# Guaranteed and robust a posteriori error estimates and stopping criteria for iterative linearizations and linear solvers

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Joint work with
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(linearization error)
*Pavel Jiránek (CERFACS, Toulouse, France), Zdeněk Strakoš (AS, Prague, Czech Republic)* (algebraic error)

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# Outline

1. Introduction
2. A class of nonlinear problems
   - Quasi-linear elliptic problems
   - Newton and fixed-point linearizations
   - Distinguishing discretization and linearization errors
3. A posteriori error estimates including linearization error
   - A guaranteed and robust a posteriori error estimate
   - Stopping criteria for linearizations
   - Adaptive strategy
   - Numerical experiments
4. A posteriori estimates including algebraic error
   - A guaranteed a posteriori estimate
   - Stopping criteria for iterative solvers
   - Numerical experiments
5. Concluding remarks and future work

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# Discretization, linearization, and algebraic solvers

**Discretization**

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

**Iterative linearization**

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

**Iterative algebraic system solution**

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

- the approximate solution $p_h^{\mathrm{a}}$ 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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# Previous results: general and algebraic error

**A posteriori estimates without algebraic error**

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

**A posteriori estimates accounting for algebraic error**

- Repin (1997)

**Stopping criteria for iterative solvers**

- Becker, Johnson, and Rannacher (1995)
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**Algebraic energy error estimation in the conjugate gradient method**

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**Continuous finite elements**

- Han (1994), general framework
- Verfürth (1994), residual estimates
- Barrett and Liu (1994), quasi-norm estimates
- Liu and Yan (2001), quasi-norm estimates
- Veeser (2002), convergence $p$-Laplacian
- Carstensen and Klose (2003), guaranteed estimates
- Chaillou and Suri (2006, 2007), distinguishing discretization and linearization errors (only fixed-point, one linearized problem (not an iterative loop))
- Diening and Kreuzer (2008), linear cvg $p$-Laplacian

**Other methods**

- Liu and Yan (2001), quasi-norm estimates for the nonconforming finite element method
- Kim (2007), guaranteed estimates for locally conservative methods

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# Previous results: error components equilibration

**Error components equilibration**

- engineering literature, since 1950's
- Ladevèze (since 1980's)
- Verfürth (2003), space and time error equilibration
- Babuška, Oden (2004), verification and validation
- Bernardi (2006), estimation and equilibration of model errors
- ...

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# Quasi-linear elliptic problem

## Quasi-linear elliptic problem

$$-\nabla\cdot\boldsymbol{\sigma}(\nabla u) = f \qquad \text{in } \Omega,$$
$$u = 0 \qquad \text{on } \partial\Omega,$$

where

- $\forall \xi \in \mathbb{R}^d$, $\boldsymbol{\sigma}(\xi) = a(|\xi|)\xi$,
- $a(x) \sim x^{p-2}$ 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** $A : V := W_0^{1,p}(\Omega) \to V'$

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

**Weak formulation**

Find $u \in V$ such that

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

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# Linearizations at $u_0 \in V$

**Linearized operator $A_L : V \to V'$**

- let $u_0 \in V$
- linearized flux $\boldsymbol{\sigma}_L : \mathbb{R}^d \to \mathbb{R}^d$ depending on $\nabla u_0$

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

**Linearized problem**

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**Fixed-point linearization**

$$\boldsymbol{\sigma}_L(\boldsymbol{\xi}) := a(|\nabla u_0|)\boldsymbol{\xi}$$

**Newton linearization**

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

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# Error measure

## Error measure

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

- based on the difference of the fluxes
- dual norm of the residual
- avoids any appearance of the ratio continuity constant / monotonicity constant
- there holds $J_u(u_{L,h}) \to 0$ if and only if $\|u - u_{L,h}\|_V \to 0$

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# Outline

# Abstract estimate

**Theorem (Abstract estimate distinguishing the discretization and linearization errors)**

*Let $u \in V$ be the weak solution, let $u_{L,h} \in V$ be arbitrary. Then*

$$\mathcal{J}_u(u_{L,h}) \leq \|A_L u_L - A_L u_{L,h}\|_{V'} + \|A_L u_{L,h} - A u_{L,h}\|_{V'}.$$

## Remarks

- result due to Chaillou and Suri (2007)
- first term: **discretization error** of a **linear problem**
- second term: **linearization error**

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# Outline

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# A posteriori error estimate

**Theorem (A posteriori error estimate)**

*Let*

- $u \in V$ *be the weak solution,*
- $u_{L,h} \in V$ *be arbitrary,*
- $\mathbf{t}_h \in \mathbf{H}^q(\mathrm{div}, \Omega)$ *be arbitrary but such that* $(\nabla \cdot \mathbf{t}_h, 1)_D = (f, 1)_D$ *for all* $D \in \mathcal{D}_h^{\mathrm{int}}$.

*Then there holds*

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

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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*

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

- *linearization estimator*

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

# 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

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

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## Local linearization stopping criterion

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

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# Local efficiency

**Theorem (Local efficiency)**

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

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

*where the constant $C$ is independent of $a$ and $p$.*

- local efficiency, but in a different norm

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- **robustness** with respect to the **nonlinearity** thanks to the choice of the dual norm

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# Outline

# Adaptive strategy

## Adaptive strategy

- choose an initial mesh $\mathcal{T}_h^0$ and an initial guess $u_{L,h}^0 \in V_h(\mathcal{T}_h^0)$
- on the mesh $\mathcal{T}_h^j$, $j \geq 0$, for $i \geq 1$, do the iterative loop:
  1) linearize the flux function at $u_{L,h}^{i-1}$
  2) solve the discrete linearized problem for $u_{L,h}^i$
  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 $\eta$
- if the desired overall **precision is reached**, then **stop**, else refine the mesh adaptively, interpolate to it the current solution, $j \leftarrow (j+1)$, and go to the second step

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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

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

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

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

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- put

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

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# Numerical experiment I

**Model problem**

- $p$-Laplacian

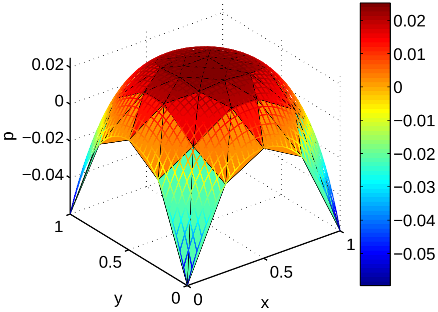
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f && \text{in } \Omega,\\ u &= u_0 && \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose a Dirichlet BC)

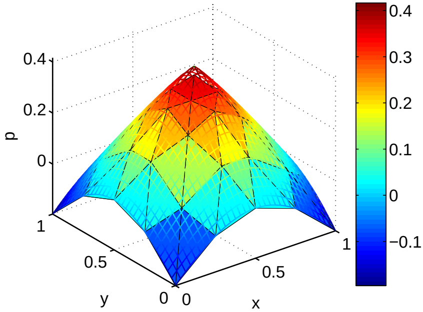
$$u_0(x,y) = -\frac{p-1}{p}\left((x-\tfrac{1}{2})^2 + (y-\tfrac{1}{2})^2\right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p}\left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

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

# Analytical and approximate solutions

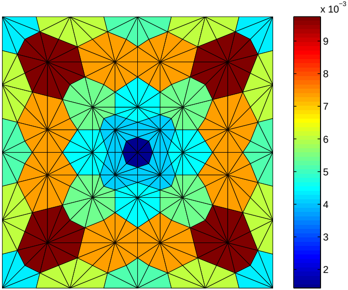



Case $p = 1.4$

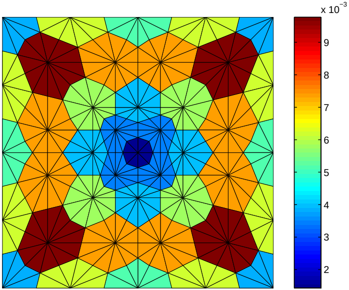



Case $p = 10$

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

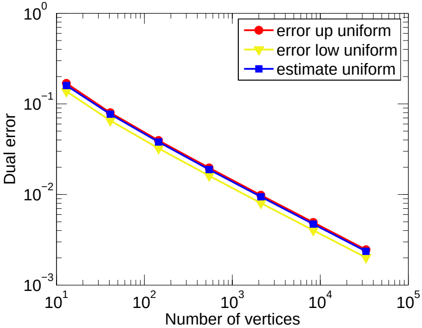



Estimated error distribution

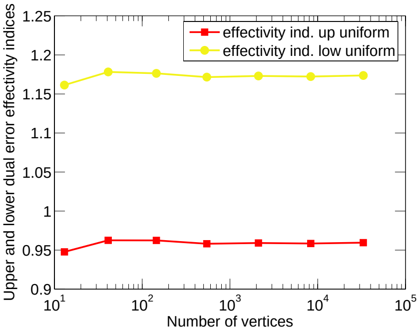



Exact error distribution

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




Estimated and actual errors




Effectivity index

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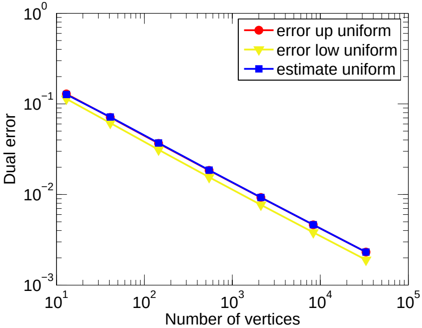
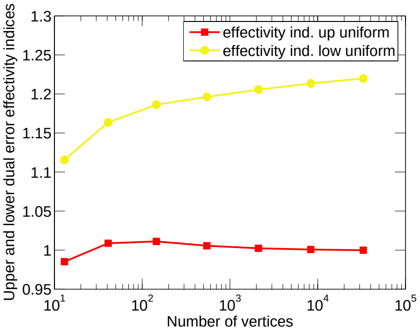



Estimated and actual errors




Effectivity index

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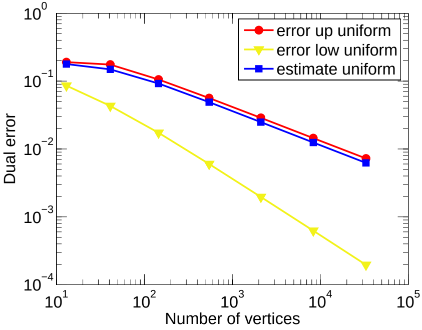
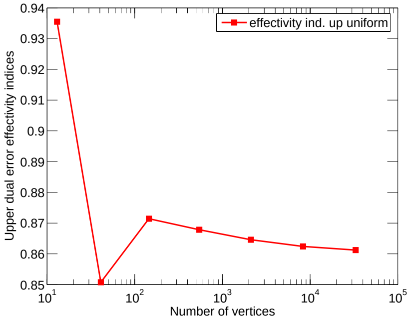
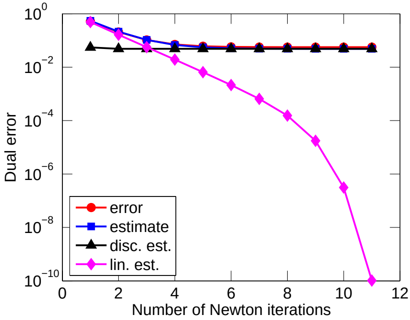



Estimated and actual errors

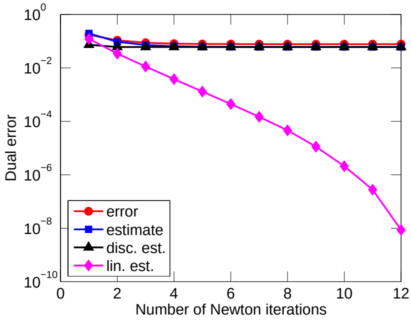



Effectivity index

# Discretization and linearization componenets

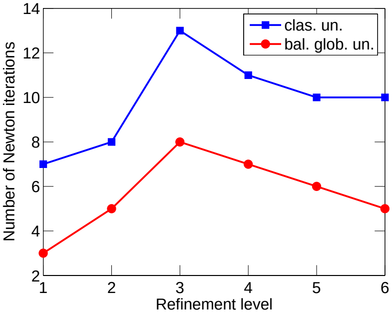



Case $p = 10$

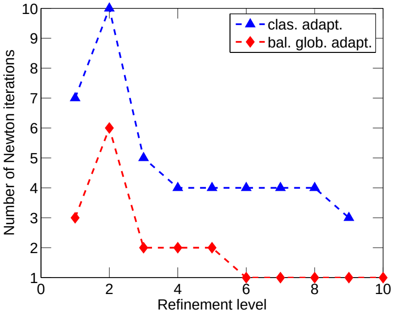



Case $p = 50$

# Evolution of Newton iterations




Classical versus balanced Newton, uniform refinement




Classical versus balanced Newton, adaptive ref.

# Numerical experiment II

**Model problem**

- $p$-Laplacian

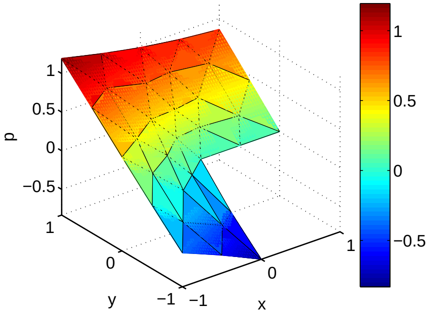
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f \qquad \text{in } \Omega, \\ u &= u_0 \qquad \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose a Dirichlet BC)

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

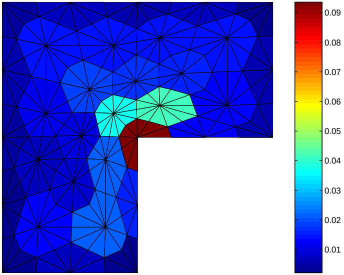
- $p = 4$, L-shape domain, singularity in the origin (Carstensen and Klose (2003))

# Analytical and approximate solutions

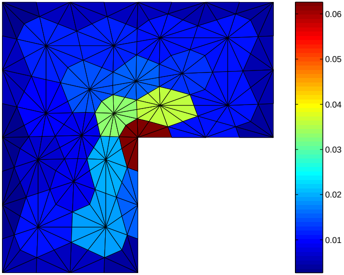



Analytical and approximate solutions

# Error distribution on a uniformly refined mesh

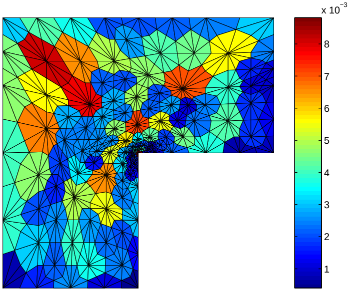



Estimated error distribution




Exact error distribution

# Error distribution on an adaptively refined mesh

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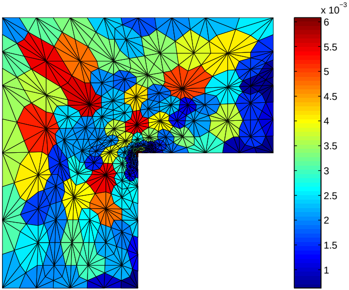
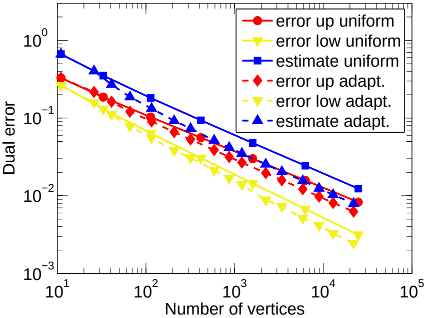



Exact error distribution

# Estimated and actual errors and the effectivity index

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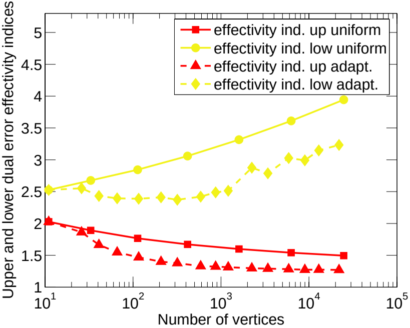


Effectivity index

# 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, $\mathbb{A}X^* \approx B$
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# A posteriori estimate including the algebraic error

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

*There holds*

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

- **nonconformity estimator**
  - $\eta_{\mathrm{NC},K} := |||\tilde{p}_h^{\mathrm{a}} - \mathcal{I}_{\mathrm{Os}}^{\Gamma}(\tilde{p}_h^{\mathrm{a}})|||_K$
  - reflects the departure of $\tilde{p}_h^{\mathrm{a}}$ from $H_\Gamma^1(\Omega)$
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# 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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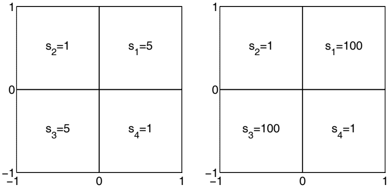
# Outline

# Discontinuous diffusion tensor

- model problem

$$-\nabla \cdot (\mathbf{S}\nabla p) = 0 \quad \text{in} \quad \Omega = (-1,1) \times (-1,1)$$

- discontinuous and inhomogeneous **S**, two cases:

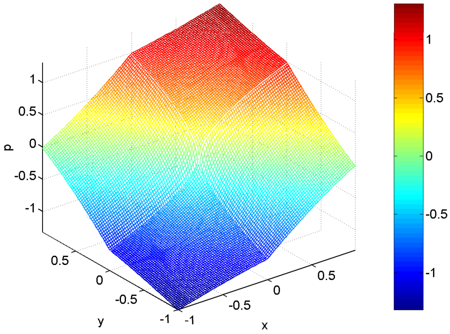



- analytical solution: singularity at the origin

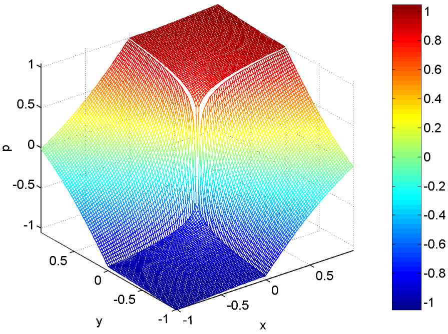
$$p(r,\theta)|_{\Omega_i} = r^\alpha(a_i \sin(\alpha\theta) + b_i \cos(\alpha\theta))$$

  - $(r,\theta)$ polar coordinates in $\Omega$
  - $a_i$, $b_i$ constants depending on $\Omega_i$
  - $\alpha$ regularity of the solution

# Analytical solutions

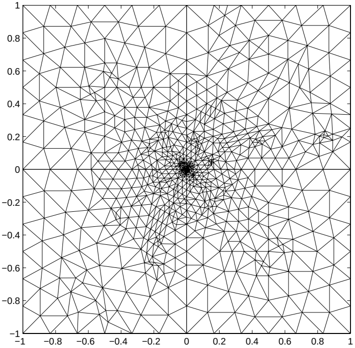



Case 1




Case 2

# Adaptively refined unstructured meshes

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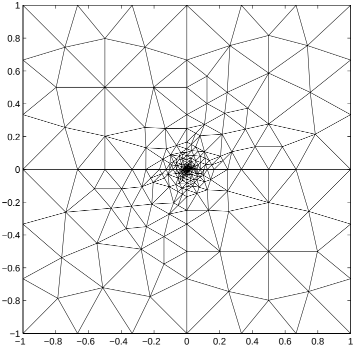
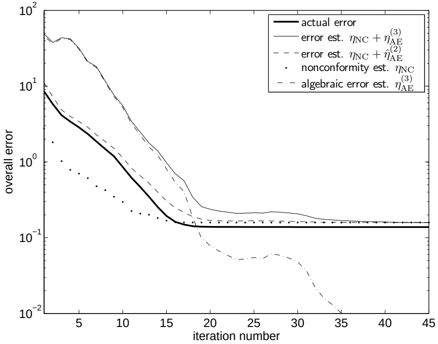



Case 2

# Overall error and overall error estimators

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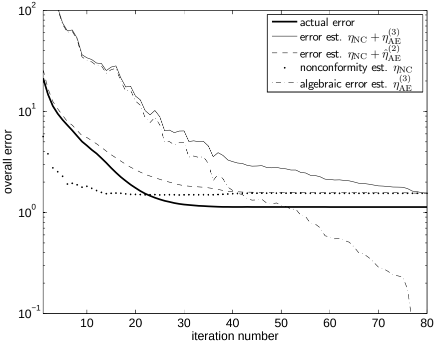
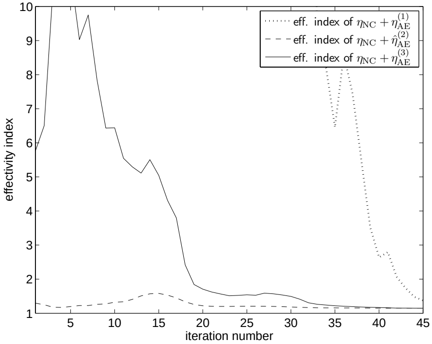
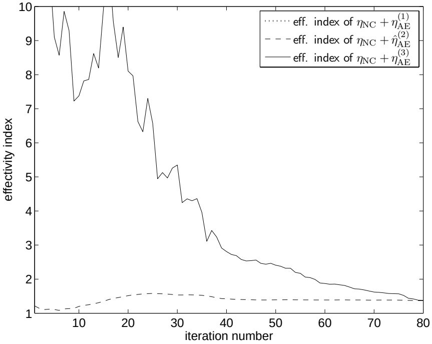



Case 2

# Effectivity indices of the overall error estimators




Case 1




Case 2

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# 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
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