

The current landscape of energy a posteriori error estimators

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INRIA Paris

28th Chemnitz FEM symposium, September 29, 2015

Outline

- 1 Introduction and the current landscape
 - Optimal properties
 - Various energy a posteriori error estimators
- 2 Equilibrated fluxes in the Laplace case
 - Guaranteed upper bound
 - Polynomial-degree-robust local efficiency
 - Applications
 - Numerical results
- 3 Adaptive inexact Newton method
 - Guaranteed a posteriori error estimate
 - Stopping criteria, efficiency, and robustness
 - Numerical results
- 4 Full adaptivity for unsteady nonlinear problems
- 5 Guaranteed bounds for Laplace eigen-values and -vectors
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What is an a posteriori error estimate

A posteriori error estimate

- Let u be a weak solution of a PDE.
- Let u_h be its approximate numerical solution.
- A priori error estimate: $\|\nabla(u - u_h)\| \leq C(u)h^k$. **Dependent on u , not computable.** Useful in theoretical assessment of convergence.
- A posteriori error estimate: $\|\nabla(u - u_h)\| \leq C\eta(u_h)$. **Only uses u_h , computable.** Great in practical calculation.

Usual form

- Element indicators $\eta_K(u_h)$, $K \in \mathcal{T}_h$.
- Can be used to determine mesh elements with large error.
- We can then refine these elements: mesh adaptivity.

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Model problem

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$$\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega \end{aligned}$$

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

Weak formulation

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

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

Finite element solution

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

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Optimal estimate

- **guaranteed upper bound:**

$$\|\nabla(u - u_h)\| \leq \left\{ \sum_{K \in \mathcal{T}_h} \eta_K(u_h)^2 \right\}^{\frac{1}{2}}$$

- **local efficiency:**

$$\eta_K(u_h) \leq C_{\text{eff}} \|\nabla(u - u_h)\|_{\omega_K} \quad \forall K \in \mathcal{T}_h$$

- **asymptotic exactness:**

$$\frac{\left\{ \sum_{K \in \mathcal{T}_h} \eta_K(u_h)^2 \right\}^{\frac{1}{2}}}{\|\nabla(u - u_h)\|} \rightarrow 1$$

- **robustness:** C_{eff} independent of the parameters (size and shape of Ω , regularity of u , refinement of \mathcal{T}_h , polynomial degree of u_h) (final time, singular perturbation ...)
- **small evaluation cost** of $\eta_K(u_h)$
- **error components identification:** discretization, algebraic (linearization, time stepping ...)

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Residual-based estimates

Theorem (Residual-based estimate, Verfürth (1989))

Let $u \in H_0^1(\Omega)$ be the weak solution and let $u_h \in V_h$ be its FE approximation. Then there exists $C_{\text{up}} > 0$ only depending on d (space dimension) and $\kappa_{\mathcal{T}_h}$ (shape-regularity of \mathcal{T}_h) such that

$$\|\nabla(u - u_h)\| \leq C_{\text{up}} \left\{ \sum_{K \in \mathcal{T}_h} \underbrace{(h_K \|f + \Delta u_h\|_K + h_K^{\frac{1}{2}} \|[\![\nabla u_h]\!] \cdot \mathbf{n}_K\|_{\partial K})^2}_{\eta_{\text{res},K}} \right\}^{\frac{1}{2}}.$$

For C_{low} additionally depending p (polynomial degree),

$$\eta_{\text{res},K} \leq C_{\text{low}} (\|\nabla(u - u_h)\|_{\omega_K} + \|f - \Pi_p f\|_{\omega_K}) \quad \forall K \in \mathcal{T}_h.$$

Properties

- ⊕ rigorous
- ⊕ cheap (explicit)
- ⊖ what is C_{up} ?
- ⊖ C_{low} depends on p

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Averaging estimates

Theorem (Averaging estimate, Zienkiewicz and Zhu (1987))

Let $u \in H_0^1(\Omega)$ and let $u_h \in V_h$ be the FE approximation. Then

$$\|\nabla(u - u_h)\| \lesssim \|\nabla u_h + \sigma_h\|,$$

where $\sigma_h \in [\mathbb{P}_{p'}(\mathcal{T}_h) \cap H^1(\Omega)]^d$ is obtained by local averaging (smoothing) of $-\nabla u_h$.

Properties

- ⊕ cheap (explicit)
- ⊕ often asymptotically exact
- problem-independent
- ⊖ upper bound (may be severely violated on coarse meshes), efficiency (under certain conditions, however, equivalence with residual-based estimates can be shown)

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Functional estimates

Theorem (Functional estimate, \approx Prager and Synge (1947), Hlaváček, Haslinger, Nečas, and Lovíšek (1979), Repin (1997))

Let $u \in H_0^1(\Omega)$ be the weak solution and let $u_h \in H_0^1(\Omega)$ be arbitrary. Let $\sigma_h \in \mathbf{H}(\text{div}, \Omega)$ be arbitrary. Then

$$\|\nabla(u - u_h)\| \leq \|\nabla u_h + \sigma_h\| + h_\Omega \|f - \nabla \cdot \sigma_h\|.$$

Properties

- ⊕ general (no requirement on u_h)
- ⊕ guaranteed upper bound
- ⊖ h_Ω may be large
- ⊖ no local efficiency
- ⊖ potentially expensive (global solve for σ_h)

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The current landscape

Estimator	Guar. bound	Loc. eff.	Asymp. exact.	Rob. data	Rob. ρ	Cost	Maximal overest.	Err. comps.
Residual	✗	✓	✗	✓	✗	explicit	✗	✗
Averaging	✗	✗	✓	✗	✗	explicit	✗	✓
Hierarchical	✗	✓	✓	✓	✓	global	✗	✗
Functional	✓	✗	✓	✗	✗	global	✗	✓
Equil. res.	✗	✓	✓	✓	✗	implicit	✗	✓
Geometric	✗	✗	✓	✗	✗	explicit	✗	✓
Equil. flux	✓	✓	✓	✓	✓	implicit	✓	✓

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Equilibrated flux a posteriori estimate

Properties of the weak solution

- $u \in H_0^1(\Omega)$ (constraint)
- $\sigma := -\nabla u$ (constitutive relation)
- $\nabla \cdot \sigma = f$ (equilibrium)
- $\sigma \in \mathbf{H}(\text{div}, \Omega)$ (constraint)

Theorem (Equilibrated flux estimate, \approx Prager and Synge (1947))

- Let $u \in H_0^1(\Omega)$ be the weak solution;
- $u_h \in H^1(\mathcal{T}_h)$ (piecewise $H^1(K)$) be arbitrary;
- $s_h \in H_0^1(\Omega)$, $\sigma_h \in \mathbf{H}(\text{div}, \Omega)$, $(\nabla \cdot \sigma_h, 1)_K = (f, 1)_K \forall K \in \mathcal{T}_h$.

Then

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

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Global potential and flux reconstructions

Ideally

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

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

- $\mathbf{V}_h \subset \mathbf{H}(\text{div}, \Omega)$, $Q_h \subset L^2(\Omega)$, $V_h \subset H_0^1(\Omega)$
- too expensive, **global minimization** problems (the hypercircle method)

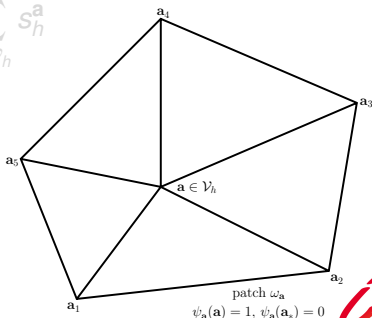
Local potential and flux reconstructions

Partition of unity localization

$$\sigma_h^{\mathbf{a}} := \arg \min_{\mathbf{v}_h \in \mathbf{V}_h^{\mathbf{a}}, \nabla \cdot \mathbf{v}_h = ?} \|\psi_{\mathbf{a}} \nabla u_h + \mathbf{v}_h\|_{\omega_{\mathbf{a}}}$$

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- cut-off by hat basis functions $\psi_{\mathbf{a}} \in \mathbb{P}_1(\mathcal{T}_h) \cap H^1(\Omega)$
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- local minimizations



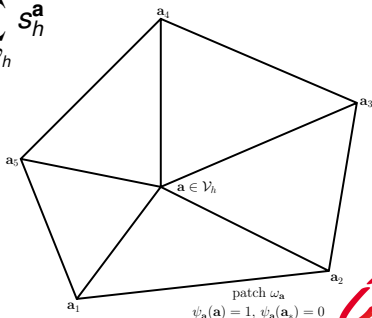
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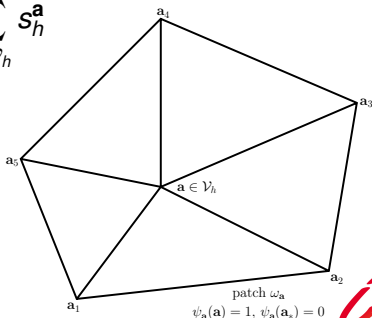
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Local equilibrated flux reconstruction

Assumption A (Galerkin orthogonality wrt hat functions)

There holds $u_h \in H^1(\mathcal{T}_h)$ and

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

$\mathbf{V}_h^{\mathbf{a}} \times Q_h^{\mathbf{a}}$: MFE spaces (hom. Neumann BC for $\mathbf{a} \in \mathcal{V}_h^{\text{int}}$, homogeneous Dirichlet BC on $\partial\omega_{\mathbf{a}} \cap \partial\Omega$ for $\mathbf{a} \in \mathcal{V}_h^{\text{ext}}$)

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$$\Updownarrow$$

$$(\sigma_h^{\mathbf{a}}, \mathbf{v}_h)_{\omega_{\mathbf{a}}} - (\bar{r}_h^{\mathbf{a}}, \nabla \cdot \mathbf{v}_h)_{\omega_{\mathbf{a}}} = -(\psi_{\mathbf{a}} \nabla u_h, \mathbf{v}_h)_{\omega_{\mathbf{a}}} \quad \forall \mathbf{v}_h \in \mathbf{V}_h^{\mathbf{a}},$$

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$V_h^{\mathbf{a}}$: FE space (hom. Dirichlet BC on $\partial\omega_{\mathbf{a}}$ for all $\mathbf{a} \in \mathcal{V}_h$)

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

Let $u_h \in H^1(\mathcal{T}_h)$. For each $\mathbf{a} \in \mathcal{V}_h$, prescribe $s_h^{\mathbf{a}} \in V_h^{\mathbf{a}}$ by solving the **local conforming finite element problem**

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Assumptions

Assumption B (Weak continuity)

There holds $\langle \llbracket u_h \rrbracket, 1 \rangle_e = 0 \quad \forall e \in \mathcal{E}_h.$

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)

Let u be the weak solution. Under *Assumptions A, B, and C*,

$$\|\nabla u_h + \sigma_h\|_K \leq C_{\text{st}} C_{\text{cont,PF}} \sum_{\mathbf{a} \in \mathcal{V}_K} \|\nabla(u - u_h)\|_{\omega_{\mathbf{a}}},$$

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Remarks

- $C_{\text{cont,PF}}$: $\approx 1 + 2/\pi$ on convex patches $\omega_{\mathbf{a}}$
- C_{st} can be bounded by solving the local Neumann problems by conforming FEs: find $r_h^{\mathbf{a}} \in V_h^{\mathbf{a}} \subset H_*^1(\omega_{\mathbf{a}})$ s.t.

$$(\nabla r_h^{\mathbf{a}}, \nabla v_h)_{\omega_{\mathbf{a}}} = -(\psi_{\mathbf{a}} \nabla u_h, \nabla v_h)_{\omega_{\mathbf{a}}} + (\psi_{\mathbf{a}} f - \nabla \psi_{\mathbf{a}} \cdot \nabla u_h, v_h)_{\omega_{\mathbf{a}}} \quad \forall v_h \in V_h^{\mathbf{a}};$$

then the first $C_{\text{st}} \leq \|\psi_{\mathbf{a}} \nabla u_h + \sigma_h^{\mathbf{a}}\|_{\omega_{\mathbf{a}}} / \|\nabla r_h^{\mathbf{a}}\|_{\omega_{\mathbf{a}}}$

- \Rightarrow maximal overestimation factor guaranteed

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- **Assumption A:** take $v_h = \psi_a$
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Discontinuous Galerkin finite elements

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Find $u_h \in V_h$ such that

$$\sum_{K \in \mathcal{T}_h} (\nabla u_h, \nabla v_h)_K - \sum_{e \in \mathcal{E}_h} \{ \langle \{\nabla u_h\} \cdot \mathbf{n}_e, [v_h] \rangle_e + \theta \langle \{\nabla v_h\} \cdot \mathbf{n}_e, [u_h] \rangle_e \} \\ + \sum_{e \in \mathcal{E}_h} \langle \alpha h_e^{-1} [u_h], [v_h] \rangle_e = (f, v_h) \quad \forall v_h \in V_h.$$

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- symmetric version:

$$\|\mathfrak{G}(u_h) + \sigma_h\|_K \leq C_{\text{st}} C_{\text{cont,PF}} \sum_{a \in \mathcal{V}_K} \|\mathfrak{G}(u - u_h)\|_{\omega_a},$$

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$$\|\mathfrak{G}(u_h) + \sigma_h\|_K \leq C_{\text{st}} C_{\text{cont,PF}} \sum_{\mathbf{a} \in \mathcal{V}_K} \|\mathfrak{G}(u - u_h)\|_{\omega_{\mathbf{a}}},$$

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

Discontinuous Galerkin finite elements

Discontinuous Galerkin finite elements

Find $u_h \in V_h$ such that

$$\sum_{K \in \mathcal{T}_h} (\nabla u_h, \nabla v_h)_K - \sum_{e \in \mathcal{E}_h} \{ \langle \{\nabla u_h\} \cdot \mathbf{n}_e, [v_h] \rangle_e + \theta \langle \{\nabla v_h\} \cdot \mathbf{n}_e, [u_h] \rangle_e \} \\ + \sum_{e \in \mathcal{E}_h} \langle \alpha h_e^{-1} [u_h], [v_h] \rangle_e = (f, v_h) \quad \forall v_h \in V_h.$$

- $V_h := \mathbb{P}_p(\mathcal{T}_h)$, $p \geq 1$
- **Assumption A:** take $v_h = \psi_{\mathbf{a}}$ for $\theta = 0$, otherwise estimates for the discrete gradient $\mathfrak{G}(u_h) := \nabla u_h - \theta \sum_{e \in \mathcal{E}_h} \iota_e([u_h])$
- NIPG, IIPG: broken Poincaré–Friedrichs inequality & jumps
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Numerics: smooth test case

Model problem

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega :=]0, 1[^2 \\ u &= u_D && \text{on } \partial\Omega \end{aligned}$$

Exact solution

$$\begin{aligned} u(\mathbf{x}) &= (c_1 + c_2(1 - x_1) + e^{-\alpha x_1})(c_1 + c_2(1 - x_2) + e^{-\alpha x_2}) \\ c_1 &= -e^{-\alpha}, \quad c_2 = -1 - c_1, \quad \alpha = 10 \end{aligned}$$

Discretization

- incomplete interior penalty discontinuous Galerkin method
- unstructured nested triangular grids
- uniform refinement

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Estimates, errors, and effectivity indices

h	p	$\ \nabla(u-u_h)\ $	$\ u-u_h\ _{DG}$	$\ \nabla u_h + \sigma_h\ $	$\ \nabla(u_h-s_h)\ $	η_{osc}	η	η_{DG}	f^{eff}	f_{DG}^{eff}
$h_0/1$	1	1.21E+00	1.22E+00	1.24E+00	1.07E-01	5.56E-02	1.30E+00	1.31E+00	1.07	1.07
$h_0/2$		6.18E-01 (0.97)	6.22E-01 (0.97)	6.38E-01 (0.96)	5.09E-02 (1.07)	7.02E-03 (2.99)	6.47E-01 (1.01)	6.50E-01 (1.01)	1.05	1.05
$h_0/4$		3.12E-01 (0.99)	3.13E-01 (0.99)	3.22E-01 (0.99)	2.43E-02 (1.07)	8.80E-04 (3.00)	3.24E-01 (1.00)	3.25E-01 (1.00)	1.04	1.04
$h_0/8$		1.56E-01 (1.00)	1.57E-01 (1.00)	1.61E-01 (1.00)	1.18E-02 (1.05)	1.10E-04 (3.00)	1.62E-01 (1.00)	1.63E-01 (1.00)	1.04	1.04
$h_0/1$	2	1.50E-01	1.53E-01	1.49E-01	2.76E-02	5.10E-03	1.56E-01	1.59E-01	1.04	1.04
$h_0/2$		3.85E-02 (1.96)	3.92E-02 (1.96)	3.83E-02 (1.96)	7.99E-03 (1.79)	3.22E-04 (3.98)	3.94E-02 (1.98)	4.01E-02 (1.98)	1.03	1.02
$h_0/4$		9.70E-03 (1.99)	9.88E-03 (1.99)	9.68E-03 (1.98)	2.12E-03 (1.92)	2.02E-05 (4.00)	9.93E-03 (1.99)	1.01E-02 (1.99)	1.02	1.02
$h_0/8$		2.43E-03 (1.99)	2.48E-03 (1.99)	2.43E-03 (1.99)	5.42E-04 (1.96)	1.26E-06 (4.00)	2.49E-03 (1.99)	2.54E-03 (1.99)	1.02	1.02
$h_0/1$	3	1.32E-02	1.34E-02	1.29E-02	2.52E-03	3.58E-04	1.35E-02	1.37E-02	1.03	1.03
$h_0/2$		1.67E-03 (2.98)	1.69E-03 (2.98)	1.65E-03 (2.97)	3.13E-04 (3.01)	1.13E-05 (4.99)	1.70E-03 (3.00)	1.71E-03 (3.00)	1.01	1.01
$h_0/4$		2.11E-04 (2.99)	2.13E-04 (2.99)	2.09E-04 (2.99)	3.83E-05 (3.03)	3.53E-07 (5.00)	2.12E-04 (3.00)	2.15E-04 (3.00)	1.01	1.01
$h_0/8$		2.64E-05 (3.00)	2.67E-05 (3.00)	2.61E-05 (3.00)	4.69E-06 (3.03)	1.10E-08 (5.00)	2.66E-05 (3.00)	2.69E-05 (3.00)	1.01	1.01
$h_0/1$	4	9.36E-04	9.54E-04	9.05E-04	2.41E-04	2.12E-05	9.57E-04	9.74E-04	1.02	1.02
$h_0/2$		5.93E-05 (3.98)	6.05E-05 (3.98)	5.77E-05 (3.97)	1.68E-05 (3.84)	3.36E-07 (5.98)	6.04E-05 (3.99)	6.16E-05 (3.98)	1.02	1.02
$h_0/4$		3.72E-06 (3.99)	3.80E-06 (3.99)	3.63E-06 (3.99)	1.10E-06 (3.94)	5.31E-09 (5.98)	3.80E-06 (3.99)	3.87E-06 (3.99)	1.02	1.02
$h_0/8$		2.33E-07 (4.00)	2.38E-07 (4.00)	2.27E-07 (4.00)	7.02E-08 (3.97)	8.30E-11 (6.00)	2.38E-07 (4.00)	2.43E-07 (3.99)	1.02	1.02
$h_0/1$	5	5.41E-05	5.50E-05	5.22E-05	1.38E-05	1.06E-06	5.50E-05	5.58E-05	1.02	1.02
$h_0/2$		1.70E-06 (4.99)	1.72E-06 (5.00)	1.65E-06 (4.98)	4.39E-07 (4.98)	9.35E-09 (6.82)	1.72E-06 (5.00)	1.74E-06 (5.00)	1.01	1.01
$h_0/4$		5.32E-08 (5.00)	5.39E-08 (5.00)	5.19E-08 (4.99)	1.40E-08 (4.97)	7.67E-11 (6.93)	5.38E-08 (5.00)	5.45E-08 (5.00)	1.01	1.01
$h_0/8$		1.66E-09 (5.00)	1.69E-09 (5.00)	1.62E-09 (5.00)	4.41E-10 (4.99)	5.99E-13 (7.00)	1.68E-09 (5.00)	1.70E-09 (5.00)	1.01	1.01

Numerics: singular test case & hp -adaptivity

Model problem

$$\begin{aligned} -\Delta u &= 0 & \text{in } \Omega := \Omega :=]-1, 1[^2 \setminus [0, 1]^2, \\ u &= u_D & \text{on } \partial\Omega \end{aligned}$$

Exact solution

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

Discretization

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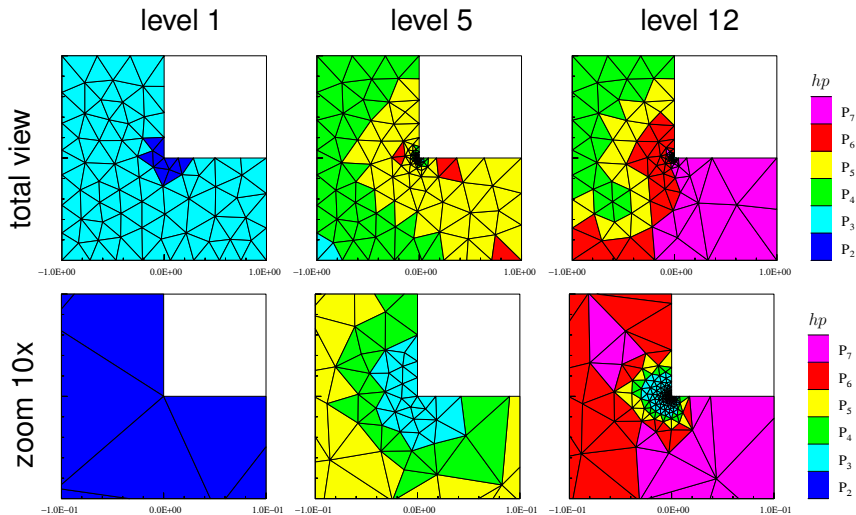
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- incomplete interior penalty discontinuous Galerkin method
- unstructured non-nested triangular grids
- hp -adaptive refinement

hp-refinement grids



Estimates, errors, and effectivity indices

lev	$ T_h $	DoF	$\ \nabla(u - u_h)\ $	$\ \nabla u_h + \sigma_h\ $	η_{osc}	$\ \nabla(u_h - s_h)\ $	η_{BC}	η	ρ^{eff}
0	114	684	6.22E-02	6.63E-02	1.89E-15	4.48E-02	3.81E-02	1.05E-01	1.69
1	122	1180	4.28E-02	4.27E-02	1.18E-14	3.08E-02	2.92E-02	7.29E-02	1.70
2	139	1919	3.28E-02	3.37E-02	8.21E-14	2.09E-02	2.12E-02	5.36E-02	1.64
3	165	2573	2.32E-02	2.30E-02	3.88E-13	1.50E-02	1.03E-02	3.41E-02	1.47
4	174	2858	1.02E-02	1.01E-02	4.48E-13	8.22E-03	9.19E-03	1.99E-02	1.96
5	199	3351	6.27E-03	6.21E-03	1.12E-12	4.81E-03	6.18E-03	1.25E-02	2.00
6	237	3926	4.21E-03	4.23E-03	1.98E-12	3.15E-03	3.29E-03	7.66E-03	1.82
7	285	4537	2.84E-03	2.91E-03	7.47E-12	2.13E-03	2.42E-03	5.33E-03	1.88
8	338	5257	2.04E-03	2.19E-03	4.63E-11	1.45E-03	1.32E-03	3.51E-03	1.72
9	372	5658	1.21E-03	1.23E-03	1.11E-11	9.07E-04	9.99E-04	2.26E-03	1.87
10	426	6500	7.70E-04	7.69E-04	5.69E-11	5.55E-04	6.95E-04	1.46E-03	1.89
11	453	7010	4.95E-04	5.04E-04	9.77E-11	3.97E-04	4.74E-04	9.91E-04	2.00
12	469	7308	3.41E-04	3.47E-04	1.13E-10	2.55E-04	2.88E-04	6.40E-04	1.88
13	463	7286	2.42E-04	2.42E-04	1.39E-10	1.73E-04	1.94E-04	4.37E-04	1.81
14	458	7215	1.69E-04	1.69E-04	1.23E-10	1.19E-04	1.53E-04	3.17E-04	1.88
15	440	6955	1.29E-04	1.31E-04	1.45E-10	9.21E-05	9.10E-05	2.24E-04	1.73
16	435	7035	9.71E-05	9.91E-05	1.39E-10	6.89E-05	7.63E-05	1.74E-04	1.79
17	434	7167	8.52E-05	8.97E-05	1.41E-10	5.76E-05	5.47E-05	1.42E-04	1.67
18	419	6960	7.51E-05	7.97E-05	1.44E-10	5.00E-05	4.15E-05	1.21E-04	1.60
19	410	6838	6.06E-05	6.35E-05	1.47E-10	3.87E-05	3.65E-05	9.69E-05	1.60

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Inexact iterative linearization

System of nonlinear algebraic equations

Nonlinear operator $\mathcal{A} : \mathbb{R}^N \rightarrow \mathbb{R}^N$, 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 $k := 1$.
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$$\mathbb{A}^{k-1} U^k \approx F^{k-1}.$$
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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**: $A(u) = f$

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

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**: $A(u) = f$

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?

Model steady problem, discretization

Quasi-linear elliptic problem

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

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

$$(\bar{\sigma}(u, \nabla u), \nabla v) = (f, v) \quad \forall v \in V$$

Numerical approximation

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

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Abstract assumptions

Assumption A (Total flux reconstruction)

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

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

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

There exist fluxes $\mathbf{d}_h^{k,i}, \mathbf{l}_h^{k,i}, \mathbf{a}_h^{k,i} \in [L^q(\Omega)]^d$ such that

- (i) $\sigma_h^{k,i} = \mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i} + \mathbf{a}_h^{k,i}$;
- (ii) as the linear solver converges, $\|\mathbf{a}_h^{k,i}\|_q \rightarrow 0$;
- (iii) as the nonlinear solver converges, $\|\mathbf{l}_h^{k,i}\|_q \rightarrow 0$.

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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

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

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Stopping criteria and efficiency

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

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

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

$$\eta_{\text{lin}}^{k,i} \leq \gamma_{\text{lin}} \eta_{\text{disc}}^{k,i}$$

Theorem (Global efficiency)

Under the global stopping criteria and the usual assumptions,

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

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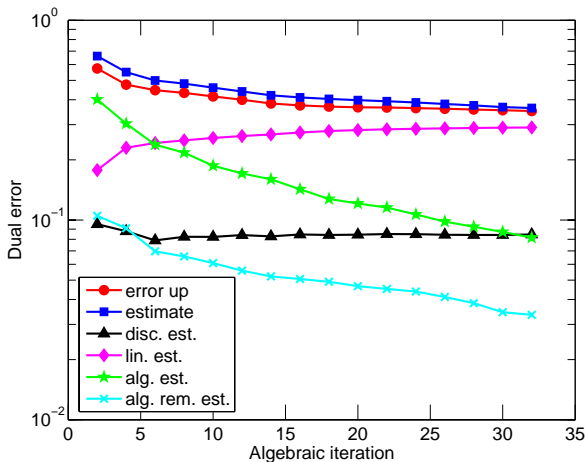
where C is *independent* of $\bar{\sigma}$ and q .

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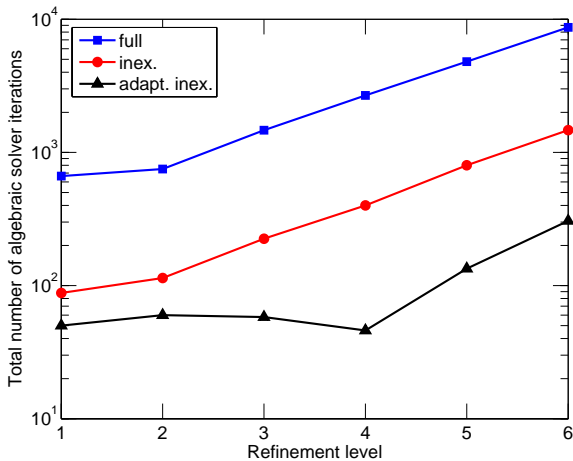
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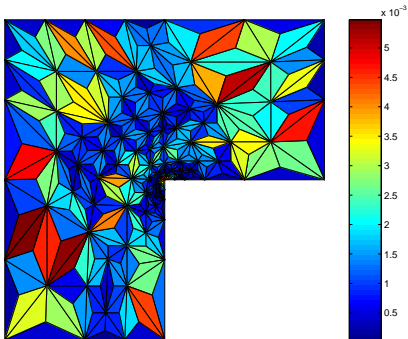
Error and estimators as a function of CG iterations, regular 10-Laplacian, 6th level mesh, 6th Newton step.



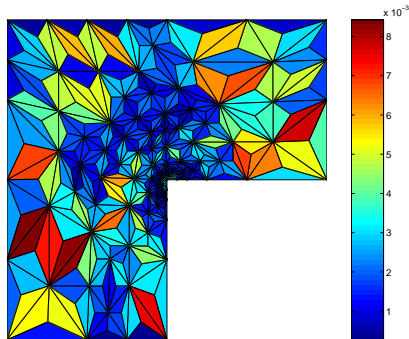
Overall algebraic solver iterations, regular 10-Laplacian



Full adaptivity, singular 4-Laplacian



Estimated error distribution



Exact error distribution

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Two-phase flow in porous media

Two-phase flow in porous media

$$\begin{aligned} \partial_t(\phi \mathbf{s}_\alpha) + \nabla \cdot \mathbf{u}_\alpha &= q_\alpha, & \alpha \in \{o, w\}, \\ -\lambda_\alpha(\mathbf{s}_w) \underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha \mathbf{g} \nabla z) &= \mathbf{u}_\alpha, & \alpha \in \{o, w\}, \\ \mathbf{s}_o + \mathbf{s}_w &= 1, \\ \rho_o - \rho_w &= \rho_c(\mathbf{s}_w) \end{aligned}$$

+ boundary & initial conditions

Mathematical issues

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

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- coupled system
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Global and complementary pressures

Global pressure

$$p(s_w, p_w) := p_w + \int_0^{s_w} \frac{\lambda_o(a)}{\lambda_w(a) + \lambda_o(a)} p'_c(a) da$$

Complementary pressure

$$q(s_w) := - \int_0^{s_w} \frac{\lambda_w(a)\lambda_o(a)}{\lambda_w(a) + \lambda_o(a)} p'_c(a) da$$

Comments

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

$$\mathbf{u}_w(s_w, p_w) := -\mathbf{K}(\lambda_w(s_w)\nabla p(s_w, p_w) + \nabla q(s_w) + \lambda_w(s_w)\rho_w g \nabla Z),$$

$$\mathbf{u}_o(s_w, p_w) := -\mathbf{K}(\lambda_o(s_w)\nabla p(s_w, p_w) - \nabla q(s_w) + \lambda_o(s_w)\rho_o g \nabla Z)$$

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Weak formulation

Energy space

$$X := L^2((0, T); H_D^1(\Omega))$$

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

Find (s_w, p_w) such that, with $s_o := 1 - s_w$,

$$s_w \in C([0, T]; L^2(\Omega)), \quad s_w(\cdot, 0) = s_w^0,$$

$$\partial_t s_w \in L^2((0, T); (H_D^1(\Omega))'),$$

$$p(s_w, p_w) \in X,$$

$$q(s_w) \in X,$$

$$\int_0^T \{ \langle \partial_t(\phi s_\alpha), \varphi \rangle - (\mathbf{u}_\alpha(s_w, p_w), \nabla \varphi) - (q_\alpha, \varphi) \} dt = 0$$

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Link energy-type error – dual norm of the residual

Dual norm of the residual on the time interval I_n

$$\mathcal{J}_{\mathbf{s}_w, \rho_w}^n(\mathbf{s}_w, h_\tau, \rho_w, h_\tau) := \left\{ \sum_{\alpha \in \{o, w\}} \left\{ \sup_{\varphi \in X_n, \|\varphi\|_{X_n} = 1} \int_{I_n} \left\{ \langle \partial_t(\phi \mathbf{s}_\alpha) - \partial_t(\phi \mathbf{s}_{\alpha, h_\tau}), \varphi \rangle - (\mathbf{u}_\alpha(\mathbf{s}_w, \rho_w) - \mathbf{u}_\alpha(\mathbf{s}_w, h_\tau, \rho_w, h_\tau), \nabla \varphi) \right\} dt \right\}^2 \right\}^{\frac{1}{2}}$$

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

Let (\mathbf{s}_w, ρ_w) be the *weak solution*. Let $(\mathbf{s}_w, h_\tau, \rho_w, h_\tau)$ be *arbitrary* such that $\mathbf{p}(\mathbf{s}_w, h_\tau, \rho_w, h_\tau) \in X$ and $\mathbf{q}(\mathbf{s}_w, h_\tau) \in X$ (and satisfying the initial and boundary conditions for simplicity). Then

$$\begin{aligned} & \|\mathbf{s}_w - \mathbf{s}_w, h_\tau\|_{L^2((0, T); H^{-1}(\Omega))} + \|\mathbf{q}(\mathbf{s}_w) - \mathbf{q}(\mathbf{s}_w, h_\tau)\|_{L^2(\Omega \times (0, T))} \\ & + \|\mathbf{p}(\mathbf{s}_w, \rho_w) - \mathbf{p}(\mathbf{s}_w, h_\tau, \rho_w, h_\tau)\|_{L^2((0, T); H_0^1(\Omega))} \\ & \leq C \left\{ \sum_{n=1}^N \mathcal{J}_{\mathbf{s}_w, \rho_w}^n(\mathbf{s}_w, h_\tau, \rho_w, h_\tau)^2 \right\}^{\frac{1}{2}}. \end{aligned}$$

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$$\mathcal{J}_{\mathbf{s}_w, \mathbf{p}_w}^n(\mathbf{s}_{w, h\tau}, \mathbf{p}_{w, h\tau}) := \left\{ \sum_{\alpha \in \{o, w\}} \left\{ \sup_{\varphi \in X_n, \|\varphi\|_{X_n} = 1} \int_{I_n} \left\{ \langle \partial_t(\phi \mathbf{s}_\alpha) - \partial_t(\phi \mathbf{s}_{\alpha, h\tau}), \varphi \rangle - (\mathbf{u}_\alpha(\mathbf{s}_w, \mathbf{p}_w) - \mathbf{u}_\alpha(\mathbf{s}_{w, h\tau}, \mathbf{p}_{w, h\tau}), \nabla \varphi) \right\} dt \right\}^2 \right\}^{\frac{1}{2}}$$

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

Let $(\mathbf{s}_w, \mathbf{p}_w)$ be the *weak solution*. Let $(\mathbf{s}_{w, h\tau}, \mathbf{p}_{w, h\tau})$ be *arbitrary* such that $\mathbf{p}(\mathbf{s}_{w, h\tau}, \mathbf{p}_{w, h\tau}) \in X$ and $\mathbf{q}(\mathbf{s}_{w, h\tau}) \in X$ (and satisfying the initial and boundary conditions for simplicity). Then

$$\begin{aligned} & \|\mathbf{s}_w - \mathbf{s}_{w, h\tau}\|_{L^2((0, T); H^{-1}(\Omega))} + \|\mathbf{q}(\mathbf{s}_w) - \mathbf{q}(\mathbf{s}_{w, h\tau})\|_{L^2(\Omega \times (0, T))} \\ & + \|\mathbf{p}(\mathbf{s}_w, \mathbf{p}_w) - \mathbf{p}(\mathbf{s}_{w, h\tau}, \mathbf{p}_{w, h\tau})\|_{L^2((0, T); H_0^1(\Omega))} \\ & \leq C \left\{ \sum_{n=1}^N \mathcal{J}_{\mathbf{s}_w, \mathbf{p}_w}^n(\mathbf{s}_{w, h\tau}, \mathbf{p}_{w, h\tau})^2 \right\}^{\frac{1}{2}}. \end{aligned}$$

Distinguishing the error components

Theorem (Distinguishing the error components)

Consider a vertex-centered finite volume / backward Euler approximation and Newton linearization. Let

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

with the approximations $(s_{w,h_T}^{n,k,i}, p_{w,h_T}^{n,k,i})$. Then

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

Error components

- $\eta_{sp}^{n,k,i}$: spatial discretization
- $\eta_{tm}^{n,k,i}$: temporal discretization
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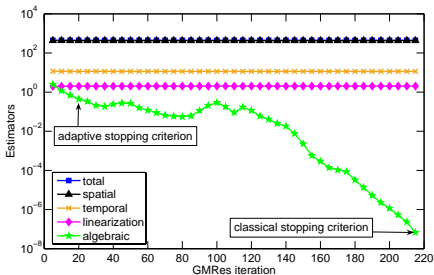
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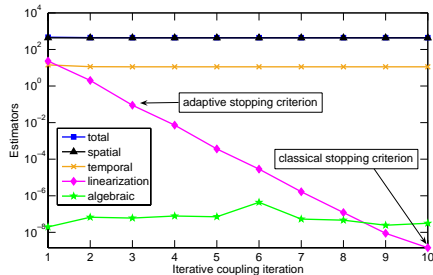
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Estimators and stopping criteria

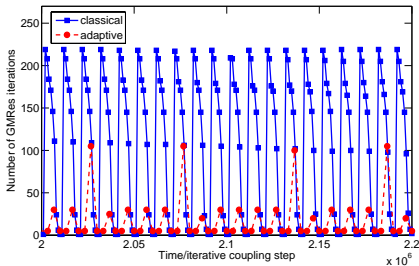


Estimators in function of GMRes iterations

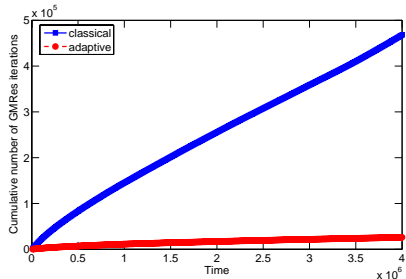


Estimators in function of iterative coupling iterations

GMRes iterations

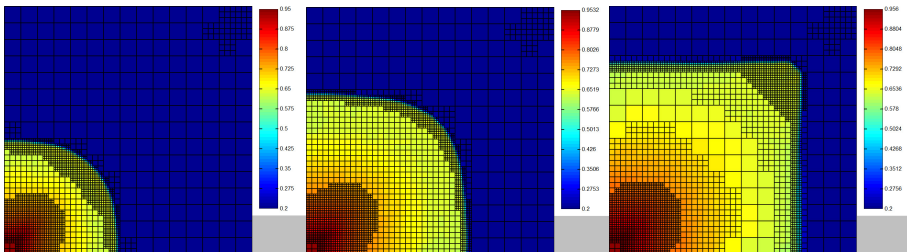


Per time and iterative
coupling step



Cumulated

Space/time/nonlinear solver/linear solver adaptivity



Fully adaptive computation

Full adaptivity

Full adaptivity

- only a **necessary number** of **algebraic/linearization solver iterations**
- adaptive **regularization**, **model adaptation**, adaptive choice of the **scheme parameters**
- **“online decisions”**: algebraic step / linearization step / space mesh refinement / time step modification
- important computational savings

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Setting

Laplace eigenvalue problem

Find **eigenvector** & **eigenvalue** pair (u, λ) such that $\|u\| = 1$ and

$$\begin{aligned} -\Delta u &= \lambda u && \text{in } \Omega \subset \mathbb{R}^d, d = 2, 3, \\ u &= 0 && \text{on } \partial\Omega. \end{aligned}$$

Full problem, weak formulation

Find $(u_k, \lambda_k) \in V := H_0^1(\Omega) \times \mathbb{R}^+$ with $\|u_k\| = 1$, $k \geq 1$, s. t.

$$(\nabla u_k, \nabla v) = \lambda_k (u_k, v) \quad \forall v \in V$$

- $0 < \lambda_1 < \lambda_2 \leq \dots \leq \lambda_k \rightarrow \infty$

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Approximate solution and assumptions

Assumption A (Conforming variational solution)

There holds

- $(u_h, \lambda_h) \in V \times \mathbb{R}^+$
- $\|u_h\| = 1$
- $(u_h, \mathbf{1}) > 0$
- $\|\nabla u_h\|^2 = \lambda_h$

Assumption B (Galerkin orthogonality of the residual to ψ_a)

There holds, for all $\mathbf{a} \in \mathcal{V}_h^{\text{int}}$,

$$\lambda_h(u_h, \psi_a)_{\omega_a} - (\nabla u_h, \nabla \psi_a)_{\omega_a} = 0.$$

Assumption C (Piecewise polynomial form)

There holds $u_h \in \mathbb{P}_p(\mathcal{T}_h)$, $p \geq 1$, and the mixed finite element spaces $\mathbf{V}_h \times Q_h$ are of degree $p + 1$.

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Guaranteed bounds for the first eigenvalue

Theorem (Eigenvalue bounds)

Let $0 < \underline{\lambda}_2 \leq \lambda_2$ and $0 < \underline{\lambda}_1 \leq \lambda_1$. Let **Assumptions A and B** hold and let $\lambda_h < \underline{\lambda}_2$. Let σ_h be an equilibrated flux and let

$$\underbrace{\beta_h}_{\downarrow 0} := \frac{1}{\sqrt{\underline{\lambda}_1}} \left(1 - \frac{\lambda_h}{\underline{\lambda}_2}\right)^{-1} \|\nabla u_h + \sigma_h\| < 1,$$

$$\underbrace{\alpha_h^2}_{\downarrow 0} := 2 \left(1 - \sqrt{1 - \beta_h^2}\right) \leq |\Omega|^{-1} (u_h, 1)^2.$$

Then

$$\lambda_1 \geq \lambda_h - \overbrace{\left(1 - \frac{\lambda_h}{\underline{\lambda}_2}\right)^{-2} \left(1 - \frac{\alpha_h^2}{4}\right)^{-1}}^{\eta^2} \|\nabla u_h + \sigma_h\|^2,$$

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Guaranteed bounds for the first eigenvector

Theorem (Eigenvector bounds)

Let the assumptions of the eigenvalue theorem be verified.

Then

$$\|\nabla(u_1 - u_h)\| \leq \eta.$$

Moreover, under Assumption C,

$$\eta \leq (d+1) C_{\text{cont,PF}} C_{\text{st}} \underbrace{\left(\frac{\|\nabla(u_1 - u_h)\|^2}{\lambda_1} + 1 \right)^{\frac{1}{2}}}_{\downarrow 1}$$

$$\underbrace{\left(1 - \frac{\lambda_h}{\lambda_2}\right)^{-1}}_{\downarrow \left(1 - \frac{\lambda_1}{\lambda_2}\right)^{-1}} \underbrace{\left(1 - \frac{\alpha_h^2}{4}\right)^{-\frac{1}{2}}}_{\downarrow 1} \|\nabla(u_1 - u_h)\|.$$

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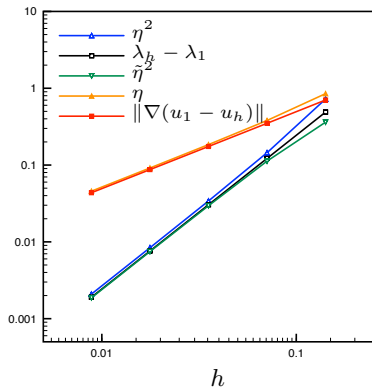
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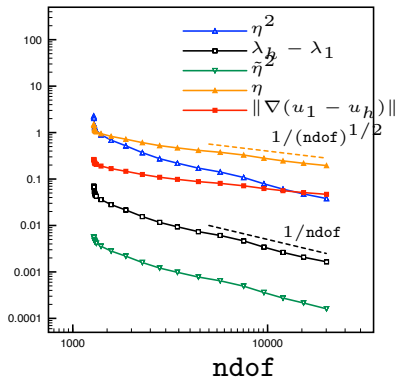
$$\eta \leq (d+1) C_{\text{cont,PF}} C_{\text{st}} \underbrace{\left(\frac{\|\nabla(u_1 - u_h)\|^2}{\lambda_1} + 1 \right)^{\frac{1}{2}}}_{\downarrow 1}$$

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Guaranteed eigenvalue and eigenvector bounds



Square, uniform refinement



L-shape, adaptive refinement

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Previous results (Laplace)

Global flux reconstructions

- Prager and Synge (1947):

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

for **any** $u_h \in H_0^1(\Omega)$ and **any** $\sigma_h \in \mathbf{H}(\text{div}, \Omega)$ s.t. $\nabla \cdot \sigma_h = f$

- Hlaváček, Haslinger, Nečas, and Lovíšek (1979), Repin (1997), . . . : **global construction** of σ_h : unprecise/costly

Local flux reconstructions

- Ladevèze and Leguillon (1983), equilibrated face fluxes
- Destuynder and Métivet (1999), discrete flux σ_h
- Luce and Wohlmuth (2004), local efficiency proof
- Kim (2007), Ainsworth (2007), Ern, Nicaise, and Vohralík (2007), discontinuous Galerkin method elementwise prescription
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Previous results (nonlinear and stopping criteria)

A posteriori error estimates for numerical discretizations of nonlinear problems

- Ladevèze (since 1990's), guaranteed upper bound
- Verfürth (1994), residual estimates
- Chaillou and Suri (2006, 2007), distinguishing discretization and linearization errors

Stopping criteria for algebraic solvers

- Becker, Johnson, and Rannacher (1995), multigrid stopping criterion
- Arioli (2000's), comparison of the algebraic and discretization errors

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Previous results (unsteady nonlinear)

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- Gallimard, Ladevèze, Pelle (1997), const. rel. estimates
- Verfürth (1998), framework for energy control, efficiency
- Ohlberger (2001), non-energy estimates, hyperbolic limit
- Akrivis, Makridakis, and Nochetto (2006), higher-order temporal discretizations

Degenerate parabolic problems

- Nochetto, Schmidt, Verdi (2000), Stefan problem

Two-phase flows

- Chen and Ewing (2003), mesh adaptivity

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Previous results (eigenproblems)

Eigenvalues

- Carstensen and Gedicke (2014): guaranteed bound, lowest-order nonconforming FEs
- Hu, Huang, Lin (2014): nonconforming FEs (saturation assumption may be necessary)
- Šebestová and Vejchodský (2014), Kuznetsov and Repin (2013): guaranteed bounds (condition on applicability, suboptimal convergence speed)
- Liu and Oishi (2013): guaranteed bound, lowest-order conforming FEs (auxiliary eigenvalue problem)

Eigenvectors

- Rannacher, Westenberger, Wollner (2010), Grubišić and Ovall (2009), Durán, Padra, Rodríguez (2003), Heuveline and Rannacher (2002), Larson (2000), Maday and Patera (2000), Verfürth (1994) (uncomputable higher-order terms)

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- CANCÈS E., DUSSON G., MADAY Y., STAMM B., VOHRALÍK M., Guaranteed and robust a posteriori bounds for Laplace eigenvalues and eigenvectors: conforming approximations, HAL Preprint 01194364.
- ERN A., VOHRALÍK M., Adaptive inexact Newton methods with a posteriori stopping criteria for nonlinear diffusion PDEs, *SIAM J. Sci. Comput.* **35** (2013), A1761–A1791.
- CANCÈS C., POP I. S., VOHRALÍK M., An a posteriori error estimate for vertex-centered finite volume discretizations of immiscible incompressible two-phase flow, *Math. Comp.* **83** (2014), 153–188.

Thank you for your attention!

