Guaranteed and robust a posteriori error estimates and balancing discretization and linearization errors for monotone nonlinear problems

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Joint work with
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Outline

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Discretization, linearization, and algebraic solvers

Discretization

- let p be the weak solution of $A(p) = F$, A nonlinear
- let p_h be its approximate numerical solution, $A_h(p_h) = F_h$

Iterative linearization

- $A_{\mathrm{L},h}^{(i-1)} p_h^{(i)} = F_{\mathrm{L},h}^{(i-1)}$: discrete Newton or fixed-point linearization
- **when do we stop?**

Iterative algebraic system solution

- $A_{\mathrm{L},h}^{(i-1)} p_h^{(i)} = F_{\mathrm{L},h}^{(i-1)}$ is a linear algebraic system
- we only solve it inexactly by, e.g., some iterative method
- **when do we stop?**

Approximate solution

- the approximate solution p_h^{a} that we have as an outcome does not solve $A_h(p_h^{\mathrm{a}}) = F_h$
- how big is the **overall error** $\|p - p_h^{\mathrm{a}}\|_\Omega$**?**

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A posteriori error estimate

- aims at estimating $\|p - p_h^{\mathrm{a}}\|_\Omega$
- but most of the existing approaches rely on $A_h(p_h^{\mathrm{a}}) = F_h$!

Aims of this work

- give a **guaranteed and robust upper bound** on the **overall error** $\|p - p_h^{\mathrm{a}}\|_\Omega$
- predict the **overall error distribution** (local efficiency)
- distinguish the algebraic/linearization errors, due to inexact solution of linear/nonlinear problems, and the discretization error, due to mesh size and numerical scheme
- **stop** the **iterative solvers** whenever algebraic/linearization errors do not affect the overall error significantly

Benefits

- **optimal computable overall error bound**
- **adaptive mesh refinement**
- **important computational savings**

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- Babuška and Rheinboldt (1978)
- Verfürth (1996, book)
- Ainsworth and Oden (2000, book)
- Luce and Wohlmuth (2004)

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- Repin (1997)

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- Han (1994), general framework
- Verfürth (1994), residual estimates
- Veeser (2002), convergence *p*-Laplacian
- Carstensen and Klose (2003), guaranteed estimates
- Chaillou and Suri (2006, 2007), distinguishing discretization and linearization errors

Other methods

- Kim (2007), guaranteed estimates for locally conservative methods

Error components equilibration

- engineering literature, since 1950's
- Ladevèze (since 1980's)
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$$-\nabla\cdot\boldsymbol{\sigma}(\nabla u) = f \qquad \text{in } \Omega,$$
$$u = 0 \qquad \text{on } \partial\Omega,$$

where

- $\forall \xi \in \mathbb{R}^d$, $\sigma(\xi) = a(|\xi|)\xi$,
- $a(x) \sim x^{p-2}$ as $x \to +\infty$, $p \in (1, +\infty)$,
- $f \in L^q(\Omega)$, $q := \frac{p}{p-1}$

Example

p-Laplacian: $a(x) = x^{p-2}$

Nonlinear operator $A : V := W_0^{1,p}(\Omega) \to V'$

$$\langle Au, v\rangle_{V',V} := (\sigma(\nabla u), \nabla v)$$

Weak formulation

Find $u \in V$ such that

$$Au = f \text{ in } V'$$

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Linearizations at $u_0 \in V$

Linearized flux function $\boldsymbol{\sigma}_{\mathrm{L},u_0}$

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- linearized flux function $\boldsymbol{\sigma}_{\mathrm{L},u_0} : \mathbb{R}^d \to \mathbb{R}^d$ depending on ∇u_0, $\boldsymbol{\sigma}_{\mathrm{L},u_0}(\nabla u)$

Fixed-point linearization

$$\boldsymbol{\sigma}_{\mathrm{L},u_0}(\boldsymbol{\xi}) := a(|\nabla u_0|)\boldsymbol{\xi}$$

Newton linearization

$$\boldsymbol{\sigma}_{\mathrm{L},u_0}(\boldsymbol{\xi}) := a(|\nabla u_0|)\boldsymbol{\xi} + a'(|\nabla u_0|)\frac{1}{|\nabla u_0|}(\nabla u_0 \otimes \nabla u_0)(\boldsymbol{\xi} - \nabla u_0)$$

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- $u_{\mathrm{L},h} \in V$
- based on the difference of the fluxes
- dual norm of the residual
- inspired from Angermann (1995), Verfürth (2005), Chaillou and Suri (2006, 2007)
- not a norm for the difference $u - u_{\mathrm{L},h}$
- avoids any appearance of the ratio continuity constant / monotonicity constant
- there holds $J_u(u_{\mathrm{L},h}) \to 0$ if and only if $\|u - u_{\mathrm{L},h}\|_V \to 0$

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Error measure

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$$\mathcal{J}_u(u_{\mathrm{L},h}) := \|Au - Au_{\mathrm{L},h}\|_{V'} = \sup_{v \in V \setminus \{0\}} \frac{(\boldsymbol{\sigma}(\nabla u) - \boldsymbol{\sigma}(\nabla u_{\mathrm{L},h}), \nabla v)}{\|\nabla v\|_p}$$

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- dual norm of the residual
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A posteriori error estimate

Assumption A (Equilibrated flux)

Let there be a mesh $\mathcal{D}_h$ *of* Ω *and* $\mathbf{t}_h \in \mathbf{H}^q(\mathrm{div}, \Omega)$ *such that*

$$(\nabla \cdot \mathbf{t}_h, 1)_D = (f, 1)_D \qquad \forall D \in \mathcal{D}_h^{\mathrm{int}}.$$

Theorem (A posteriori error estimate)

Let

- $u \in V$ *be the weak solution,*
- $u_{\mathrm{L},h} \in V$ *be arbitrary,*
- *Assumption A hold.*

Then there holds

$$\mathcal{J}_u(u_{\mathrm{L},h}) \leq \eta := \left\{ \sum_{D \in \mathcal{D}_h} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^q \right\}^{1/q} + \left\{ \sum_{D \in \mathcal{D}_h} \eta_{\mathrm{L},D}^q \right\}^{1/q}.$$

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Estimators

Estimators

- *residual estimator*

$$\eta_{\mathrm{R},D} := C_{\mathrm{P/F},p,D} h_D \|f - \nabla\cdot\mathbf{t}_h\|_{q,D}$$

- *diffusive flux estimator*

$$\eta_{\mathrm{DF},D} := \|\boldsymbol{\sigma}_{\mathrm{L}}(\nabla u_{\mathrm{L},h}) + \mathbf{t}_h\|_{q,D}$$

- *linearization estimator*

$$\eta_{\mathrm{L},D} := \|\boldsymbol{\sigma}(\nabla u_{\mathrm{L},h}) - \boldsymbol{\sigma}_{\mathrm{L}}(\nabla u_{\mathrm{L},h})\|_{q,D}$$

Outline

Balancing the discretization and linearization errors

Global linearization stopping criterion

- stop the Newton (or fixed-point) linearization whenever

$$\eta_{\mathrm{L}} \leq \gamma\, \eta_{\mathrm{D}},$$

where

$$\eta_{\mathrm{L}} := \left\{ \sum_{D \in \mathcal{D}_h} \eta_{\mathrm{L},D}^q \right\}^{1/q} \quad \text{linearization error},$$

$$\eta_{\mathrm{D}} := \left\{ \sum_{D \in \mathcal{D}_h} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^q \right\}^{1/q} \quad \text{discretization error}$$

Local linearization stopping criterion

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Local efficiency

Assumption B (Approximation property)

There holds, for all $D \in \mathcal{D}_h$,

$$\eta_{\mathrm{DF},D} \lesssim \left\{ \sum_{T \in \mathcal{S}_D} h_T^q \| f + \nabla \cdot \boldsymbol{\sigma}_{\mathrm{L}}(\nabla u_{\mathrm{L},h}) \|_{q,T}^q + \sum_{F \in \mathcal{G}_D^{\mathcal{T}}} h_F \| [\![\boldsymbol{\sigma}_{\mathrm{L}}(\nabla u_{\mathrm{L},h}) \cdot \mathbf{n}]\!] \|_{q,F}^q \right\}^{\frac{1}{q}}.$$

Theorem (Local efficiency)

Let the mesh $\mathcal{T}_h$ be shape-regular and let the local stopping criterion, with γ_D small enough, hold. Let Assumption B hold. Then

$$\eta_{\mathrm{L},D} + \eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D} \le C \| \boldsymbol{\sigma}(\nabla u) - \boldsymbol{\sigma}(\nabla u_{\mathrm{L},h}) \|_{q,D},$$

where the constant C is independent of a and p.

- local efficiency, but in a different norm

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Let the mesh $\mathcal{T}_h$ be shape-regular and let the global stopping criterion, with γ small enough, hold. Let Assumption B hold. Recall that $\mathcal{J}_u(u_{\mathrm{L},h}) \leq \eta$. Then

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Outline

Adaptive strategy

Adaptive strategy

- choose an initial mesh $\mathcal{T}_h^0$ and an initial guess $u_{\mathrm{L},h}^0 \in V_h(\mathcal{T}_h^0)$
- on the mesh $\mathcal{T}_h^j$, $j \geq 0$, for $i \geq 1$, do the iterative loop:
  1) linearize the flux function at $u_{\mathrm{L},h}^{i-1}$
  2) solve the discrete linearized problem for $u_{\mathrm{L},h}^i$
  3) if the linearization stopping criterion is reached, then stop the linearization, else set $i \leftarrow (i+1)$ and go to step 1)
- evaluate the overall a posteriori error estimate η
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Outline

The conforming finite element method

Application to the conforming finite element method

- $V_h \subset V$, continuous piecewise linears
- discrete linearized problem: find $u_{\mathrm{L},h} \in V_h$ such that

$$(\sigma_{\mathrm{L}}(\nabla u_{\mathrm{L},h}), \nabla v_h) = (f, v_h) \quad \forall v_h \in V_h$$

- verify Assumptions A and B

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Construction of $\mathbf{t}_h$

- $\mathcal{D}_h$: dual mesh around nodes
- $\mathcal{S}_h$: simplicial submesh of both $\mathcal{T}_h$ and $\mathcal{D}_h$ (as in Luce and Wohlmuth (2004))
- definition of $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{S}_h)$ by direct prescription:

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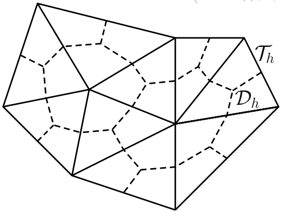

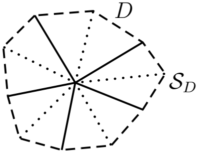

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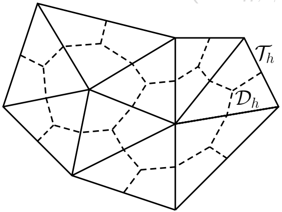

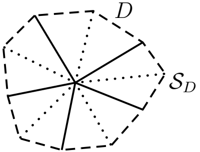

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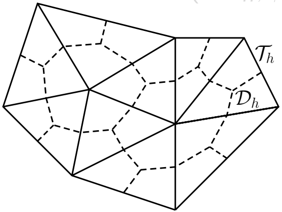

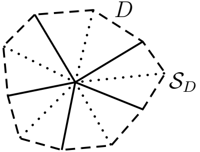

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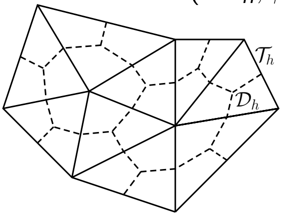

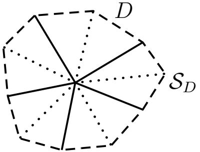

Outline

Computable upper and lower bounds on the dual norm

Computable upper and lower bounds on the dual norm

- recall that

$$\|Au - Au_{\mathrm{L},h}\|_{V'} = \sup_{v \in V \setminus \{0\}} \frac{(\sigma(\nabla u) - \sigma(\nabla u_{\mathrm{L},h}), \nabla v)}{\|\nabla v\|_p}$$

- following Chaillou and Suri (2006), there exist computable upper and lower bounds for $\|Au - Au_{\mathrm{L},h}\|_{V'}$:

$$\mathcal{J}_u(u_{\mathrm{L},h}) \leq \mathcal{J}_u^{\mathrm{up}}(u_{\mathrm{L},h}) := \|\sigma(\nabla u) - \sigma(\nabla u_{\mathrm{L},h})\|_q,$$

$$\mathcal{J}_u(u_{\mathrm{L},h}) \geq \mathcal{J}_u^{\mathrm{low}}(u_{\mathrm{L},h}) := \frac{(\sigma(\nabla u) - \sigma(\nabla u_{\mathrm{L},h}), \nabla(u - u_{\mathrm{L},h}))}{\|\nabla(u - u_{\mathrm{L},h})\|_p}$$

- put

$$\mathcal{I}^{\mathrm{up}} := \frac{\eta}{\mathcal{J}_u^{\mathrm{up}}(u_{\mathrm{L},h})} \quad \text{and} \quad \mathcal{I}^{\mathrm{low}} := \frac{\eta}{\mathcal{J}_u^{\mathrm{low}}(u_{\mathrm{L},h})}$$

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$$\mathcal{J}_u(u_{\mathrm{L},h}) \leq \mathcal{J}_u^{\mathrm{up}}(u_{\mathrm{L},h}) := \|\sigma(\nabla u) - \sigma(\nabla u_{\mathrm{L},h})\|_q,$$

$$\mathcal{J}_u(u_{\mathrm{L},h}) \geq \mathcal{J}_u^{\mathrm{low}}(u_{\mathrm{L},h}) := \frac{(\sigma(\nabla u) - \sigma(\nabla u_{\mathrm{L},h}), \nabla(u - u_{\mathrm{L},h}))}{\|\nabla(u - u_{\mathrm{L},h})\|_p}$$

- put

$$\mathcal{I}^{\mathrm{up}} := \frac{\eta}{\mathcal{J}_u^{\mathrm{up}}(u_{\mathrm{L},h})} \quad \text{and} \quad \mathcal{I}^{\mathrm{low}} := \frac{\eta}{\mathcal{J}_u^{\mathrm{low}}(u_{\mathrm{L},h})}$$

Computable upper and lower bounds on the dual norm

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- recall that

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Numerical experiment I

Model problem

- p-Laplacian

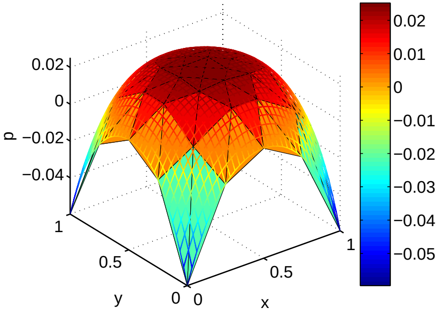
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) = f \quad & \text{in } \Omega, \\ u = u_0 \quad & \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose a Dirichlet BC)

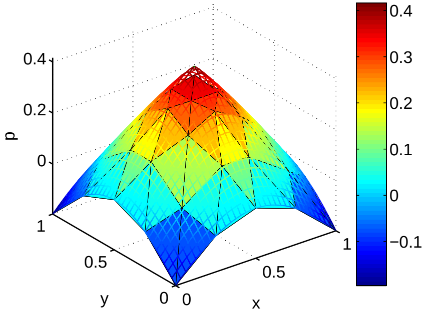
$$u_0(x,y) = -\frac{p-1}{p}\left((x-\tfrac{1}{2})^2 + (y-\tfrac{1}{2})^2\right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p}\left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

- tested values $p = 1.4, 3, 10, 50$

Analytical and approximate solutions

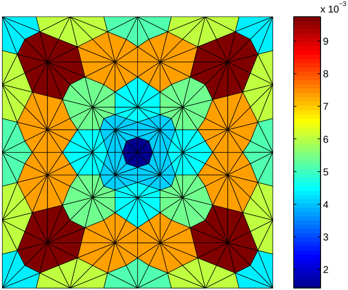


Case $p = 1.4$

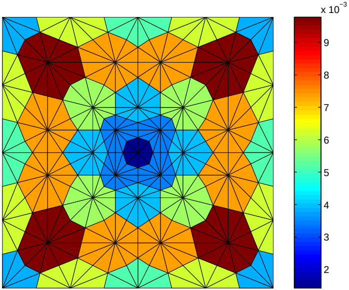


Case $p = 10$

Error distribution on a uniformly refined mesh, $p = 3$

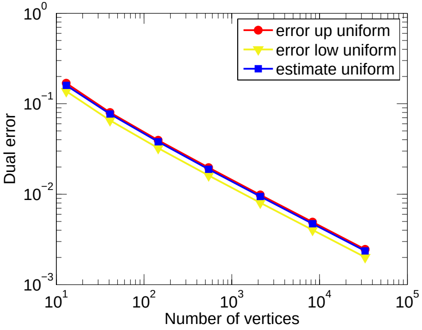


Estimated error distribution

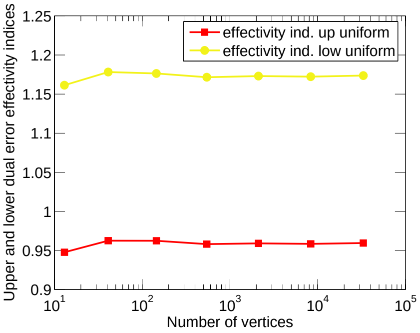


Exact error distribution

Estimated and actual errors and the eff. index, $p = 1.4$

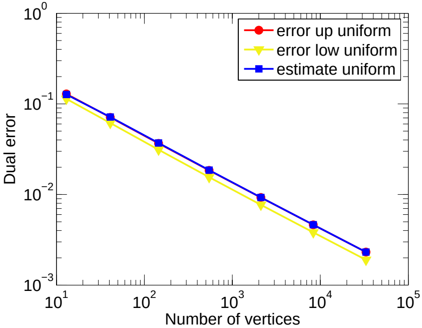


Estimated and actual errors

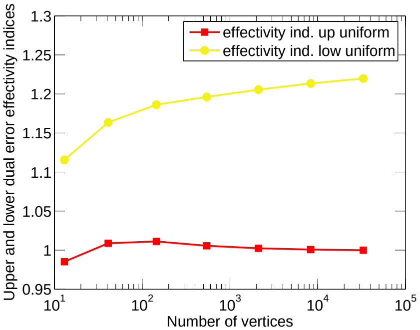


Effectivity index

Estimated and actual errors and the eff. index, $p = 3$

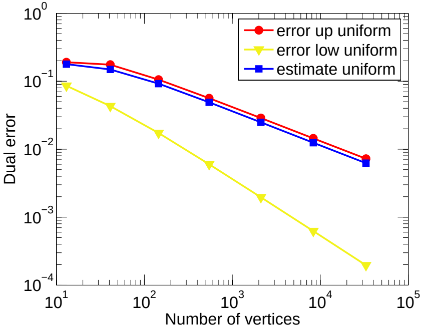


Estimated and actual errors

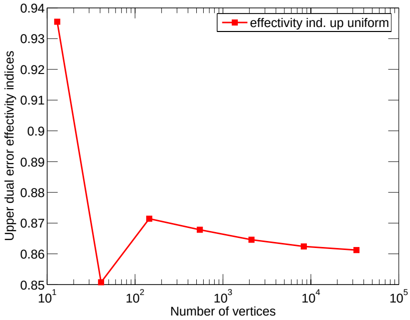


Effectivity index

Estimated and actual errors and the eff. index, $p = 10$

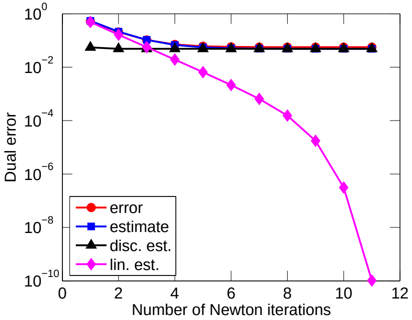


Estimated and actual errors

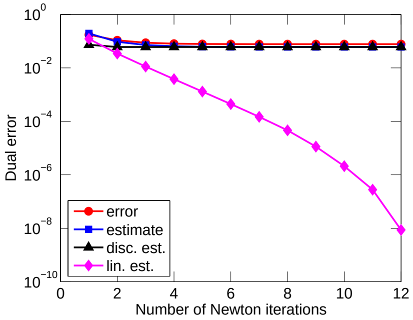


Effectivity index

Discretization and linearization componenets

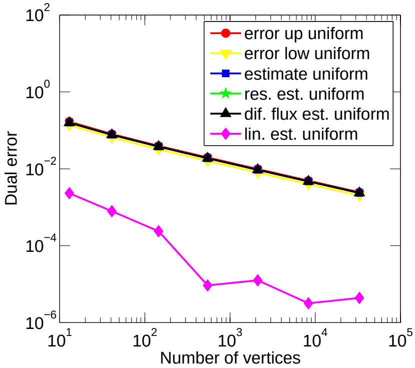


Case $p = 10$

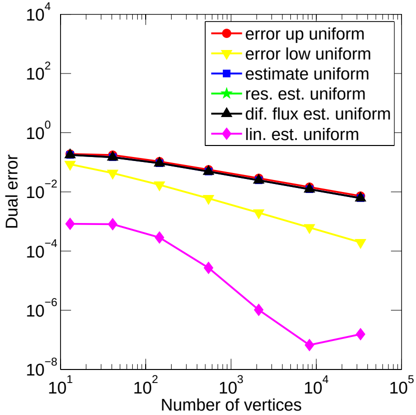


Case $p = 50$

Different error components

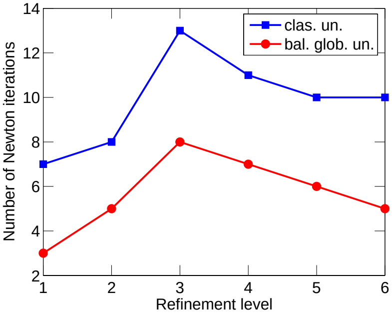


Case $p = 1.4$

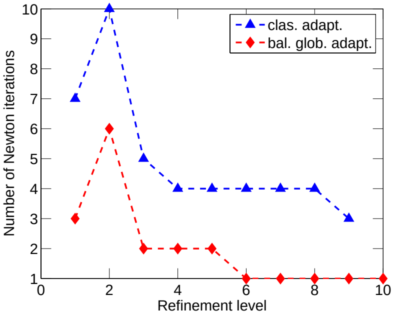


Case $p = 10$

Evolution of Newton iterations



Classical versus balanced Newton, uniform refinement



Classical versus balanced Newton, adaptive ref.

Numerical experiment II

Model problem

- p-Laplacian

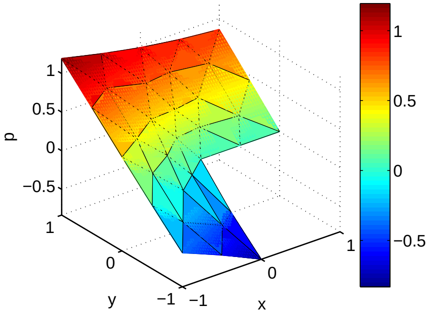
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f \qquad \text{in } \Omega, \\ u &= u_0 \qquad \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose a Dirichlet BC)

$$u_0(r,\theta) = r^{\frac{7}{8}} \sin(\theta \tfrac{7}{8})$$

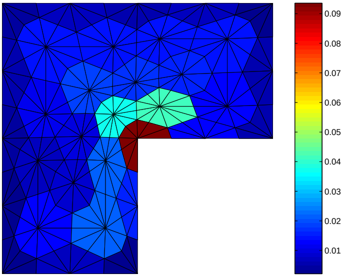
- $p = 4$, L-shape domain, singularity in the origin (Carstensen and Klose (2003))

Analytical and approximate solutions

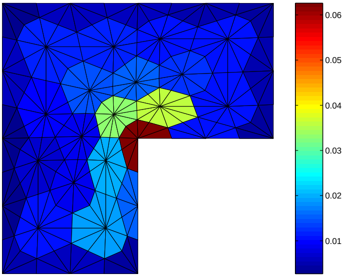


Analytical and approximate solutions

Error distribution on a uniformly refined mesh

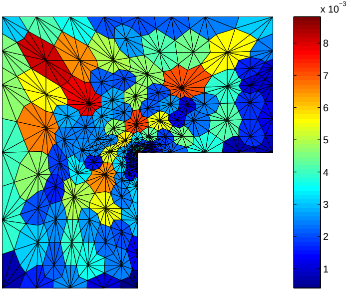


Estimated error distribution

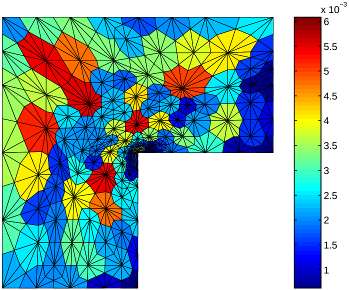


Exact error distribution

Error distribution on an adaptively refined mesh

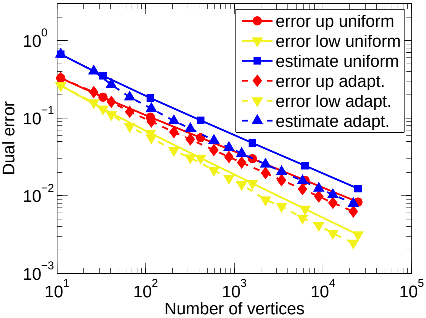


Estimated error distribution

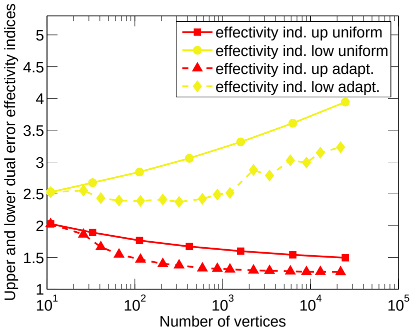


Exact error distribution

Estimated and actual errors and the effectivity index



Estimated and actual errors



Effectivity index

Outline

A model elliptic problem

A model elliptic problem

$$\begin{aligned} -\nabla\cdot(\mathbf{S}\nabla p) &= f \quad \text{in } \Omega, \\ p &= g \quad \text{on } \Gamma := \partial\Omega \end{aligned}$$

Algebraic problem

- at some point, we shall solve $\mathbb{A}X = B$
- we only solve it inexactly, $\mathbb{A}X^* \approx B$
- we know the algebraic residual, $R := B - \mathbb{A}X^*$

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Outline

A posteriori estimate including the algebraic error

Theorem (Estimate including the algebraic error, FVs/MFEs)

There holds

$$|||p - \tilde{p}_h^{\mathrm{a}}||| \leq \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{NC},K}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{R},K}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{AE},K}^2 \right\}^{\frac{1}{2}}.$$

Outline

Stopping criteria for iterative solvers

Global stopping criterion

- stop the iterative solver whenever

$$\eta_{\mathrm{AE}} \leq \gamma\, \eta_{\mathrm{NC}},$$

where

$$\eta_{\mathrm{AE}} = \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{AE},K}^2 \right\}^{\frac{1}{2}}, \quad \eta_{\mathrm{NC}} = \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{NC},K}^2 \right\}^{\frac{1}{2}}$$

Local stopping criterion

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$$\eta_{\mathrm{AE},K} \leq \gamma_K\, \eta_{\mathrm{NC},K} \qquad \forall K \in \mathcal{T}_h$$

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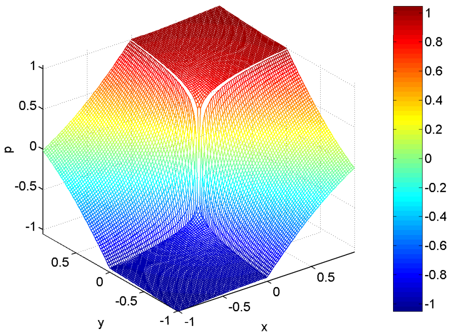
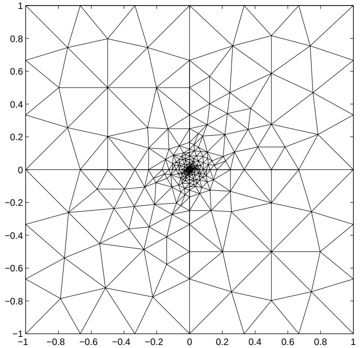
Analytical solution and adaptively refined mesh

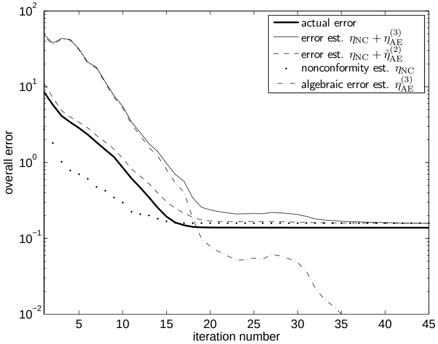


Analytical solution

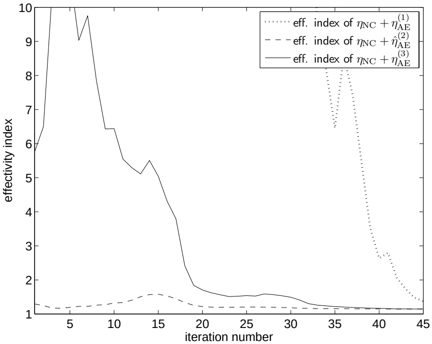


Adaptively refined mesh

Error, estimate, and effectivity index



Error and algebraic and discretization estimates



Effectivity index

Outline

Concluding remarks and future work

Concluding remarks

- linear/nonlinear systems are never solved exactly in practical large scale computations
- present estimates: **certified overall error bound**
- linear/nonlinear sts should be solved inexactly on purpose
  - balancing discretization and algebraic/linearization errors by stopping criteria
  - useless to make an extensive number of iterations after the algebraic/linearization error drops below the discretization one
  - **important computational savings**
- local efficiency: suitable for **adaptive mesh refinement**
- guaranteed, robust, locally computable estimates

Future work

- nonlinear case for nonconforming methods
- systems of nonlinear PDEs

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Bibliography

Bibliography

- El Alaoui L., Ern. A, Vohralík M., Guaranteed and robust a posteriori error estimates and balancing discretization and linearization errors for monotone nonlinear problems, *Comput. Methods Appl. Mech. Engrg.* DOI 10.1016/j.cma.2010.03.024 (2010).
- Jiránek P., Strakoš Z., Vohralík M., A posteriori error estimates including algebraic error and stopping criteria for iterative solvers, *SIAM J. Sci. Comput.* **32** (2010), 1567–1590.

Thank you for your attention!

Bibliography

Bibliography

- EL ALAOUI L., ERN. A, VOHRALÍK M., Guaranteed and robust a posteriori error estimates and balancing discretization and linearization errors for monotone nonlinear problems, *Comput. Methods Appl. Mech. Engrg.* DOI 10.1016/j.cma.2010.03.024 (2010).
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Thank you for your attention!