A posteriori error estimates robust with respect to the strength of nonlinearities

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Inria Paris & Ecole des Ponts

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Outline

A posteriori error estimates: certify the error in a FE discretization

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

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

Guaranteed error upper bound (reliability)

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

Error lower bound (efficiency)

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

- C_{eff} a generic constant independent of Ω, u, u_ℓ and namely of the number of mesh elements $|\mathcal{T}_\ell|$ (h if $\mathcal{T}_\ell$ uniform) and of the polynomial degree p

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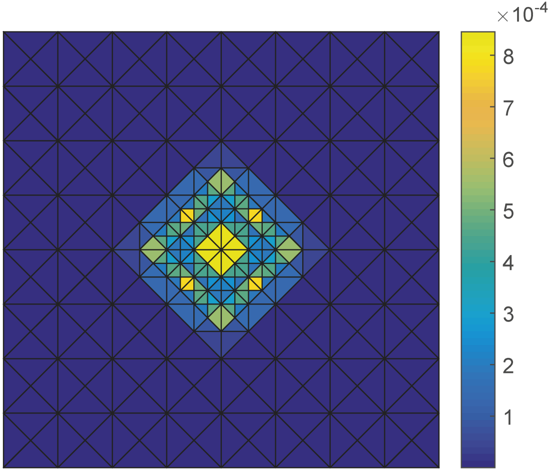
How **large** is the error? (steady linear Darcy, known solution)

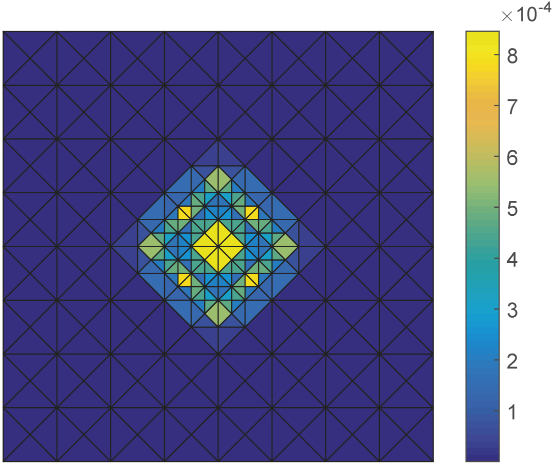
$h \approx 1/\|\mathcal{T}_\ell\|^{\frac{1}{2}}$	p	relative error estimate $\frac{\eta(u_\ell)}{\|\nabla u_\ell\|}$	relative error $\frac{\|\nabla(u-u_\ell)\|}{\|\nabla u_\ell\|}$	effectivity index $\frac{\eta(u_\ell)}{\|\nabla(u-u_\ell)\|}$
h_0	1	28%	24%	**1.17**
$\approx h_0/2$		14%	13%	**1.09**
$\approx h_0/4$		7.0%	6.6%	**1.06**
$\approx h_0/8$		3.3%	3.1%	**1.04**
$\approx h_0/2$	2	9.5×10^{-1}%	9.2×10^{-1}%	**1.04**
$\approx h_0/4$	3	5.9×10^{-3}%	5.9×10^{-3}%	**1.01**
$\approx h_0/8$	4	5.9×10^{-6}%	5.8×10^{-6}%	**1.01**

A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

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



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



Exact local error $\|\nabla(u - u_\ell)\|_K$

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

Goals

Error control

a posteriori error estimates

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

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Guaranteed a posteriori error estimates

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Guaranteed a posteriori error estimates **efficient**

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

Goals

Error control

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

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

Goals

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

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

Goals

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

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

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Usage

- provide sharp **computable bounds** in **physically-based error measures**

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Usage

- provide sharp **computable bounds** in **physically-based error measures**
- predict the **error localization** (in discretization, in linearization, in linear solver)
- **adapt** the **nonlinear solver** and the **linear solver** (balancing error components), **adaptive mesh refinement** ...

Outline

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A model steady nonlinear problem

Nonlinear elliptic problem

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

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

- $\Omega \subset \mathbb{R}^d$, $1 \leq d \leq 3$, open bounded polytope with Lipschitz boundary $\partial\Omega$
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Assumption (Nonlinear function a)

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

$$|a(|\boldsymbol{x}|)\boldsymbol{x} - a(|\boldsymbol{y}|)\boldsymbol{y}| \leq a_c|\boldsymbol{x} - \boldsymbol{y}| \qquad \text{(Lipschitz continuity)},$$
$$(a(|\boldsymbol{x}|)\boldsymbol{x} - a(|\boldsymbol{y}|)\boldsymbol{y}) \cdot (\boldsymbol{x} - \boldsymbol{y}) \geq a_m|\boldsymbol{x} - \boldsymbol{y}|^2 \qquad \text{(strong monotonicity)}.$$

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\end{aligned}
$$

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

Example of the nonlinear function a

Example (Mean curvature nonlinearity)

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

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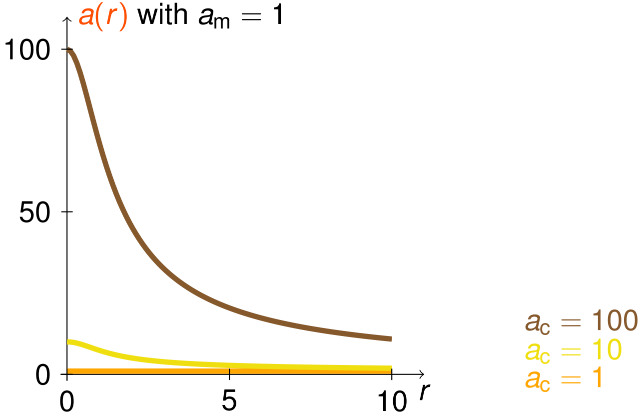

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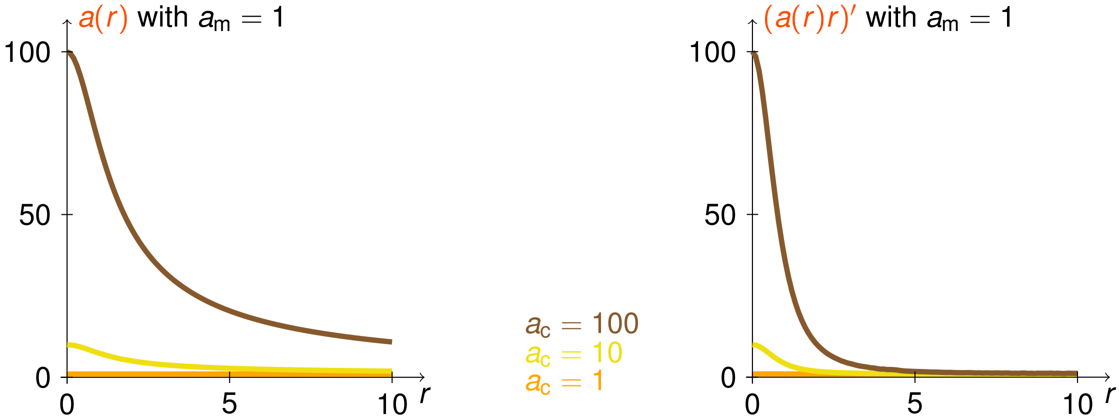

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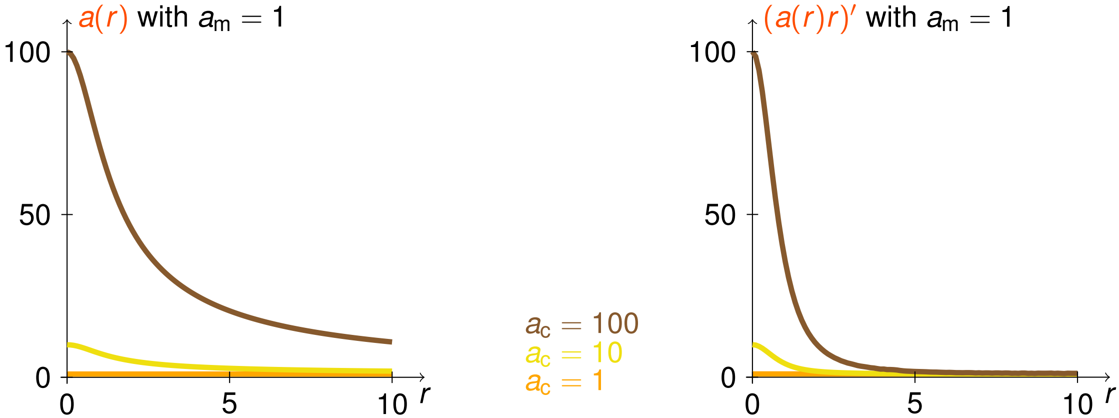
Strength of the nonlinearity

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



Outline

Weak solution

Definition (Weak solution)

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

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

Energy

Definition (Energy functional)

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

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

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

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

Equivalently

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

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Finite element approximation

Definition (Finite element approximation)

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

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

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

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

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

Outline

Known results

Energy difference (not robust wrt $\frac{a_c}{a_m}$)

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

- Zeidler (1992), Han (1994), Repin (1997), Ladevèze & Moës (1997), Diening & Kreuzer (2008), Bartels & Milicevic (2020), . . .

Sobolev norm

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

Dual norm of the residual

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

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Dual norm of the residual (**robust** wrt $\frac{a_c}{a_m}$), "bypasses" the nonlinearity

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

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

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Known results

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Outline

Iterative linearization

Need to solve a nonlinear system

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

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Definition (Linearized finite element approximation)

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

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

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

Examples

Example (Picard (fixed-point))

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

Example (Zarantonello)

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

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

Example (Newton)

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

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Equivalently

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

Outline

A posteriori error estimates for an augmented energy difference

Theorem (A posteriori estimate of augmented energy)

For all linearization steps $k \geq 1$, $\mathcal{E}_\ell^k \leq \eta_\ell^k.$

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

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Practically

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

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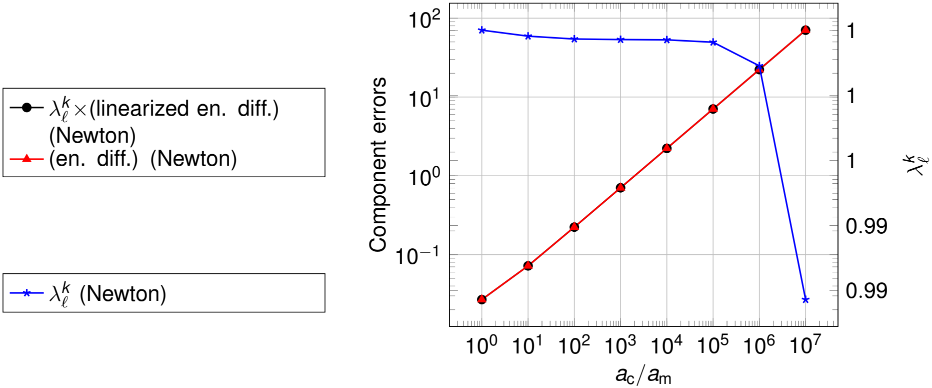

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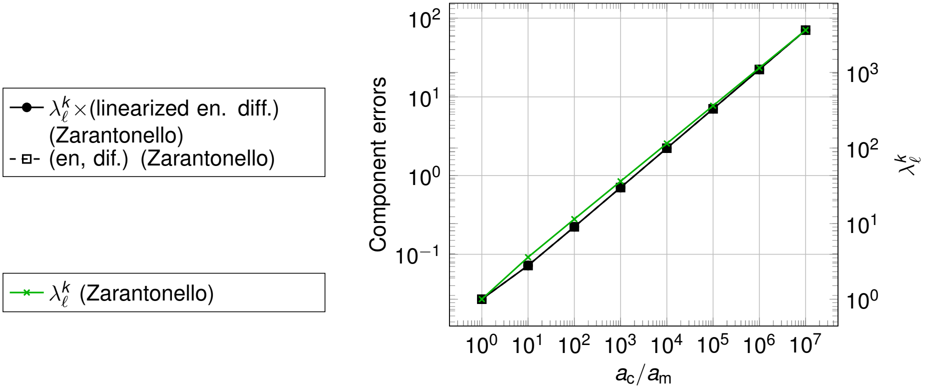

Outline

Fenchel conjugate, dual energy, flux equilibration, estimator

Definition (Fenchel conjugate)

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

Definition (Dual energy)

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

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

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

Definition (Estimator)

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

Fenchel conjugate, dual energy, flux equilibration, estimator

Definition (Fenchel conjugate)

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

Definition (Dual energy)

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

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

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Outline

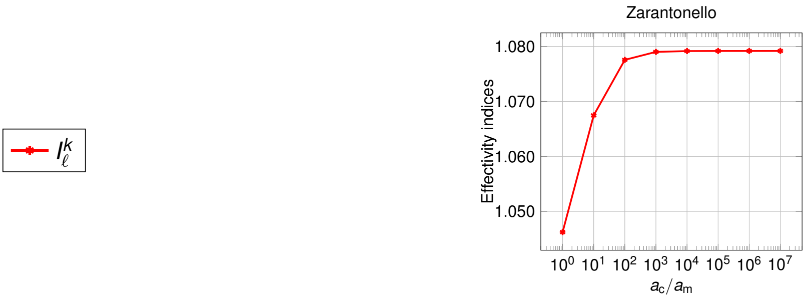
Smooth solution

Setting

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

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

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



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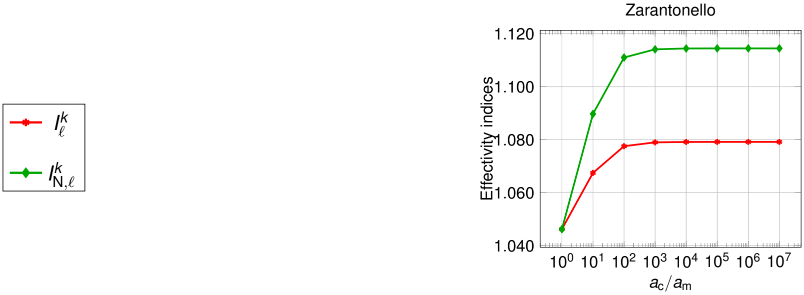

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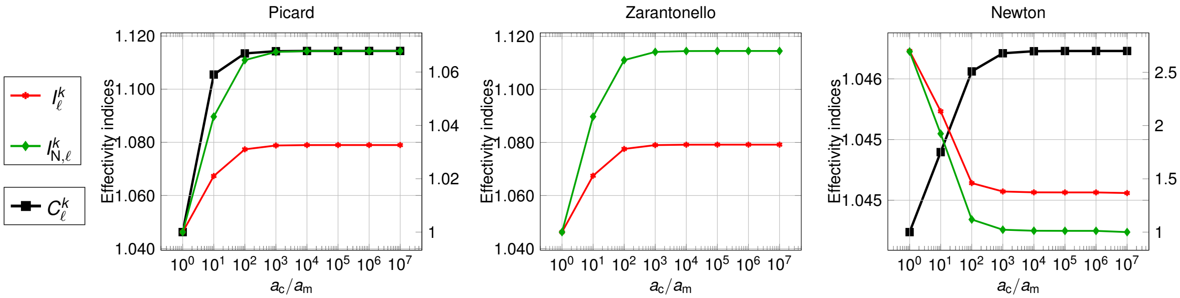

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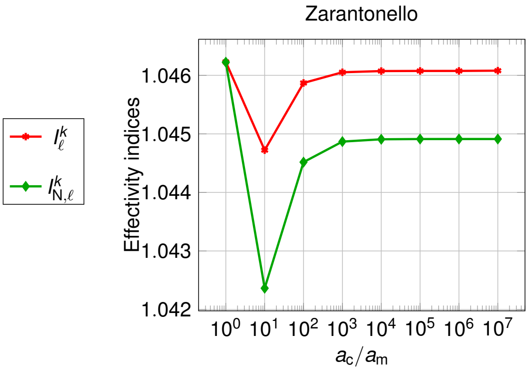
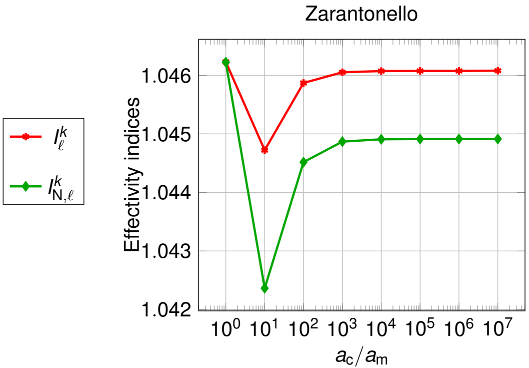
How **large** is the error? **Robustness** wrt the nonlinearities

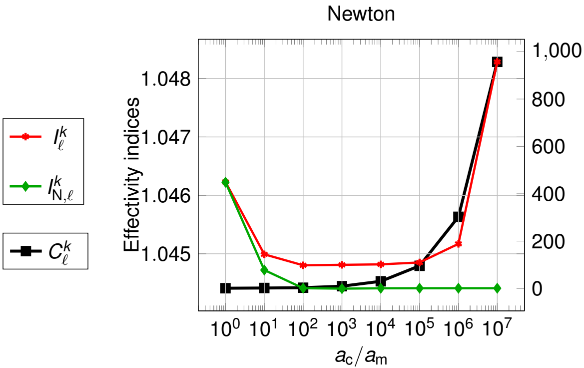
$$\left(a(r) = a_{\mathrm{m}} + (a_{\mathrm{c}} - a_{\mathrm{m}})\frac{1-e^{-\frac{3}{2}r^2}}{1+2e^{-\frac{3}{2}}}\right)$$



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

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





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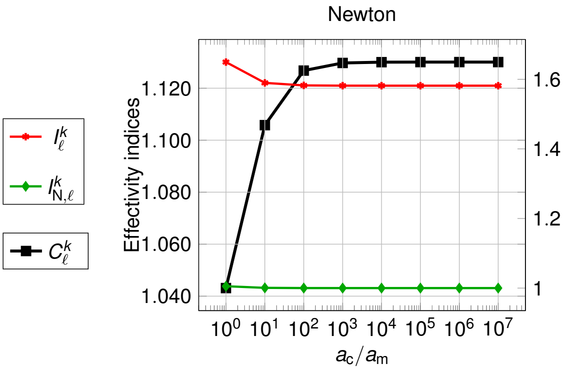
Singular solution

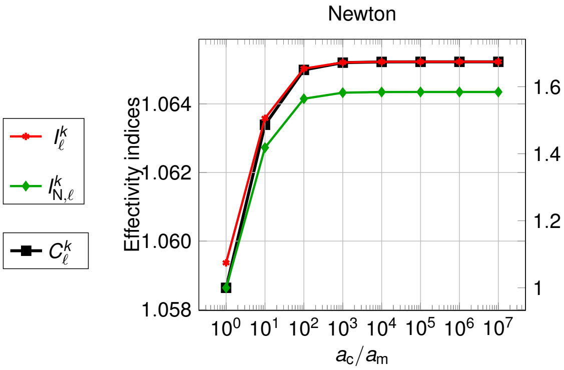
Setting

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

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



Uniform mesh refinement



Adaptive mesh refinement

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

Outline

1. Introduction
2. Gradient-dependent nonlinearities
   - Setting
   - Previous results
   - Iterative linearization
   - A posteriori error estimates for an augmented energy difference
   - Fenchel conjugate, dual energy, flux equilibration, estimator
   - Numerical experiments
3. Gradient-independent nonlinearities
   - Setting
   - A posteriori error estimates for an iteration-dependent norm
   - Numerical experiments
4. Conclusions

Observation

Observation

Not all nonlinear problems admit an energy minimization structure.

A model steady nonlinear problem

Nonlinear elliptic problem

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

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

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

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

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

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

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

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

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Outline

Finite element discretization and iterative linearization

Definition (Linearized finite element approximation)

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

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

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

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

Iteration-dependent norm

- $$|||v|||^2_{1,u_\ell^{k-1}} := ((v, v))_{u_\ell^{k-1}} = \|(L_\ell^{k-1})^{1/2} v\|^2 + \|(A_\ell^{k-1})^{1/2} \nabla v\|^2, \qquad v \in H_0^1(\Omega)$$
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An orthogonal decomposition of the total residual/error

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

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

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

- **orthogonal decomposition**
- **error components**
- $u^k_{\langle\ell\rangle} \in H^1_0(\Omega)$ such that

$$((u^k_{\langle\ell\rangle} - u_\ell^{k-1}, v))_{u_\ell^{k-1}} = \underbrace{-\langle\mathcal{R}(u_\ell^{k-1}), v\rangle}_{\text{residual}} \qquad \forall v \in H^1_0(\Omega)$$

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Outline

A posteriori error estimates for an iteration-dependent norm

Theorem (A posteriori estimate of iteration-dependent norm)

For all linearization steps $k \geq 1$,

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

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For all linearization steps $k \geq 1$,

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

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

$$\eta(u_\ell^k) \leq C_{\mathrm{eff}}(d, \kappa_{\mathcal{T}}, p) C_\ell^k |||\mathcal{R}(u_\ell^{k-1})|||_{-1,u_\ell^{k-1}} \quad + \textit{quadrature error terms},$$

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

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where

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

A posteriori error estimates for 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*

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

where

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

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

A posteriori error estimates for an iteration-dependent norm

Theorem (A posteriori estimate of iteration-dependent norm)

For all linearization steps $k \geq 1$,

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

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

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

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- ✓ **local efficiency**

Outline

One time step of the Richards equation

Setting

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

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

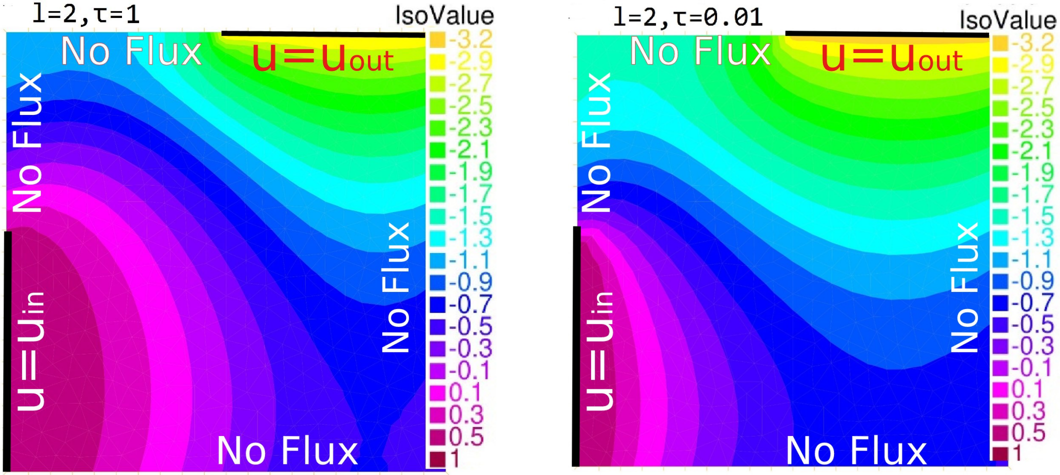
$$\boldsymbol{K} = \begin{bmatrix} 1 & 0.2 \\ 0.2 & 1 \end{bmatrix}, \quad \boldsymbol{g} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

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

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

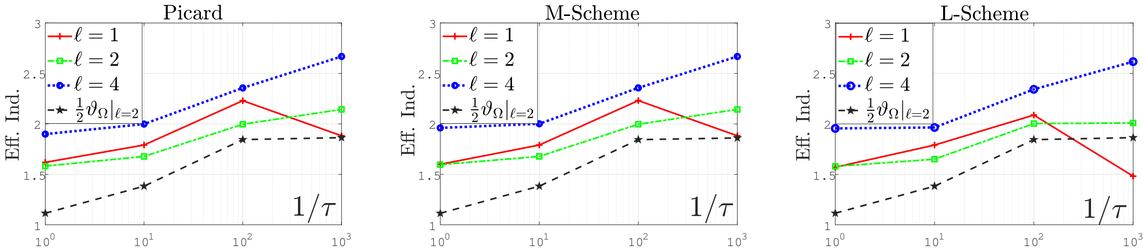
- time step length $\tau \in [10^{-3}, 1]$

One time step of the Richards equation: saturation u



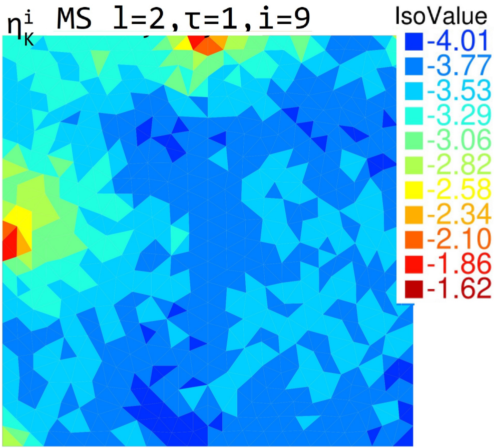
Time step length $\tau = 1$ Time step length $\tau = 0.01$

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

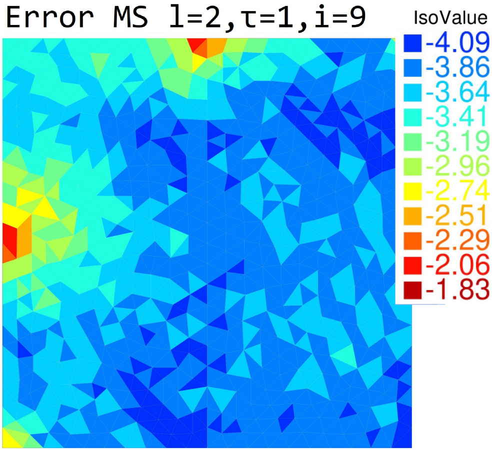


K. Mitra, M. Vohralík, to be sumbitted (2023)

Where is the error **localized**?



Estimated local error, $\tau = 1$



Exact local error, $\tau = 1$

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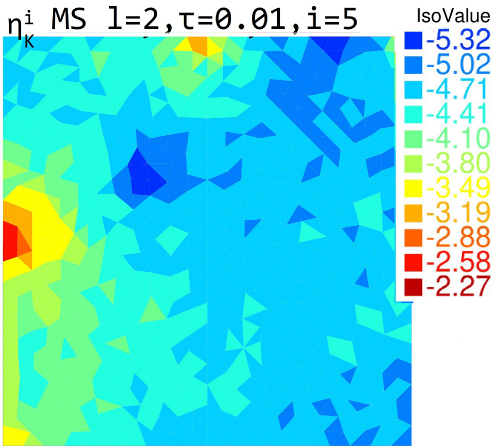
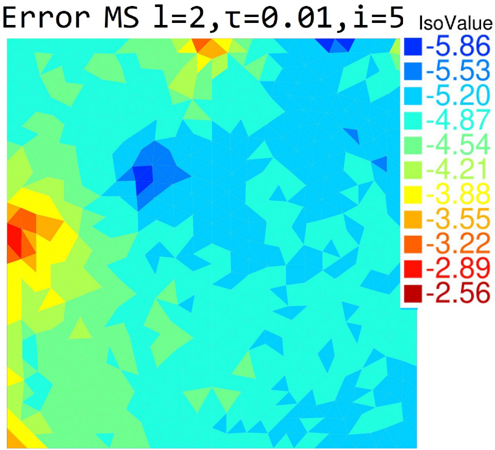


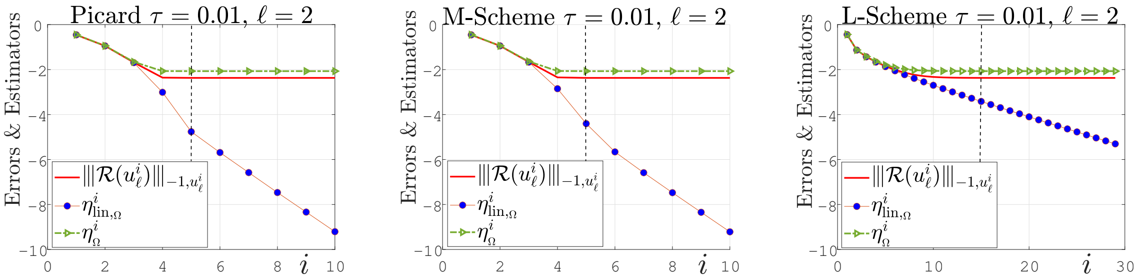
Estimated local error, $\tau = 0.01$



Exact local error, $\tau = 0.01$

K. Mitra, M. Vohralík, to be sumbitted (2023)

Error components and adaptivity via **stopping criteria**



Time step length $\tau = 0.01$

K. Mitra, M. Vohralík, to be sumbitted (2023)

Outline

Conclusions

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- a posteriori **certification** of the **error** for nonlinear problems
- **robustness** with respect to the **strength of nonlinearities** for model cases
- augmenting the energy difference by the (discretization) error on the given linearization step
- employing iteration-dependent norms

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Thank you for your attention!

Outline

Sobolev space and error

Sobolev space

$$H_0^1(\Omega)$$

Sobolev norm error

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

Residual and its dual norm

Definition (Residual)

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

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

Definition (Dual norm of the finite element residual)

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

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

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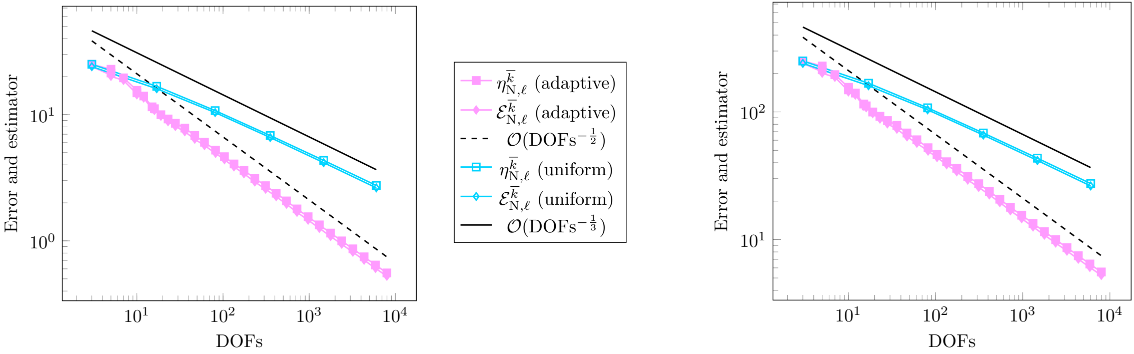
Outline

5 Other error measures

6 Adaptivity

7 Equilibrated flux reconstruction

Decreasing the **error efficiently**: **optimal decay rate** wrt DoFs



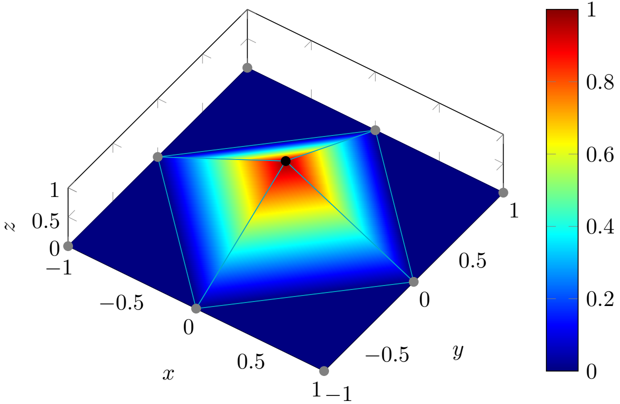
$\frac{a_c}{a_m} = 10^3$

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

Outline

Partition of unity

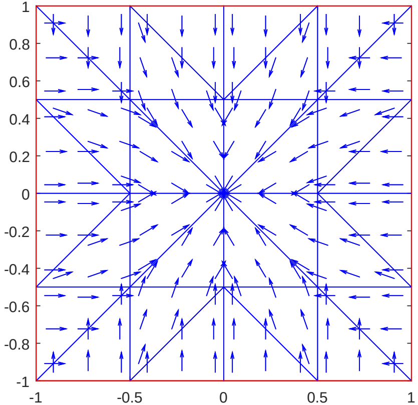
$$\sum_{\boldsymbol{a}\in\mathcal{V}_\ell} \psi^{\boldsymbol{a}} = 1$$



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

Equilibrated flux reconstruction

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



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

Equilibrated flux reconstruction

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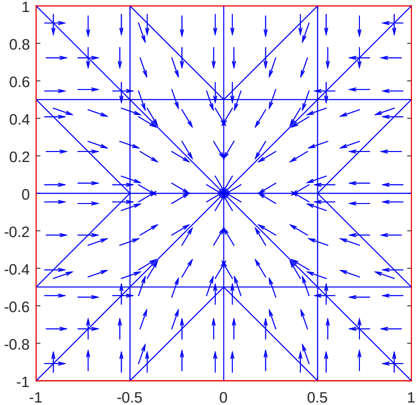

Flux $\boldsymbol{\iota}_\ell \notin \boldsymbol{H}(\mathrm{div})$, $\nabla \cdot \boldsymbol{\iota}_\ell \neq f$

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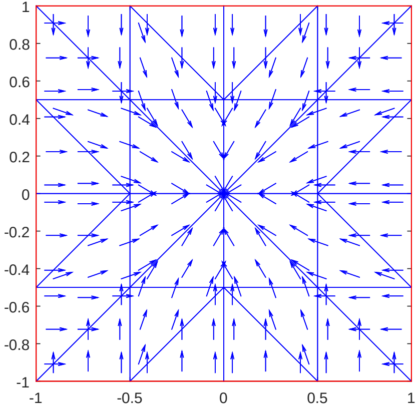

Flux $\boldsymbol{\iota}_\ell \notin \boldsymbol{H}(\mathrm{div})$, $\nabla{\cdot}\boldsymbol{\iota}_\ell \neq f$

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

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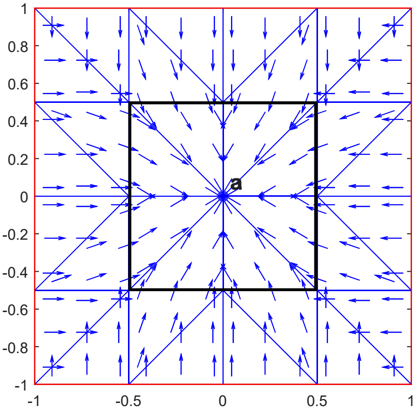

Flux $\boldsymbol{\iota}_\ell \notin \mathbf{H}(\mathrm{div})$, $\nabla\cdot\boldsymbol{\iota}_\ell \neq f$

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

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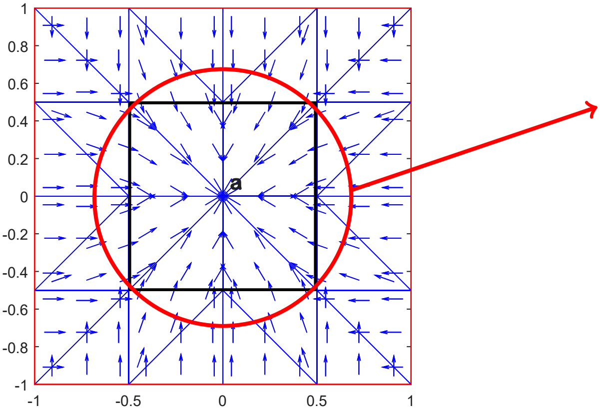

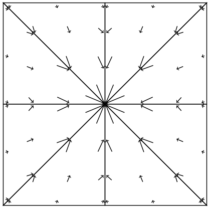

$\psi^{\boldsymbol{a}} \boldsymbol{\iota}_\ell$

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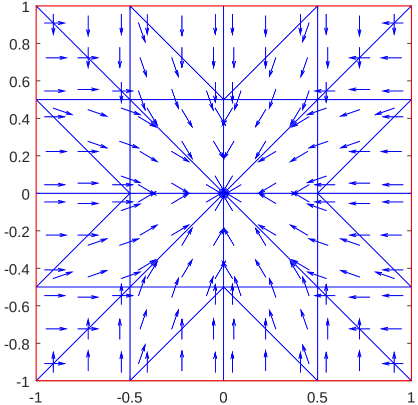

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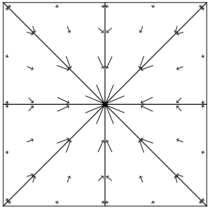

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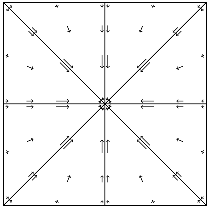

$\boldsymbol{\sigma}_\ell^{\boldsymbol{a}}$

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

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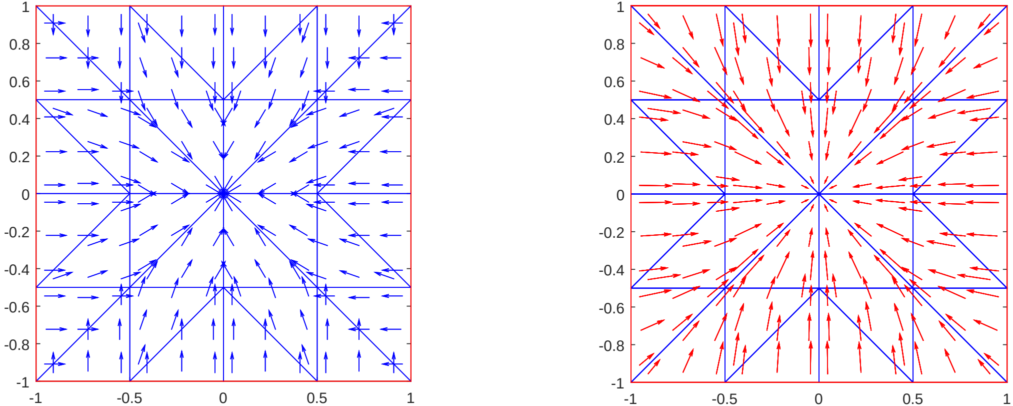

Flux $\boldsymbol{\iota}_\ell \notin \boldsymbol{H}(\mathrm{div})$, $\nabla\cdot\boldsymbol{\iota}_\ell \neq f$

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

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

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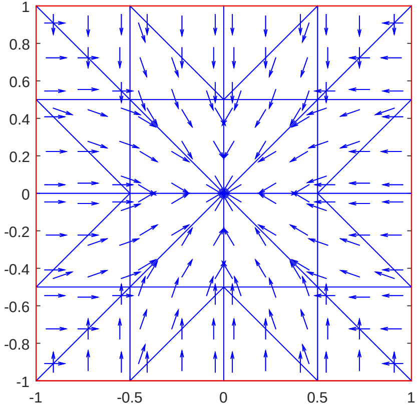

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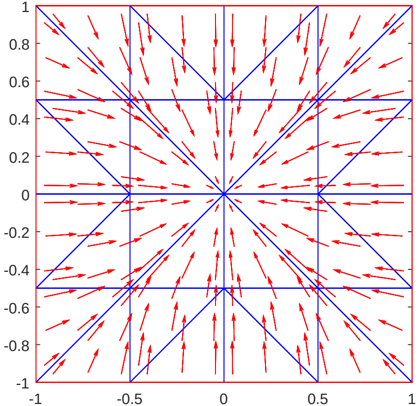

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Equilibrated flux reconstruction

Use

- **a posteriori error estimates**
  - comparison of the original & reconstructed flux $\|\nabla u_\ell + \sigma_\ell\|$: discretization error
  - error component fluxes: linearization and algebraic errors
- recovery of **mass conservative fluxes**
  - local on patches of mesh elements from FE-type approximations
  - local on elements from FV- & DG-type approximations
  - inexact nonlinear solvers (still local)
  - inexact linear solvers (price of one MG iteration)

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