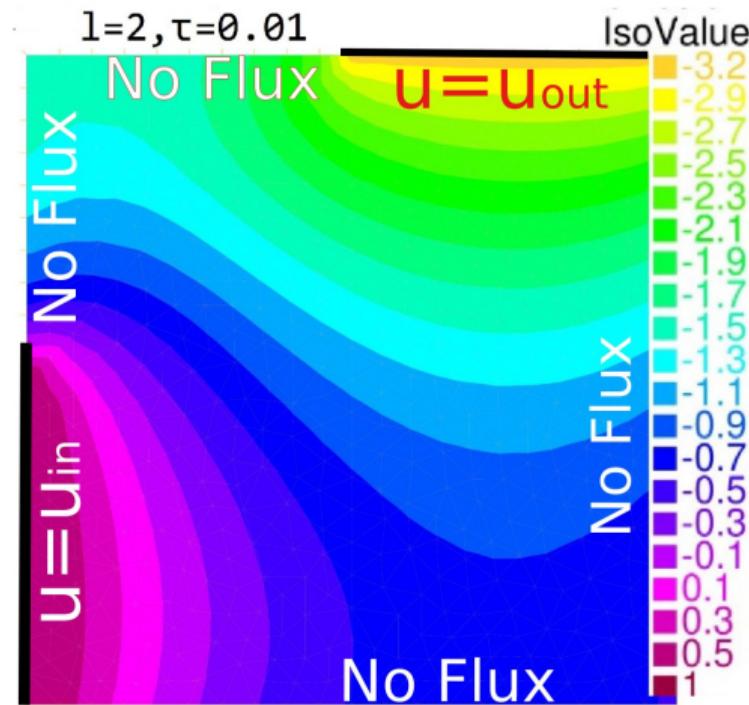
$$S(u) := \left(1 + (2 - u)^{\frac{1}{1-\lambda}}\right)^{-\lambda}, \quad \kappa(s) := \sqrt{s} \left(1 - (1 - s^{\frac{1}{\lambda}})^\lambda\right)^2, \quad \lambda = 0.5$$

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

Solution u

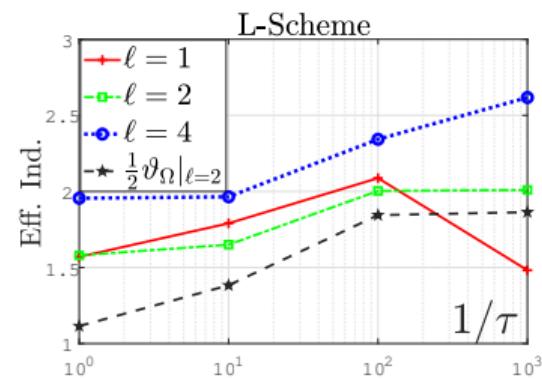
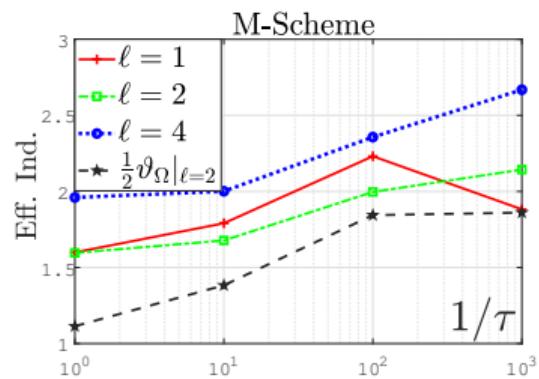
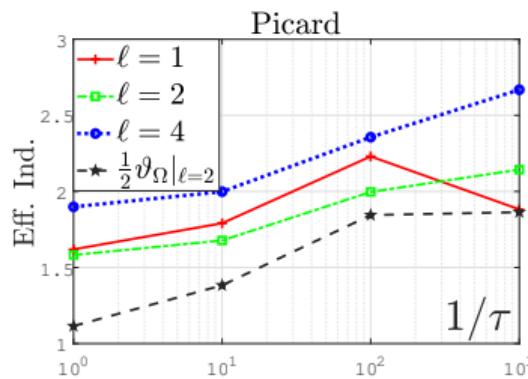


Time step length $\tau = 1$



Time step length $\tau = 0.01$

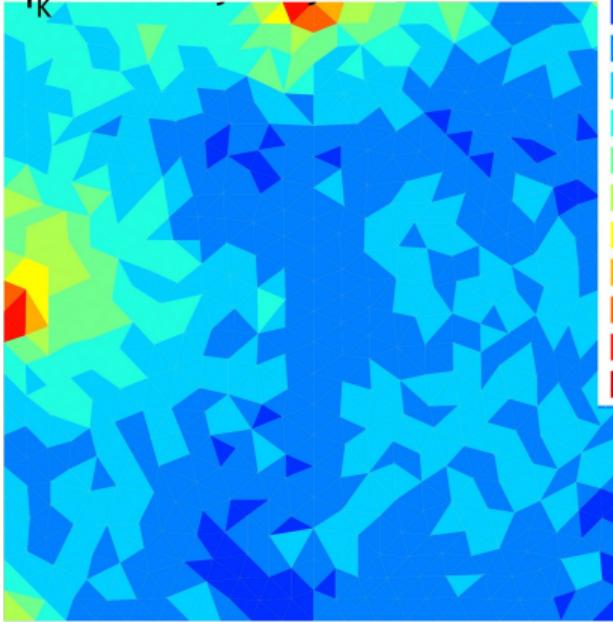
How large is the error? Robustness wrt the nonlinearities



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Where is the error **localized**?

η_K^i MS $l=2, \tau=1, i=9$

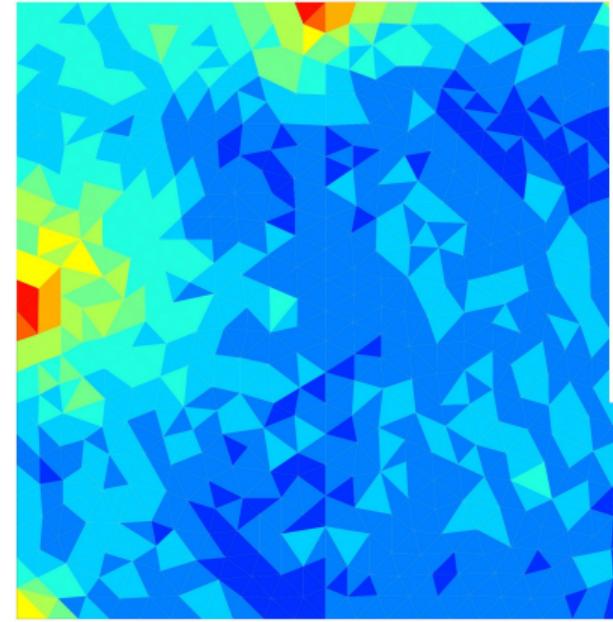


Estimated error, $\tau = 1$

IsoValue

-4.01
-3.77
-3.53
-3.29
-3.06
-2.82
-2.58
-2.34
-2.10
-1.86
-1.62

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

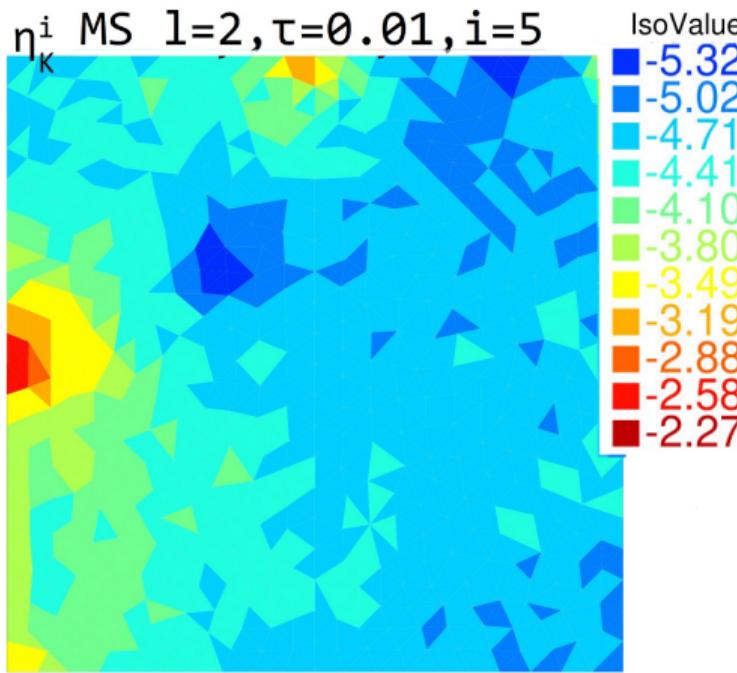
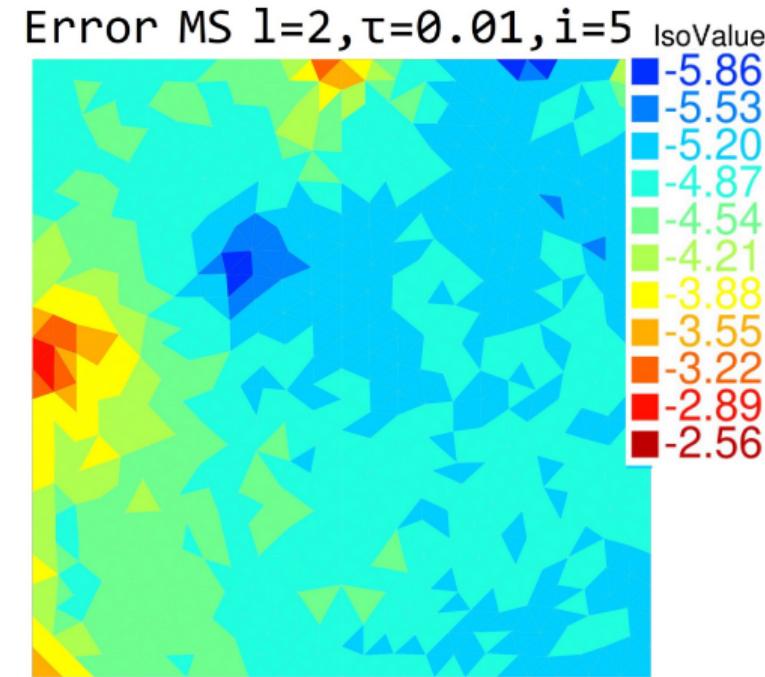


Exact error, $\tau = 1$

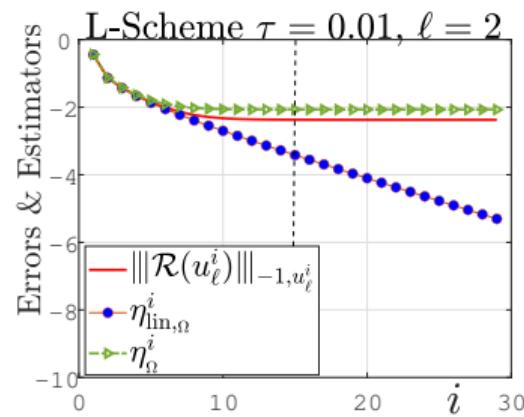
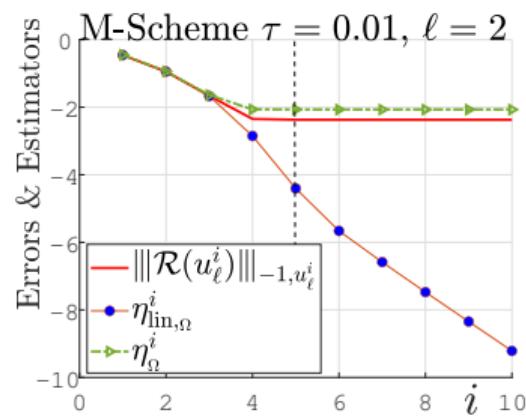
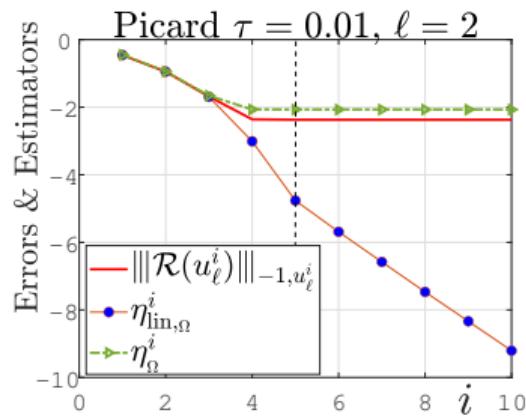
IsoValue

-4.09
-3.86
-3.64
-3.41
-3.19
-2.96
-2.74
-2.51
-2.29
-2.06
-1.83

Where is the error **localized**?

Estimated error, $\tau = 0.01$ Exact error, $\tau = 0.01$

Error components and adaptivity via stopping criteria



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A model nonlinear problem

Nonlinear elliptic problem

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

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

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

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Assumption (Gradient-dependent diffusivity)

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

$$|a(|\mathbf{x}|)\mathbf{x} - a(|\mathbf{y}|)\mathbf{y}| \leq a_c |\mathbf{x} - \mathbf{y}| \quad (\text{Lipschitz continuity}),$$

$$(a(|\mathbf{x}|)\mathbf{x} - a(|\mathbf{y}|)\mathbf{y}) \cdot (\mathbf{x} - \mathbf{y}) \geq a_m |\mathbf{x} - \mathbf{y}|^2 \quad (\text{strong monotonicity}).$$

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- $a_m \leq a(r) \leq a_c$, $a_m \leq (a(r)r)' \leq a_c$

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Weak solution

Definition (Weak solution)

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

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

Energy and energy minimization

Definition (Energy functional)

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

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

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

$$\phi(r) := \int_0^r a(s)s \, ds.$$

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Equivalently

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

Finite element approximation

Definition (Finite element approximation)

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

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

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Equivalently

$$u_\ell = \arg \min_{v_\ell \in V_\ell} \mathcal{J}(v_\ell)$$

Energy difference

Energy difference

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

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

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Iterative linearization

Definition (Linearized finite element approximation)

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

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

Iterative linearization

Definition (Linearized finite element approximation)

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- $u_\ell^0 \in V_\ell$ a given initial guess
- iterative linearization index $k \geq 1$
- $\mathbf{A}_\ell^{k-1}: \Omega \rightarrow \mathbb{R}^{d \times d}$ matrix-valued function constructed from u_ℓ^{k-1} ,
- $\mathbf{b}_\ell^{k-1}: \Omega \rightarrow \mathbb{R}^d$ vector-valued function constructed from u_ℓ^{k-1}

Examples

Example (Picard (fixed-point))

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

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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**.

Examples

Example (Picard (fixed-point))

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

Example (Zarantonello)

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

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

Example (Newton)

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

$$\mathbf{b}_\ell^{k-1} = \mathbf{a}'(|\nabla u_\ell^{k-1}|) |\nabla u_\ell^{k-1}| \nabla u_\ell^{k-1}.$$

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Main idea

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Apply in the **a posteriori analysis** and in **adaptivity**, to define the way how we measure the error, the **iterative linearization** on the **discrete level**.

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$$\mathcal{J}_\ell^{k-1}(v) := \frac{1}{2} \left\| (\mathbf{A}_\ell^{k-1})^{\frac{1}{2}} \nabla v \right\|^2 - (f, v) - (\mathbf{b}_\ell^{k-1}, \nabla v), \quad v \in H_0^1(\Omega).$$

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

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Continuous minimizer of the linearized energy functional

$$u_{\langle \ell \rangle}^k := \arg \min_{v_\ell \in H_0^1(\Omega)} \mathcal{J}_\ell^{k-1}(v)$$

Augmented energy difference

Augmented energy difference

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

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$$\mathcal{E}_\ell^k := \frac{1}{2} \left(\underbrace{\mathcal{J}(u_\ell^k) - \mathcal{J}(u)}_{\text{energy difference}} \right) + \lambda_\ell^k \frac{1}{2} \left(\underbrace{\mathcal{J}_\ell^{k-1}(u_\ell^k) - \mathcal{J}_\ell^{k-1}(u_{\langle \ell \rangle}^k)}_{\text{linearized energy difference}} \right)$$

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

$$\mathcal{E}_\ell^k := \frac{1}{2} \left(\underbrace{\mathcal{J}(u_\ell^k) - \mathcal{J}(u)}_{\text{energy difference} \leq \eta_{N,\ell}^k} \right) + \lambda_\ell^k \frac{1}{2} \left(\underbrace{\mathcal{J}_\ell^{k-1}(u_\ell^k) - \mathcal{J}_\ell^{k-1}(u_{\langle \ell \rangle}^k)}_{\text{linearized energy difference} \leq \eta_{L,\ell}^k} \right)$$

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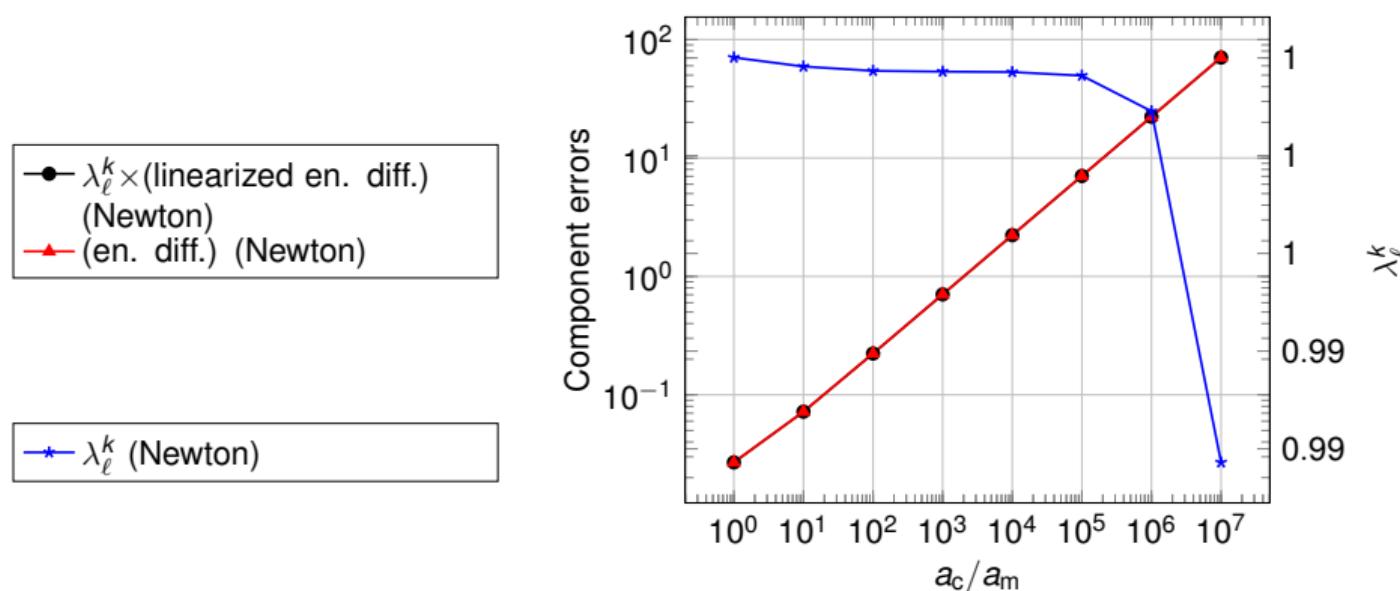
Practically

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

Augmented energy difference

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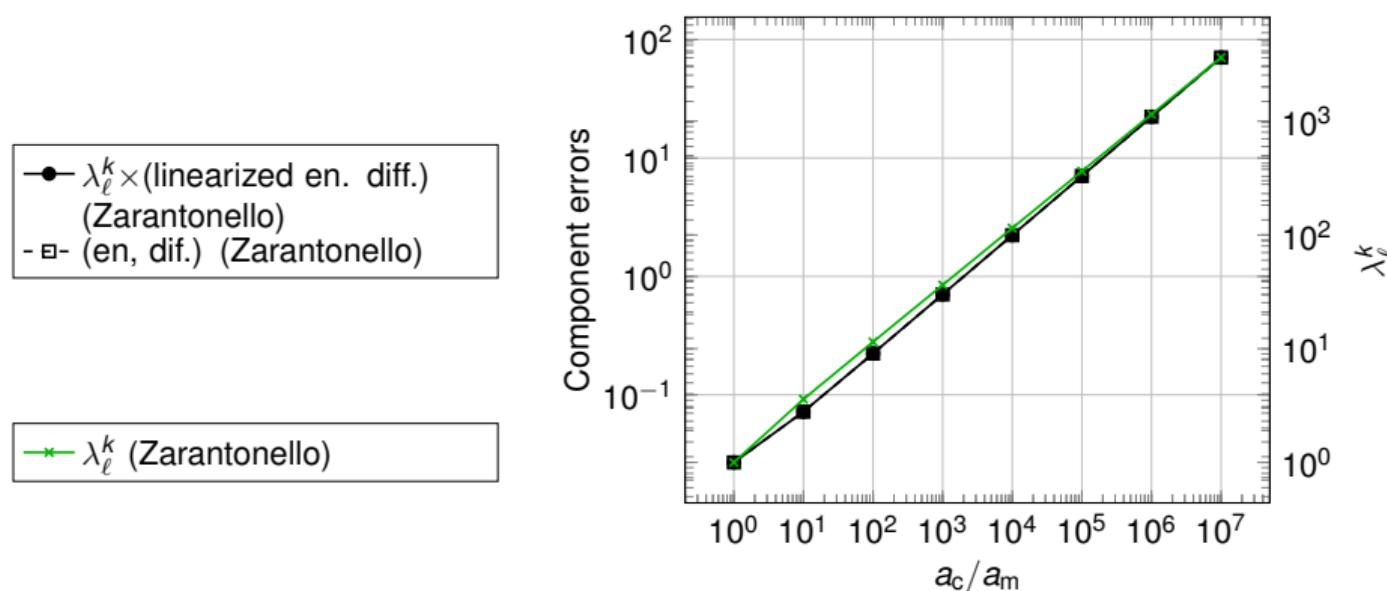
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A posteriori error estimates for an augmented energy difference

Theorem (A posteriori estimate of augmented energy)

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

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Fenchel conjugate, dual energy, estimator, flux equilibration

Definition (Fenchel conjugate)

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

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

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$$\eta_{\ell}^k := \underbrace{\frac{1}{2}(\mathcal{J}(u_{\ell}^k) - \mathcal{J}^*(\sigma_{\ell}^k))}_{\text{en. diff. estimate}} + \lambda_{\ell}^k \underbrace{\frac{1}{2}(\mathcal{J}_{\ell}^{k-1}(u_{\ell}^k) - \mathcal{J}_{\ell}^{*, k-1}(\sigma_{\ell}^k))}_{\text{linearized en. diff. estimate}}$$

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Definition (Flux equilibration: $\sigma_{\ell}^k = \sum_{\mathbf{a} \in \mathcal{V}_{\ell}} \sigma_{\ell}^{\mathbf{a}, k}$)

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

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Smooth solution

Setting

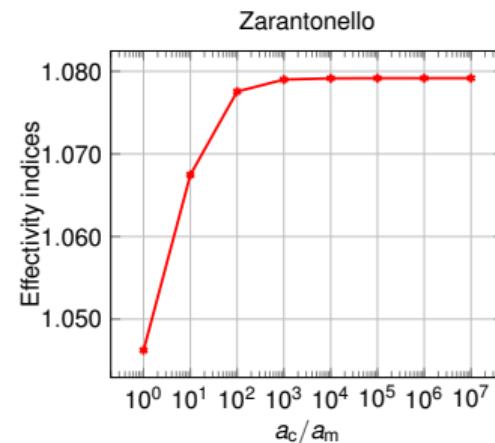
- unit square $\Omega = (0, 1)^2$
- known smooth solution $u(x, y) := 10x(x - 1)y(y - 1)$
- $p = 1$
- effectivity indices

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

How large is the error? Robustness wrt the nonlinearities

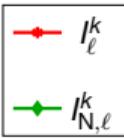
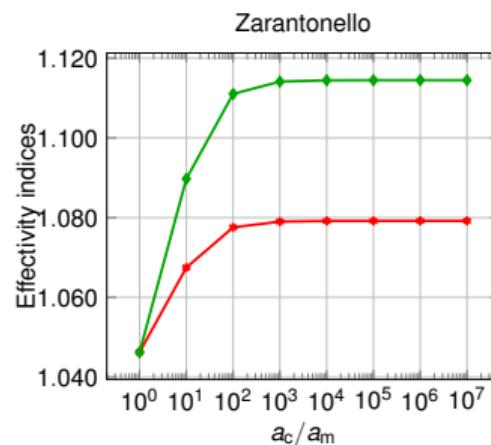
$$(a(r) = a_m + \frac{a_c - a_m}{\sqrt{1+r^2}})$$

—♦— I_ℓ^k



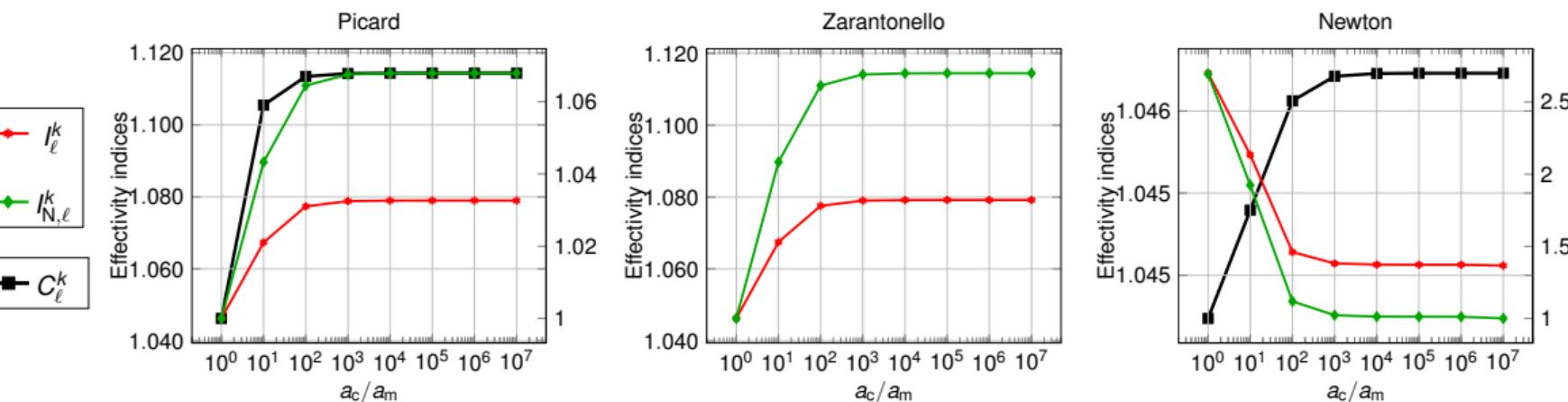
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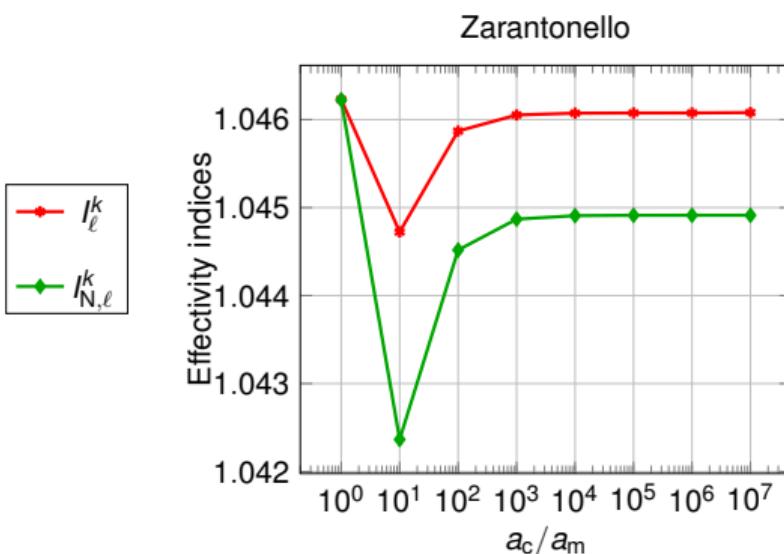
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A. Harnist, K. Mitra, A. Rappaport, M. Vohralík, preprint (2023)

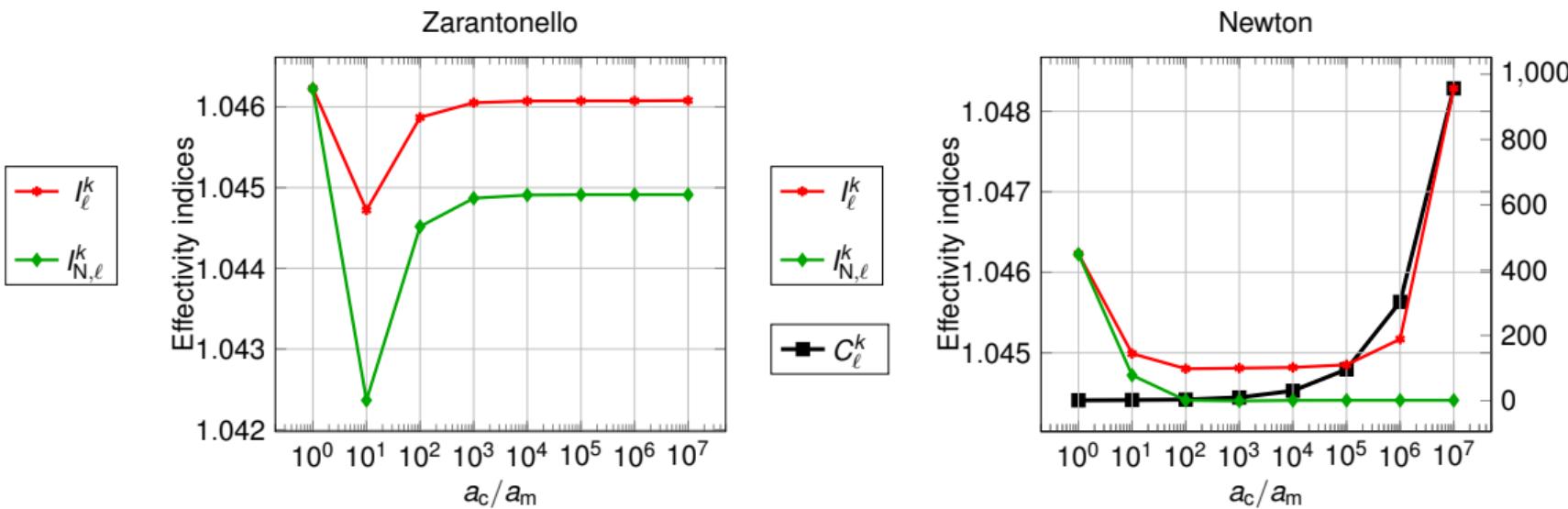
How large is the error? Robustness wrt the nonlinearities

$$(a(r) = a_m + (a_c - a_m) \frac{1 - e^{-\frac{3}{2}r^2}}{1 + 2e^{-\frac{3}{2}r^2}})$$



How large is the error? Robustness wrt the nonlinearities

$$(a(r) = a_m + (a_c - a_m) \frac{1 - e^{-\frac{3}{2}r^2}}{1 + 2e^{-\frac{3}{2}r^2}}, \text{ robustness only for Zarantonello})$$



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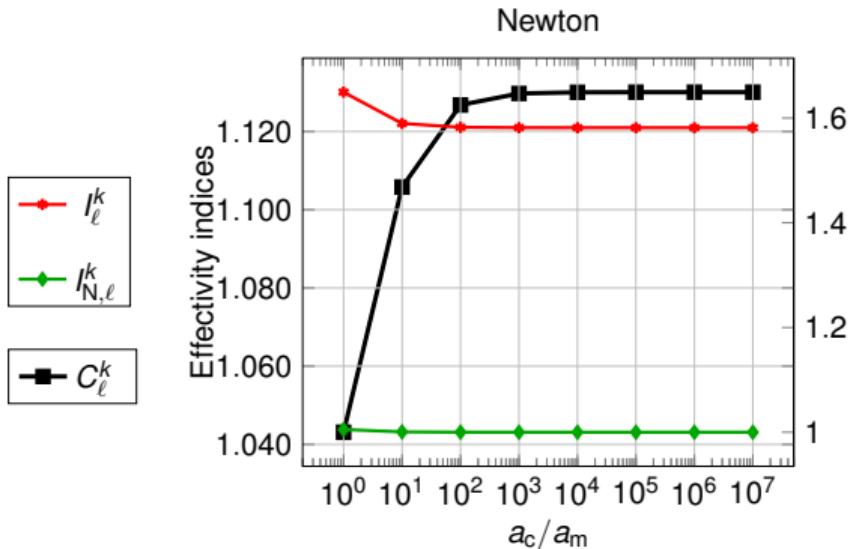
Singular solution

Setting

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

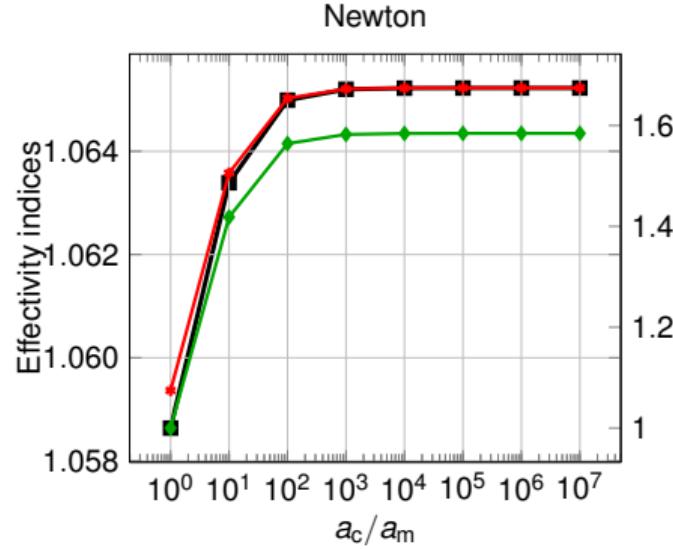
How large is the error? Robustness wrt the nonlinearities

Newton



Uniform mesh refinement

Newton



Adaptive mesh refinement

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

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- employing **iteration-dependent norms**
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Thank you for your attention!

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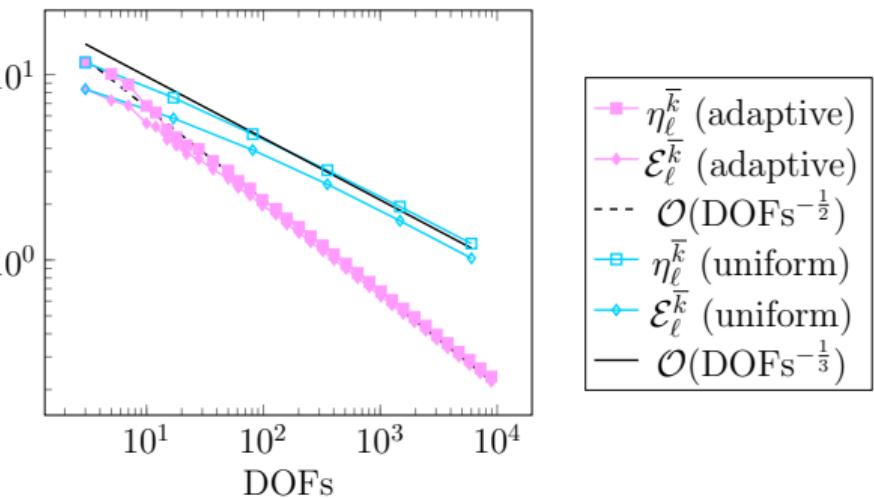
Adaptivity

6

Equilibrated flux reconstruction

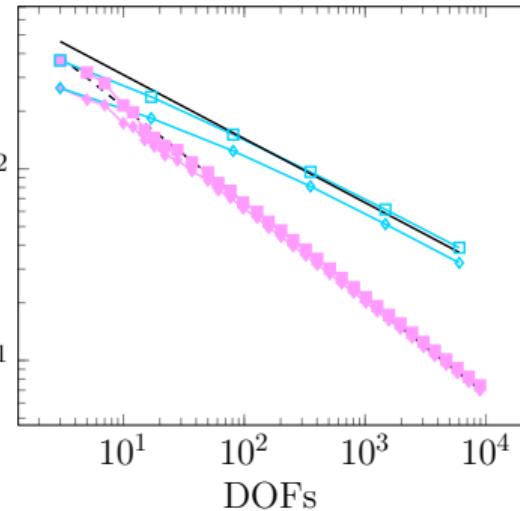
Decreasing the error efficiently: optimal decay rate wrt DoFs

Error and estimator



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

Error and estimator



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

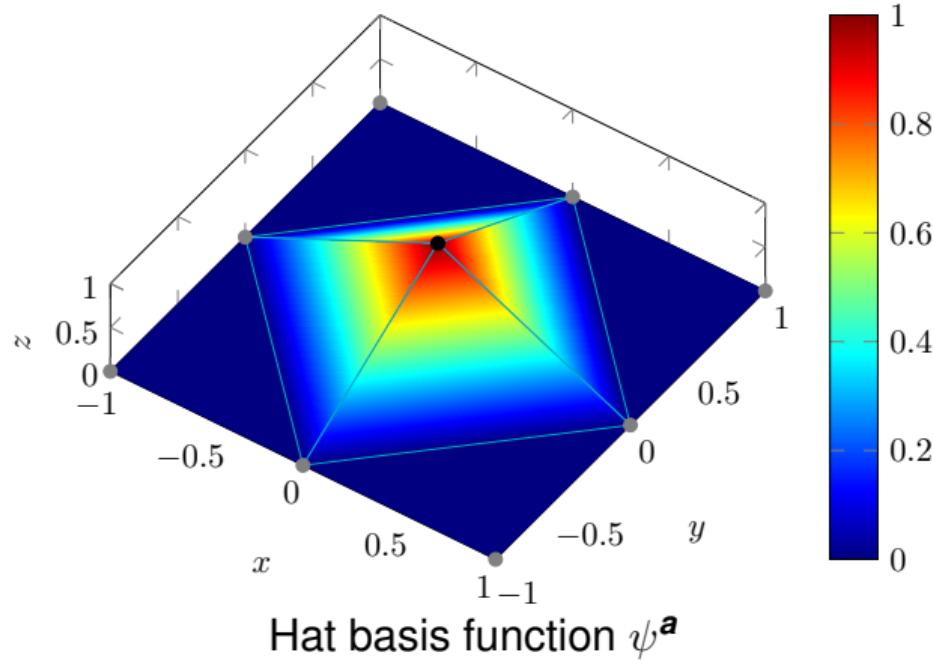
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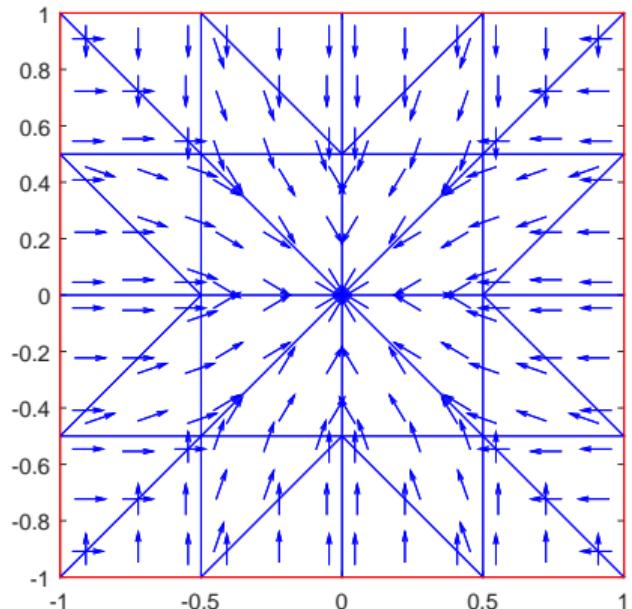
Partition of unity

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



Equilibrated flux reconstruction

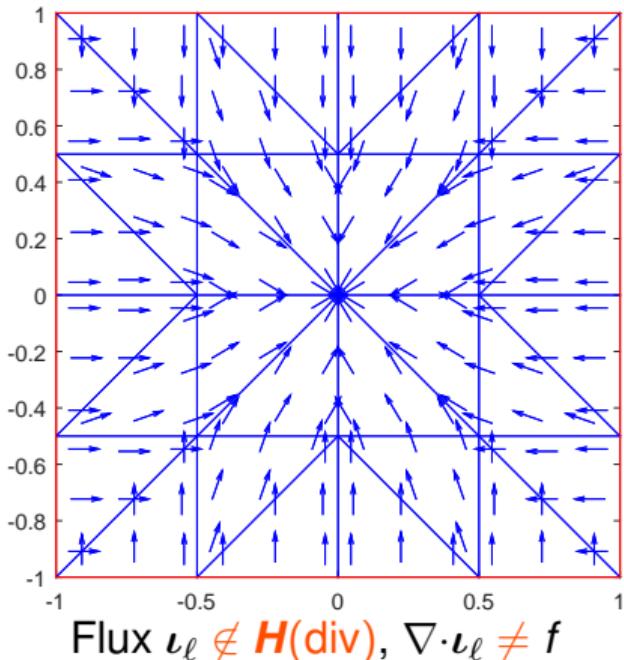
Destuynder and Métivet (1998), Braess & Schöberl (2008), Ern & Vohralík (2013)



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

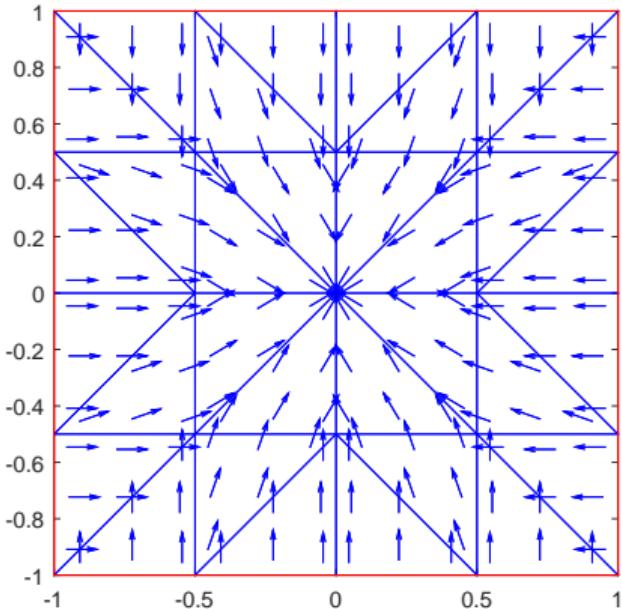
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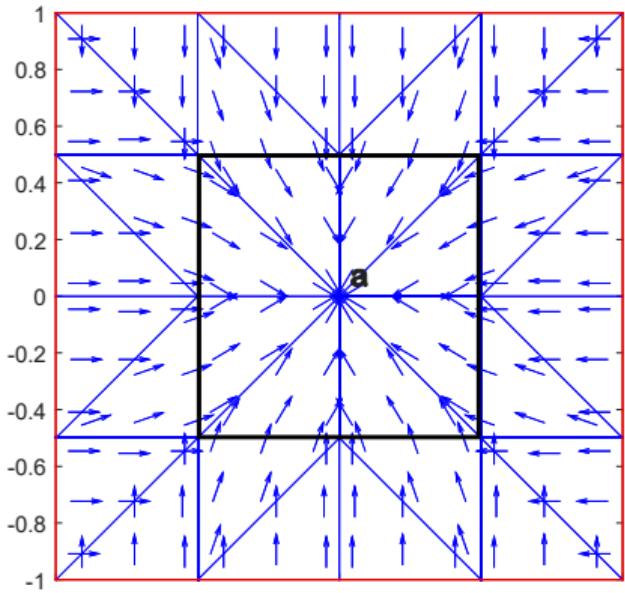


Flux $\boldsymbol{\iota}_\ell \notin \mathbf{H}(\text{div})$, $\nabla \cdot \boldsymbol{\iota}_\ell \neq f$

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

Equilibrated flux reconstruction

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



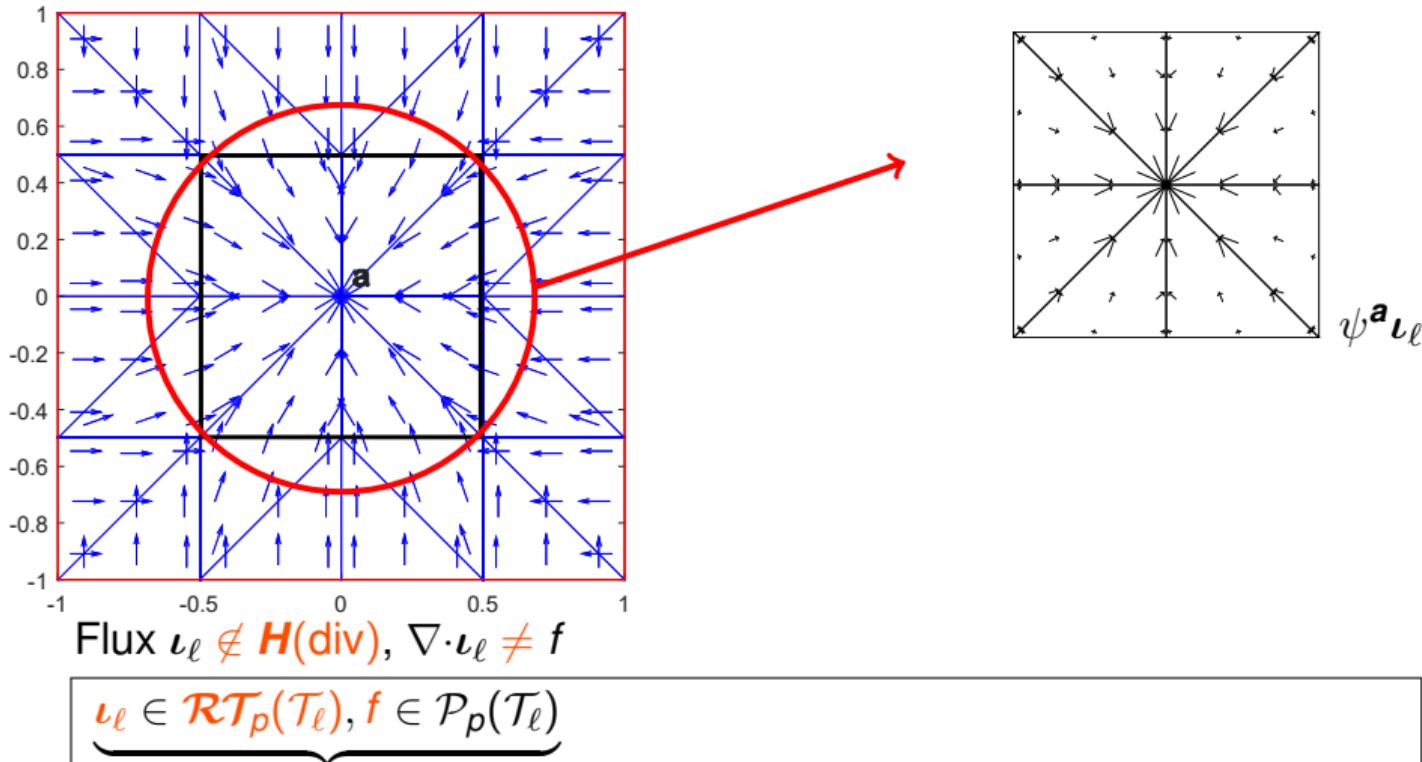
Flux $\boldsymbol{\iota}_\ell \notin \mathbf{H}(\text{div})$, $\nabla \cdot \boldsymbol{\iota}_\ell \neq f$

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

$$(f, \psi^{\mathbf{a}})_{\omega_{\mathbf{a}}} + (\boldsymbol{\iota}_\ell, \nabla \psi^{\mathbf{a}})_{\omega_{\mathbf{a}}} = 0 \quad \forall \mathbf{a} \in \mathcal{V}_\ell^{\text{int}}$$

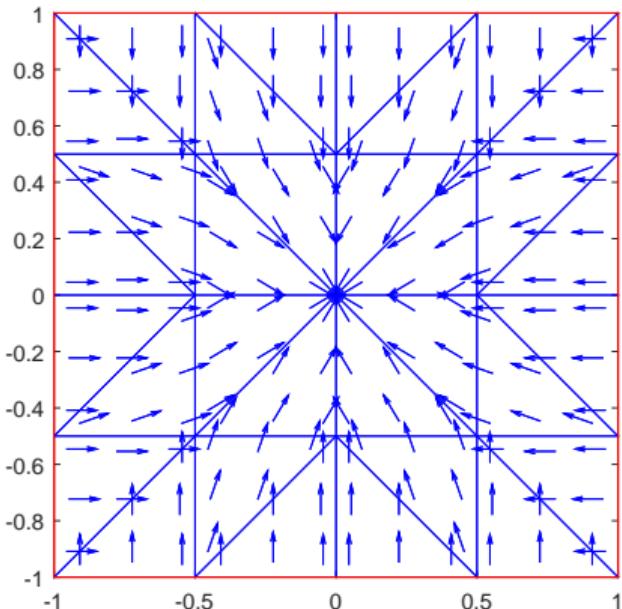
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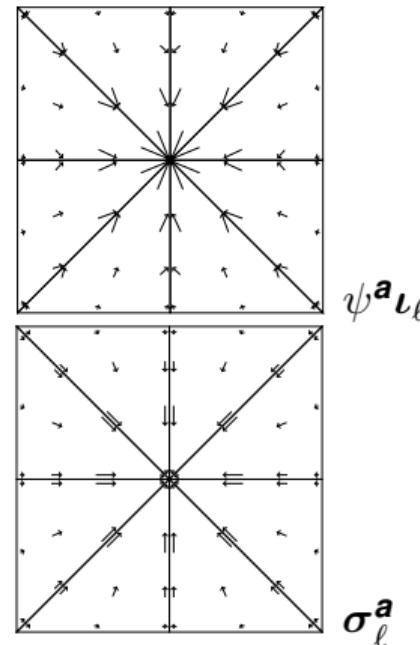


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Flux $\boldsymbol{\iota}_\ell \notin \mathbf{H}(\text{div})$, $\nabla \cdot \boldsymbol{\iota}_\ell \neq f$



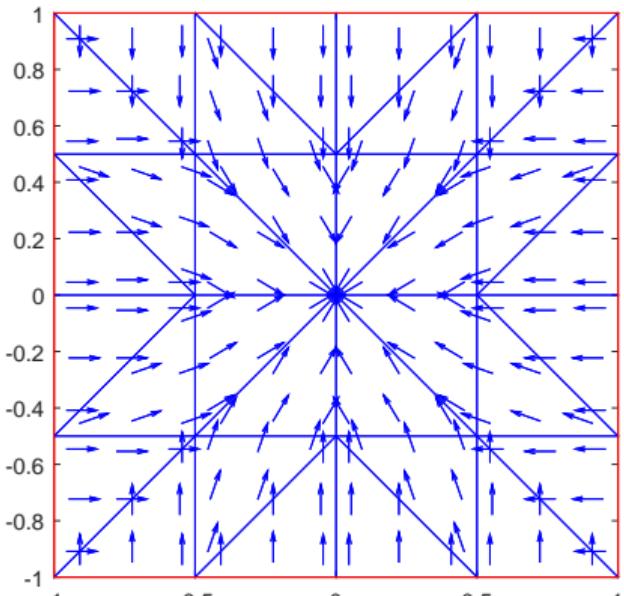
$\boldsymbol{\iota}_\ell \in \mathcal{RT}_p(\mathcal{T}_\ell)$, $f \in \mathcal{P}_p(\mathcal{T}_\ell)$

$$\sigma^{\mathbf{a}} := \arg \min_{\mathbf{v}_\ell \in \mathcal{RT}_{p+1}(\mathcal{T}_\ell) \cap H_0(\text{div}, \omega_\mathbf{a})} \|\psi^{\mathbf{a}} \boldsymbol{\iota}_\ell - \mathbf{v}_\ell\|_{\omega_\mathbf{a}}^2$$

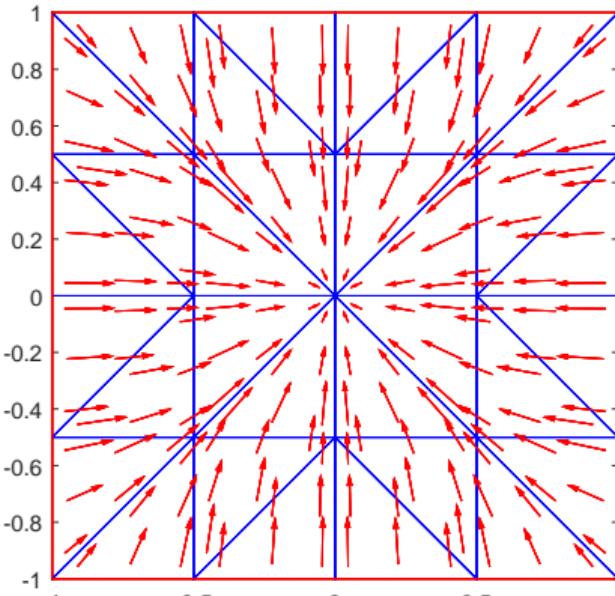
$$\nabla \cdot \mathbf{v}_\ell = f \psi^{\mathbf{a}} + \boldsymbol{\iota}_\ell \cdot \nabla \psi^{\mathbf{a}}$$

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



Equilibrated flux $\boldsymbol{\sigma}_\ell \in \mathbf{H}(\text{div})$, $\nabla \cdot \boldsymbol{\sigma}_\ell = f$

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

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