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

André Harnist, Koondanibha Mitra, Ari Rappaport, and Martin Vohralík

Inria Paris & Ecole des Ponts

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Outline

- Introduction
 - Numerical approximation of partial differential equations
 - A posteriori error estimates
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 - Setting (gradient-dependent case)
 - Error measures
 - Known results
- Iterative linearization
- A posteriori error estimates for an augmented energy difference
- Mumerical experiments
- 6 Extensions
 - Setting (gradient-independent case)
 - A posteriori error estimates for an iteration-dependent norm
 - Numerical experiments
- Conclusions



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Numerical approximation of partial differential equations

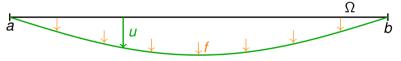
Numerical methods

- mathematically-based algorithms evaluated by computers
- deliver approximate solutions
- conception: more effort ⇒ closer to the unknown solution
- example: elastic string



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Numerical approximation u_{h_0} and its convergence to u

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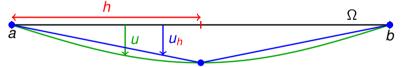


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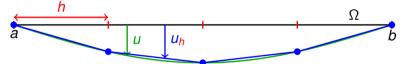
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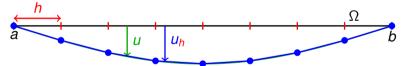


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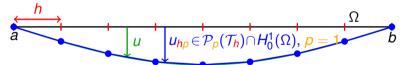


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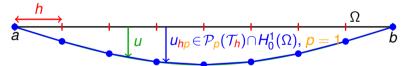
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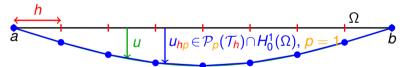
Numerical approximation u_{hp} and its convergence to u

Error
$$\|\nabla(u-u_{hp})\| = \left\{ \int_a^b |(u-u_{hp})'|^2 \right\}^{\frac{1}{2}}$$



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Numerical approximation u_{hp} and its convergence to u

Error
$$\|\nabla(u-u_{hp})\| = \left\{ \int_a^b |(u-u_{hp})'|^2 \right\}^{\frac{1}{2}}$$

Need to solve a linear system

$$\mathbb{A}_{hp}\mathsf{U}_{hp}=\mathsf{F}_{hp}$$



Crucial questions

- How large is the overall error?



3 crucial questions

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- Where (model/space/time/linearization/algebra) is it localized?



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- Can we decrease it efficiently?



3 crucial questions & suggested answers

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Suggested answers

A posteriori error estimates.



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- A posteriori error estimates.
- Identification of error components.



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- Where (model/space/time/linearization/algebra) is it localized?
- Oan we decrease it efficiently?

Suggested answers

- A posteriori error estimates.
- Identification of error components.
- Balancing error components, adaptivity (working where needed).



CDG Terminal 2E collapse in 2004 (opened in 2003)



- no earthquake, flooding, tsunami, heavy rain, extreme temperature
- deterministic, steady problem, PDE known, data known, implementation OK



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Y. El Kamari *, W. Raphael *, *, A. Chateauneuf b,c

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probably numerical simulations done with insufficient precision, I believe without error certification by a posteriori error estimates





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

$$-\nabla \cdot (\nabla u) = f \quad \text{in} \quad \Omega,$$

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

Guaranteed error upper bound (reliability)

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

Error lower bound (efficiency)

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

• 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}_{ℓ} uniform) and of the polynomial degree n (for d < 3)



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

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- C_{eff} only depends on mesh shape regularity $\kappa_{\mathcal{T}}$, d, and possibly p (if $d \geq 4$)
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How large is the overall error?

$h \approx 1/ \mathcal{T}_{\ell} ^{\frac{1}{2}}$	р	$\eta(U_\ell)$	rel. error estimate $\frac{\eta(u_\ell)}{\ \nabla u_\ell\ }$	$\ \nabla(u-u_\ell)\ $	rel. error $\frac{\ \nabla(u-u_\ell)\ }{\ \nabla u_\ell\ }$	$I^{ ext{eff}} = rac{\eta(u_{\ell})}{\ abla(u-u_{\ell})\ }$
h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$	2	4.23×10^{-1}				
$\approx h_0/4$	3	2.62 × 10=				
$\approx h_0/8$	4	2.60 × 10=				



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h_0	1	1.25	28%	1.07	24%	1.17
		6.07×10^{-1}				
$\approx h_0/2$	2	4.23×10^{-2}	$9.6 \times 10^{-1}\%$	4.07 × 10		
$\approx h_0/4$	3	2.62×10^{-4}		2.60 × 10 =		
$\approx h_0/8$	4	2.60×10^{-7}	5.9 × 10 ⁻¹ %			



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$\approx h_0/2$	2	4.23×10^{-2}	$9.5 \times 10^{-1}\%$	4.07×10^{-6}	9.2 × 10 1%	
$\approx h_0/4$	3	2.62×10^{-4}	$5.9 \times 10^{-3}\%$	2.60 × 10	5.9 × 10 ⁻³ %	
$\approx h_0/8$	4	2.60×10^{-7}	$5.9 \times 10^{-6}\%$	2.58×10^{-7}	5.8 × 10 ⁻⁹ %	



How large is the overall error? (model pb, known smooth solution)

$h \approx 1/ \mathcal{T}_{\ell} ^{\frac{1}{2}}$	$\rho \mid \eta(u_\ell)$	rel. error estimate $\frac{\eta(u_\ell)}{\ \nabla u_\ell\ }$	$\ \nabla(u-u_\ell)\ $	rel. error $\frac{\ \nabla(u-u_\ell)\ }{\ \nabla u_\ell\ }$	$I^{\text{eff}} = \frac{\eta(u_\ell)}{\ \nabla(u - u_\ell)\ }$
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	$6.07 \times 10^{-}$		5.56×10^{-1}		
$\approx h_0/2$	$2 ext{ } 4.23 imes 10^{-}$	9.5×10^{-1} %	4.07×10^{-2}	9.2 × 10 ⁻¹ %	
$\approx h_0/4$	3 2.62 × 10 ⁻	4 5.9 \times 10 ⁻³ %	2.60×10^{-4}	5.9 × 10 ⁻³ %	
$\approx h_0/8$	$4 2.60 \times 10^{-}$	$7 5.9 \times 10^{-6}\%$	2.58×10^{-7}		



How large is the overall error? (model pb, known smooth solution)

$h pprox 1/ \mathcal{T}_\ell ^{rac{1}{2}}$	$\eta(u_\ell)$	rel. error estimate $\frac{\eta(u_\ell)}{\ abla u_\ell\ }$	$\ \nabla(u-u_\ell)\ $	rel. error $\frac{\ \nabla(u-u_\ell)\ }{\ \nabla u_\ell\ }$	$I^{eff} = rac{\eta(u_\ell)}{\ abla(u-u_\ell)\ }$
h_0	1.25	28%	1.07	24%	1.17
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$\approx h_0/8$	$1.2.60 \times 10^{-7}$	5.9×10^{-6} %	2.58×10^{-7}	$5.8 \times 10^{-6}\%$	



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



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$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	1.04
$\approx h_0/2$	2	4.23×10^{-2}		4.07×10^{-2}	$9.2 \times 10^{-1}\%$	1.04
$\approx h_0/4$	3	2.62×10^{-4}	$5.9 \times 10^{-3}\%$	2.60×10^{-4}	$5.9 \times 10^{-3}\%$	1.01
$\approx h_0/8$	4	2.60×10^{-7}	$5.9 \times 10^{-6}\%$	2.58×10^{-7}	$5.8 \times 10^{-6}\%$	1.01

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



$h pprox 1/ \mathcal{T}_\ell ^{rac{1}{2}}$	p	$\eta(u_\ell)$	rel. error estimate $\frac{\eta(u_\ell)}{\ \nabla u_\ell\ }$	$\ \nabla(u-u_\ell)\ $	rel. error $\frac{\ \nabla(u-u_\ell)\ }{\ \nabla u_\ell\ }$	$I^{ ext{eff}} = rac{\eta(u_\ell)}{\ abla(u-u_\ell)\ }$
h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$		6.07×10^{-1}	14%	5.56×10^{-1}	13%	1.09
$\approx h_0/4$		3.10×10^{-1}	7.0%	2.92×10^{-1}	6.6%	1.06
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	1.04
$\approx h_0/2$	2	4.23×10^{-2}		4.07×10^{-2}	$9.2 \times 10^{-1}\%$	1.04
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A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015) V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)



Linear problems

A posteriori error estimates **robust** with respect to the **discretization parameters** $|\mathcal{T}_{\ell}|$ (h if \mathcal{T}_{ℓ} uniform) and p ($d \leq 3$).

Nonlinear problems

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



Linear problems

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Nonlinear problems

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



Setting Iterative linearization Estimates Numerics Extensions C Numerical approximation of PDEs A posteriori error estimates



- Numerical approximation of partial differential equations
- A posteriori error estimates
- Setting and known results
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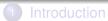
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A model nonlinear problem

Nonlinear elliptic problem

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

$$-\nabla \cdot (\mathbf{a}(|\nabla \mathbf{u}|)\nabla \mathbf{u}) = f \quad \text{in} \quad \Omega,$$

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

- $\Omega \subset \mathbb{R}^d$, d > 1, open polytope with Lipschitz boundary $\partial \Omega$
- $f \in L^2(\Omega)$

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

$$|a(|x|)x - a(|y|)y| \le a_c|x - y|$$
 (Lipschitz continuity),
 $(a(|x|)x - a(|y|)y) \cdot (x - y) \ge a_m|x - y|^2$ (strong monotonicity)

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



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Assumption (Nonlinear function a)

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

$$|a(|\mathbf{x}|)\mathbf{x} - a(|\mathbf{y}|)\mathbf{y}| \le \frac{\mathsf{a_c}}{|\mathbf{x} - \mathbf{y}|}$$
 (Lipschitz continuity),

$$(a(|\mathbf{x}|)\mathbf{x} - a(|\mathbf{y}|)\mathbf{y}) \cdot (\mathbf{x} - \mathbf{y}) \ge \frac{\mathbf{a}_{\mathsf{m}}}{\mathbf{a}_{\mathsf{m}}}|\mathbf{x} - \mathbf{y}|^2$$

(strong monotonicity).





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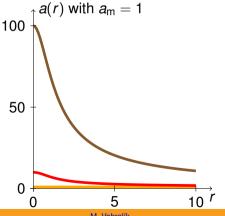
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$$a_{\rm m} \le a(r) \le a_{\rm c}, \ a_{\rm m} \le (a(r)r)'(r) \le a_{\rm c}$$



Strength of the nonlinearity, $0 < a_m < a_c < \infty$ real parameters

Example (Mean curvature nonlinearity)

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

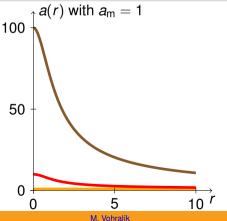


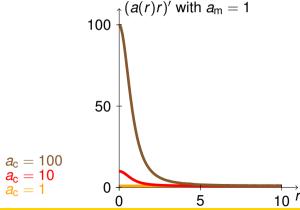
$$a_{c} = 100$$
 $a_{c} = 10$
 $a_{c} = 1$

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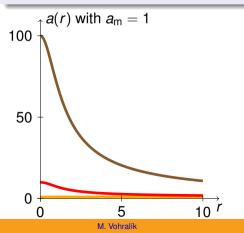


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Strength of the nonlinearity, $0 < a_m < a_c < \infty$ real parameters

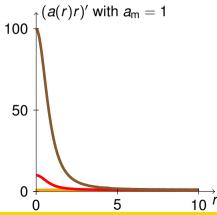
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Strength of the nonlinearity

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



Definition (Weak solution)

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

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

$$(a(|
abla u_\ell|)
abla u_\ell,
abla v_\ell) = (f, v_\ell) \qquad orall v_\ell \in V^p_\ell$$

- \mathcal{T}_{ℓ} simplicial mesh of Ω
- p > 1 polynomial degree
- conforming finite elements
- $V_{\ell}^{p} := \mathcal{P}_{p}(\mathcal{T}_{\ell}) \cap H_{0}^{1}(\Omega)$

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



Definition (Weak solution)

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

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

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}_{ℓ} simplicial mesh of Ω
- $p \ge 1$ polynomial degree
- conforming finite elements
- $V_{\ell}^{p} := \mathcal{P}_{p}(\mathcal{T}_{\ell}) \cap H_{0}^{1}(\Omega)$

Need to **solve** a **nonlinear system**

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



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Sobolev space and error

Sobolev space

$$H_0^1(\Omega)$$

Sobolev norm error

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



Energy and energy differences

Definition (Energy functional)

$$\mathcal{J}: H^1_0(\Omega) \to \mathbb{R}$$

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

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

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

$$u = \arg\min_{v \in H_0^1(\Omega)} \mathcal{J}(v), \qquad u_\ell = \arg\min_{v_\ell \in V_\ell^p} \mathcal{J}(v_\ell)$$

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



Energy and energy differences

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$${\color{red} {\mathcal J}}: H^1_0(\Omega) o {\mathbb R}$$

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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

$$u = \arg\min_{\mathbf{v} \in H^1_{\epsilon}(\Omega)} \mathcal{J}(\mathbf{v}), \qquad u_{\ell} = \arg\min_{\mathbf{v}_{\ell} \in V^{\rho}_{\ell}} \mathcal{J}(\mathbf{v}_{\ell}).$$

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

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



Energy and energy differences

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Energy difference

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

- $\mathcal{J}(u_{\ell}) \mathcal{J}(u) \geq 0$, $\mathcal{J}(u_{\ell}) \mathcal{J}(u) = 0$ if and only if $u_{\ell} = u$
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Residual and its dual norm

Definition (Residual)

$$\mathcal{R}: H^1_0(\Omega) \to H^{-1}(\Omega);$$
 for $w \in H^1_0(\Omega), \mathcal{R}(w) \in H^{-1}(\Omega)$ is given by
$$\langle \mathcal{R}(w), v \rangle := (a(|\nabla w|)\nabla w, \nabla v) - (f, v), \quad v \in H^1_0(\Omega).$$

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

- $|||\mathcal{R}(u_{\ell})|||_{-1} > 0$, $|||\mathcal{R}(u_{\ell})|||_{-1} = 0$ 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: $|||v||| := ||\nabla v||$
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Residual and its dual norm

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Definition (Dual norm of the finite element residual)

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

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Sobolev norm

$$\|a_{\mathsf{m}}\|\nabla(u_{\ell}-u)\| \leq \eta(u_{\ell}) \leq \frac{C_{\mathsf{eff}}}{2} \|\nabla(u_{\ell}-u)\|$$

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

Energy difference

$$\mathcal{J}(u_{\ell}) - \mathcal{J}(u) \leq \frac{1}{2} \eta(u_{\ell})^2 \leq C_{\text{eff}}^2 \frac{a_{\text{C}}^2}{a_{\text{m}}^2} \big(\mathcal{J}(u_{\ell}) - \mathcal{J}(u) \big)$$



Sobolev norm

$$\|a_{\mathsf{m}}\|\nabla(u_{\ell}-u)\| \leq \eta(u_{\ell}) \leq \frac{C_{\mathsf{eff}}a_{\mathsf{c}}}{C_{\mathsf{eff}}a_{\mathsf{c}}}\|\nabla(u_{\ell}-u)\|$$

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

Strength of the nonlinearity Not robust with respect to $\frac{\partial c}{\partial m}$.



Sobolev norm

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

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 & Kreuzer (2008), Bartels & Milicevic (2020), . . .

Strength of the nonlinearity

Not robust with respect to 40 mm.



Sobolev norm

$$|a_{\mathsf{m}}||\nabla(u_{\ell}-u)|| \leq \eta(u_{\ell}) \leq \frac{C_{\mathsf{eff}}}{2} ||\nabla(u_{\ell}-u)||$$

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

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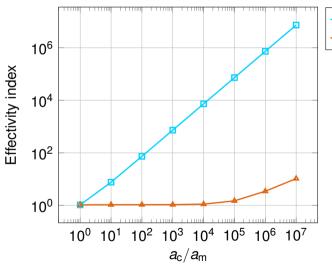
Zeidler (1992), Han (1994), Repin (1997), Ladevèze & Moës (1997), Diening
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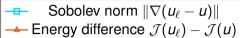
Strength of the nonlinearity

Not robust with respect to $\frac{a_0}{a_0}$.



Non-robustness







Dual norm of the residual

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

 Chaillou & Suri (2006), El Alaoui, Ern, & Vohralík (2011), Blechta, Málek, & Vohralík (2020), ...

- **Robust** with respect to $\frac{a_c}{a_m}$ if $|||v||| = ||\nabla v||$.



Dual norm of the residual

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

 Chaillou & Suri (2006), El Alaoui, Ern, & Vohralík (2011), Blechta, Málek, & Vohralík (2020), ...

Strength of the nonlinearity

- Robust with respect to $\frac{\partial c}{\partial v}$ if $|||v||| = ||\nabla v||$.
- $|||\mathcal{R}(u_{\ell})|||_{-1}$ **localizes** over patches of elements.



Known results

Dual norm of the residual

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

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- Robust with respect to $\frac{\partial c}{\partial v}$ if $|||v||| = ||\nabla v||$.
- $|||\mathcal{R}(u_{\ell})|||_{-1}$ localizes over patches of elements.
- Does not see the nonlinearity $(H^{-1}(\Omega))$ residual norm)



Known results

Dual norm of the residual

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

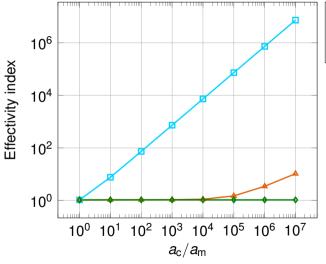
 Chaillou & Suri (2006), El Alaoui, Ern, & Vohralík (2011), Blechta, Málek, & Vohralík (2020), ...

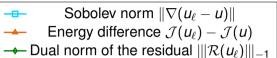
Strength of the nonlinearity

- Robust with respect to $\frac{\partial c}{\partial v}$ if $|||v||| = ||\nabla v||$.
- $|||\mathcal{R}(u_{\ell})|||_{-1}$ **localizes** over patches of elements.
- Does not see the nonlinearity $(H^{-1}(\Omega))$ residual norm) (essentially estimates the **flux error** $||a(|\nabla u_{\ell}|)\nabla u_{\ell} - a(|\nabla u|)\nabla u||$).



Non-robustness







Nonlinear problems

A posteriori error estimates **robust** with respect to the **strength of nonlinearities** in more **physically-based error measures**?



Iterative linearization

Addressing iterative linearization

Chaillou & Suri (2006), Ern & Vohralík (2013), Bernardi, Dakroub, Mansour, & Sayah (2015), Gantner, Haberl, Praetorius, & Stiftner (2018), Heid & Wihler (2020), Botti & Riedlbeck (2020), . . .

Observation

None of the above approaches employ in the analysis, to define norms, the iterative linearization, i.e., how do we solve the nonlinear system $\mathcal{A}_{\ell}(U_{\ell}) = F_{\ell}$.



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Setting Iterative linearization Estimates Numerics Extensions C

Outline



- Numerical approximation of partial differential equations
- A posteriori error estimates
- Setting and known results
 - Setting (gradient-dependent case)
 - Error measures
 - Known results
- Iterative linearization
- A posteriori error estimates for an augmented energy difference
- 5 Numerical experiments
- **6** Extensions
 - Setting (gradient-independent case)
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- Conclusions



etting Iterative linearization Estimates Numerics Extensions C

Iterative linearization

Definition (Linearized finite element approximation)

 $u_{\ell}^{\mathbf{k}} \in V_{\ell}^{p}$ such that

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

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

Definition (Linearized energy functional)

$$\begin{split} \mathcal{J}_{\ell}^{k-1} : H_0^1(\Omega) \to \mathbb{R} \\ \mathcal{J}_{\ell}^{k-1}(v) := \frac{1}{n} \left\| (\boldsymbol{A}_{\ell}^{k-1})^{\frac{1}{2}} \nabla v \right\|^2 - (f, v) - (\boldsymbol{b}_{\ell}^{k-1}, \nabla v), \quad v \in H_0^1(\Omega) \end{split}$$

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



g Iterative linearization Estimates Numerics Extensions C

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Definition (Linearized finite element approximation)

 $u_\ell^{m{k}} \in V_\ell^p$ such that

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

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Examples

Example (Picard (fixed-point))

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

Example (Zarantonello)

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

with $\gamma \geq \frac{a_0^2}{a_m}$ a constant parameter.

Example ((Damped) Newton)

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

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Theorem (A posteriori estimate of energy)

Let $f \in \mathcal{P}_{p-1}(\mathcal{T}_{\ell})$ for simplicity. For all linearization steps $k \geq 1$,

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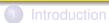
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Smooth solution

Setting

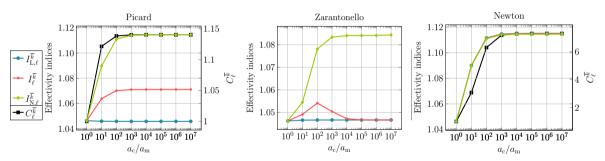
- unit square $\Omega = (0, 1)^2$
- known smooth solution u(x, y) := 10 x(x 1)y(y 1)
- mean curvature or exponential nonlinearity

$$a(r) = a_{\mathsf{m}} + rac{a_{\mathsf{c}} - a_{\mathsf{m}}}{\sqrt{1 + r^2}} \qquad ext{or} \qquad a(r) = a_{\mathsf{m}} + (a_{\mathsf{c}} - a_{\mathsf{m}}) rac{1 - e^{-rac{3}{2}r^2}}{1 + 2e^{-rac{3}{2}}}$$

- p = 1,3969 DOFs
- stopping iteration \overline{k} such that $\|\nabla(u_{\ell}^{\overline{k}-1}-u_{\ell}^{\overline{k}})\|<10^{-6}$
- effectivity indices

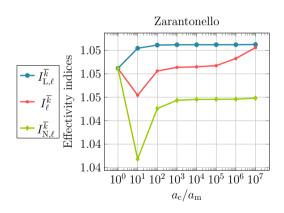
$$\underbrace{I_{\ell}^{k} := \left(\frac{\eta_{\ell}^{k}}{\mathcal{E}_{\ell}^{k}}\right)^{\frac{1}{2}}}_{\text{total}}, \quad I_{N,\ell}^{k} := \underbrace{\left(\frac{\mathcal{J}(u_{\ell}^{k}) - \mathcal{J}^{*}(\sigma_{\ell}^{k})}{\mathcal{J}(u_{\ell}^{k}) - \mathcal{J}(u)}\right)^{\frac{1}{2}}}_{\text{energy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

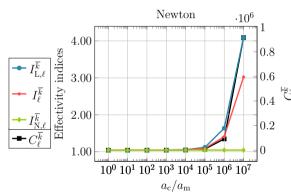
Error certification robust wrt the nonlinearities (mean curvature)



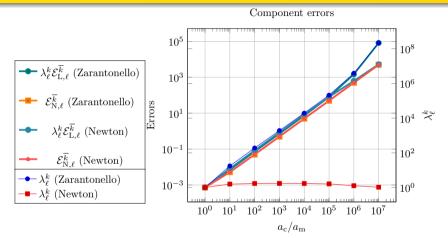


Error certification robust wrt the nonlinearities (exponential, robustness only for Zarantonello)





Error certification robust wrt the nonlinearities (exponential)



Components of $\mathcal{E}^{\overline{k}}_{\ell}$: the energy difference $\mathcal{E}^{\overline{k}}_{N,\ell} = \mathcal{J}(u^{\overline{k}}_{\ell}) - \mathcal{J}(u)$, the energy difference of the linearized problem $\mathcal{E}^{\overline{k}}_{L,\ell} = \mathcal{J}^{\overline{k}-1}_{\ell}(u^{\overline{k}}_{\ell}) - \mathcal{J}^{\overline{k}-1}_{\ell}(u^{\overline{k}}_{\ell})$, & the weight λ^k_{ℓ}

Singular solution

Setting

- L-shaped domain $\Omega = (-1,1)^2 \setminus ([0,1) \times (-1,0])$
- known singular solution $u(\rho,\theta) = \rho^{\frac{2}{3}} \sin(\frac{2}{3}\theta)$
- exponential nonlinearity

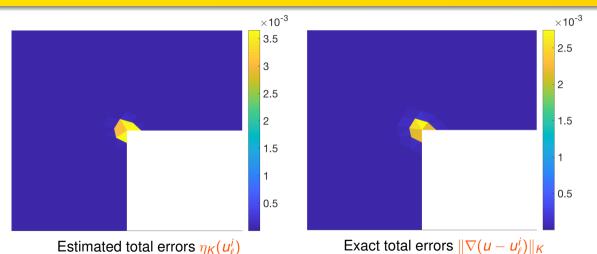
$$a(r) = a_{\mathsf{m}} + (a_{\mathsf{c}} - a_{\mathsf{m}}) \frac{1 - e^{-\frac{3}{2}r^2}}{1 + 2e^{-\frac{3}{2}}}$$

 \bullet p = 1, uniform or adaptive mesh refinement



tting Iterative linearization Estimates Numerics Extensions C

Where is the error localized?

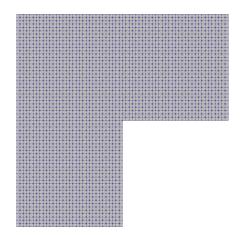


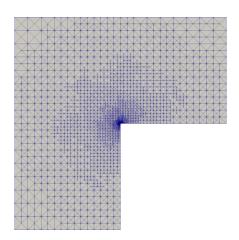
J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)



Setting Iterative linearization Estimates Numerics Extensions C

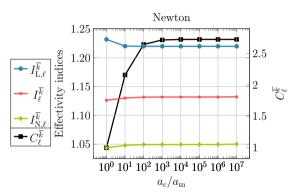
Adaptive mesh refinement



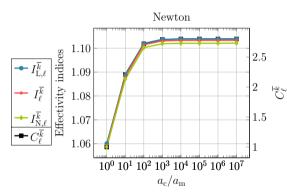




Error certification robust wrt the nonlinearities



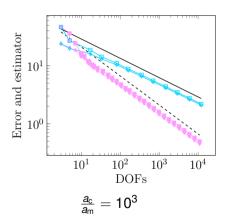
Uniform mesh refinement

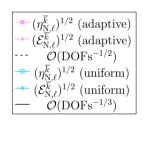


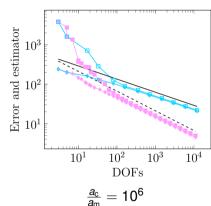
Adaptive mesh refinement



Decreasing the error efficiently: optimal decay rate wrt DoFs









Setting Iterative linearization Estimates Numerics Extensions C Setting (gradient-independent nonlinearities) Estimates Numerics

Outline



- Numerical approximation of partial differential equations
- A posteriori error estimates
- Setting and known results
 - Setting (gradient-dependent case)
 - Error measures
 - Known results
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- Numerical experiments
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A model nonlinear problem

Nonlinear elliptic problem

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

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

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

 \bullet $\tau > 0$ a parameter (time step size in transient problems)

$$\begin{aligned} |\mathcal{D}(\pmb{x}_1,\xi_1) - \mathcal{D}(\pmb{x}_2,\xi_2)| &\leq \mathcal{D}_{\mathsf{M}}(|\pmb{x}_1 - \pmb{x}_2| + |\xi_1 - \xi_2|) \quad \forall \pmb{x}_1,\pmb{x}_2 \in \Omega \ \textit{and} \ \xi_1,\xi_2 \in \mathcal{R}, \\ 0 &\leq f(\pmb{x},\xi_2) - f(\pmb{x},\xi_1) \leq f_{\mathsf{M}} \left(\xi_2 - \xi_1\right) \quad \forall \pmb{x} \in \Omega \ \textit{and} \ \xi_2 \geq \xi_1, \\ \pmb{q} \ \textit{is "small" wrt} \ \pmb{K}\mathcal{D}. \end{aligned}$$



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

$$\begin{split} |\mathcal{D}(\boldsymbol{x}_1,\xi_1) - \mathcal{D}(\boldsymbol{x}_2,\xi_2)| &\leq \mathcal{D}_{M}(|\boldsymbol{x}_1 - \boldsymbol{x}_2| + |\xi_1 - \xi_2|) \quad \forall \boldsymbol{x}_1,\boldsymbol{x}_2 \in \Omega \text{ and } \xi_1,\xi_2 \in \mathcal{R}, \\ 0 &\leq f(\boldsymbol{x},\xi_2) - f(\boldsymbol{x},\xi_1) \leq f_{M}\left(\xi_2 - \xi_1\right) \quad \forall \boldsymbol{x} \in \Omega \text{ and } \xi_2 \geq \xi_1, \\ \boldsymbol{q} \text{ is "small" wrt } \underline{\boldsymbol{K}}\mathcal{D}. \end{split}$$



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Strength of the nonlinearity ratio a_c/a_m



Definition (Linearized finite element approximation)

 $u_{\ell}^{\mathbf{k}} \in V_{\ell}^{\mathbf{p}}$ such that

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

linearization: reaction-diffusion scalar product

$$((w, v))_{u_{\ell}^{k-1}} := (\underbrace{L(x, u_{\ell}^{k-1})}_{\text{reaction coef}} w, v) + (\underbrace{\mathfrak{a}(x, u_{\ell}^{k-1})}_{\text{diffusion coef}} \nabla w, \nabla v), \quad w, v \in H_0^1(\Omega)$$

covers many linearization schemes: Picard (fixed-point), L & M-schemes, ...

$$|||v|||_{1,u_{\ell}^{k-1}} := ((v, v))_{u_{\ell}^{k-1}}^{\frac{1}{2}}, \quad v \in H_0^1(\Omega)$$



Iterative linearization

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$$|||v|||_{1,u_{\rho}^{k-1}} := ((v, v))^{\frac{1}{2}}_{u_{\rho}^{k-1}}, \quad v \in H_0^1(\Omega)$$

induced by the linearization scalar product



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Iteration-dependent norm

$$|||v|||_{1,u_{\ell}^{k-1}} := ((v, v))^{\frac{1}{2}}_{u_{\ell}^{k-1}}, \quad v \in H_0^1(\Omega)$$

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 $k \ge 1$, there holds

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

- orthogonal decomposition



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- orthogonal decomposition
- error components



Setting Iterative linearization Estimates Numerics Extensions C Setting (gradient-independent nonlinearities) Estimates Numerics

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Theorem (A posteriori estimate of iteration-dependent norm)

For all linearization steps $k \ge 1$,

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

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

$$\eta_\ell^k \leq \textcolor{red}{C_{\text{eff}}(\textit{d},\kappa_{\mathcal{T}},\textit{p})C_\ell^k|||\mathcal{R}(u_\ell^{k-1})|||_{-1,u_\ell^{k-1}} + \textit{quadrature terms} + \textit{data oscillation terms},$$

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$$C_{\ell}^{k}$$

$$\begin{cases} = 1 & Zarantonello \end{cases}$$

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 Zarantonello

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Theorem (A posteriori estimate of iteration-dependent norm)

For all linearization steps k > 1.

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

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

$$\eta_\ell^k \leq \textit{C}_{\text{eff}}(\textit{d},\kappa_{\mathcal{T}},\textit{p}) C_\ell^k |||\mathcal{R}(u_\ell^{k-1})|||_{-1,u_\ell^{k-1}} + \textit{quadrature terms} + \textit{data oscillation terms},$$

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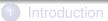
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- C_{ℓ}^{k} given by **local** (patch) **properties**: typically **much better** than a_{c}/a_{m} C_{ℓ}^{k} **computable**: we can affirm **robustness** *a posteriori*, for the given case
- also local efficiency

Setting Iterative linearization Estimates Numerics Extensions C Setting (gradient-independent nonlinearities) Estimates Numerics

Outline



- Numerical approximation of partial differential equations
- A posteriori error estimates
- Setting and known results
 - Setting (gradient-dependent case)
 - Error measures
 - Known results
- Iterative linearization
- A posteriori error estimates for an augmented energy difference
- Numerical experiments
- 6 Extensions
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The Richards equation

Setting

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

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

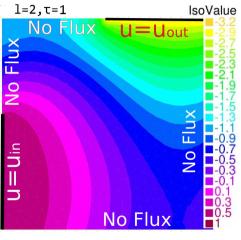
$$\underline{\mathbf{K}} = \begin{bmatrix} 1 & 0.2 \\ 0.2 & 1 \end{bmatrix}, \quad \mathbf{g} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- time step length $\tau \in [10^{-3}, 1]$
- van Genuchten saturation and permeability laws

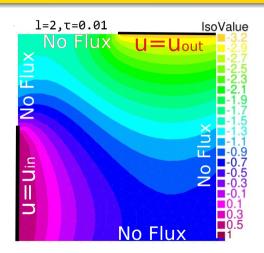
$$S(\xi) := \left(1 + (2-\xi)^{rac{1}{1-\lambda}}
ight)^{-\lambda}, \quad \kappa(s) := \sqrt{s}\left(1 - (1-s^{rac{1}{\lambda}})^{\lambda}
ight)^2, \quad \lambda = 0.5$$



One time step of the Richards equation with realistic data



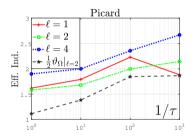
Time step length $\tau = 1$

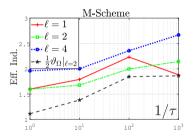


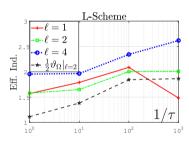
Time step length $\tau = 0.01$



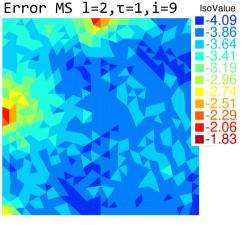
Error certification robust wrt the nonlinearities



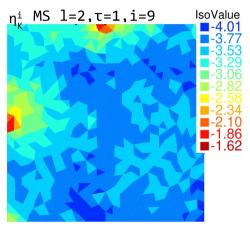








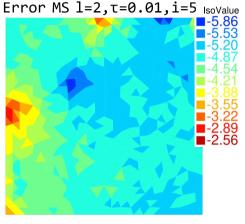
Error, $\tau = 1$



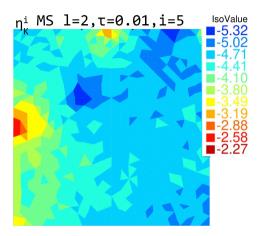
Estimate, $\tau = 1$



Where is the error **localized?**



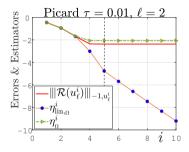
Error, $\tau = 0.01$

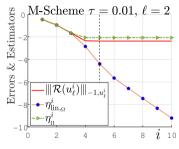


Estimate, $\tau = 0.01$



Error components and adaptivity via stopping criteria





L-Scheme $\tau = 0.01$, $\ell = 2$ Storm -2

Storm

Time step length $\tau = 0.01$



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- a posteriori certification of the error for nonlinear problems
- robustness with respect to the strength of nonlinearities
- 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!

