A posteriori error estimates and solver adaptivity in numerical simulations

Martin Vohralík

in collaboration with

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Outline

Inexact iterative linearization

System of nonlinear algebraic equations

Nonlinear operator $\mathcal{A}: \mathbb{R}^N \to \mathbb{R}^N$, vector $F \in \mathbb{R}^N$: find $U \in \mathbb{R}^N$ s.t.

$$\mathcal{A}(U) = F$$

Algorithm (Inexact iterative linearization)

1. *Choose initial vector U^0. Set $k := 1$.*
2. $U^{k-1} \Rightarrow$ *matrix $\mathbb{A}^{k-1}$ and vector F^{k-1}: find U^k s.t.*

   $$\mathbb{A}^{k-1} U^k \approx F^{k-1}.$$

3.
   1. *Set $U^{k,0} := U^{k-1}$ and $i := 1$.*
   2. *Do an algebraic solver step $\Rightarrow U^{k,i}$ s.t. ($R^{k,i}$ algebraic res.)*

      $$\mathbb{A}^{k-1} U^{k,i} = F^{k-1} - R^{k,i}.$$

   3. *Convergence? OK $\Rightarrow U^k := U^{k,i}$. KO $\Rightarrow i := i + 1$, back to 3.2.*
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Approximate solution

- approximate solution $U^{k,i}$ does not solve $\mathcal{A}(U^{k,i}) = F$

Numerical method

- underlying numerical method: the vector $U^{k,i}$ is associated with a (piecewise polynomial) approximation $u_h^{k,i}$

Partial differential equation

- underlying PDE, u its weak solution: $A(u) = f$

Question (Stopping criteria)

- *What is a good stopping criterion for the linear solver?*
- *What is a good stopping criterion for the nonlinear solver?*

Question (Error)

- *How big is the error $\|u - u_h^{k,i}\|$ on Newton step k and algebraic solver step i, how is it distributed?*

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1. Introduction
2. A posteriori estimates based on potential & flux reconstruction
   - Potential and flux reconstructions
   - Polynomial-degree-robust local efficiency
   - Applications and numerical illustration
3. Algebraic estimates and stopping criteria for iterative solvers
   - Multilevel (multigrid) setting
   - Domain decomposition methods
4. Adaptive inexact Newton method
   - Stopping criteria, efficiency, and nonlinearity-robustness
   - Applications and numerical illustration
5. Application to complex porous media flows
6. Conclusions and outlook

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Laplace model problem

Model problem

$$-\Delta u = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \partial\Omega$$

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ polygon/polyhedron
- $f \in L^2(\Omega)$

Weak formulation

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

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

Properties of the weak solution

- $u \in H_0^1(\Omega)$ (primal variable constraint)
- $\sigma := -\nabla u$ (constitutive relation)
- $\nabla \cdot \sigma = f$ (equilibrium)
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Theorem (A guaranteed a posteriori error estimate, Prager and Synge (1947), Dari, Durán, Padra, and Vampa (1996), Ainsworth (2005), Kim (2007), Vohralík (2007), ...**)**

- *Let $u \in H_0^1(\Omega)$ be the weak solution;*
- *$u_h \in H^1(\mathcal{T}_h) := \{v \in L^2(\Omega),\ v|_K \in H^1(K) \quad \forall K \in \mathcal{T}_h\}$ be arbitrary (thus $u_h \notin H_0^1(\Omega)$ and $-\nabla u_h \notin \mathbf{H}(\mathrm{div}, \Omega)$);*
- *$s_h \in H_0^1(\Omega)$ and $\boldsymbol{\sigma}_h \in \mathbf{H}(\mathrm{div}, \Omega)$ be such that*

$$(\nabla\cdot\boldsymbol{\sigma}_h, 1)_K = (f, 1)_K \text{ for all } K \in \mathcal{T}_h.$$

Then

$$\|\nabla(u - u_h)\|^2 \leq \sum_{K\in\mathcal{T}_h} \Big(\underbrace{\|\nabla u_h + \boldsymbol{\sigma}_h\|_K}_{\text{constitutive relation}} + \underbrace{\frac{h_K}{\pi}\|f - \nabla\cdot\boldsymbol{\sigma}_h\|_K}_{\text{equilibrium}} \Big)^2 + \sum_{K\in\mathcal{T}_h} \underbrace{\|\nabla(u_h - s_h)\|_K^2}_{\text{primal constraint}}.$$

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- define $s \in H_0^1(\Omega)$ by

$$(\nabla s, \nabla v) = (\nabla u_h, \nabla v) \qquad \forall v \in H_0^1(\Omega)$$

- develop (Pythagoras)

$$\|\nabla(u - u_h)\|^2 = \|\nabla(u - s)\|^2 + \|\nabla(s - u_h)\|^2$$

- projection definition of s:

$$\|\nabla(s - u_h)\|^2 = \underbrace{\min_{v \in H_0^1(\Omega)} \|\nabla(v - u_h)\|^2}_{\text{distance of } u_h \text{ to } H_0^1(\Omega)}$$

- dual norm characterization, definition of s:

$$\|\nabla(u - s)\|^2 = \underbrace{\sup_{\varphi \in H_0^1(\Omega);\, \|\nabla \varphi\| = 1} (\nabla(u - \ ), \nabla \varphi)^2}_{\text{dual norm of the residual}}$$

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Proof (continuation).

- nonconformity upper bound:

$$\min_{v\in H_0^1(\Omega)} \|\nabla(v-u_h)\| \le \|\nabla(u_h - s_h)\|$$

- weak solution definition, equilibrated flux, Green theorem:

$$(\nabla(u-u_h),\nabla\varphi) = (f,\varphi) - (\nabla u_h,\nabla\varphi)$$
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- nonconformity upper bound:

$$\min_{v \in H_0^1(\Omega)} \|\nabla(v - u_h)\| \leq \|\nabla(u_h - s_h)\|$$

- weak solution definition, equilibrated flux, Green theorem:

$$(\nabla(u - u_h), \nabla\varphi) = (f, \varphi) - (\nabla u_h, \nabla\varphi)$$
$$= (f - \nabla\cdot\boldsymbol{\sigma}_h, \varphi) - (\nabla u_h + \boldsymbol{\sigma}_h, \nabla\varphi)$$

- Cauchy–Schwarz and Poincaré inequalities, equilibration:

$$-(\nabla u_h + \boldsymbol{\sigma}_h, \nabla\varphi) \leq \sum_{K \in \mathcal{T}_h} \|\nabla u_h + \boldsymbol{\sigma}_h\|_K \|\nabla\varphi\|_K,$$

$$(f - \nabla\cdot\boldsymbol{\sigma}_h, \varphi) = \sum_{K \in \mathcal{T}_h} (f - \nabla\cdot\boldsymbol{\sigma}_h, \varphi - \varphi_K)_K$$
$$\leq \sum_{K \in \mathcal{T}_h} \frac{h_K}{\pi} \|f - \nabla\cdot\boldsymbol{\sigma}_h\|_K \|\nabla\varphi\|_K$$

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Outline

Global potential and flux reconstructions

Ideally

$$\boldsymbol{\sigma}_h := \arg \min_{\mathbf{v}_h \in \mathbf{V}_h,\, \nabla\cdot\mathbf{v}_h = \Pi_{Q_h} f} \|\nabla u_h + \mathbf{v}_h\|$$

$$s_h := \arg \min_{v_h \in V_h} \|\nabla(u_h - v_h)\|$$

- $\mathbf{V}_h \subset \mathbf{H}(\mathrm{div}, \Omega)$, $Q_h \subset L^2(\Omega)$, $V_h \subset H^1_0(\Omega)$
- too expensive, **global** minimization problems (the hypercircle method . . .)

Local potential and flux reconstructions

Definition (Constr. of $\boldsymbol{\sigma}_h$, Destuynder and Métivet (1999) & Braess and Schöberl (2008))

For each $\mathbf{a} \in \mathcal{V}_h$, solve the **local mixed FE problem**

$$\boldsymbol{\sigma}_h^{\mathbf{a}} := \arg \min_{\mathbf{v}_h \in \mathbf{V}_h^{\mathbf{a}},\, \nabla\cdot\mathbf{v}_h = \Pi_{Q_h^{\mathbf{a}}}(\psi_{\mathbf{a}} f - \nabla\psi_{\mathbf{a}}\cdot\nabla u_h)} \|\psi_{\mathbf{a}}\nabla u_h + \mathbf{v}_h\|_{\omega_{\mathbf{a}}}.$$

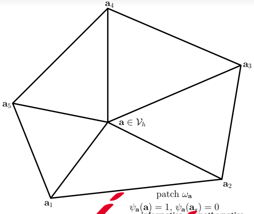
Definition (Construction of s_h, $\approx$ Carstensen and Merdon (2013), EV (2015))

For each $\mathbf{a} \in \mathcal{V}_h$, solve the **local conforming FE problem**

$$s_h^{\mathbf{a}} := \arg \min_{v_h \in V_h^{\mathbf{a}}} \|\nabla(\psi_{\mathbf{a}} u_h - v_h)\|_{\omega_{\mathbf{a}}}.$$

Key ideas

- **local** minimizations
- cut-off by hat basis functions $\psi_{\mathbf{a}}$
- $\boldsymbol{\sigma}_h := \sum_{\mathbf{a}\in\mathcal{V}_h} \boldsymbol{\sigma}_h^{\mathbf{a}}, \quad s_h := \sum_{\mathbf{a}\in\mathcal{V}_h} s_h^{\mathbf{a}}$



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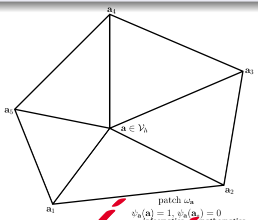

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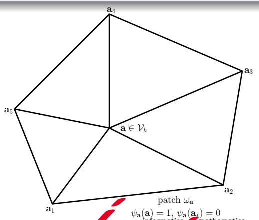
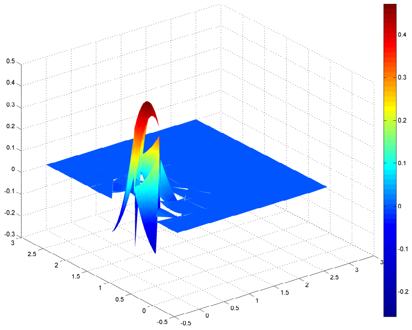
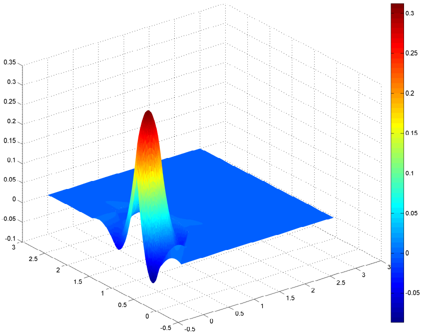


Potential reconstruction

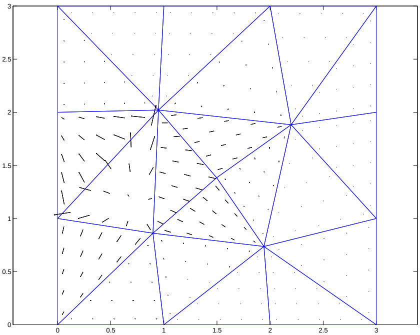


Potential u_h

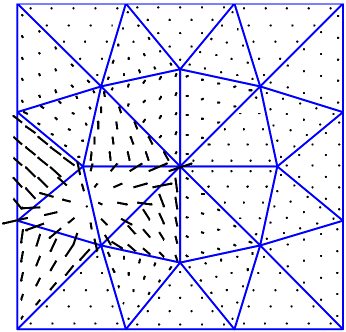


Potential reconstruction s_h

Equilibrated flux reconstruction



Flux $-\nabla u_h$



Flux reconstruction $\boldsymbol{\sigma}_h$

Outline

Continuous-level patch problems

Definition (Continuous-level flux reconstruction)

For each $\mathbf{a} \in \mathcal{V}_h$, set

$$\boldsymbol{\sigma}^{\mathbf{a}} := \arg \min_{\substack{\mathbf{v} \in \mathbf{H}(\mathrm{div},\omega_{\mathbf{a}}),\ \nabla\cdot\mathbf{v} = (\psi_{\mathbf{a}} f - \nabla\psi_{\mathbf{a}}\cdot\nabla u_h) \\ \mathbf{v}\cdot\mathbf{n}_{\omega_{\mathbf{a}}} = 0 \text{ on } \partial\omega_{\mathbf{a}}\ (\setminus\partial\Omega)}} \|\psi_{\mathbf{a}}\nabla u_h + \mathbf{v}\|_{\omega_{\mathbf{a}}}.$$

Definition (Continuous-level potential reconstruction)

For each $\mathbf{a} \in \mathcal{V}_h$, set

$$s^{\mathbf{a}} := \arg \min_{v \in H^1_0(\omega_{\mathbf{a}})} \|\nabla(\psi_{\mathbf{a}} u_h - v)\|_{\omega_{\mathbf{a}}}.$$

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Assumptions

Assumption A (Galerkin orthogonality wrt hat functions)

There holds

$$(\nabla u_h, \nabla \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} = (f, \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} \qquad \forall \mathbf{a} \in \mathcal{V}_h^{\mathrm{int}}.$$

Assumption B (Weak continuity)

There holds $\langle [\![u_h]\!], 1 \rangle_e = 0 \qquad \forall e \in \mathcal{E}_h.$

Assumption C (Piecewise polynomials, data, and meshes)

The approximation u_h and the datum f are piecewise polynomial. The degrees of the MFE reconstructions σ_h and s_h are chosen correspondingly. The meshes $\mathcal{T}_h$ are shape-regular.

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Polynomial-degree-robust efficiency

Theorem (Polynomial-degree-robust efficiency via MFE / FE / continuous stability Braess, Pillwein, and Schöberl (2009); Costabel and McIntosh (2010); Demkowicz, Gopalakrishnan, and Schöberl (2012), EV (2015)**)**

Let u be the weak solution and let Assumptions A, B, and C hold. Then there exists constants $C_{\rm st}$, $C_{\rm cont,PF}$, $C_{\rm cont,bPF} > 0$ only depending on the shape-regularity parameter $\kappa_{\mathcal{T}}$ such that

$$\|\boldsymbol{\sigma}_h^{\mathbf{a}} + \psi_{\mathbf{a}} \nabla u_h\|_{\omega_{\mathbf{a}}} \leq C_{\rm st} \|\boldsymbol{\sigma}^{\mathbf{a}} + \psi_{\mathbf{a}} \nabla u_h\|_{\omega_{\mathbf{a}}} \leq C_{\rm st} C_{\rm cont,PF} \|\nabla(u - u_h)\|_{\omega_{\mathbf{a}}};$$

$$\|\nabla(\psi_{\mathbf{a}} u_h - s_h^{\mathbf{a}})\|_{\omega_{\mathbf{a}}} \leq C_{\rm st} \|\nabla(\psi_{\mathbf{a}} u_h - s^{\mathbf{a}})\|_{\omega_{\mathbf{a}}} \leq C_{\rm st} C_{\rm cont,bPF} \|\nabla(u - u_h)\|_{\omega_{\mathbf{a}}}.$$

Remarks

- $C_{\rm st}$ can be bounded by solving the local Neumann problems by conforming FEs
- $\Rightarrow$ maximal overestimation factor guaranteed

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Outline

Conforming finite elements

Conforming finite elements

Find $u_h \in V_h$ such that

$$(\nabla u_h, \nabla v_h) = (f, v_h) \qquad \forall v_h \in V_h.$$

- $V_h := \mathbb{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega)$, $p \geq 1$
- Assumption A: take $v_h = \psi_{\mathbf{a}}$
- $V_h \subset H_0^1(\Omega)$: $s_h := u_h$, no need for Assumption B
- Assumption C: technical, always satisfied

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Mixed finite elements

Mixed finite elements

Find a couple $(\boldsymbol{\sigma}_h, \bar{u}_h) \in \mathbf{V}_h \times Q_h$ such that

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- postprocessed solution $u_h \in V_h$, $V_h := \mathbb{P}_p(\mathcal{T}_h)$, $p \geq 1$; $v_h \in V_h$ satisfy

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Numerics: smooth case

Model problem

$$-\Delta u = f \quad \text{in } \Omega := (0,1)^2,$$
$$u = 0 \quad \text{on } \partial\Omega$$

Exact solution

$$u(x,y) = \sin(2\pi x)\sin(2\pi y)$$

Discretization

- symmetric interior penalty discontinuous Galerkin method
- unstructured triangular grids
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Uniform refinement: **asymptotic exactness**

h	p	$\|\nabla_{\rm d}(u-u_h)\|$	$\|u-u_h\|_{\rm DG}$	$\|\nabla_{\rm d}u_h+\boldsymbol{\sigma}_h\|$	$\eta_{\rm osc}$	$\|\nabla_{\rm d}(u_h-s_h)\|$	η	$\eta_{\rm DG}$	$I^{\rm eff}$	$I^{\rm eff}_{\rm DG}$
h_0	1	1.07E-00	1.09E-00	1.12E-00	5.55E-02	4.16E-01	1.25E-00	1.26E-00	1.17	1.16
$\approx h_0/2$		5.56E-01	5.61E-01	5.71E-01	7.42E-03	1.82E-01	6.07E-01	6.11E-01	1.09	1.09
$\approx h_0/4$		2.92E-01	2.93E-01	2.96E-01	1.04E-03	8.77E-02	3.10E-01	3.11E-01	1.06	1.06
$\approx h_0/8$		1.39E-01	1.39E-01	1.40E-01	1.10E-04	3.85E-02	1.45E-01	1.45E-01	1.04	1.04
h_0	2	1.54E-01	1.55E-01	1.55E-01	5.10E-03	3.05E-02	1.63E-01	1.64E-01	1.06	1.06
$\approx h_0/2$		4.07E-02	4.09E-02	4.13E-02	3.53E-04	7.55E-03	4.23E-02	4.26E-02	1.04	1.04
$\approx h_0/4$		1.10E-02	1.11E-02	1.12E-02	2.51E-05	1.97E-03	1.14E-02	1.15E-02	1.03	1.03
$\approx h_0/8$		2.50E-03	2.52E-03	2.54E-03	1.30E-06	4.21E-04	2.57E-03	2.59E-03	1.03	1.03
h_0	3	1.37E-02	1.37E-02	1.37E-02	3.58E-04	1.74E-03	1.41E-02	1.41E-02	1.03	1.03
$\approx h_0/2$		1.85E-03	1.85E-03	1.85E-03	1.26E-05	2.10E-04	1.88E-03	1.88E-03	1.01	1.01
$\approx h_0/4$		2.60E-04	2.60E-04	2.60E-04	4.73E-07	2.54E-05	2.62E-04	2.62E-04	1.01	1.01
$\approx h_0/8$		2.75E-05	2.75E-05	2.75E-05	1.15E-08	2.55E-06	2.76E-05	2.76E-05	1.01	1.01
h_0	4	9.87E-04	9.87E-04	9.84E-04	2.12E-05	1.11E-04	1.01E-03	1.01E-03	1.02	1.02
$\approx h_0/2$		6.92E-05	6.93E-05	6.92E-05	3.96E-07	7.44E-06	7.00E-05	7.00E-05	1.01	1.01
$\approx h_0/4$		5.04E-06	5.04E-06	5.04E-06	7.58E-09	4.98E-07	5.07E-06	5.07E-06	1.01	1.01
$\approx h_0/8$		2.58E-07	2.59E-07	2.58E-07	8.96E-11	2.47E-08	2.60E-07	2.60E-07	1.01	1.01
h_0	5	5.64E-05	5.64E-05	5.63E-05	1.06E-06	4.50E-06	5.75E-05	5.75E-05	1.02	1.02
$\approx h_0/2$		2.01E-06	2.01E-06	2.01E-06	9.88E-09	1.46E-07	2.03E-06	2.03E-06	1.01	1.01
$\approx h_0/4$		7.74E-08	7.74E-08	7.73E-08	1.01E-10	4.35E-09	7.76E-08	7.76E-08	1.00	1.00
$\approx h_0/8$		1.86E-09	1.86E-09	1.86E-09	1.70E-12	1.00E-10	1.86E-09	1.86E-09	1.00	1.00
h_0	6	2.85E-06	2.85E-06	2.85E-06	4.70E-08	2.18E-07	2.90E-06	2.90E-06	1.02	1.02
$\approx h_0/2$		5.42E-08	5.42E-08	5.42E-08	2.40E-10	4.02E-09	5.46E-08	5.46E-08	1.01	1.01
$\approx h_0/4$		1.07E-09	1.07E-09	1.07E-09	1.03E-11	6.90E-11	1.08E-09	1.08E-09	1.01	1.01

Numerics: singular case

Model problem

$$\begin{aligned} -\Delta u &= 0 \quad \text{in } \Omega := (-1,1)^2 \setminus [0,1]^2, \\ u &= u_{\mathrm{D}} \quad \text{on } \partial\Omega \end{aligned}$$

Exact solution

$$u(r,\phi) = r^{2/3} \sin(2\phi/3)$$

Discretization

- incomplete interior penalty discontinuous Galerkin method
- unstructured non-nested triangular grids
- *hp*-adaptive refinement

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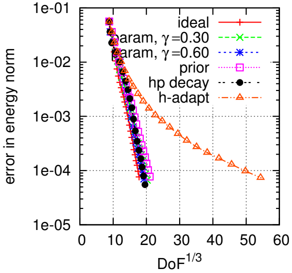
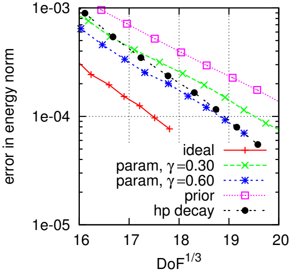
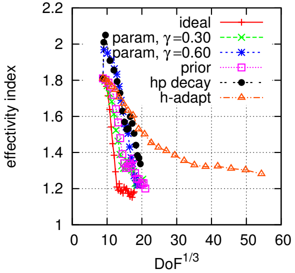
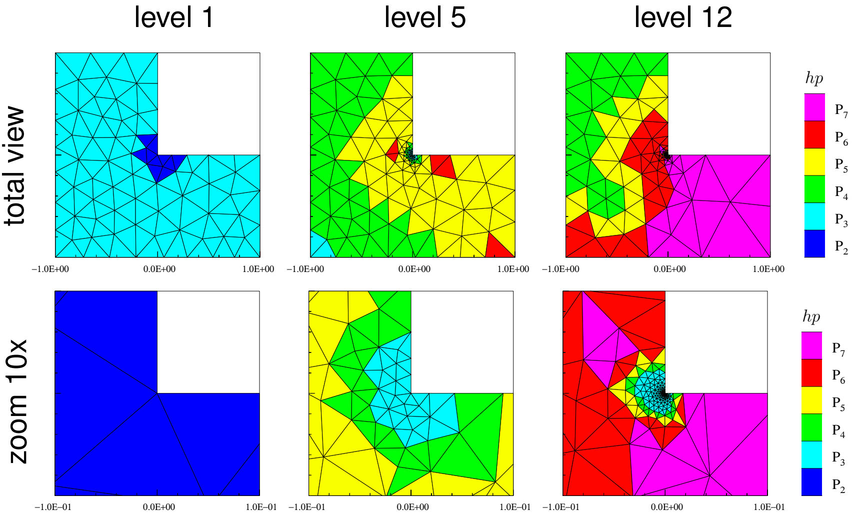
hp-adaptive refinement: **exponential convergence**







hp-refinement grids



Outline

Including iterative algebraic solver

Finite element approximation of the Laplace problem

Find $u_h \in V_h := \mathbb{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega)$, $p \geq 1$, such that

$$(\nabla u_h, \nabla v_h) = (f, v_h) \qquad \forall v_h \in V_h.$$

Linear algebraic system

Find $U_h \in \mathbb{R}^N$ such that

$$\mathbb{A}_h U_h = F_h$$

Algebraic solver (iterative)

On each iteration $i \geq 1$: approximate vector $U_h^i \in \mathbb{R}^N$ such that

$$\mathbb{A}_h U_h^i = F_h - R_h^i \qquad (R_h^i := F_h - \mathbb{A}_h U_h^i)$$

Algebraic error representer

On each iteration $i \geq 1$: approximate solution $u_h^i \in V_h$ such that

$$(\nabla u_h^i, \nabla \psi_l) = (f, \psi_l) - (r_h^i, \psi_l) \qquad \forall l = 1, \ldots, N,$$

where the algebraic error representer $r_h^i \in L^2(\Omega)$ is such that $(r_h^i, \psi_l) = (R_h^i)_l$, $l = 1, \ldots, N$;

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$$\Rightarrow (\nabla(u_h - u_h^i), \nabla v_h) = (r_h^i, v_h) \qquad \forall v_h \in V_h.$$

Outline

Algebraic error upper bound

Theorem (Upper bound via algebraic error flux reconstruction)

Let $\boldsymbol{\sigma}^i_{h,\mathrm{alg}} \in \mathbf{H}(\mathrm{div}, \Omega)$ *be such that* $\nabla\cdot\boldsymbol{\sigma}^i_{h,\mathrm{alg}} = r^i_h$. *Then*

$$\underbrace{\|\nabla(u_h - u^i_h)\|}_{\text{algebraic error}} \leq \underbrace{\|\boldsymbol{\sigma}^i_{h,\mathrm{alg}}\|}_{\text{upper algebraic est.}}.$$

Proof.

$$\|\nabla(u_h - u^i_h)\| = \sup_{v_h \in V_h, \|\nabla v_h\|=1} (\nabla(u_h - u^i_h), \nabla v_h);$$

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Constructions of $\sigma^i_{h,\mathrm{alg}}$

1. sequential sweep trough $\mathcal{T}_h$, local min. (JSV (2010))
2. approximate by precomputing ν iterations (EV (2013))
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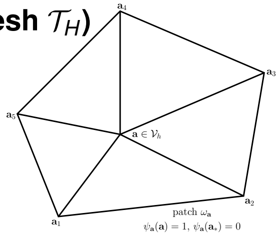
Algebraic error flux reconstruction

Coarse grid Riesz representer (coarse mesh $\mathcal{T}_H$)

$$\mathbb{A}_H \Upsilon_H^i = R_H^i$$

$$\Leftrightarrow$$

$$(\nabla \upsilon_H^i, \nabla \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} = (r_h^i, \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} \quad \forall \mathbf{a} \in \mathcal{V}_H$$



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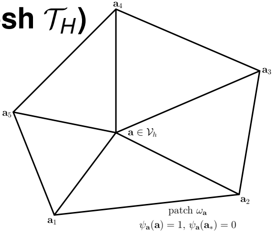

Homogeneous Neumann pbs on coarse patches $\omega_{\mathbf{a}}$, mixed FE space (Destuynder & Métivet (1999), Braess & Schöberl (2008), EV (2013))

$$\boldsymbol{\sigma}_{h,\mathrm{alg}}^{\mathbf{a},i} := \arg \min_{\mathbf{v}_h \in \mathbf{V}_h^{\mathbf{a}},\ \nabla\cdot\mathbf{v}_h = \Pi_{Q_h^{\mathbf{a}}}(\psi_{\mathbf{a}} r_h^i - \nabla\psi_{\mathbf{a}}\cdot\nabla\upsilon_H^i)} \|\mathbf{v}_h\|_{\omega_{\mathbf{a}}},$$

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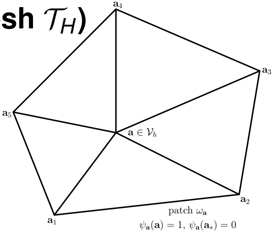

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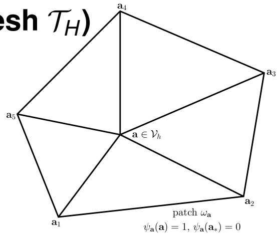

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every fine grid element $K \in \mathcal{T}_h$ lies exactly in $(d+1)$ coarse patches $\omega_{\mathbf{a}}$, $\mathbf{a} \in \mathcal{V}_H$ & partition of unity $\sum_{\mathbf{a}\in\mathcal{V}_H, K\subset\overline{\omega_{\mathbf{a}}}} \psi^{\mathbf{a}} = 1|_K$:

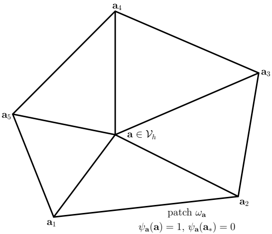
$$\nabla\cdot\boldsymbol{\sigma}^i_{h,\mathrm{alg}}|_K = \sum_{\mathbf{a}\in\mathcal{V}_H, K\subset\overline{\omega_{\mathbf{a}}}} \nabla\cdot\boldsymbol{\sigma}^{\mathbf{a},i}_{h,\mathrm{alg}}|_K = \sum_{\mathbf{a}\in\mathcal{V}_H, K\subset\overline{\omega_{\mathbf{a}}}} \Pi_{Q_h}(\psi_{\mathbf{a}} r^i_h - \nabla\psi_{\mathbf{a}}\cdot\nabla v^i_H)|_K = r^i_h|_K$$

European Research Council

Algebraic error lower bound

Setting

- coarse vertices $\mathbf{a} \in \mathcal{V}_H$ and patches $\omega_{\mathbf{a}}$
- $X_h^{\mathbf{a}} := \mathbb{P}_p(\mathcal{T}_h) \cap H_0^1(\omega_{\mathbf{a}})$
  conforming FE space



Algebraic error lower bound

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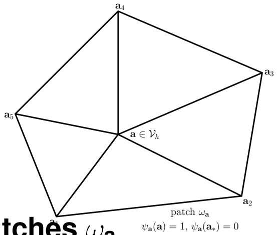

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Homogeneous Dirichlet pbs on coarse patches $\omega_{\mathbf{a}}$

(Babuška and Strouboulis (2001), Repin (2008))

$$v_h^{\mathbf{a},i} \in X_h^{\mathbf{a}} \text{ s.t. } (\nabla v_h^{\mathbf{a},i}, \nabla v_h)_{\omega_{\mathbf{a}}} = (r_h^i, v_h)_{\omega_{\mathbf{a}}} \ \forall v_h \in X_h^{\mathbf{a}},$$

Algebraic error lower bound

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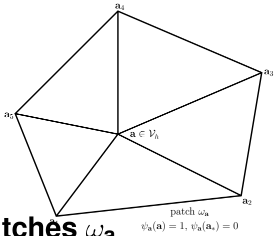

Homogeneous **Dirichlet** pbs on coarse patches $\omega_{\mathbf{a}}$

(Babuška and Strouboulis (2001), Repin (2008))

$$v_h^{\mathbf{a},i} \in X_h^{\mathbf{a}} \text{ s.t. } (\nabla v_h^{\mathbf{a},i}, \nabla v_h)_{\omega_{\mathbf{a}}} = (r_h^i, v_h)_{\omega_{\mathbf{a}}} \quad \forall v_h \in X_h^{\mathbf{a}}, \qquad v_h^i := \sum_{\mathbf{a}\in\mathcal{V}_H} v_h^{\mathbf{a},i}$$

Theorem (Lower bound via algebraic residual liftings)

There holds

$$\underbrace{\|\nabla(u_h - u_h^i)\|}_{\text{algebraic error}} \geq \underbrace{\frac{\sum_{\mathbf{a}\in\mathcal{V}_H} \|\nabla v_h^{\mathbf{a},i}\|_{\omega_{\mathbf{a}}}^2}{\|\nabla v_h^i\|}}_{\text{lower algebraic est.}}.$$

Numerical illustration

Peak $\Omega = (0,1) \times (0,1)$, $u(x,y) = x(x-1)y(y-1)\exp(-100(x-0.5)^2 - 100(y-117/1000)^2)$

L-shape $(-1,1) \times (-1,1) \setminus [0,1] \times [-1,0]$, $u(r,\theta) = r^{2/3} \sin(2\theta/3)$

Discretization

- conforming finite elements with $p = 1, \ldots, 5$
- unstructured triangular meshes
- 4 uniform refinements
- stopping criterion $\eta^i_{\mathrm{alg}} \leq 0.1(\eta^i_{\mathrm{disc}} + \eta_{\mathrm{osc}})$

Multigrid setting

- geometric multigrid V-cycle
- 5 pre-smoothing steps of Gauss–Seidel

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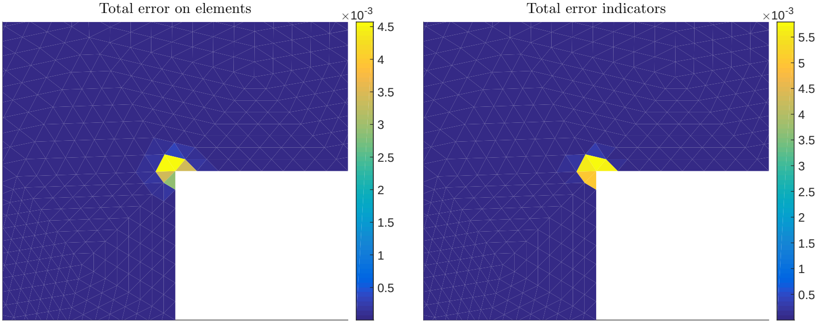
Peak problem, multigrid

p	MG iter	algebraic error	algebraic eff. UB	algebraic eff. LB	total error	total eff. UB	total eff. LB	discretization error	discretization eff. UB	discretization eff. LB
1 (2.55×10^3)	1	8.1×10^{-3}	1.14	1.10^{-1}	1.0×10^{-2}	1.63	1.19^{-1}	6.1×10^{-3}	2.42	—
	2	4.3×10^{-4}	1.13	1.12^{-1}	6.1×10^{-3}	1.13	1.05^{-1}		1.13	1.06^{-1}
2 (1.03×10^4)	1	8.8×10^{-3}	1.17	1.08^{-1}	8.8×10^{-3}	1.72	1.18^{-1}	3.9×10^{-4}	3.28×10^1	—
	2	6.1×10^{-4}	1.19	1.03^{-1}	7.2×10^{-4}	1.75	1.12^{-1}		2.89	—
	3	2.0×10^{-5}	1.19	1.03^{-1}	3.9×10^{-4}	1.08	1.04^{-1}		1.08	1.04^{-1}
3 (2.34×10^4)	1	4.9×10^{-3}	1.14	1.06^{-1}	4.9×10^{-3}	1.59	1.26^{-1}	1.9×10^{-5}	3.33×10^2	—
	3	2.7×10^{-5}	1.17	1.04^{-1}	3.3×10^{-5}	1.69	1.17^{-1}		2.60	—
	5	1.6×10^{-7}	1.15	1.04^{-1}	1.9×10^{-5}	1.02	1.09^{-1}		1.02	1.09^{-1}
4 (4.17×10^4)	1	5.8×10^{-3}	1.22	1.05^{-1}	5.8×10^{-3}	1.83	1.17^{-1}	8.1×10^{-7}	1.12×10^4	—
	3	1.0×10^{-4}	1.16	1.03^{-1}	1.0×10^{-4}	1.71	1.08^{-1}		1.76×10^2	—
	5	2.4×10^{-6}	1.14	1.03^{-1}	2.5×10^{-6}	1.62	1.10^{-1}		4.12	—
	7	6.7×10^{-8}	1.13	1.03^{-1}	8.2×10^{-7}	1.10	1.16^{-1}		1.10	1.16^{-1}
5 (6.52×10^4)	1	4.8×10^{-3}	1.19	1.04^{-1}	4.8×10^{-3}	1.74	1.19^{-1}	3.1×10^{-8}	2.21×10^5	—
	3	2.1×10^{-4}	1.14	1.03^{-1}	2.1×10^{-4}	1.63	1.09^{-1}		8.78×10^3	—
	5	1.5×10^{-5}	1.11	1.02^{-1}	1.5×10^{-5}	1.55	1.07^{-1}		5.57×10^2	—
	7	1.4×10^{-6}	1.12	1.02^{-1}	1.4×10^{-6}	1.57	1.05^{-1}		5.34×10^1	—
	9	1.4×10^{-7}	1.14	1.01^{-1}	1.4×10^{-7}	1.65	1.06^{-1}		6.06	—
	11	1.3×10^{-8}	1.16	1.01^{-1}	3.4×10^{-8}	1.41	1.38^{-1}		1.47	1.62^{-1}
	13	1.2×10^{-9}	1.16	1.01^{-1}	3.1×10^{-8}	1.05	1.21^{-1}		1.05	1.21^{-1}

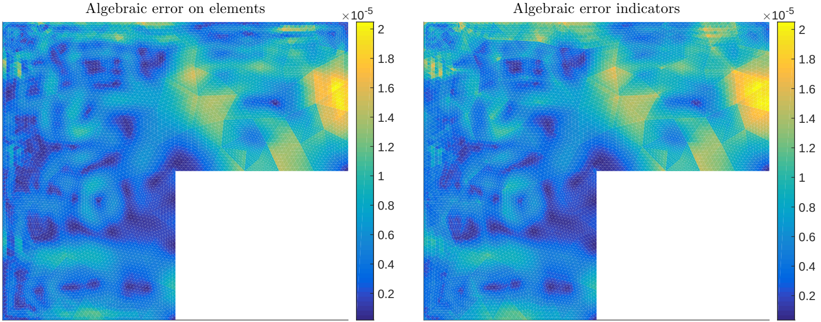
L-shape problem, PCG

p	PCG iter	algebraic error	algebraic eff. UB	algebraic eff. LB	total error	total eff. UB	total eff. LB	discretization error	discretization eff. UB	discretization eff. LB
1 (7.97×10^3)	2	2.9×10^{-1}	1.25	4.08^{-1}	2.9×10^{-1}	1.38	6.15^{-1}	3.6×10^{-2}	1.11×10^1	—
	4	1.2×10^{-3}	1.24	4.17^{-1}	3.6×10^{-2}	1.24	1.12^{-1}		1.24	1.12^{-1}
2 (3.22×10^4)	3	2.1×10^{-1}	1.14	3.62^{-1}	2.1×10^{-1}	1.26	6.03^{-1}	1.4×10^{-2}	1.76×10^1	—
	6	2.5×10^{-3}	1.18	3.17^{-1}	1.5×10^{-2}	1.47	1.32^{-1}		1.49	1.35^{-1}
	9	9.2×10^{-6}	1.17	3.53^{-1}	1.4×10^{-2}	1.29	1.30^{-1}		1.29	1.30^{-1}
3 (7.27×10^4)	4	1.3	1.06	4.53^{-1}	1.3	1.10	1.08×10^{1} $^{-1}$	8.6×10^{-3}	1.58×10^2	—
	8	9.9×10^{-2}	1.10	3.55^{-1}	10.0×10^{-2}	1.24	6.02^{-1}		1.41×10^1	—
	12	1.2×10^{-2}	1.10	3.58^{-1}	1.5×10^{-2}	1.71	2.67^{-1}		2.99	—
	16	8.2×10^{-4}	1.10	3.55^{-1}	8.6×10^{-3}	1.51	1.42^{-1}		1.52	1.43^{-1}
4 (1.29×10^5)	5	1.7×10^{-1}	1.24	2.34^{-1}	1.7×10^{-1}	1.42	3.35^{-1}	6.2×10^{-3}	3.66×10^1	—
	10	2.4×10^{-3}	1.22	2.79^{-1}	6.6×10^{-3}	1.78	1.83^{-1}		1.90	2.93^{-1}
	15	2.3×10^{-5}	1.27	2.33^{-1}	6.2×10^{-3}	1.44	1.62^{-1}		1.44	1.62^{-1}
5 (2.02×10^5)	6	1.1	1.09	4.14^{-1}	1.1	1.16	7.42^{-1}	4.7×10^{-3}	2.71×10^2	—
	12	8.5×10^{-2}	1.11	3.75^{-1}	8.5×10^{-2}	1.23	5.77^{-1}		2.19×10^1	—
	18	7.5×10^{-3}	1.15	3.12^{-1}	8.9×10^{-3}	1.76	3.43^{-1}		3.31	—
	24	3.9×10^{-4}	1.15	3.17^{-1}	4.7×10^{-3}	1.56	1.80^{-1}		1.57	1.82^{-1}

L-shape problem, $p = 3$, total error, 16th PCG iteration



L-shape problem, $p = 3$, alg. error, 16th PCG iteration



Outline

Numerical illustration

Model problem with tensor diffusion

$$-\nabla\cdot(\underline{\mathbf{K}}\nabla u) = f \quad \text{in } \Omega := (0,1)^2,$$
$$u = 0 \quad \text{on } \partial\Omega$$

$$\underline{\mathbf{K}} := \begin{cases} 15 - 10\sin(10\pi x)\sin(10\pi y) & x, y \in (0,1/2) \text{ or } (1/2,1) \\ 15 - 10\sin(2\pi x)\sin(2\pi y) & \text{otherwise} \end{cases}$$

Exact solution

$$u(x,y) = x(1-x)y(1-y)$$

Setting

- Schwarz domain decomposition
- 9 subdomains
- Robin transmission conditions
- lowest-order mixed finite element discretization

Error components and stopping criteria

- distinction of discretization and algebraic (DD) error
- stopping criterion $\eta^i_{\mathrm{DD}} \le 0.1(\eta^i_{\mathrm{disc}} + \eta_{\mathrm{osc}})$

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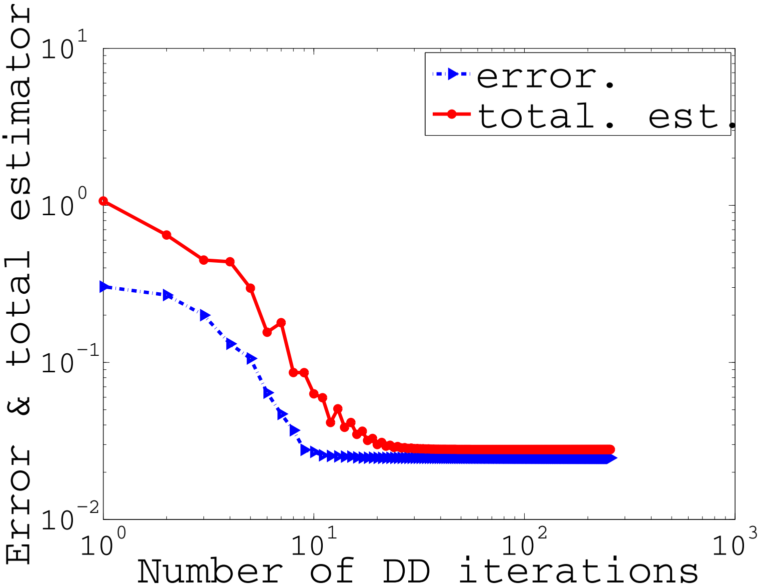
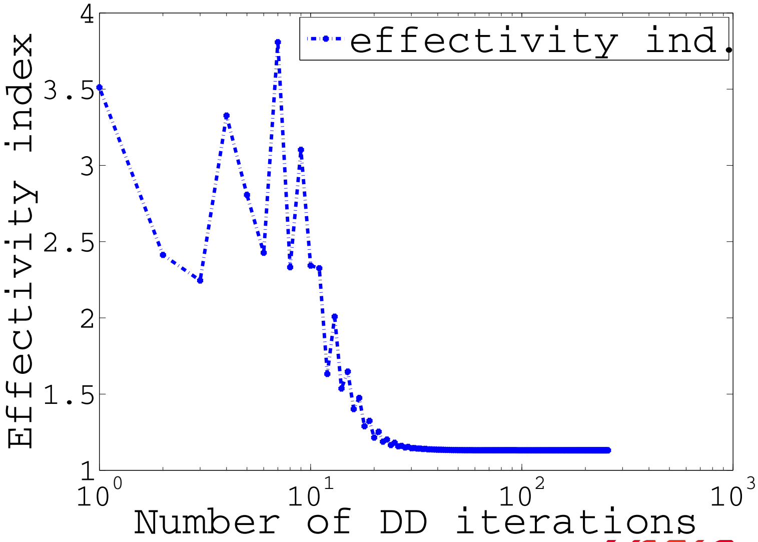
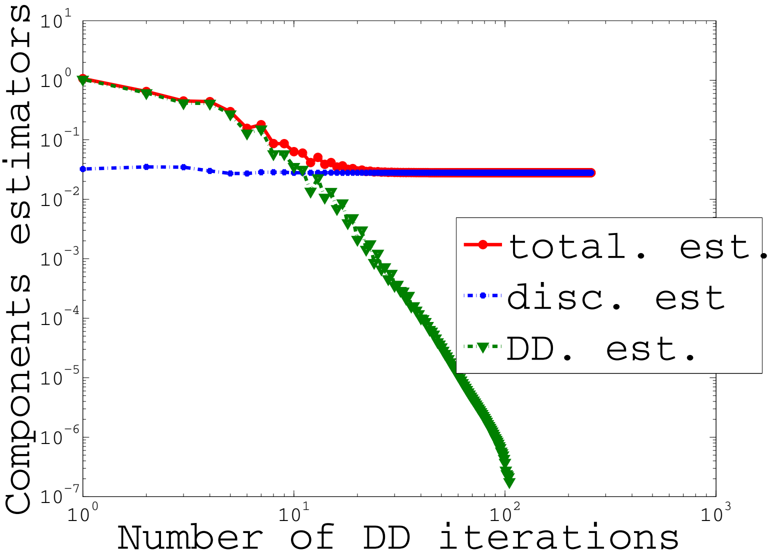
Error and estimate



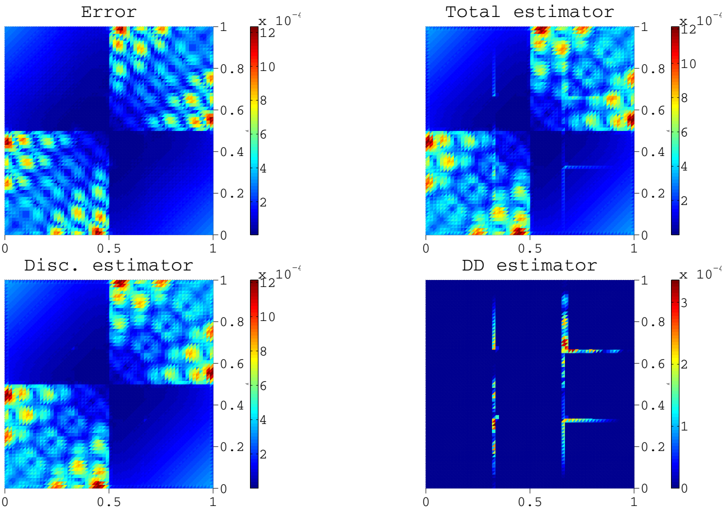
Effectivity index



DD stopping criterion



Error and estimators distribution, 20th DD iteration



Outline

Model nonlinear problem, discretization

Quasi-linear elliptic problem

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

- $p > 1$, $q := \frac{p}{p-1}$, $f \in L^q(\Omega)$
- example: p-Laplacian with $\overline{\boldsymbol{\sigma}}(u, \nabla u) = |\nabla u|^{p-2} \nabla u$
- f piecewise polynomial for simplicity
- weak solution: $u \in V := W_0^{1,p}(\Omega)$ such that

$$(\overline{\boldsymbol{\sigma}}(u, \nabla u), \nabla v) = (f, v) \qquad \forall v \in V$$

Numerical approximation

- simplicial mesh $\mathcal{T}_h$, linearization step k, algebraic step i
- $u_h^{k,i} \in V(\mathcal{T}_h) := \{v \in L^p(\Omega), v|_K \in W^{1,p}(K) \quad \forall K \in \mathcal{T}_h\} \not\subset V$

Model nonlinear problem, discretization

Quasi-linear elliptic problem

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

- $p > 1$, $q := \frac{p}{p-1}$, $f \in L^q(\Omega)$
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Abstract assumptions

Assumption A (Total flux reconstruction)

There exists $\boldsymbol{\sigma}_h^{k,i} \in \mathbf{H}^q(\mathrm{div}, \Omega)$ *and* $\rho_h^{k,i} \in L^q(\Omega)$ *such that*

$$\nabla \cdot \boldsymbol{\sigma}_h^{k,i} = f - \underbrace{\rho_h^{k,i}}_{\text{algebraic remainder}}.$$

Assumption B (Discretization, linearization, and alg. fluxes)

There exist fluxes $\boldsymbol{\sigma}_{h,\mathrm{dis}}^{k,i}, \boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i}, \boldsymbol{\sigma}_{h,\mathrm{alg}}^{k,i} \in [L^q(\Omega)]^d$ *such that*

(i) $\boldsymbol{\sigma}_h^{k,i} = \boldsymbol{\sigma}_{h,\mathrm{dis}}^{k,i} + \boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i} + \boldsymbol{\sigma}_{h,\mathrm{alg}}^{k,i}$;

(ii) *as the linear solver converges,* $\|\boldsymbol{\sigma}_{h,\mathrm{alg}}^{k,i}\|_q \to 0$;

(iii) *as the nonlinear solver converges,* $\|\boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i}\|_q \to 0$.

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Estimate distinguishing error components

Theorem (Estimate distinguishing different error components)

Let

- $u \in V$ *be the weak solution,*
- $u_h^{k,i} \in V(\mathcal{T}_h)$ *be arbitrary,*
- *Assumptions A and B hold.*

Then there holds

$$\underbrace{\mathcal{J}_u(u_h^{k,i})}_{\text{dual norm of the residual + NC}} \leq \eta_{\mathrm{disc}}^{k,i} + \underbrace{\eta_{\mathrm{lin}}^{k,i}}_{\|\boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i}\|_q} + \underbrace{\eta_{\mathrm{alg}}^{k,i}}_{\|\boldsymbol{\sigma}_{h,\mathrm{alg}}^{k,i}\|_q} + \underbrace{\eta_{\mathrm{rem}}^{k,i}}_{h_\Omega \|\rho_h^{k,i}\|_{q,K}} + \eta_{\mathrm{quad}}^{k,i}.$$

Outline

Stopping criteria and efficiency

Global stopping criteria $\gamma_{\rm rem}, \gamma_{\rm alg}, \gamma_{\rm lin} \approx 0.1$

$$\eta_{\rm rem}^{k,i} \leq \gamma_{\rm rem} \max\{\eta_{\rm disc}^{k,i}, \eta_{\rm lin}^{k,i}, \eta_{\rm alg}^{k,i}\},$$
$$\eta_{\rm alg}^{k,i} \leq \gamma_{\rm alg} \max\{\eta_{\rm disc}^{k,i}, \eta_{\rm lin}^{k,i}\},$$
$$\eta_{\rm lin}^{k,i} \leq \gamma_{\rm lin}\eta_{\rm disc}^{k,i}$$

Theorem (Global efficiency)

Under the global stopping criteria and usual assumptions,

$$\eta_{\rm disc}^{k,i} + \eta_{\rm lin}^{k,i} + \eta_{\rm alg}^{k,i} + \eta_{\rm rem}^{k,i} \leq C(\mathcal{J}_u(u_h^{k,i}) + \eta_{\rm quad}^{k,i}),$$

where C is independent of $\overline{\sigma}$ and q.

- local (elementwise) stopping criteria $\Rightarrow$ **local** efficiency
- **robustness** with respect to the **nonlinearity** thanks to the choice of $\mathcal{J}_u$ as error measure

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$$\eta_{\text{alg}}^{k,i} \le \gamma_{\text{alg}} \max\{\eta_{\text{disc}}^{k,i}, \eta_{\text{lin}}^{k,i}\},$$
$$\eta_{\text{lin}}^{k,i} \le \gamma_{\text{lin}} \eta_{\text{disc}}^{k,i}$$

Theorem (Global efficiency)

Under the global stopping criteria and usual assumptions,

$$\eta_{\text{disc}}^{k,i} + \eta_{\text{lin}}^{k,i} + \eta_{\text{alg}}^{k,i} + \eta_{\text{rem}}^{k,i} \le C(\mathcal{J}_u(u_h^{k,i}) + \eta_{\text{quad}}^{k,i}),$$

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Applications

Discretization methods

- conforming finite elements
- nonconforming finite elements
- discontinuous Galerkin
- various finite volumes
- mixed finite elements

Linearizations

- fixed point
- Newton

Linear solvers

- independent of the linear solver

...all Assumptions A to D verified

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Numerical experiment I

Model problem

- p-Laplacian

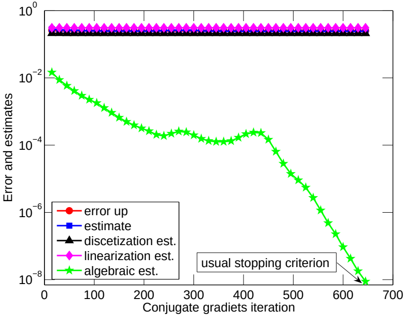
$$\nabla\cdot(|\nabla u|^{p-2}\nabla u) = f \quad \text{in } \Omega,$$
$$u = u_{\mathrm{D}} \quad \text{on } \partial\Omega$$

- weak solution (used to impose the Dirichlet BC)

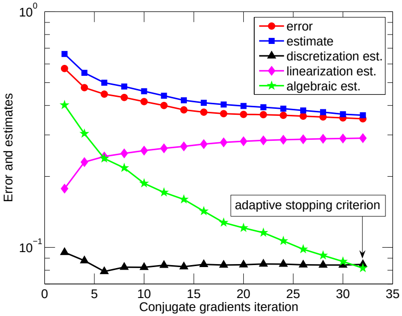
$$u(x,y) = -\frac{p-1}{p}\left((x-\tfrac{1}{2})^2 + (y-\tfrac{1}{2})^2\right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p}\left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

- tested values $p = 1.5$ and 10
- Crouzeix–Raviart nonconforming finite elements

Error and estimators as a function of CG iterations, $p = 10$, 6th level mesh, 6th Newton step.

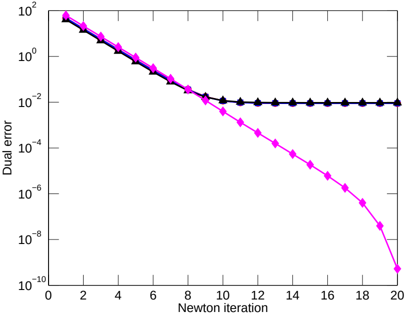


Usual stopping criterion

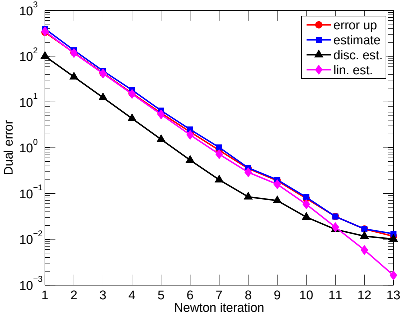


Adaptive stopping criterion

Error and estimators as a function of Newton iterations, $p = 10$, 6th level mesh

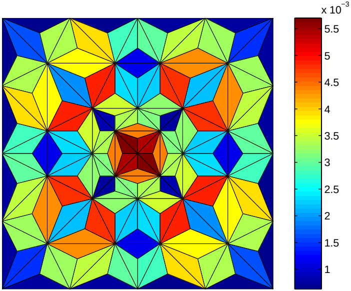


Usual stopping criterion

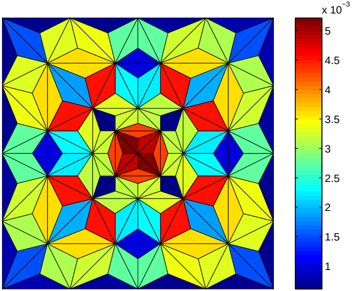


Adaptive stopping criterion

Predicting the **error distribution**

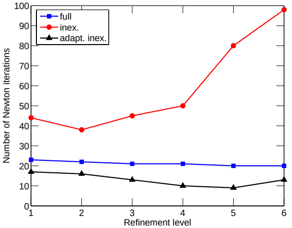


Estimated error distribution

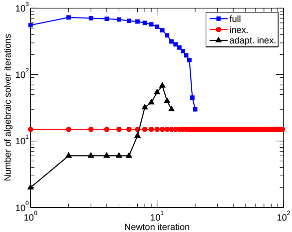


Exact error distribution

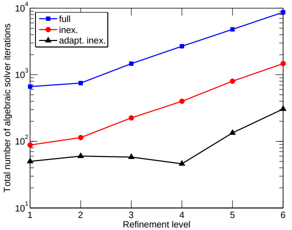
Newton and algebraic iterations: **huge savings**



Newton it. / refinement

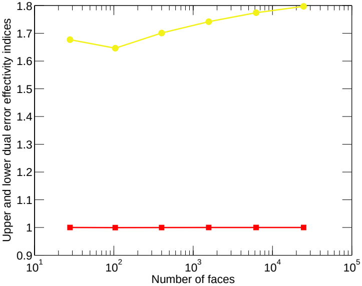


alg. it. / Newton step

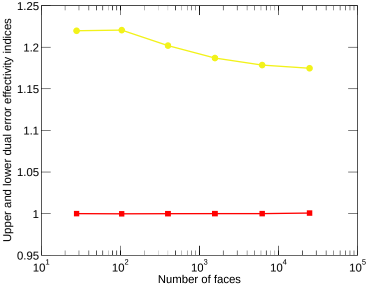


alg. it. / refinement

Effectivity indices, $p = 10$ vs $p = 1.5$: **robustness**



$p = 10$



$p = 1.5$

Numerical experiment II

Model problem

- p-Laplacian

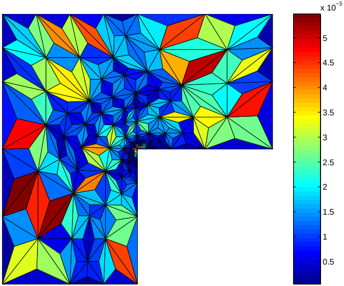
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f && \text{in } \Omega, \\ u &= u_{\mathrm{D}} && \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

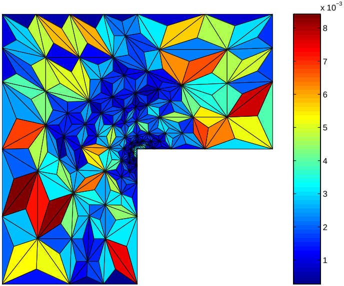
$$u(r,\theta) = r^{\frac{7}{8}} \sin(\theta \tfrac{7}{8})$$

- $p = 4$, L-shape domain, singularity in the origin (Carstensen and Klose (2003))
- Crouzeix–Raviart nonconforming finite elements

Error distribution on an adaptively refined mesh

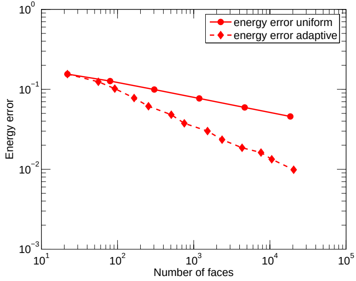


Estimated error distribution

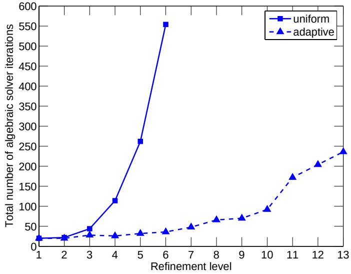


Exact error distribution

Energy error and overall performance



Energy error



Overall performance

Outline

Multiphase, multi-compositional flows

Two-phase immiscible incompressible flow

$$\begin{aligned} \partial_t(\phi s_\alpha) + \nabla\cdot\mathbf{u}_\alpha &= q_\alpha, & \alpha \in \{\mathrm{o}, \mathrm{w}\}, \\ -\lambda_\alpha(s_\mathrm{w})\underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha g \nabla z) &= \mathbf{u}_\alpha, & \alpha \in \{\mathrm{o}, \mathrm{w}\}, \\ s_\mathrm{o} + s_\mathrm{w} &= 1, \\ p_\mathrm{o} - p_\mathrm{w} &= p_\mathrm{c}(s_\mathrm{w}) \end{aligned}$$

+ boundary & initial conditions

Mathematical issues

- coupled system
- unsteady, nonlinear
- elliptic–degenerate parabolic type
- dominant advection

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Distinguishing the error components

Theorem (Distinguishing the error components)

Let

- *n be the time step,*
- *k be the linearization step,*
- *i be the algebraic solver step,*

with the approximations $(s_{\mathrm{w},h\tau}^{n,k,i}, p_{\mathrm{w},h\tau}^{n,k,i})$. Then

$$\mathcal{J}_{s_{\mathrm{w}},p_{\mathrm{w}}}^{n}(s_{\mathrm{w},h\tau}^{n,k,i}, p_{\mathrm{w},h\tau}^{n,k,i}) \leq \eta_{\mathrm{sp}}^{n,k,i} + \eta_{\mathrm{tm}}^{n,k,i} + \eta_{\mathrm{lin}}^{n,k,i} + \eta_{\mathrm{alg}}^{n,k,i}.$$

Error components

- $\eta_{\mathrm{sp}}^{n,k,i}$: spatial discretization
- $\eta_{\mathrm{tm}}^{n,k,i}$: temporal discretization
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- $\eta_{\mathrm{alg}}^{n,k,i}$: algebraic solver

Full adaptivity

- only a **necessary number** of all **solver iterations**
- **"online decisions"**: algebraic step / linearization step / space mesh refinement / time step modification

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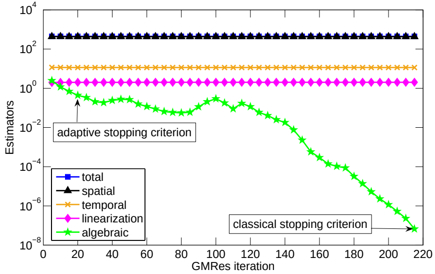
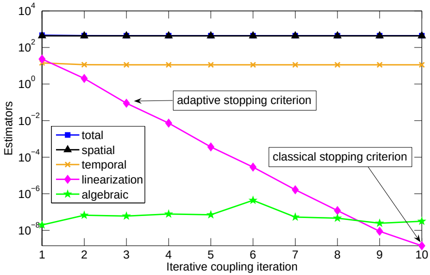
Estimators and stopping criteria

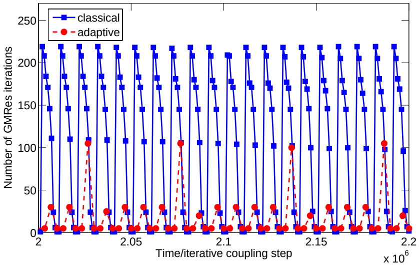


Estimators in function of GMRes iterations

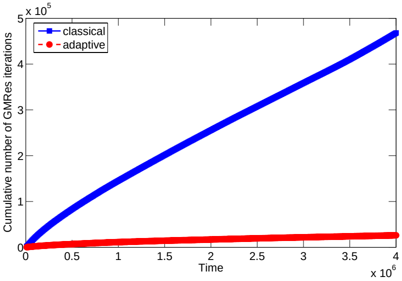


Estimators in function of iterative coupling iterations

GMRes iterations

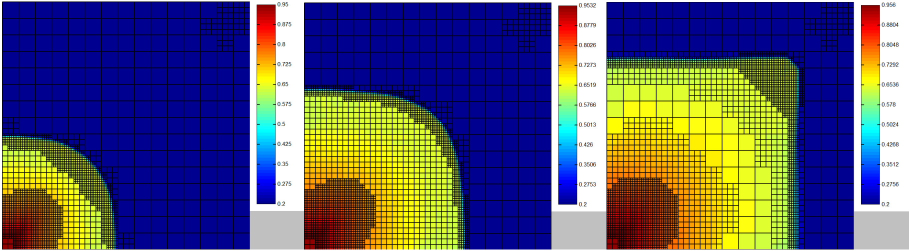


Per time and iterative coupling step



Cumulated

Space/time/nonlinear solver/linear solver adaptivity



Fully adaptive computation

Outline

Conclusions and outlook

Conclusions

- guaranteed energy error estimates
- robustness (polynomial degree, nonlinearity)
- full adaptivity (linear solver, nonlinear solver, mesh)
- unified framework for all classical numerical schemes

Ongoing work

- convergence and optimality
- higher-order time discretizations
- DD for nonlinear problems (CEMRACS ApostDD project)

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Thank you for your attention!