Guaranteed a posteriori error bounds and discretization–linearization–algebraic resolution adaptivity in numerical approximations of model PDEs

Martin Vohralík

en collaboration avec S. Ali Hassan, C. Cancès, E. Cancès, P. Daniel, V. Dolejší, G. Dusson, A. Ern, C. Japhet, M. Kern, Y. Maday, J. Papež, I. S. Pop, U. Rüde, I. Smears, B. Stamm, M. F. Wheeler, & B. Wohlmuth

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Outline

Optimal a posteriori error estimate

Guaranteed upper bound

- $\|u - u_h\|_{?,\Omega}^2 \leq \sum_{K \in \mathcal{T}_h} \eta_K(u_h)^2$
- no undetermined constant: **error control**

Local efficiency

- $\eta_K(u_h) \leq C_{\text{eff}} \|u - u_h\|_{?,\text{neighbors of } K}$
- **local** error lower bound (optimal space mesh refinement)

Robustness

- C_{eff} independent of data (diffusion, reaction), **nonlinearity**, domain Ω, meshes, solution u, **polynomial degree** of u_h

Asymptotic exactness

- $\sum_{K \in \mathcal{T}_h} \eta_K(u_h)^2 / \|u - u_h\|_{?,\Omega}^2 \searrow 1$
- overestimation factor goes to one with increasing effort

Small evaluation cost

- estimators $\eta_K(u_h)$ can be evaluated cheaply (locally)

Error components identification

- $\eta_K(u_h)$ can distinguish different error components

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   - Applications & numerical results
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3. Nonlinear Laplace equation: adaptive stopping criteria
   - Adaptive inexact Newton method
   - Applications & numerical results
4. Laplace eigenvalues and eigenvectors: guaranteed bounds
   - Applications & numerical results
5. Two-phase flow in porous media: industrial application
6. Conclusions and outlook

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)
- $\sigma \in \mathbf{H}(\mathrm{div}, \Omega)$ (dual variable constraint)

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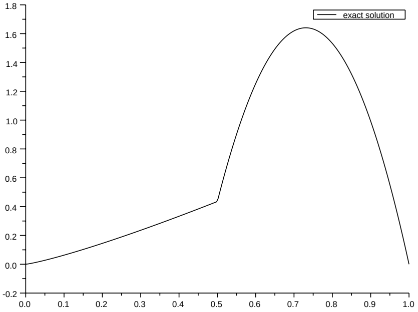
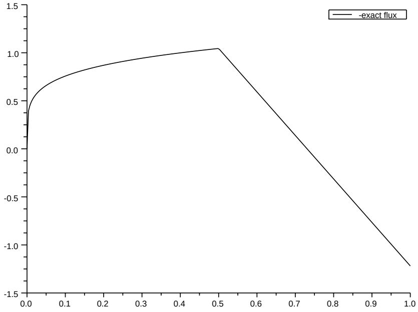
Exact solution and flux

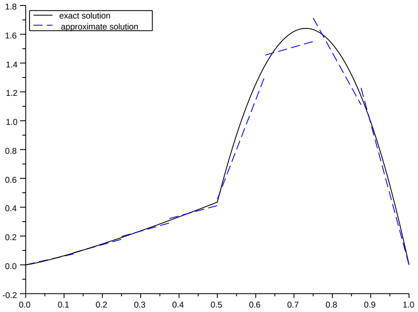


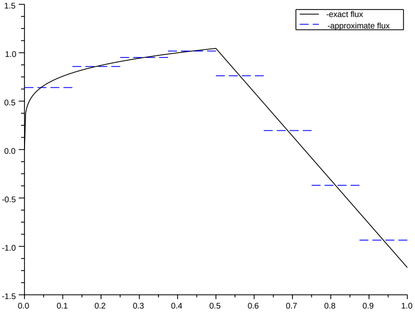


Solution u is continuous

Flux $\boldsymbol{\sigma} := -\underline{\mathbf{K}}\nabla u$ is continuous

Approximate solution and flux

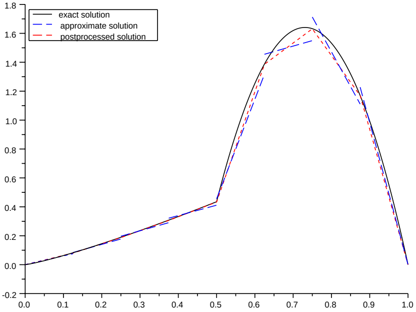




Approximate solution u_h is not necessarily continuous

Approximate flux $-\underline{\mathbf{K}}\nabla u_h$ is not necessarily continuous

Potential and flux reconstructions



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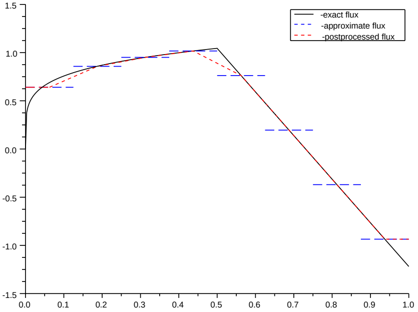

Flux reconstruction

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Theorem (A guaranteed a posteriori error estimate, Prager and Synge (1947), Ladevèze (1975), Dari, Durán, Padra, & Vampa (1996), Ainsworth (2005), Kim (2007), Vohralík (2007), ...)

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

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

Then

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

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Global potential and flux reconstructions

Ideally

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

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

✓ computable, discrete spaces $V_h \subset H_0^1(\Omega)$, $\mathbf{V}_h \subset \mathbf{H}(\mathrm{div}, \Omega)$, $Q_h \subset L^2(\Omega)$

✗ too expensive, **global** minimization problems (the hypercircle method ...)

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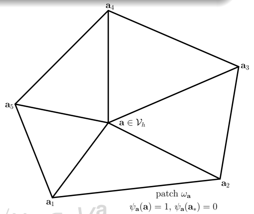
Local potential reconstruction

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**

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



Equivalent form

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Key ideas

- **local** minimizations
- cut-off by hat basis functions $\psi_{\mathbf{a}}$
- $V_h^{\mathbf{a}} \subset H_0^1(\omega_{\mathbf{a}})$: homogeneous Dirichlet BC on $\partial\omega_{\mathbf{a}}$
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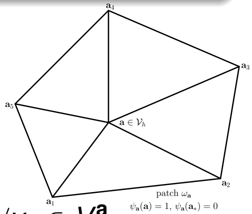

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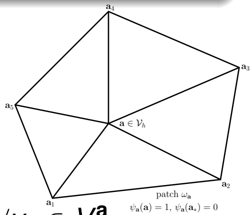

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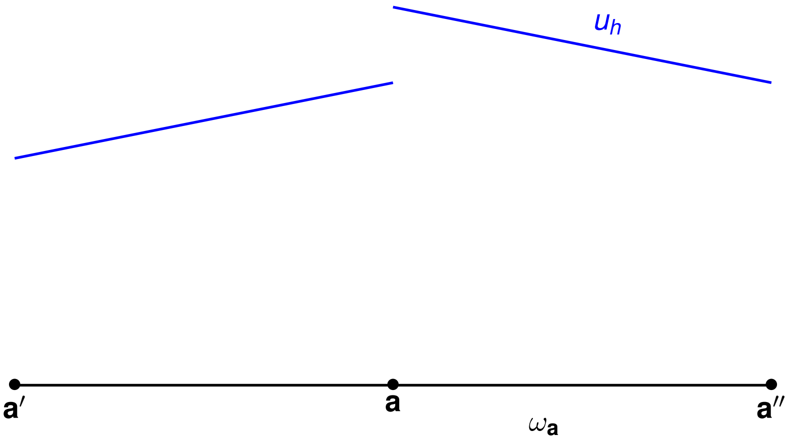

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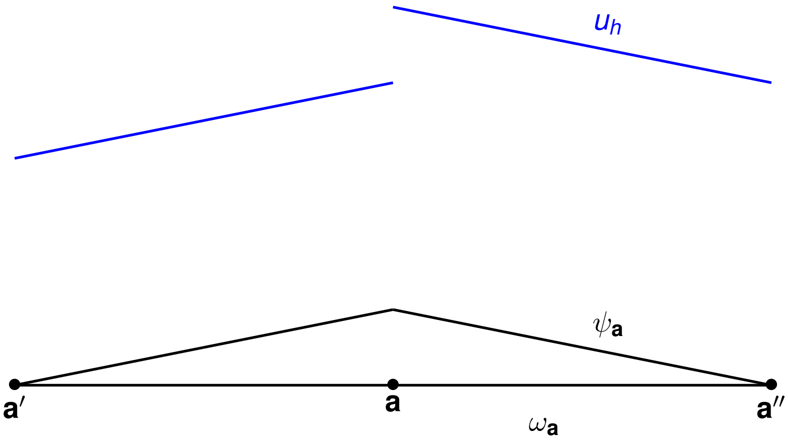

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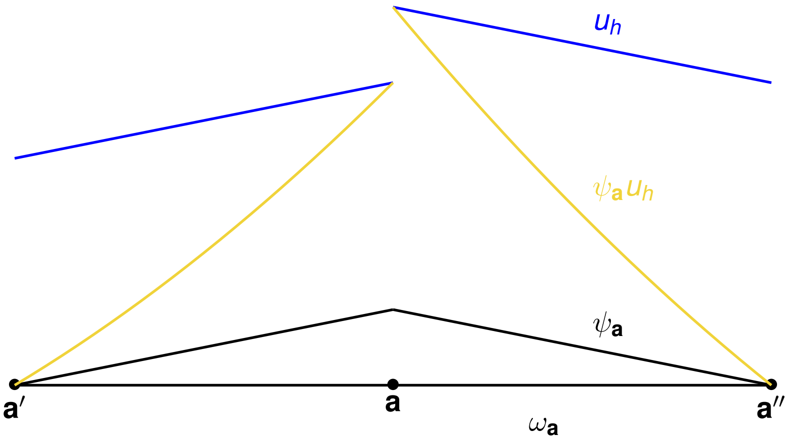

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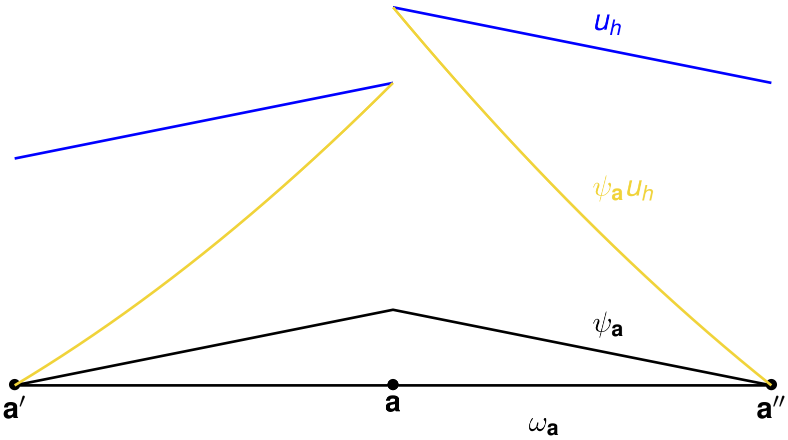
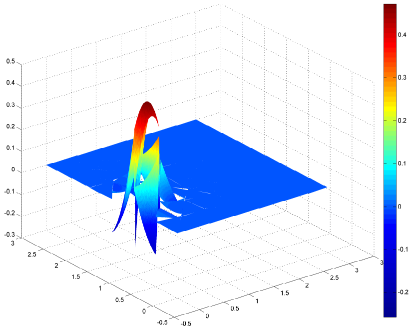


Potential reconstruction in 2D



Potential u_h

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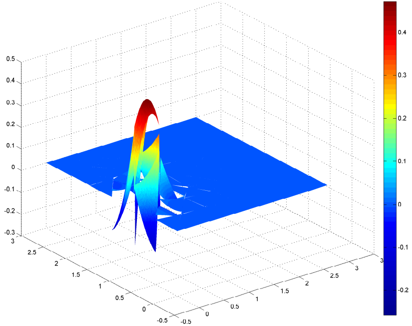
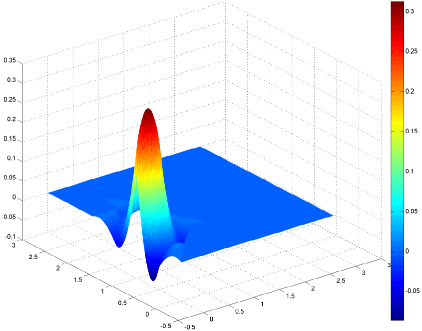


Potential u_h



Potential reconstruction s_h

Local flux reconstructions

Assumption A (Galerkin orthogonality wrt hat functions)

There holds

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

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**

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

Key points

- $\mathbf{V}_h^{\mathbf{a}} \subset \mathbf{H}(\mathrm{div}, \omega_{\mathbf{a}})$: homogeneous Neumann BC on $\partial\omega_{\mathbf{a}}$
- $\boldsymbol{\sigma}_h := \sum_{\mathbf{a}\in\mathcal{V}_h} \boldsymbol{\sigma}_h^{\mathbf{a}}$

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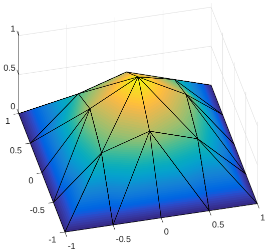
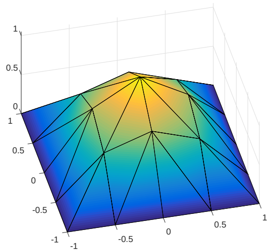
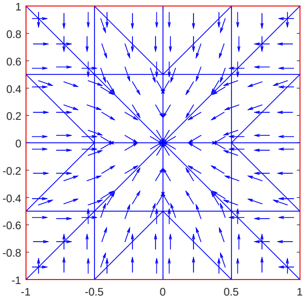
Equilibrated flux reconstruction



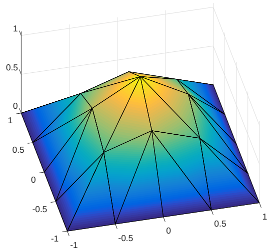
Equilibrated flux reconstruction

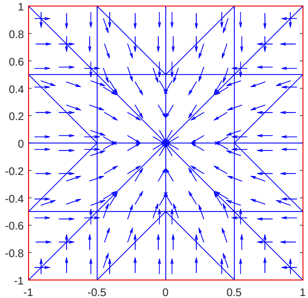




Flux $-\nabla u_h$

Equilibrated flux reconstruction





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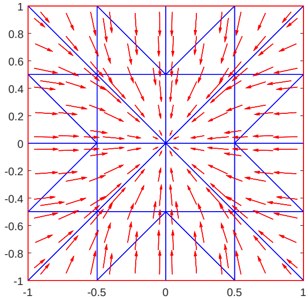

Flux reconstruction $\boldsymbol{\sigma}_h$

Outline

Polynomial-degree-robust efficiency

Assumption B (Piecewise polynomials, data, and meshes)

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

Theorem (Polynomial-degree-robust efficiency Braess, Pillwein, and Schöberl (2009); Costabel and McIntosh (2010); Demkowicz, Gopalakrishnan, and Schöberl (2012), EV (2015, 2016)**)**

Let u be the weak solution and let Assumptions A and B 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

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

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

Remarks

- equivalence error–estimate
- maximal overestimation factor guaranteed

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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 $v_h = \psi_{\mathbf{a}}$

✓ Assumption B: technical, always satisfied

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$$\langle [\![v_h]\!], q_h \rangle_e = 0 \qquad \forall q_h \in \mathbb{P}_{p-1}(e), \forall e \in \mathcal{E}_h$$

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Discontinuous Galerkin finite elements

Discontinuous Galerkin finite elements

Find $u_h \in V_h$ such that

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

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- estimates for the discrete gradient

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

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- $\Rightarrow$ modified Galerkin orthogonality

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Numerics: smooth case

Model problem

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

Exact solution

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

Discretization

- symmetric interior penalty discontinuous Galerkin method: $u_h \notin H_0^1(\Omega)$
- unstructured triangular grids
- uniform h and p refinement

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How large is the overall error? (model pb, known sol.)

h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\|\nabla u_h\|}$	$\|\nabla(u-u_h)\|$	rel. error $\frac{\|\nabla(u-u_h)\|}{\|\nabla u_h\|}$	$I^{\mathrm{eff}} = \frac{\eta(u_h)}{\|\nabla(u-u_h)\|}$
h_0	1	1.3	$2.8 \times 10^{1}\%$	1.1	$2.4 \times 10^{1}\%$	1.17
$\approx h_0/2$		6.1×10^{-1}	$1.4 \times 10^{1}\%$	5.6×10^{-1}	$1.3 \times 10^{1}\%$	1.09
$\approx h_0/4$		3.1×10^{-1}	7.0%	2.9×10^{-1}	6.6%	1.06
$\approx h_0/8$		1.5×10^{-1}	3.3%	1.4×10^{-1}	3.1%	1.04
h_0	2	1.6×10^{-1}	3.7%	1.5×10^{-1}	3.5%	1.06
$\approx h_0/2$	2	4.2×10^{-2}	$9.5 \times 10^{-1}\%$	4.1×10^{-2}	$9.2 \times 10^{-1}\%$	1.04
h_0	3	1.4×10^{-2}	$3.2 \times 10^{-1}\%$	1.4×10^{-2}	$3.1 \times 10^{-1}\%$	1.03
$\approx h_0/4$	3	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	1.01
h_0	4	1.0×10^{-3}	$2.3 \times 10^{-2}\%$	9.9×10^{-4}	$2.2 \times 10^{-2}\%$	1.02
$\approx h_0/8$	4	2.6×10^{-7}	$5.9 \times 10^{-6}\%$	2.6×10^{-7}	$5.8 \times 10^{-6}\%$	1.01

A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

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h_0	2	1.6×10^{-1}	3.7%	1.5×10^{-1}	3.5%	1.06
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Numerics: smooth case with localized features

Model problem

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\begin{aligned}
-\Delta u &= f \quad \text{in } \Omega := (-1,1)^2, \\
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$$

Exact solution

$$u(x,y) = (x^2-1)(y^2-1)\exp\left(-100(x^2+y^2)\right)$$

Discretization

- conforming finite elements: $u_h \in H^1(\Omega)$
- unstructured nested triangular grids
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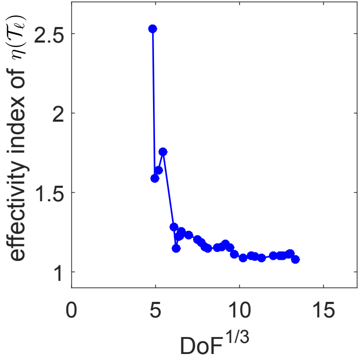
How precise are the estimates?



Effectivity indices on *hp* meshes

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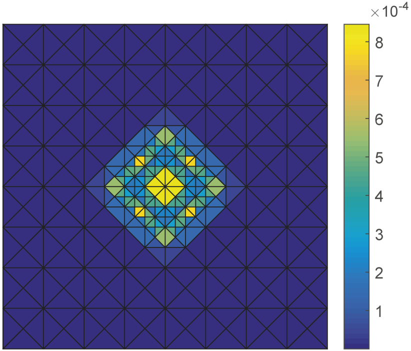
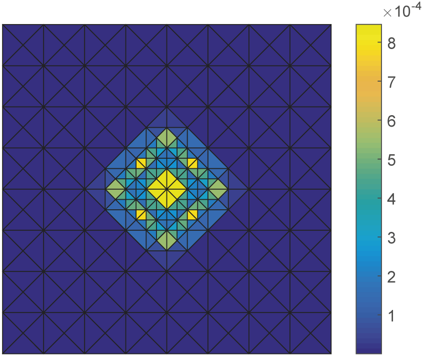
Where (in space) is the error localized?



Estimated error distribution

$\eta_K(u_h)$



Exact error distribution

$\|\nabla(u - u_h)\|_K$

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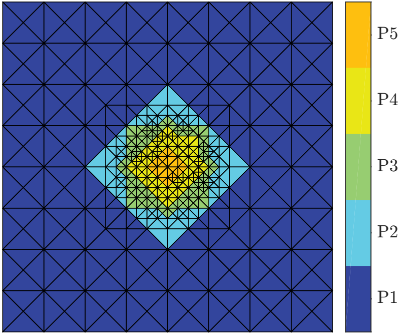
Can we decrease the error efficiently?



Mesh $\mathcal{T}_h$ and pol. degrees p_K

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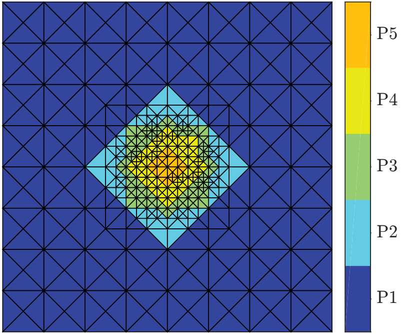
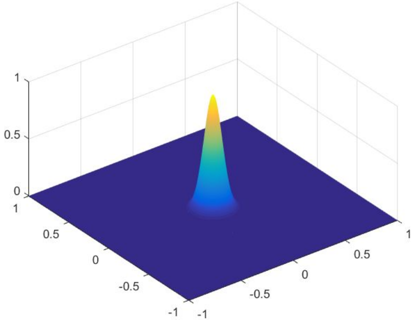


Mesh $\mathcal{T}_h$ and pol. degrees p_K



Exact solution

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

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

- conforming finite elements: $u_h \in H^1(\Omega)$
- unstructured nested triangular grids
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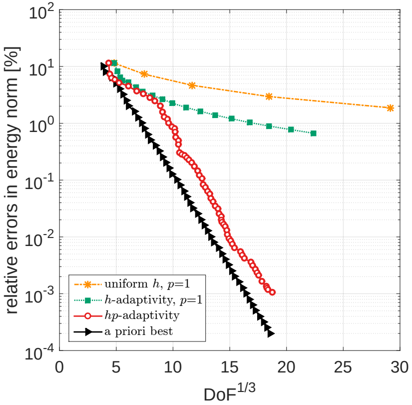

Relative error as a function of no. of unknowns

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

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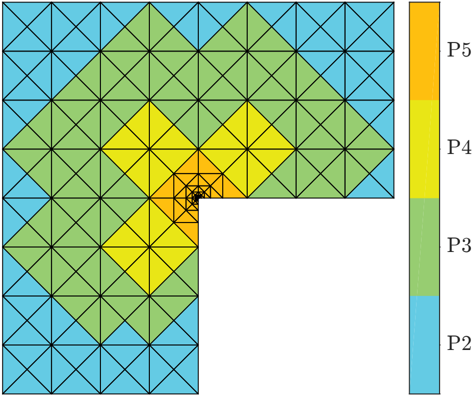
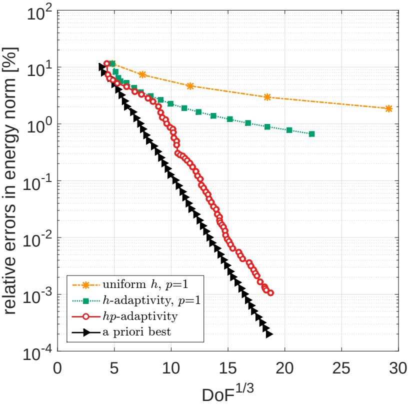


Mesh $\mathcal{T}_h$ and polynomial degrees p_K



Relative error as a function of no. of unknowns

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

Outline

Setting

Laplace problem

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

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

Conforming finite element approximation

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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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

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

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

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Goals

$$\|\nabla(u - u_h^i)\|$$

$$\|\nabla(u_h - u_h^i)\|$$

$$\|\nabla(u - u_h)\|$$

Goals: find **a posteriori estimates** for **any** $i \geq 1$

Total error $\underline{\eta}^i_{\mathrm{tot}} \leq \|\nabla(u - u_h^i)\| \leq \eta^i_{\mathrm{tot}}$

Algebraic error $\underline{\eta}^i_{\mathrm{alg}} \leq \|\nabla(u_h - u_h^i)\| \leq \eta^i_{\mathrm{alg}}$

Discretization error $\underline{\eta}^i_{\mathrm{dis}} \leq \|\nabla(u - u_h)\| \leq \eta^i_{\mathrm{dis}}$

Goals: find **a posteriori estimates** for **any** $i \geq 1$

Total error $\underline{\eta}_{\mathrm{tot}}^{i} \leq \|\nabla(u - u_h^i)\| \leq \eta_{\mathrm{tot}}^{i}$

Algebraic error $\underline{\eta}_{\mathrm{alg}}^{i} \leq \|\nabla(u_h - u_h^i)\| \leq \eta_{\mathrm{alg}}^{i}$

Discretization error $\underline{\eta}_{\mathrm{dis}}^{i} \leq \|\nabla(u - u_h)\| \leq \eta_{\mathrm{dis}}^{i}$

Further goals

- estimate the **distribution** of the errors (local efficiency)
- design reliable (local) **stopping criteria**

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- estimate the **distribution** of the errors (local efficiency)
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Tools

- **flux** and **potential reconstructions**
- **local Neumann** MFE & **local Dirichlet** FE problems
- **multilevel hierarchy** (algebraic components)

Numerical illustration

Peak

$$\Omega = (0,1) \times (0,1),$$

$$u(x,y) = x(x-1)y(y-1)e^{-100(x-0.5)^2-100(y-117/1000)^2}$$

L-shape

$$\Omega = (-1,1) \times (-1,1) \setminus \ [0,1] \times [-1,0],$$

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

Discretization

- conforming finite elements, $p = 1, \ldots, 5$
- unstructured triangular meshes
- 4 uniform refinements

Multigrid

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

PCG

- incomplete Cholesky with drop-off tolerance 1e-4 prec.

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Peak problem, multigrid

p (unknowns)	iter	**alg.** error	eff. UB	eff. LB	**tot.** error	eff. UB	eff. LB	**disc.** error	eff. UB	eff. LB
1 (9.31×10^3)	1	6.09×10^{-3}	1.13	1.02^{-1}	6.93×10^{-3}	1.61	1.21^{-1}	3.32×10^{-3}	2.84	—
	2	1.90×10^{-4}	1.13	1.03^{-1}	3.32×10^{-3}	1.10	1.03^{-1}		1.10	1.03^{-1}
2 (3.76×10^4)	1	7.49×10^{-3}	1.13	1.00^{-1}	7.49×10^{-3}	1.61	1.23^{-1}	1.11×10^{-4}	8.53×10^1	—
	3	8.11×10^{-6}	1.17	1.01^{-1}	1.12×10^{-4}	1.10	1.03^{-1}		1.10	1.03^{-1}
3 (8.48×10^4)	1	4.94×10^{-3}	1.10	1.00^{-1}	4.94×10^{-3}	1.40	1.44^{-1}	2.87×10^{-6}	1.68×10^3	—
	5	7.79×10^{-9}	1.17	1.00^{-1}	2.87×10^{-6}	1.01	1.11^{-1}		1.01	1.11^{-1}
4 (1.51×10^5)	1	4.45×10^{-3}	1.09	1.00^{-1}	4.45×10^{-3}	1.44	1.37^{-1}	6.33×10^{-8}	7.28×10^4	—
	6	1.06×10^{-9}	1.11	1.00^{-1}	6.33×10^{-8}	1.02	1.15^{-1}		1.02	1.15^{-1}

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L-shape problem, PCG

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1 (2.50×10^4)	4	8.86×10^{-2}	1.02	1.00^{-1}	9.13×10^{-2}	1.26	4.33^{-1}	2.22×10^{-2}	3.35	—
	8	3.82×10^{-4}	1.01	1.00^{-1}	2.22×10^{-2}	1.22	1.12^{-1}		1.22	1.12^{-1}
2 (1.01×10^5)	4	6.24×10^{-1}	1.01	1.00^{-1}	6.24×10^{-1}	1.07	9.06^{-1}	8.93×10^{-3}	2.61×10^1	—
	12	1.87×10^{-4}	1.01	1.00^{-1}	8.93×10^{-3}	1.33	1.28^{-1}		1.33	1.28^{-1}
3 (2.27×10^5)	7	1.02	1.00	1.00^{-1}	1.02	1.05	10.0^{-1}	5.29×10^{-3}	6.29×10^1	—
	28	9.58×10^{-5}	1.00	1.00^{-1}	5.29×10^{-3}	1.46	1.41^{-1}		1.46	1.41^{-1}
4 (4.04×10^5)	7	1.17	1.01	1.00^{-1}	1.17	1.08	7.56^{-1}	3.77×10^{-3}	1.30×10^2	—
	28	1.84×10^{-4}	1.01	1.00^{-1}	3.77×10^{-3}	1.52	1.60^{-1}		1.52	1.60^{-1}

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	8	3.82×10^{-4}	1.01	1.00^{-1}	2.22×10^{-2}	1.22	1.12^{-1}		1.22	1.12^{-1}
2 (1.01×10^5)	4	6.24×10^{-1}	1.01	1.00^{-1}	6.24×10^{-1}	1.07	9.06^{-1}	8.93×10^{-3}	2.61×10^1	—
	12	1.87×10^{-4}	1.01	1.00^{-1}	8.93×10^{-3}	1.33	1.28^{-1}		1.33	1.28^{-1}
3 (2.27×10^5)	7	1.02	1.00	1.00^{-1}	1.02	1.05	10.0^{-1}	5.29×10^{-3}	6.29×10^1	—
	28	9.58×10^{-5}	1.00	1.00^{-1}	5.29×10^{-3}	1.46	1.41^{-1}		1.46	1.41^{-1}
4 (4.04×10^5)	7	1.17	1.01	1.00^{-1}	1.17	1.08	7.56^{-1}	3.77×10^{-3}	1.30×10^2	—
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L-shape problem, PCG

p (unknowns)	iter	**alg.** error	eff. UB	eff. LB	**tot.** error	eff. UB	eff. LB	**disc.** error	eff. UB	eff. LB
1 (2.50×10^4)	4	8.86×10^{-2}	1.02	1.00^{-1}	9.13×10^{-2}	1.26	4.33^{-1}	2.22×10^{-2}	3.35	—
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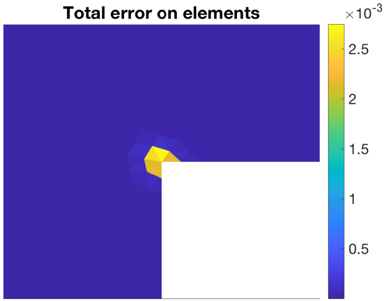
L-shape problem, $p = 3$, total error, 28th PCG iteration



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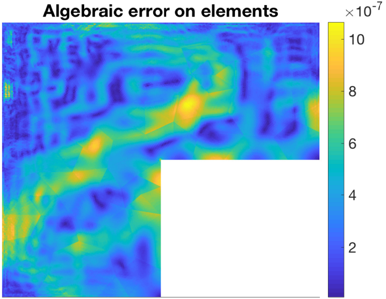
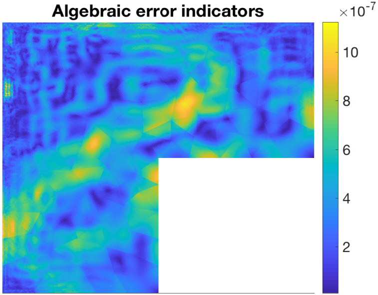
L-shape problem, $p = 3$, alg. error, 28th PCG iteration





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Domain decomposition method & 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 $\eta^i_{\rm DD} \le 0.1(\eta^i_{\rm disc} + \eta_{\rm osc})$

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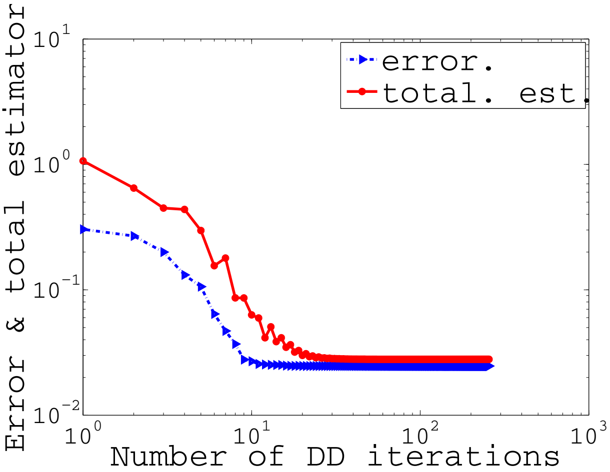
Error and estimate



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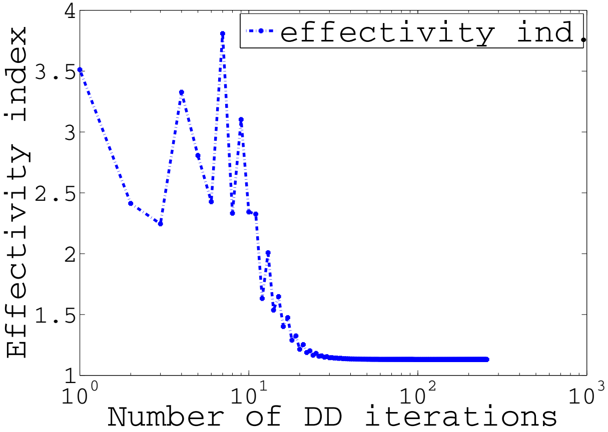
Effectivity index



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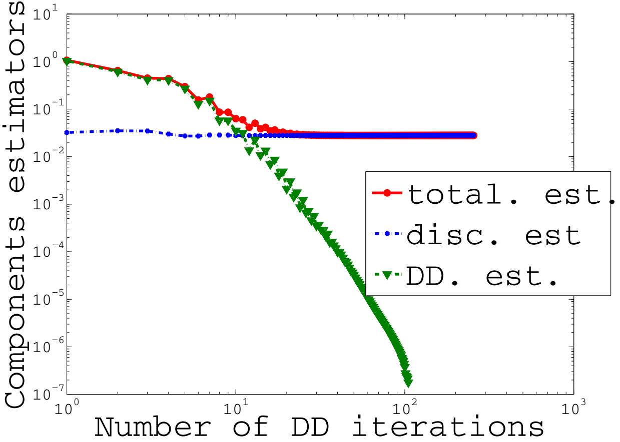
DD stopping criterion



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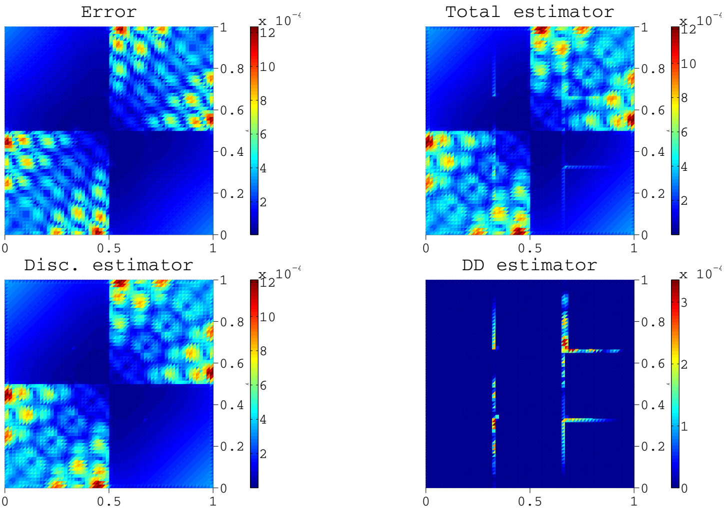
Error and estimators distribution, 20th DD iteration



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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* $i := 1$.
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   $$\mathbb{A}^{k-1} U^{k,i} = F^{k-1} - R^{k,i}.$$
   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: $A(u) = f$

Question (Stopping criteria Eisenstat and Walker (1990's), Becker, Johnson, and Rannacher (1995), Deuflhard (2004 book), Arioli (2000's)**)**

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

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Abstract assumptions

Quasi-linear elliptic problem

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$$u = 0 \quad \text{on } \partial\Omega$$

Assumption A (Total flux reconstruction)

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

$$\nabla\cdot\boldsymbol{\sigma}_h^{k,i} = f.$$

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

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

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

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

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Abstract assumptions

Quasi-linear elliptic problem

$$-\nabla\cdot\overline{\boldsymbol{\sigma}}(u, \nabla u) = f \quad \text{in } \Omega,$$
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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 (up to quadrature and data oscillation)

$$\underbrace{\mathcal{J}_u(u_h^{k,i})}_{\text{weak flux + potential nonconformity error}} \leq \eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i}.$$

Estimators

- *discretization* estimator

$$\eta_{\mathrm{disc},K}^{k,i} := 2^{\frac{1}{p}} \left(\|\overline{\boldsymbol{\sigma}}(u_h^{k,i}, \nabla u_h^{k,i}) + \boldsymbol{\sigma}_{h,\mathrm{dis}}^{k,i}\|_{q,K} + \left\{ \sum_{e \in \mathcal{E}_K} h_e^{1-q} \| [\![u_h^{k,i}]\!] \|_{q,e}^q \right\}^{1/q} \right)$$

- *linearization* estimator

$$\eta_{\mathrm{lin},K}^{k,i} := \|\boldsymbol{\sigma}_{h,\mathrm{lin}}^{k,i}\|_{q,K}$$

- *algebraic* estimator

$$\eta_{\mathrm{alg},K}^{k,i} := \|\boldsymbol{\sigma}_{h,\mathrm{alg}}^{k,i}\|_{q,K}$$

- $\eta_{\cdot}^{k,i} := \left\{ \sum_{K \in \mathcal{T}_h} \left(\eta_{\cdot,K}^{k,i} \right)^q \right\}^{1/q}$

Local stopping criteria and local efficiency

Local stopping criteria

- for $\gamma_{\mathrm{alg},K}, \gamma_{\mathrm{lin},K} \approx 0.1$, stop whenever:

$$\eta_{\mathrm{alg},K}^{k,i} \leq \gamma_{\mathrm{alg},K} \max\{\eta_{\mathrm{disc},K}^{k,i}, \eta_{\mathrm{lin},K}^{k,i}\} \qquad \forall K \in \mathcal{T}_h,$$

$$\eta_{\mathrm{lin},K}^{k,i} \leq \gamma_{\mathrm{lin},K} \eta_{\mathrm{disc},K}^{k,i} \qquad \forall K \in \mathcal{T}_h$$

Comments

✓ same physical units (fluxes), naturally relative

✓ proper $[L^q(\Omega)]^d$ framework $\times$ l_2 norms of algebraic vectors

Theorem (Local efficiency under local stopping criteria)

Let the Assumptions C and D be satisfied. Then

$$\eta_{\mathrm{disc},K}^{k,i} + \eta_{\mathrm{lin},K}^{k,i} + \eta_{\mathrm{alg},K}^{k,i} \leq C \mathcal{J}_{u,\mathfrak{T}_K}(u_h^{k,i}) \qquad \forall K \in \mathcal{T}_h.$$

✓ **robustness** with respect to the **nonlinearity** thanks to the choice of $\mathcal{J}_u$ as error measure

✓ local efficiency since the weak flux error (**dual residual** norm) can be **localized** Ciarlet, V. (2015); Blechta, Málek, V. (2016)

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Applications

Discretization methods

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

Linearizations

- ✓ fixed point
- ✓ Newton

Linear solvers

- ✓ independent of the linear solver

. . . all Assumptions A to D verified

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Numerical experiment I

Model problem

- p-Laplacian

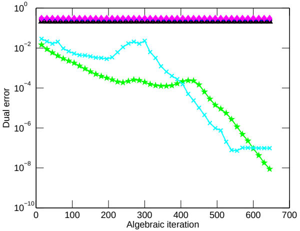
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f \qquad \text{in } \Omega, \\ u &= u_{\mathrm{D}} \qquad \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

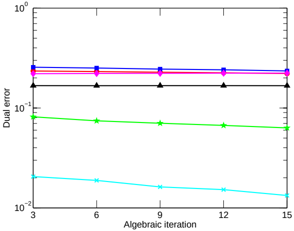
$$u(x,y) = -\frac{p-1}{p}\left((x-\tfrac{1}{2})^2 + (y-\tfrac{1}{2})^2\right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p}\left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

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

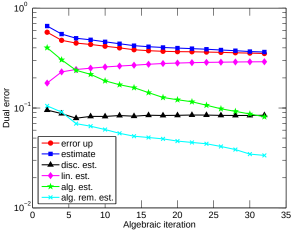
Error and estimators as a function of CG iterations, $p = 10$, 6th level mesh, 6th Newton step



Newton



inexact Newton



ad. inexact Newton

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

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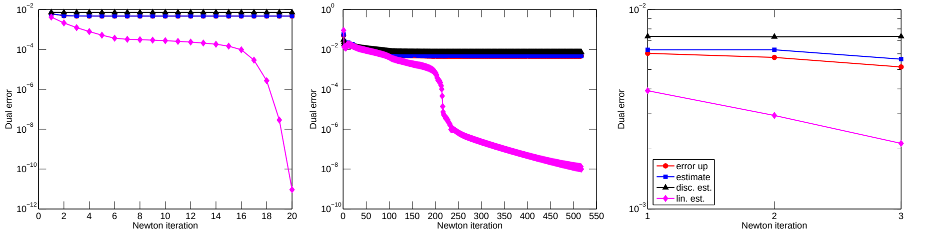

Newton   inexact Newton   ad. inexact Newton

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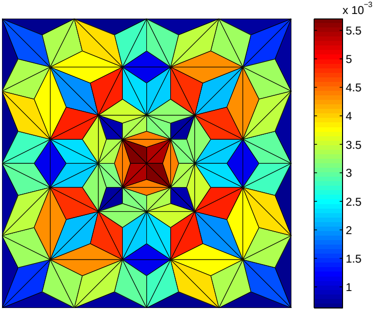
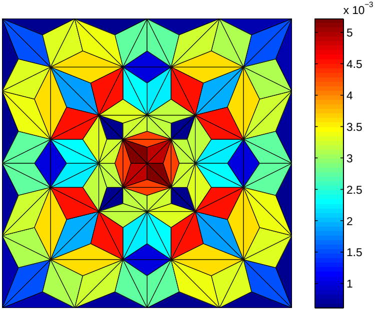
Error distribution, $p = 10$



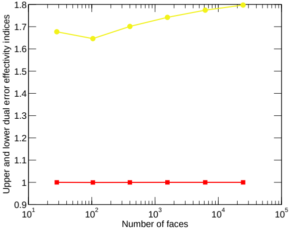
Estimated error distribution



Exact error distribution

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

Effectivity indices, $p = 10$



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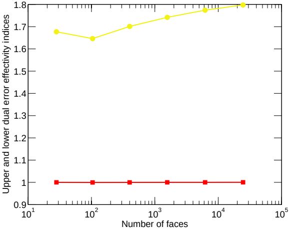

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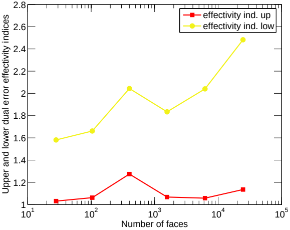

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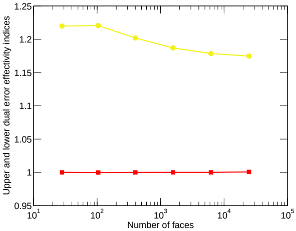

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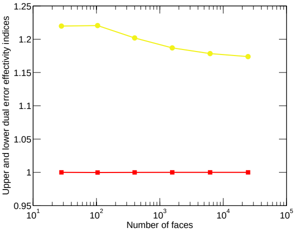

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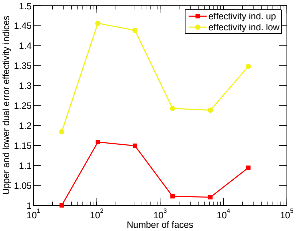

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Laplace eigenvalue problem

Problem

Find eigenvector & eigenvalue pair (u, λ) such that

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

Weak formulation

Find $(u_i, \lambda_i) \in V \times \mathbb{R}^+$, $i \geq 1$, with $\|u_i\| = 1$, such that

$$(\nabla u_i, \nabla v) = \lambda_i (u_i, v) \qquad \forall v \in V.$$

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Main results (conforming setting)

Assumption A (Conforming variational solution)

There holds

- $(u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+$
- $\|u_{ih}\| = 1$
- $\|\nabla u_{ih}\|^2 = \lambda_{ih}$ $\quad (\Rightarrow \lambda_{1h} \geq \lambda_1)$

We bound

2. i-th eigenvector energy error

$$\|\nabla(u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih}) \leq C_{\mathrm{eff},i} \|\nabla(u_i - u_{ih})\|$$

✓ $C_{\mathrm{eff},i}$ only depends on mesh shape regularity and on $\max\left\{\left(\frac{\lambda_i}{\lambda_{i-1}} - 1\right)^{-1}, \left(1 - \frac{\lambda_i}{\lambda_{i+1}}\right)^{-1}\right\} \frac{\lambda_i}{\lambda_1}$

✓ we give computable upper bounds on $C_{\mathrm{eff},i}$

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Outline

Numerical experiments

Unit square: smooth eigenvectors

- $\Omega = (0,1)^2$
- $\lambda_1 = 2\pi^2$, $\lambda_2 = 5\pi^2$ known explicitly
- $u_1(x,y) = \sin(\pi x)\sin(\pi y)$ known explicitly

L-shape: singular eigenvectors

- $\Omega := (-1,1)^2 \setminus [0,1] \times [-1,0]$
- $\lambda_1 \approx 9.6397238440$

Effectivity indices

- recall $\tilde{\eta}_i^2 \leq \lambda_{ih} - \lambda_i \leq \eta_i^2$

$$I^{\mathrm{lb}}_{\lambda,\mathrm{eff}} := \frac{\lambda_{ih} - \lambda_i}{\tilde{\eta}_i^2}, \qquad I^{\mathrm{ub}}_{\lambda,\mathrm{eff}} := \frac{\eta_i^2}{\lambda_{ih} - \lambda_i}$$

- recall $\|\nabla(u_i - u_{ih})\| \leq \eta_i$

$$I^{\mathrm{ub}}_{u,\mathrm{eff}} := \frac{\eta_i}{\|\nabla(u_i - u_{ih})\|}$$

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- $\Omega := (-1,1)^2 \setminus [0,1] \times [-1,0]$
- $\lambda_1 \approx 9.6397238440$

Effectivity indices

- recall $\tilde{\eta}_i^2 \leq \lambda_{ih} - \lambda_i \leq \eta_i^2$

$$I_{\lambda,\mathrm{eff}}^{\mathrm{lb}} := \frac{\lambda_{ih} - \lambda_i}{\tilde{\eta}_i^2}, \qquad I_{\lambda,\mathrm{eff}}^{\mathrm{ub}} := \frac{\eta_i^2}{\lambda_{ih} - \lambda_i}$$

- recall $\|\nabla(u_i - u_{ih})\| \leq \eta_i$

$$I_{u,\mathrm{eff}}^{\mathrm{ub}} := \frac{\eta_i}{\|\nabla(u_i - u_{ih})\|}$$

Numerical experiments

Unit square: smooth eigenvectors

- $\Omega = (0,1)^2$
- $\lambda_1 = 2\pi^2$, $\lambda_2 = 5\pi^2$ known explicitly
- $u_1(x,y) = \sin(\pi x)\sin(\pi y)$ known explicitly

L-shape: singular eigenvectors

- $\Omega := (-1,1)^2 \setminus [0,1] \times [-1,0]$
- $\lambda_1 \approx 9.6397238440$

Effectivity indices

- recall $\tilde{\eta}_i^2 \le \lambda_{ih} - \lambda_i \le \eta_i^2$

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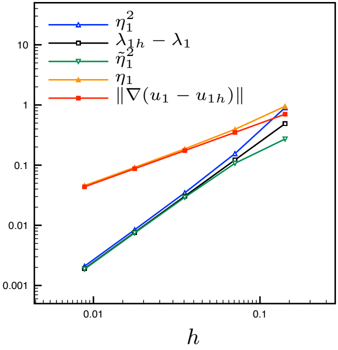
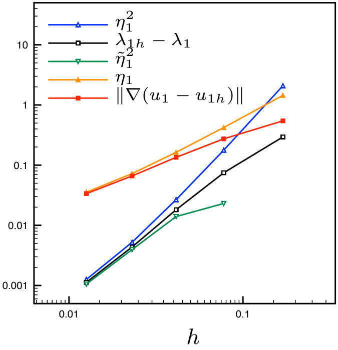
Unit square, conforming finite elements, $p = 1$



Structured meshes



Unstructured meshes

E. Cancès, G. Dusson, Y. Maday, B. Stamm, M. Vohralík, SIAM Journal on Numerical Analysis (2017)

Unit square, conforming finite elements, $p = 1$

N	h	ndof	λ_1	λ_{1h}	$\lambda_{1h} - \eta_1^2$	$\lambda_{1h} - \tilde{\eta}_1^2$	$I^{\mathrm{lb}}_{\lambda,\mathrm{eff}}$	$I^{\mathrm{ub}}_{\lambda,\mathrm{eff}}$	$E_{\lambda,\mathrm{rel}}$	$I^{\mathrm{ub}}_{u,\mathrm{eff}}$
10	0.1414	121	19.7392	20.2284	19.5054	19.8667	1.35	1.48	1.84E-02	1.21
20	0.0707	441	19.7392	19.8611	19.7164	19.7486	1.08	1.19	1.63E-03	1.09
40	0.0354	1,681	19.7392	19.7696	19.7356	19.7401	1.03	1.12	2.28E-04	1.06
80	0.0177	6,561	19.7392	19.7468	19.7384	19.7393	1.02	1.10	4.56E-05	1.05
160	0.0088	25,921	19.7392	19.7411	19.7390	19.7392	1.02	1.10	1.01E-05	1.05

Structured meshes

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10	0.1698	143	19.7392	20.0336	18.8265	–	–	4.10	–	2.02
20	0.0776	523	19.7392	19.8139	19.6820	19.7682	1.63	1.77	4.37E-03	1.33
40	0.0413	1,975	19.7392	19.7573	19.7342	19.7416	1.15	1.28	3.75E-04	1.13
80	0.0230	7,704	19.7392	19.7436	19.7386	19.7395	1.07	1.14	4.56E-05	1.07
160	0.0126	30,666	19.7392	19.7403	19.7391	19.7393	1.06	1.10	1.01E-05	1.05

Unstructured meshes

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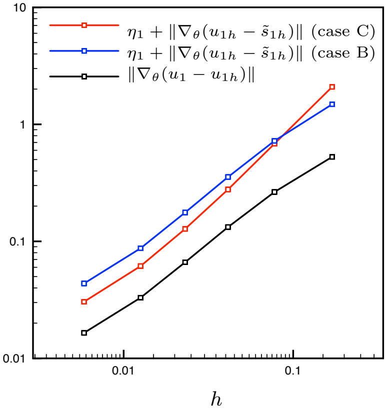
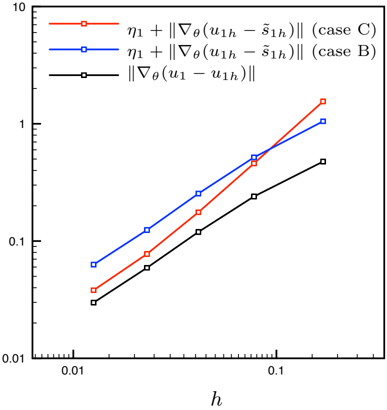
Unstructured meshes

E. Cancès, G. Dusson, Y. Maday, B. Stamm, M. Vohralík, SIAM Journal on Numerical Analysis (2017)

Unit square, nonconforming FEs & DG's, $p = 1$



Nonconforming finite elements



Discontinuous Galerkin

E. Cancès, G. Dusson, Y. Maday, B. Stamm, M. Vohralík, Numerische Mathematik (2018)

Unit square, nonconforming FEs & DG's, $p = 1$

N	h	ndof	λ_1	λ_{1h}	$\frac{\|\nabla s_{1h}\|^2}{\|s_{1h}\|^2} - \eta_1^2$	$\frac{\|\nabla s_{1h}\|^2}{\|s_{1h}\|^2}$	$E_{\lambda,\mathrm{rel}}$	$I_{u,\mathrm{eff}}^{\mathrm{ub}}$
10	0.1414	320	19.7392	19.6850	18.8966	19.8262	4.80e-02	2.68
20	0.0707	1240	19.7392	19.7257	19.6495	19.7616	5.69e-03	2.11
40	0.0354	4880	19.7392	19.7358	19.7246	19.7448	1.02e-03	1.91
80	0.0177	19360	19.7392	19.7384	19.7361	19.7406	2.29e-04	1.85
160	0.0088	77120	19.7392	19.7390	19.7385	19.7396	5.53e-05	1.83
320	0.0044	307840	19.7392	19.7392	19.7390	19.7393	1.37e-05	1.83

Nonconforming finite elements

N	h	ndof	λ_1	λ_{1h}	$\frac{\|\nabla s_{1h}\|^2}{\|s_{1h}\|^2} - \eta_1^2$	$\frac{\|\nabla s_{1h}\|^2}{\|s_{1h}\|^2}$	$E_{\lambda,\mathrm{rel}}$	$I_{u,\mathrm{eff}}^{\mathrm{ub}}$
10	0.1698	732	19.7392	19.9432	17.8788	19.9501	1.10e-01	3.26
20	0.0776	2892	19.7392	19.7928	19.6264	19.7939	8.50e-03	1.91
40	0.0413	11364	19.7392	19.7526	19.7295	19.7529	1.18e-03	1.47
80	0.0230	45258	19.7392	19.7425	19.7381	19.7426	2.28e-04	1.31
160	0.0126	182070	19.7392	19.7400	19.7390	19.7401	5.35e-05	1.28

SIP discontinuous Galerkin

Unit square, nonconforming FEs & DG's, $p = 1$

N	h	ndof	λ_1	λ_{1h}	$\frac{\|\nabla s_{1h}\|^2}{\|s_{1h}\|^2} - \eta_1^2$	$\frac{\|\nabla s_{1h}\|^2}{\|s_{1h}\|^2}$	$E_{\lambda,\mathrm{rel}}$	$I_{u,\mathrm{eff}}^{\mathrm{ub}}$
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Unit square, nonconforming FEs & DG's, $p = 1$

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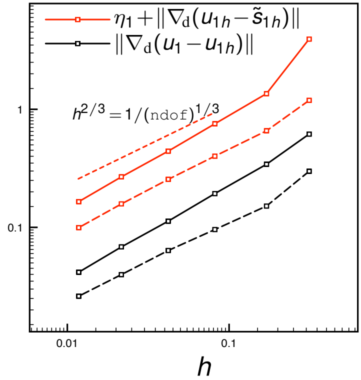
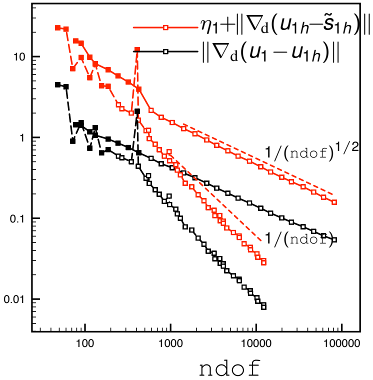
SIP discontinuous Galerkin

E. Cancès, G. Dusson, Y. Maday, B. Stamm, M. Vohralík, Numerische Mathematik (2018)

L-shape, DG's, $p = 1$ and $p = 2$, adaptivity



Uniform mesh refinement



Adaptive mesh refinement

$p = 1$ full lines, $p = 2$ dashed lines

E. Cancès, G. Dusson, Y. Maday, B. Stamm, M. Vohralík, Numerische Mathematik (2018)

Outline

1. Introduction
2. Laplace equation: potential & flux reconstructions
   - Guaranteed upper bound in a unified framework
   - Polynomial-degree-robust local efficiency
   - Applications & numerical results
   - Taking into account the algebraic error
3. Nonlinear Laplace equation: adaptive stopping criteria
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5. Two-phase flow in porous media: industrial application
6. Conclusions and outlook

Industrial problem

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

Industrial problem

Two-phase immiscible incompressible flow

$$
\begin{aligned}
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+ boundary & initial conditions

Mathematical issues

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

Distinguishing the error components

Theorem (Distinguishing the error components)

Let

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

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

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

Error components

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

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

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Full adaptivity

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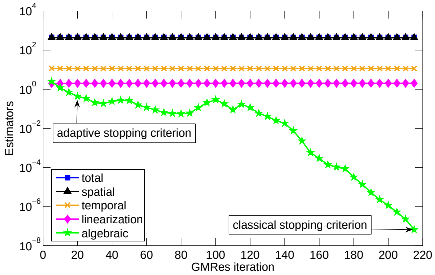
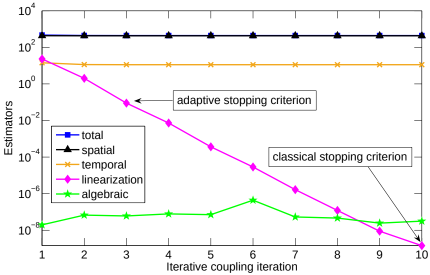
Estimators and stopping criteria



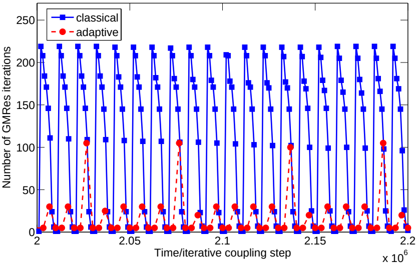
Estimators in function of GMRes iterations



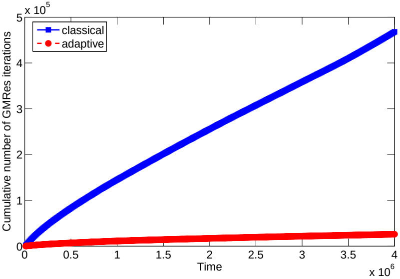
Estimators in function of iterative coupling iterations

M. F. Wheeler, M. Vohralík, Computational Geosciences (2013)

GMRes iterations



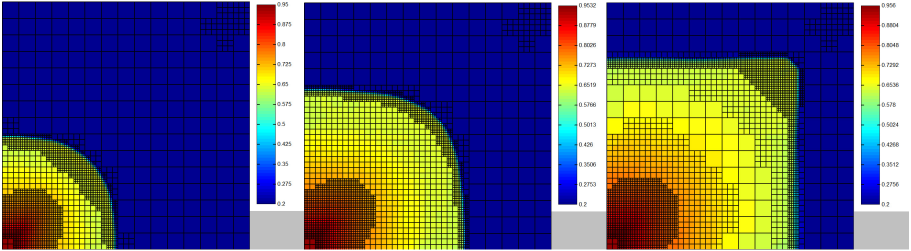
Per time and iterative coupling step



Cumulated

M. F. Wheeler, M. Vohralík, Computational Geosciences (2013)

Space/time/nonlinear solver/linear solver adaptivity



Fully adaptive computation

M. F. Wheeler, M. Vohralík, Computational Geosciences (2013)

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Conclusions and outlook

Conclusions

- ✓ guaranteed energy error estimates
- ✓ robustness (polynomial degree, nonlinearity, reaction-dominance, final time)
- ✓ local (space-time) efficiency
- ✓ unified framework for all classical numerical schemes
- ✓ discretization–linearization–algebraic resolution adaptivity
- ✓ cover the set of basic model problems (also variational inequalities, Stokes, changing coefficients, H^{-1} source terms. . .)

Ongoing work

- guaranteed reduction factor for *hp* refinement strategies
- convergence and optimality

Conclusions and outlook

Conclusions

- ✓ guaranteed energy error estimates
- ✓ robustness (polynomial degree, nonlinearity, reaction-dominance, final time)
- ✓ local (space-time) efficiency
- ✓ unified framework for all classical numerical schemes
- ✓ discretization–linearization–algebraic resolution adaptivity
- ✓ cover the set of basic model problems (also variational inequalities, Stokes, changing coefficients, H^{-1} source terms. . .)

Ongoing work

- guaranteed reduction factor for *hp* refinement strategies
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Merci de votre attention !

Outline

Proof I

Proof.

- 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 (continuation).

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$$(f, \varphi) - (\nabla u_h, \nabla \varphi) = (f - \nabla\cdot\sigma_h, \varphi) - (\nabla u_h + \sigma_h, \nabla\varphi)$$

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$$-(\nabla u_h + \sigma_h, \nabla\varphi)$$

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Outline

Potentials (Demkowicz, Gopalakrishnan, Schöberl (2009), EV 2016)

Lemma (H^1 polynomial extension on a tetrahedron)

Let $K \in \mathcal{T}_h$, $\mathcal{E}_K^{\mathrm{D}} \subset \mathcal{E}_K$. Let $r \in \mathbb{P}_p(\mathcal{E}_K^{\mathrm{D}})$ be continuous on $\mathcal{E}_K^{\mathrm{D}}$. Then for C only depending on the shape regularity of K,

$$\min_{\substack{v_h \in \mathbb{P}_p(K) \\ v_h = r_e \text{ on all } e \in \mathcal{E}_K^{\mathrm{D}}}} \|\nabla v_h\|_K \leq C \underbrace{\min_{\substack{v \in H^1(K) \\ v = r_e \text{ on all } e \in \mathcal{E}_K^{\mathrm{D}}}} \|\nabla v\|_K}_{\|r\|_{H^{1/2}(\partial K)}} .$$

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$$\begin{aligned} -\Delta \zeta_K &= 0 && \text{in } K, \\ \zeta_K &= r_e && \text{on all } e \in \mathcal{E}_K^{\mathrm{D}}, \\ -\nabla \zeta_K \cdot \mathbf{n}_K &= 0 && \text{on all } e \in \mathcal{E}_K \setminus \mathcal{E}_K^{\mathrm{D}}. \end{aligned}$$

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Fluxes (Costabel, McIntosh (2010), Demkowicz, Gopalakrishnan, Schöberl (2012), EV 2016)

Lemma ($\mathbf{H}(\mathrm{div})$ polynomial extension on a tetrahedron)

Let $K \in \mathcal{T}_h$, $\mathcal{E}_K^{\mathrm{N}} \subset \mathcal{E}_K$. Let $r \in \mathbb{P}_p(\mathcal{E}_K^{\mathrm{N}}) \times \mathbb{P}_p(K)$, satisfying $\sum_{e \in \mathcal{E}_K} (r_e, 1)_e = (r_K, 1)_K$ if $\mathcal{E}_K^{\mathrm{N}} = \mathcal{E}_K$. Then for $C = C(\kappa_K) > 0$,

$$\min_{\substack{\mathbf{v}_h \in \mathbf{RTN}_p(K) \\ \mathbf{v}_h \cdot \mathbf{n}_K = r_e \ \forall e \in \mathcal{E}_K^{\mathrm{N}} \\ \nabla \cdot \mathbf{v}_h = r_K}} \|\mathbf{v}_h\|_K \leq C \min_{\substack{\mathbf{v} \in \mathbf{H}(\mathrm{div}, K) \\ \mathbf{v} \cdot \mathbf{n}_K = r_e \ \forall e \in \mathcal{E}_K^{\mathrm{N}} \\ \nabla \cdot \mathbf{v} = r_K}} \|\mathbf{v}\|_K .$$

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Set $\xi_K := -\nabla \zeta_K$.

Outline

Model steady problem, discretization

Quasi-linear elliptic problem

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

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

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

Numerical approximation

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

Model steady problem, discretization

Quasi-linear elliptic problem

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

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

Energy error in the Laplace case

$$\|\nabla(u-u_h)\|^2 = \underbrace{\sup_{\varphi \in H_0^1(\Omega);\, \|\nabla\varphi\|=1} (\nabla(u-u_h), \nabla\varphi)^2}_{\text{dual norm of the residual, weak flux error}} + \underbrace{\min_{v \in H_0^1(\Omega)} \|\nabla(v-u_h)\|^2}_{\text{distance of } u_h \text{ to } H_0^1(\Omega)}$$

Intrinsic error measure

$$\mathcal{J}_u(u_h^{k,i}) := \underbrace{\sup_{\varphi \in V;\, \|\nabla\varphi\|_p=1} (\overline{\sigma}(u,\nabla u) - \overline{\sigma}(u_h^{k,i}, \nabla u_h^{k,i}), \nabla\varphi)}_{\text{dual norm of the residual}}$$

$$+ \underbrace{\left\{ \sum_{K\in\mathcal{T}_h} \sum_{e\in\mathcal{E}_K} h_e^{1-q} \|[\![u - u_h^{k,i}]\!]\|_{q,e}^q \right\}^{1/q}}_{\text{distance of } u_h \text{ to } V}$$

✓ there holds $\mathcal{J}_u(u_h^{k,i}) = 0$ if and only if $u = u_h^{k,i}$

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Outline

7 Proof Laplace

8 Tools

9 Nonlinear Laplace

10 Heat equation: robustness wrt final time & local efficiency

Model parabolic problem

The heat equation

$$\begin{aligned} \partial_t u - \Delta u &= f \quad \text{in } \Omega \times (0,T), \\ u &= 0 \quad \text{on } \partial\Omega \times (0,T), \\ u(0) &= u_0 \quad \text{in } \Omega \end{aligned}$$

Spaces

$$\begin{aligned} X &:= L^2(0,T; H_0^1(\Omega)), \\ \|v\|_X^2 &:= \int_0^T \|\nabla v\|^2 \,\mathrm{d}t, \\ Y &:= L^2(0,T; H_0^1(\Omega)) \cap H^1(0,T; H^{-1}(\Omega)), \\ \|v\|_Y^2 &:= \int_0^T \|\partial_t v\|_{H^{-1}(\Omega)}^2 + \|\nabla v\|^2 \,\mathrm{d}t + \|v(T)\|^2 \end{aligned}$$

Weak solution

Find $u \in Y$ with $u(0) = u_0$ such that

$$\int_0^T \langle \partial_t u, v \rangle + (\nabla u, \nabla v) \,\mathrm{d}t = \int_0^T (f, v) \,\mathrm{d}t \qquad \forall v \in X.$$

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Error and residual in the unsteady case

Theorem (Parabolic inf–sup identity)

For every $\varphi \in Y$, we have

$$\|\varphi\|_Y^2 = \left[\sup_{v \in X,\, \|v\|_X = 1} \int_0^T \langle \partial_t \varphi, v \rangle + (\nabla \varphi, \nabla v)\, \mathrm{d}t \right]^2 + \|\varphi(0)\|^2.$$

Residual of $u_{h\tau} \in Y$

- $\mathcal{R}(u_{h\tau}) \in X'$, the misfit of $u_{h\tau}$ in the weak formulation:

$$\langle \mathcal{R}(u_{h\tau}), v \rangle := \int_0^T (f, v) - \langle \partial_t u_{h\tau}, v \rangle - (\nabla u_{h\tau}, \nabla v)\, \mathrm{d}t$$

- dual norm of the residual

$$\|\mathcal{R}(u_{h\tau})\|_{X'} := \sup_{v \in X,\, \|v\|_X = 1} \langle \mathcal{R}(u_{h\tau}), v \rangle$$

Y norm error is the dual X norm of the residual + IC error

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A posteriori estimate

Guaranteed upper bound

- ✓ $\|u - u_{h\tau}\|^2_{\mathcal{E}_Y,\Omega\times(0,T)} \leq \sum_{n=1}^{N} \sum_{K\in\mathcal{T}_h^n} \eta_K^n(u_{h\tau})^2$
- ✓ no undetermined constant: **error control**

Local space-time efficiency

- ✓ $\eta_K^n(u_{h\tau}) \leq C_{\rm eff}\|u - u_{h\tau}\|_{\mathcal{E}_Y,\text{neighbors of } K\times(t^{n-1},t^n)}$
- ✓ optimal space-time mesh refinement
- ✓ **local** in **time** and in **space** error lower bound

Robustness

- ✓ $C_{\rm eff}$ independent of data, domain Ω, **final time** T, meshes, solution u, **polynomial degrees** of $u_{h\tau}$ in space and in time

Asymptotic exactness

- ✓ $\sum_{n=1}^{N} \sum_{K\in\mathcal{T}_h^n} \eta_K^n(u_{h\tau})^2 / \|u - u_{h\tau}\|^2_{\mathcal{E}_Y,\Omega\times(0,T)} \searrow 1$
- ✓ overestimation factor goes to one with meshes size

Small evaluation cost

- ✓ estimators can be evaluated cheaply (locally)

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