A posteriori error estimates and adaptive error components balancing 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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Context and questions

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: $A(u) = f$ in Ω

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 in Ω?*

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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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A posteriori error estimate

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 $-\nabla u_h \notin \mathbf{H}(\mathrm{div}, \Omega)$ in gen.);*
- *$s_h \in H_0^1(\Omega)$ 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

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

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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:

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

- dual norm characterization, definition of s, definition of u:

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

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Proof II

Proof (continuation).

- nonconformity upper bound:

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

- adding and subtracting equilibrated flux, Green theorem:

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

- Cauchy–Schwarz and Poincaré inequalities, equilibration:

$$-(\nabla u_h + \boldsymbol{\sigma}_h, \nabla \varphi)$$

$$(f - \nabla\cdot\boldsymbol{\sigma}_h, \varphi) = \sum_{K \in \mathcal{T}_h} (f - \nabla\cdot\boldsymbol{\sigma}_h, \varphi \qquad)_K$$

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$$\le \sum_{K \in \mathcal{T}_h} \frac{h_K}{\pi} \|f - \nabla\cdot\boldsymbol{\sigma}_h\|_K \|\nabla \varphi\|_K$$

Proof II

Proof (continuation).

- nonconformity upper bound:

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

- adding and subtracting equilibrated flux, Green theorem:

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

- Cauchy–Schwarz and Poincaré inequalities, equilibration:

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

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

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Outline

Global potential and flux reconstructions

Ideally

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

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

- $\mathbf{V}_h \subset \mathbf{H}(\mathrm{div}, \Omega)$, $Q_h \subset L^2(\Omega)$, $V_h \subset H_0^1(\Omega)$
- 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, ≈ Carstensen and Merdon (2013), EV (2015))

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

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Key ideas

- **local** minimizations
- cut-off by hat basis functions $\psi_{\mathbf{a}}$
- $\mathbf{V}_h^{\mathbf{a}}$: homogeneous Neumann BC on $\partial\omega_{\mathbf{a}}$ & $V_h^{\mathbf{a}}$: homogeneous Dirichlet BC on $\partial\omega_{\mathbf{a}}$
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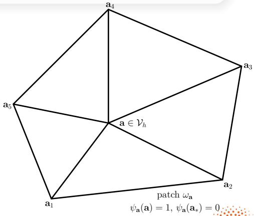

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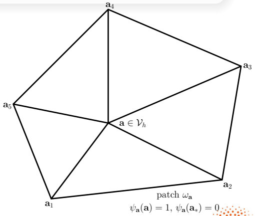

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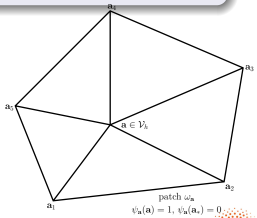

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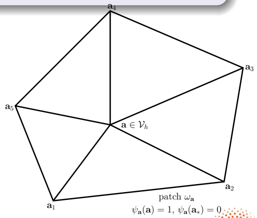
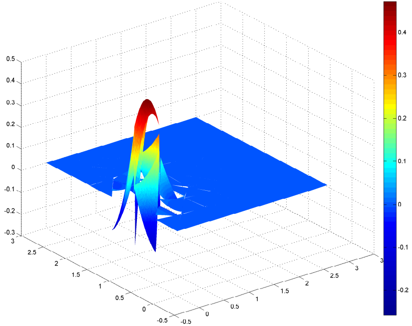
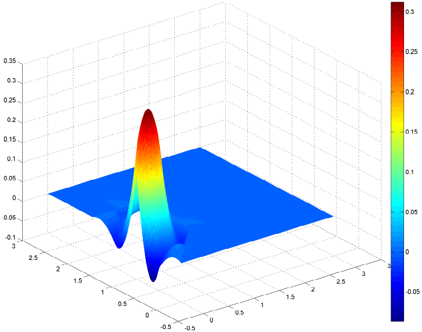


Potential reconstruction



Potential u_h



Potential reconstruction s_h

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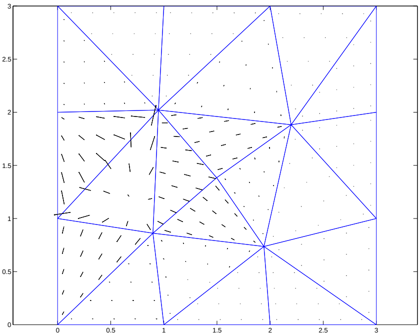
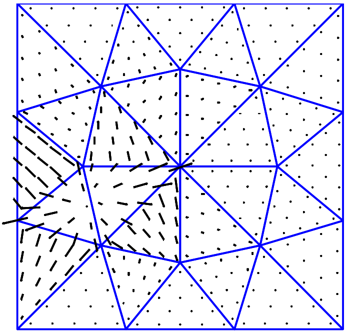
Equilibrated flux reconstruction



Flux $-\nabla u_h$



Flux reconstruction σ_h

Comments

$\mathbf{H}(\mathrm{div},\Omega)$-conformity

- $\boldsymbol{\sigma}_h^{\mathbf{a}} \in \mathbf{H}(\mathrm{div},\Omega) \Rightarrow \boldsymbol{\sigma}_h = \sum_{\mathbf{a}\in\mathcal{V}_h} \boldsymbol{\sigma}_h^{\mathbf{a}} \in \mathbf{H}(\mathrm{div},\Omega)$

Neumann compatibility condition

- for $\mathbf{a} \in \mathcal{V}_h^{\mathrm{int}}$, one needs $(\psi_{\mathbf{a}} f - \nabla\psi_{\mathbf{a}}\cdot\nabla u_h, 1)_{\omega_{\mathbf{a}}} = 0 \Rightarrow$

Assumption A (Galerkin orthogonality wrt hat functions)

There holds

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

Divergence

- Neumann compatibility condition gives

$$\nabla\cdot\boldsymbol{\sigma}_h^{\mathbf{a}}|_K = \Pi_{Q_h}(\psi_{\mathbf{a}} f - \nabla\psi_{\mathbf{a}}\cdot\nabla u_h)|_K \qquad \forall K \in \mathcal{T}_h$$

- the fact that $\boldsymbol{\sigma}_h|_K = \sum_{\mathbf{a}\in\mathcal{V}_K} \boldsymbol{\sigma}_h^{\mathbf{a}}|_K$ and the partition of unity $\sum_{\mathbf{a}\in\mathcal{V}_K} \psi^{\mathbf{a}}|_K = 1|_K$ yield

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Outline

Continuous-level patch problems

Definition (Continuous-level flux reconstruction)

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

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

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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Definition (Continuous-level potential reconstruction)

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

$$s^{\mathbf{a}} := \arg \min_{v \in H_0^1(\omega_{\mathbf{a}})} \|\nabla(\psi_{\mathbf{a}} u_h - v)\|_{\omega_{\mathbf{a}}}.$$

Assumptions for efficiency

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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Remarks

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

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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Discontinuous Galerkin finite elements

Discontinuous Galerkin finite elements

Find $u_h \in V_h$ such that

$$\sum_{K\in\mathcal{T}_h}(\nabla u_h, \nabla v_h)_K - \sum_{e\in\mathcal{E}_h}\{\langle\{\!\{\nabla u_h\}\!\}\cdot\mathbf{n}_e, [\![v_h]\!]\rangle_e + \theta\langle\{\!\{\nabla v_h\}\!\}\cdot\mathbf{n}_e, [\![u_h]\!]\rangle_e\}$$

$$+\sum_{e\in\mathcal{E}_h}\langle\alpha h_e^{-1}[\![u_h]\!], [\![v_h]\!]\rangle_e = (f, v_h) \qquad \forall v_h \in V_h.$$

- $V_h := \mathbb{P}_p(\mathcal{T}_h)$, $p \geq 1$
- Assumption A: take $v_h = \psi_{\mathbf{a}}$ for $\theta = 0$, otherwise:
  - estimates for the discrete gradient

$$\mathfrak{G}(u_h) := \nabla u_h - \theta\sum_{e\in\mathcal{E}_h}\mathfrak{l}_e([\![u_h]\!])$$

  - jumps lifting operator $\mathfrak{l}_e : L^2(e) \to [\mathbb{P}_0(\mathcal{T}_e)]^2$

$$(\mathfrak{l}_e([\![u_h]\!]), \mathbf{v}_h) = \langle\{\!\{\mathbf{v}_h\}\!\}\cdot\mathbf{n}_e, [\![u_h]\!]\rangle_e \qquad \forall \mathbf{v}_h \in [\mathbb{P}_0(\mathcal{T}_e)]^2$$

  - $\Rightarrow$ modified Galerkin orthogonality

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

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Discontinuous Galerkin finite elements: Assumption B

Nonsymmetric and incomplete versions

- broken Poincaré–Friedrichs inequality with jumps:

$$\|\nabla(\psi_{\mathbf{a}}(\tilde{u} - u_h))\|_{\omega_{\mathbf{a}}} \leq (1 + C_{\mathrm{bPF},\omega_{\mathbf{a}}} h_{\omega_{\mathbf{a}}} \|\nabla \psi_{\mathbf{a}}\|_{\infty,\omega_{\mathbf{a}}}) \|\nabla(u - u_h)\|_{\omega_{\mathbf{a}}} + C_{\mathrm{bPF},\omega_{\mathbf{a}}} h_{\omega_{\mathbf{a}}} \|\nabla \psi_{\mathbf{a}}\|_{\infty,\omega_{\mathbf{a}}} \left\{ \sum_{e \in \mathcal{E}_h,\, \mathbf{a} \in e} h_e^{-1} \|\Pi_e^0 [\![u_h]\!] \|_e^2 \right\}^{1/2}$$

- include the jump terms in the error and estimators

Symmetric version

- discrete gradient $\mathfrak{G}$ satisfies

$$(\mathfrak{G}(u_h), \mathrm{R}_{\frac{\pi}{2}} \nabla \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} = 0 \qquad \forall \mathbf{a} \in \mathcal{V}_h$$

- modified potential reconstruction: local MFE problems with data $\tau_h^{\mathbf{a}} := \psi_{\mathbf{a}} \mathrm{R}_{\frac{\pi}{2}} \mathfrak{G}(u_h)$ and $g^{\mathbf{a}} := (\mathrm{R}_{\frac{\pi}{2}} \nabla \psi_{\mathbf{a}}) \cdot \mathfrak{G}(u_h)$
- local efficiency

$$\|\mathfrak{G}(u_h - s_h)\|_K \leq C_{\mathrm{st}} C_{\mathrm{cont,P}} \sum_{\mathbf{a} \in \mathcal{V}_K} \|\mathfrak{G}(u - u_h)\|_{\omega_{\mathbf{a}}}$$

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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

$$\begin{aligned} (\boldsymbol{\sigma}_h, \mathbf{v}_h) - (\bar{u}_h, \nabla\cdot\mathbf{v}_h) &= 0 \qquad \forall \mathbf{v}_h \in \mathbf{V}_h, \\ (\nabla\cdot\boldsymbol{\sigma}_h, q_h) &= (f, q_h) \qquad \forall q_h \in Q_h. \end{aligned}$$

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

$$\langle [\![v_h]\!], q_h \rangle_e = 0 \qquad \forall q_h \in \mathbb{P}_{p'}(e), \ \forall e \in \mathcal{E}_h$$

- Assumption A: no need for flux reconstruction, $\boldsymbol{\sigma}_h$ comes from the discretization
- Assumption B satisfied, building requirement for the space V_h

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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
- uniform h refinement

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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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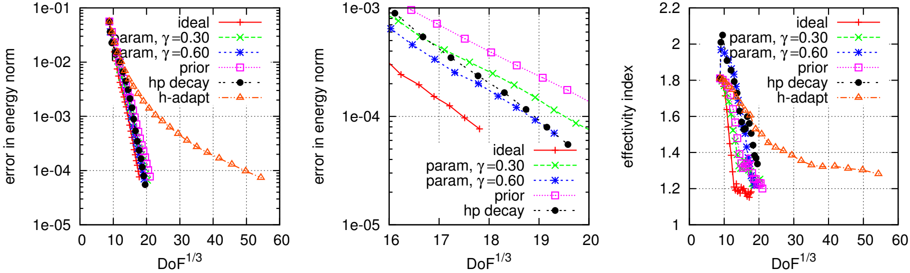
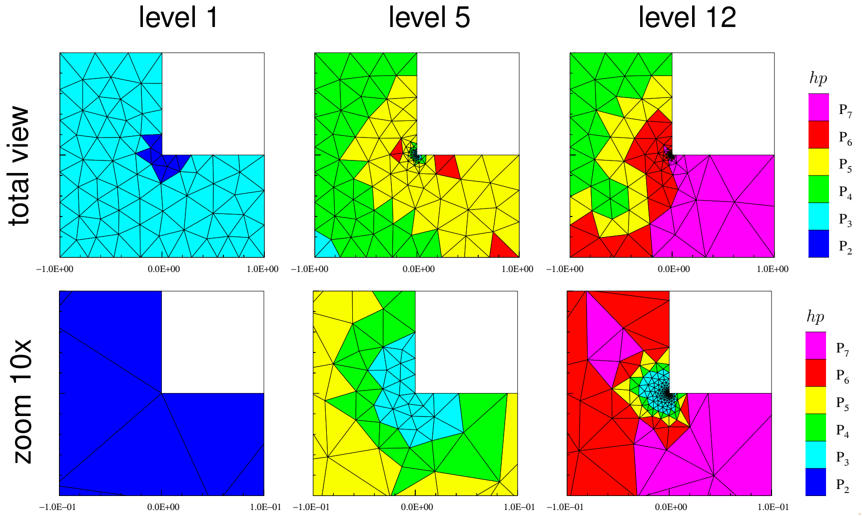
hp-adaptive refinement: **exponential convergence**



hp-refinement grids



Outline

Including iterative algebraic solver (conforming FEs)

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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Finite element approximation of the Laplace problem

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

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 $(r_h^i, \psi_l) = (R_h^i)_l$, $l = 1, \ldots, N$;

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

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.

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

$$(\nabla(u_h - u^i_h), \nabla v_h) = (r^i_h, v_h) = (\nabla\cdot\boldsymbol{\sigma}^i_{h,\mathrm{alg}}, v_h) = -(\boldsymbol{\sigma}^i_{h,\mathrm{alg}}, \nabla v_h).$$

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

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

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Algebraic error flux reconstruction, two-level setting

Definition (Coarse grid Riesz representer)

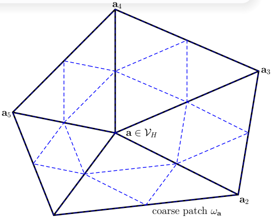
Find $v_H^i \in V_H := \mathbb{P}_1(\mathcal{T}_H) \cap H_0^1(\Omega)$ such that

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

Definition (Algebraic error flux reconstruction)

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

- homogeneous Neumann problems
- mixed FE spaces
- fine meshes of coarse patches $\omega_{\mathbf{a}}$
- Riesz representer (solve on $\mathcal{T}_H$) $\Rightarrow$ hat function orthogonality on $\mathcal{T}_H$
- extends to arbitrary number of levels



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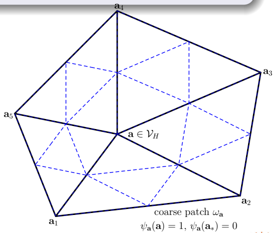

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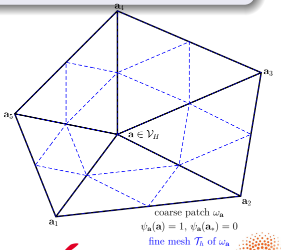

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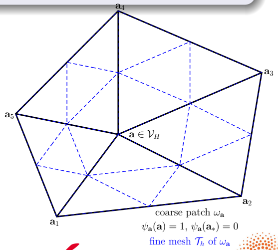

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Divergence of the algebraic error flux reconstruction

Lemma (Divergence of $\boldsymbol{\sigma}_{h,\mathrm{alg}}^{\mathbf{a},i}$)

There holds $\nabla{\cdot}\boldsymbol{\sigma}_{h,\mathrm{alg}}^{i} = r_h^i$.

Proof.

- 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 $\sum_{\mathbf{a}\in\mathcal{V}_H, K\subset\overline{\omega_{\mathbf{a}}}} \psi^{\mathbf{a}} = 1|_K$
-

$$\nabla{\cdot}\boldsymbol{\sigma}_{h,\mathrm{alg}}^{i}|_K = \sum_{\mathbf{a}\in\mathcal{V}_H, K\subset\overline{\omega_{\mathbf{a}}}} \nabla{\cdot}\boldsymbol{\sigma}_{h,\mathrm{alg}}^{\mathbf{a},i}|_K$$

$$= \sum_{\mathbf{a}\in\mathcal{V}_H, K\subset\overline{\omega_{\mathbf{a}}}} \Pi_{Q_h}(\psi_{\mathbf{a}} r_h^i - \nabla\psi_{\mathbf{a}}{\cdot}\nabla v_H^i)|_K = r_h^i|_K$$

Divergence of the algebraic error flux reconstruction

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Algebraic residual lifting

Definition (Algebraic residual lifting, ≈ Babuška and Strouboulis (2001), Repin (2008))

Find $v_h^{\mathbf{a},i} \in X_h^{\mathbf{a}} := \mathbb{P}_p(\mathcal{T}_h) \cap H_0^1(\omega_{\mathbf{a}})$ such that

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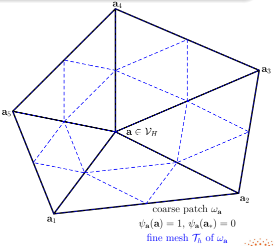

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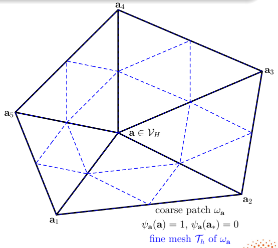

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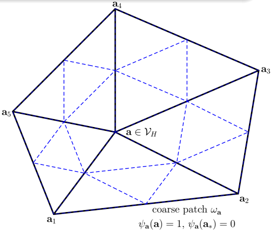

Algebraic error lower bound

Theorem (Lower bound via algebraic residual liftings)

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

Proof.

$$\|\nabla(u_h - u_h^i)\| = \sup_{v_h\in V_h, \|\nabla v_h\|=1} (r_h^i, v_h)$$

$$\geq \frac{(r_h^i, \upsilon_h^i)}{\|\nabla \upsilon_h^i\|} = \frac{\sum_{\mathbf{a}\in\mathcal{V}_H}(r_h^i, \upsilon_h^{\mathbf{a},i})_{\omega_\mathbf{a}}}{\|\nabla \upsilon_h^i\|}$$

$$= \frac{\sum_{\mathbf{a}\in\mathcal{V}_H}\|\nabla \upsilon_h^{\mathbf{a},i}\|^2_{\omega_\mathbf{a}}}{\|\nabla \upsilon_h^i\|}.$$

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Proof.

$$
\begin{aligned}
\|\nabla(u_h - u_h^i)\| &= \sup_{v_h \in V_h, \|\nabla v_h\|=1} (r_h^i, v_h)\\
&\geq \frac{(r_h^i, v_h^i)}{\|\nabla v_h^i\|} = \frac{\sum_{\mathbf{a}\in\mathcal{V}_H} (r_h^i, v_h^{\mathbf{a},i})_{\omega_{\mathbf{a}}}}{\|\nabla v_h^i\|}\\
&= \frac{\sum_{\mathbf{a}\in\mathcal{V}_H} \|\nabla v_h^{\mathbf{a},i}\|^2_{\omega_{\mathbf{a}}}}{\|\nabla v_h^i\|}.
\end{aligned}
$$

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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 $\eta^i_{\rm alg} \leq 0.1(\eta^i_{\rm disc} + \eta_{\rm osc})$

Multigrid setting

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

PCG setting

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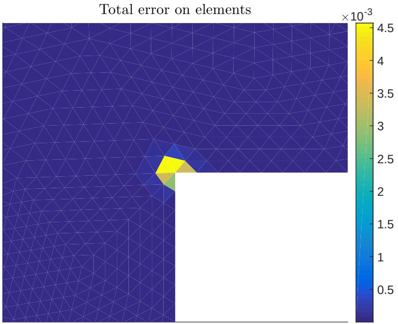
Peak problem, multigrid

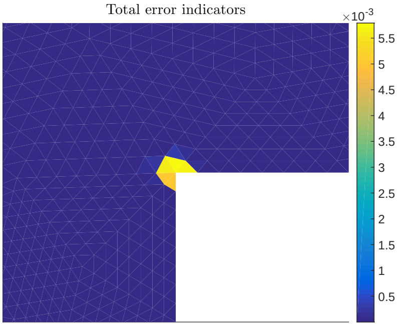
p	MG iter	algebraic error	algebraic eff. UB	algebraic eff. LB	total error	total eff. UB	total eff. LB	discretization error	discretization eff. UB	discretization eff. LB
1 (2.55×10^3)	1	8.1×10^{-3}	1.14	1.10^{-1}	1.0×10^{-2}	1.63	1.19^{-1}	6.1×10^{-3}	2.42	—
	2	4.3×10^{-4}	1.13	1.12^{-1}	6.1×10^{-3}	1.13	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

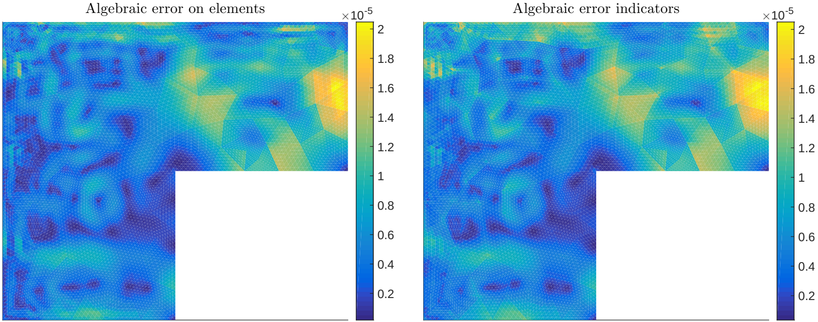
p	PCG iter	algebraic error	algebraic eff. UB	algebraic eff. LB	total error	total eff. UB	total eff. LB	discretization error	discretization eff. UB	discretization eff. LB
1 (7.97×10^3)	2	2.9×10^{-1}	1.25	4.08^{-1}	2.9×10^{-1}	1.38	6.15^{-1}	3.6×10^{-2}	1.11×10^1	—
	4	1.2×10^{-3}	1.24	4.17^{-1}	3.6×10^{-2}	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	$1.08 \times 10^{1}\,^{-1}$	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 (mixed FEs)

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 $\eta^i_{\mathrm{DD}} \leq 0.1(\eta^i_{\mathrm{disc}} + \eta_{\mathrm{osc}})$

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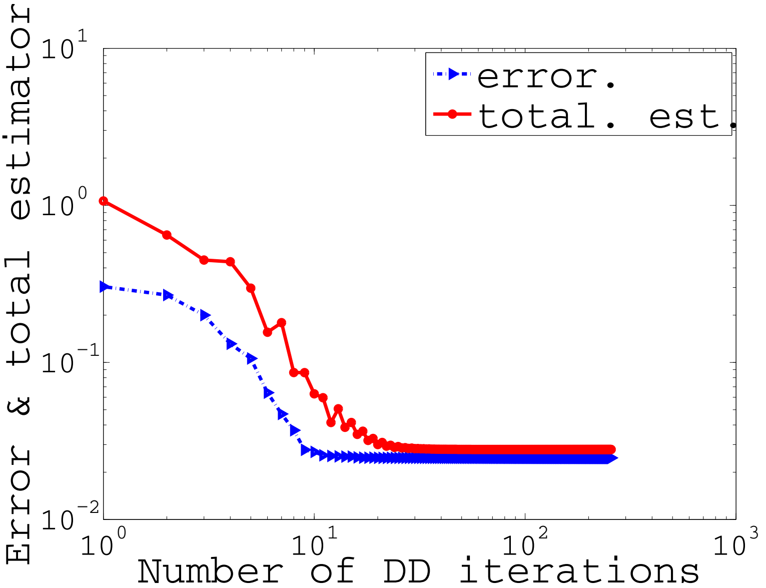
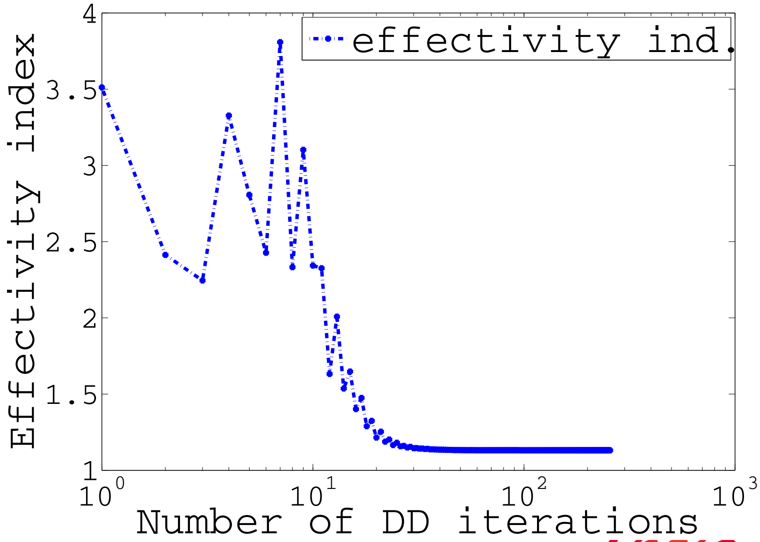
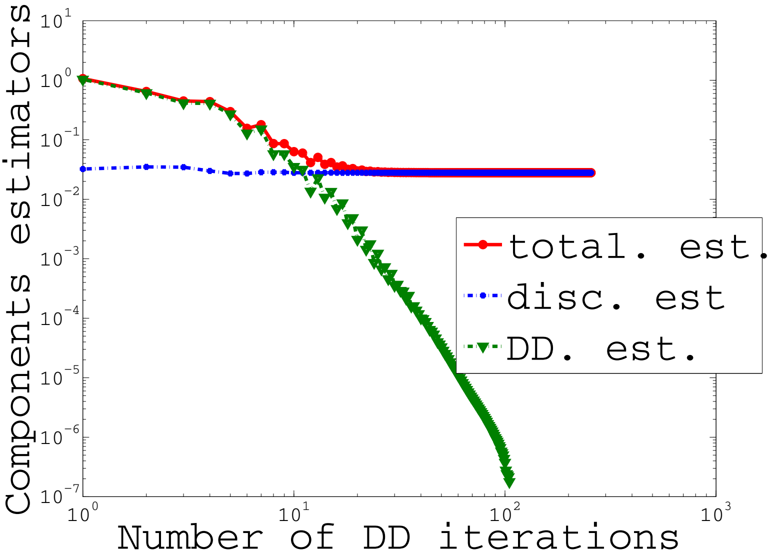
Error and estimate



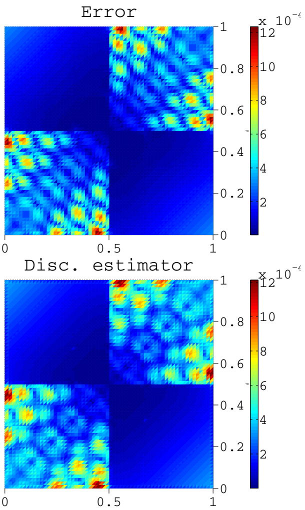
Effectivity index



DD stopping criterion



Error and estimators distribution, 20th DD iteration



Outline

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

Model nonlinear problem, discretization

Quasi-linear elliptic problem

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

- $p > 1$, $q := \frac{p}{p-1}$, $f \in L^q(\Omega)$
- 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
- $u_h^{k,i} \in V(\mathcal{T}_h) := \{v \in L^p(\Omega),\, v|_K \in W^{1,p}(K) \quad \forall K \in \mathcal{T}_h\} \not\subset V$

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Abstract assumptions

Assumption A (Total flux reconstruction)

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

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

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

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

(i) $\sigma_h^{k,i} = \sigma_{h,\mathrm{dis}}^{k,i} + \sigma_{h,\mathrm{lin}}^{k,i} + \sigma_{h,\mathrm{alg}}^{k,i}$;

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

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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

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

Outline

Stopping criteria and efficiency

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

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

Theorem (Global efficiency)

Under the global stopping criteria and usual assumptions,

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

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

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

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Outline

Nonconforming finite elements for the p-Laplacian

Discretization

Find $u_h \in V_h$ such that

$$(\overline{\sigma}(\nabla u_h), \nabla v_h) = (f, v_h) \qquad \forall v_h \in V_h.$$

- $\overline{\sigma}(\nabla u_h) = |\nabla u_h|^{p-2} \nabla u_h$
- $V_h \not\subset V$ the Crouzeix–Raviart space
- leads to the system of nonlinear algebraic equations

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

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Linearization

Linearization

Find $u_h^k \in V_h$ such that

$$(\overline{\sigma}^{k-1}(\nabla u_h^k), \nabla \psi_e) = (f, \psi_e) \qquad \forall e \in \mathcal{E}_h^{\mathrm{int}}.$$

- $u_h^0 \in V_h$ yields the initial vector U^0
- fixed-point linearization

$$\overline{\sigma}^{k-1}(\xi) := |\nabla u_h^{k-1}|^{p-2} \xi$$

- Newton linearization

$$\overline{\sigma}^{k-1}(\xi) := |\nabla u_h^{k-1}|^{p-2} \xi + (p-2)|\nabla u_h^{k-1}|^{p-4} (\nabla u_h^{k-1} \otimes \nabla u_h^{k-1})(\xi - \nabla u_h^{k-1})$$

- leads to the system of linear algebraic equations

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

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Algebraic solution

Algebraic solution

Find $u_h^{k,i} \in V_h$ such that

$$(\overline{\boldsymbol{\sigma}}^{k-1}(\nabla u_h^{k,i}), \nabla \psi_e) = (f, \psi_e) - R_e^{k,i} \qquad \forall e \in \mathcal{E}_h^{\mathrm{int}}.$$

- algebraic residual vector $R^{k,i} = \{R_e^{k,i}\}_{e \in \mathcal{E}_h^{\mathrm{int}}}$
- discrete system

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Flux reconstructions

Definition (Construction of $(\boldsymbol{\sigma}_{h,\mathrm{dis}}^{k,i} + \boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i})$)

For all $K \in \mathcal{T}_h$,

$$(\boldsymbol{\sigma}_{h,\mathrm{dis}}^{k,i} + \boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i})|_K := -\overline{\boldsymbol{\sigma}}^{k-1}(\nabla u_h^{k,i})|_K + \frac{f|_K}{d}(\mathbf{x} - \mathbf{x}_K) - \sum_{e \in \mathcal{E}_K} \frac{R_e^{k,i}}{d|D_e|}(\mathbf{x} - \mathbf{x}_K)|_{K_e},$$

where $R_e^{k,i} = (f, \psi_e) - (\overline{\boldsymbol{\sigma}}^{k-1}(\nabla u_h^{k,i}), \nabla \psi_e) \qquad \forall e \in \mathcal{E}_h^{\mathrm{int}}$.

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Definition (Construction of $\boldsymbol{\sigma}_{h,\mathrm{alg}}^{k,i}$)

Set $\boldsymbol{\sigma}_{h,\mathrm{alg}}^{k,i} := (\mathbf{d}_h^{k,i+\nu} + \mathbf{l}_h^{k,i+\nu}) - (\boldsymbol{\sigma}_{h,\mathrm{dis}}^{k,i} + \boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i})$ for (adaptively chosen) $\nu > 0$ additional algebraic solvers steps; $R^{k,i+\nu} \rightsquigarrow \rho_h^{k,i}$.

Flux reconstructions

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Set $\boldsymbol{\sigma}_{h,\mathrm{alg}}^{k,i} := (\mathbf{d}_h^{k,i+\nu} + \mathbf{l}_h^{k,i+\nu}) - (\boldsymbol{\sigma}_{h,\mathrm{dis}}^{k,i} + \boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i})$ for (adaptively chosen) $\nu > 0$ additional algebraic solvers steps; $R^{k,i+\nu} \rightsquigarrow \rho_h^{k,i}$.

Flux reconstructions

Definition (Construction of $(\boldsymbol{\sigma}_{h,\mathrm{dis}}^{k,i} + \boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i})$)

For all $K \in \mathcal{T}_h$,

$$(\boldsymbol{\sigma}_{h,\mathrm{dis}}^{k,i}+\boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i})|_K := -\overline{\boldsymbol{\sigma}}^{k-1}(\nabla u_h^{k,i})|_K + \frac{f|_K}{d}(\mathbf{x}-\mathbf{x}_K) - \sum_{e\in\mathcal{E}_K} \frac{R_e^{k,i}}{d|D_e|}(\mathbf{x}-\mathbf{x}_K)|_{K_e},$$

where $R_e^{k,i} = (f,\psi_e) - (\overline{\boldsymbol{\sigma}}^{k-1}(\nabla u_h^{k,i}), \nabla\psi_e) \qquad \forall e \in \mathcal{E}_h^{\mathrm{int}}$.

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Summary

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 verified

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Numerical experiment I

Model problem

- p-Laplacian

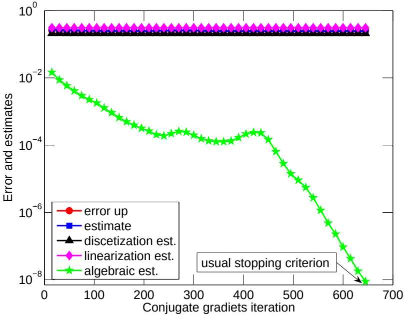
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f && \text{in } \Omega, \\ u &= u_{\mathrm{D}} && \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

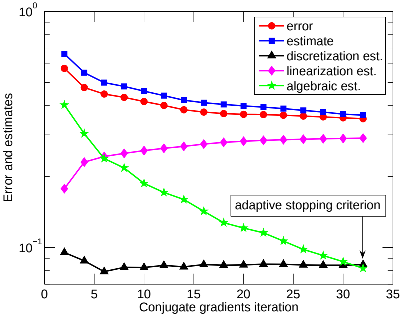
$$u(x,y) = -\frac{p-1}{p}\left((x-\tfrac{1}{2})^2 + (y-\tfrac{1}{2})^2\right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p}\left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

- 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.

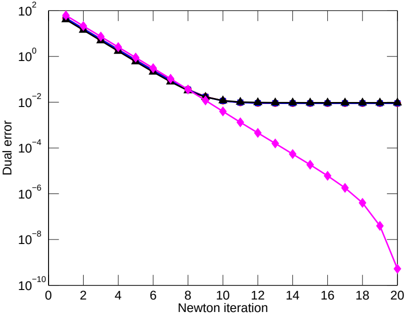


Usual stopping criterion



Adaptive stopping criterion

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



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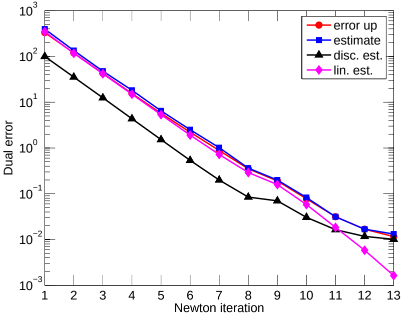
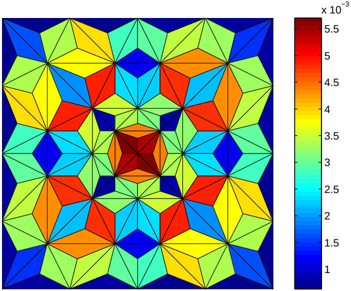
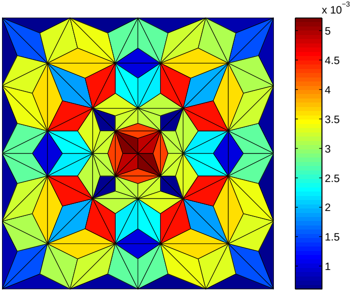


Adaptive stopping criterion

Predicting the **error distribution**

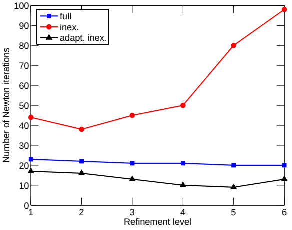


Estimated error distribution

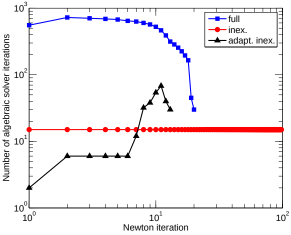


Exact error distribution

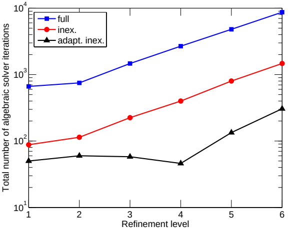
Newton and algebraic iterations: **huge savings**



Newton it. / refinement

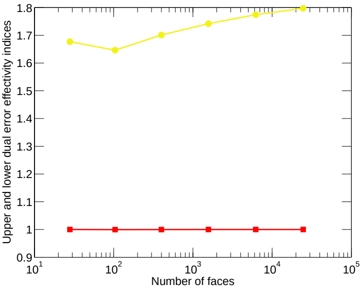


alg. it. / Newton step

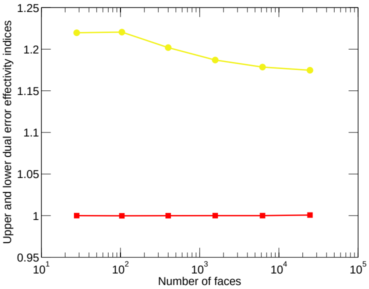


alg. it. / refinement

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



$p = 10$



$p = 1.5$

Numerical experiment II

Model problem

- p-Laplacian

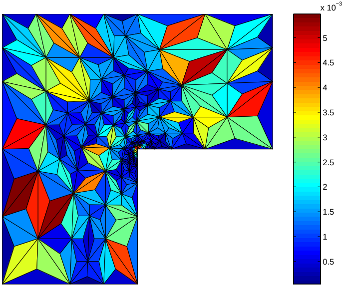
$$\nabla\cdot(|\nabla u|^{p-2}\nabla u) = f \quad \text{in } \Omega,$$
$$u = u_{\mathrm{D}} \quad \text{on } \partial\Omega$$

- weak solution (used to impose the Dirichlet BC)

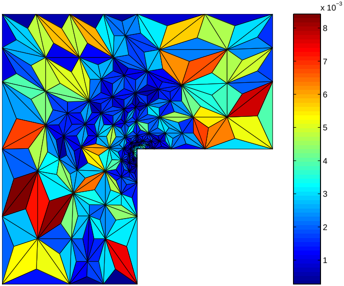
$$u(r,\theta) = r^{\frac{7}{8}} \sin(\theta \tfrac{7}{8})$$

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

Error distribution on an adaptively refined mesh

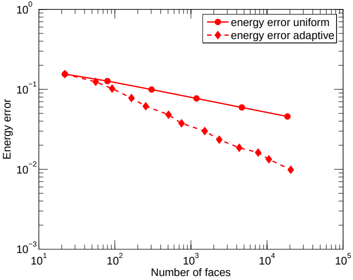


Estimated error distribution

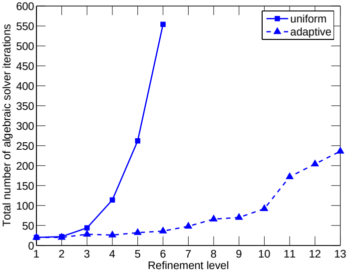


Exact error distribution

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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Global and complementary pressures

Global pressure

$$\mathfrak{p}(s_{\rm w}, p_{\rm w}) := p_{\rm w} + \int_0^{s_{\rm w}} \frac{\lambda_{\rm o}(a)}{\lambda_{\rm w}(a) + \lambda_{\rm o}(a)} p_{\rm c}'(a) {\rm d}a$$

Complementary pressure

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Comments

- necessary for the correct definition of the weak solution
- equivalent Darcy velocities expressions

$$\mathbf{u}_{\rm w}(s_{\rm w}, p_{\rm w}) := -\mathbf{K}(\lambda_{\rm w}(s_{\rm w})\nabla\mathfrak{p}(s_{\rm w}, p_{\rm w}) + \nabla\mathfrak{q}(s_{\rm w}) + \lambda_{\rm w}(s_{\rm w})\rho_{\rm w} g\nabla z),$$
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Weak formulation

Energy space

$$X := L^2((0,T); H^1_{\mathrm{D}}(\Omega))$$

Definition (Weak solution (Arbogast 1992, Chen 2001))

Find $(s_{\mathrm{w}}, p_{\mathrm{w}})$ such that, with $s_{\mathrm{o}} := 1 - s_{\mathrm{w}}$,

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Link energy-type error – dual norm of the residual

Dual norm of the residual on the time interval I_n

$$\mathcal{J}^n_{s_{\rm w},p_{\rm w}}(s_{{\rm w},h\tau},p_{{\rm w},h\tau}) := \left\{\sum_{\alpha\in\{{\rm o},{\rm w}\}}\left\{\sup_{\varphi\in X_n,\,\|\varphi\|_{X_n}=1}\int_{I_n}\{\langle\partial_t(\phi s_\alpha)-\partial_t(\phi s_{\alpha,h\tau}),\varphi\rangle - (\mathbf{u}_\alpha(s_{\rm w},p_{\rm w})-\mathbf{u}_\alpha(s_{{\rm w},h\tau},p_{{\rm w},h\tau}),\nabla\varphi)\}{\rm d}t\right\}^2\right\}^{\frac{1}{2}}$$

Theorem (Link energy-type error – dual norm of the residual)

Let $(s_{\rm w},p_{\rm w})$ be the weak solution. Let $(s_{{\rm w},h\tau},p_{{\rm w},h\tau})$ be arbitrary such that $\mathfrak{p}(s_{{\rm w},h\tau},p_{{\rm w},h\tau})\in X$ and $\mathfrak{q}(s_{{\rm w},h\tau})\in X$ (and satisfying the initial and boundary conditions for simplicity). Then

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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*

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Error components

- $\eta_{\mathrm{sp}}^{n,k,i}$: spatial discretization
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Full adaptivity

- only a **necessary number** of all **solver iterations**
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- 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*

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

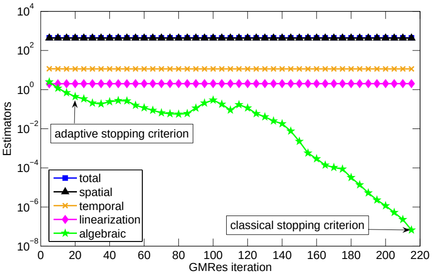
Error components

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

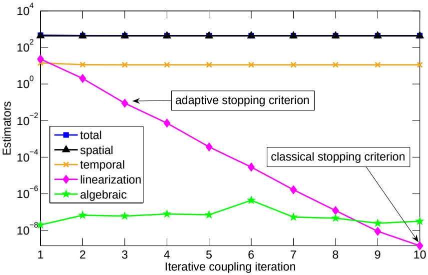
Full adaptivity

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

Estimators and stopping criteria

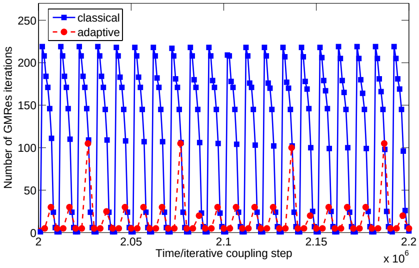


Estimators in function of GMRes iterations

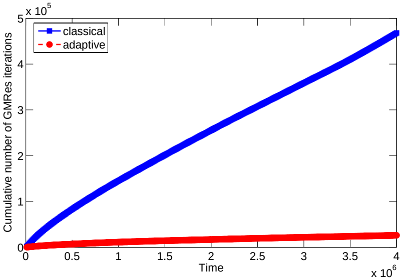


Estimators in function of iterative coupling iterations

GMRes iterations

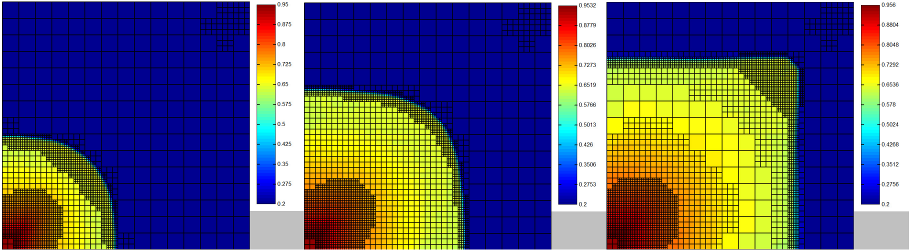


Per time and iterative coupling step



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
- nonlinear problems

Conclusions and outlook

Conclusions

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Ongoing work

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Thank you for your attention!