A posteriori error estimates and adaptivity taking into account algebraic errors

Martin Vohralík

in collaboration with J. Blechta, M. Čermák, P. Daniel, A. Ern, F. Hecht, J. Málek, A. Miraçi, J. Papež, U. Rüde, Z. Strakoš, Z. Tang, B. Wohlmuth, & S. Yousef

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Outline

1. A coarse solution as an approximation to a fine one

Setting

- $-\Delta u = f$ in $\Omega := (0,1)^d$, $d = 1,2,3$, $u = 0$ on $\partial\Omega$
- $u = \sum_{i=1}^d x_i(1 - x_i)$
- u_h: exact finite element solution on a regular simplicial mesh $\mathcal{T}_h = \mathrm{ref}(\mathcal{T}_H)$
- approximation of u_h given by u_H: exact finite element solution on $\mathcal{T}_H$

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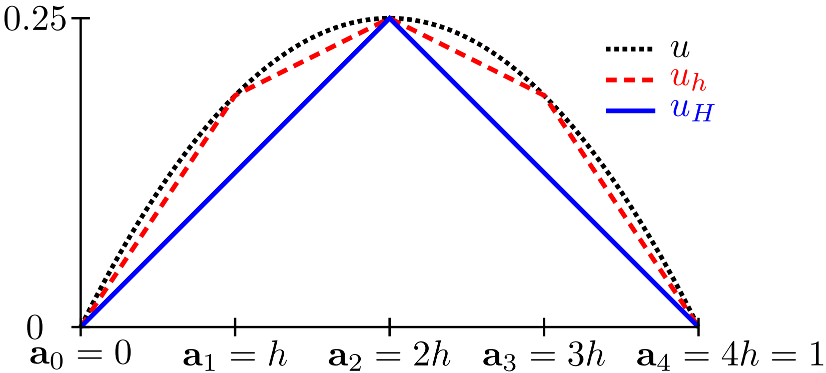
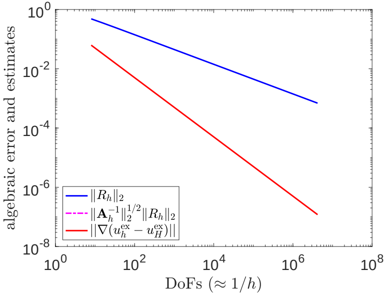


Euclidean norm of the algebraic residual vector is highly misleading



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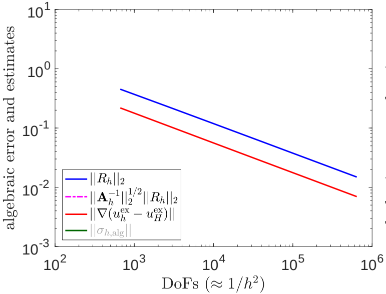

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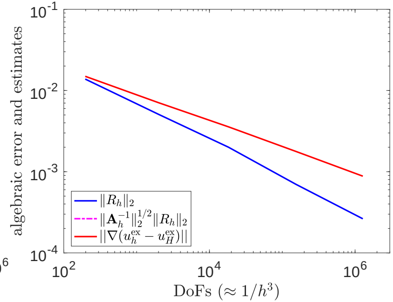

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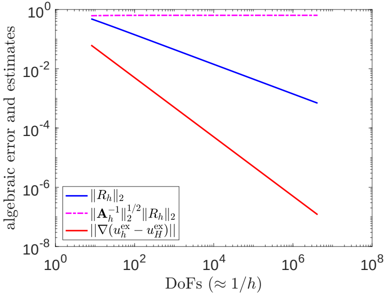

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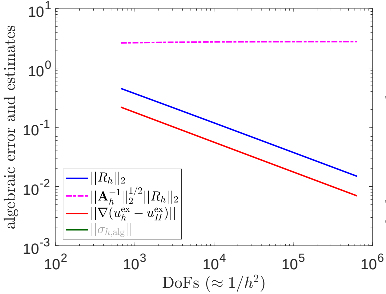

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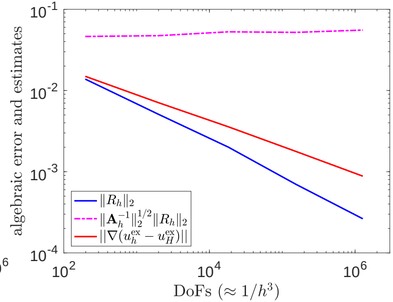

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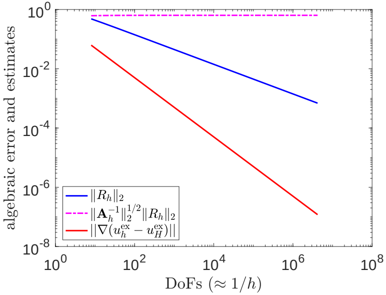

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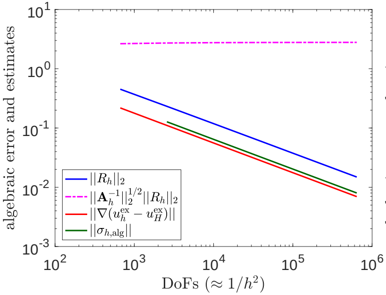

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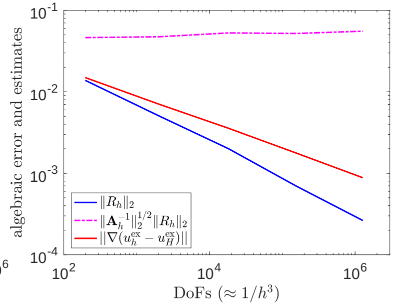

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J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, HAL Preprint 01662944 (2017)

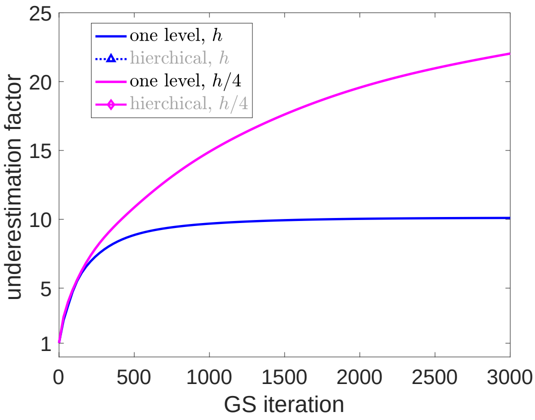
2. Slowly-converging Gauss–Seidel solver

Setting

- L-shape problem
- regular triangular mesh
- random initial guess
- an algebraic estimator based on local Dirichlet FE problems on the finest level
- local Dirichlet FE problems on a mesh hierarchy
- underestimating factor

$$\frac{\|\nabla(u_h^{\mathrm{ex}} - u_h)\|}{\text{algebraic estimate}} \geq 1$$

Precision of the finest-level-only estimator deteriorates with *i* and *h*



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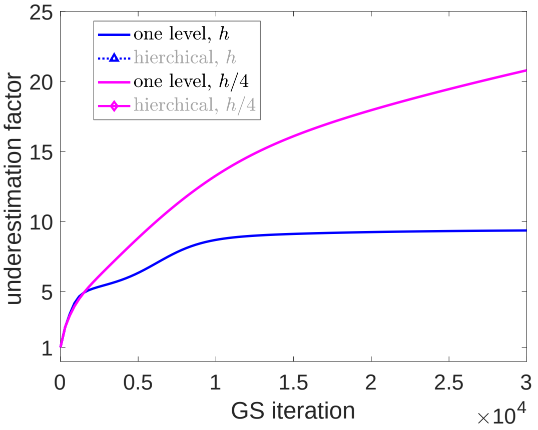

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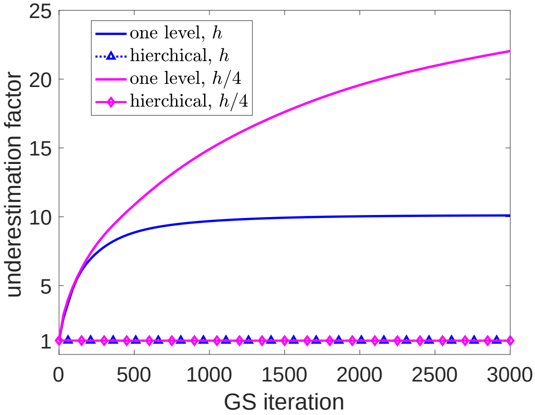

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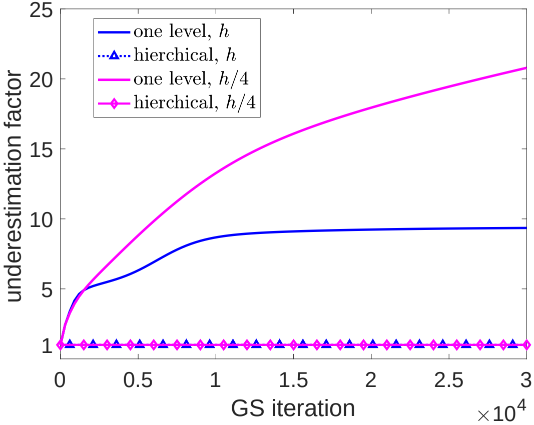

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1. Introduction: two warning examples
2. Guaranteed upper & lower bounds on total, algebraic, and discretization errors
   - Guaranteed upper and lower bounds
   - Stopping criteria and efficiency
   - Numerical illustration
3. *hp*-refinement with inexact solvers and guaranteed computable contraction
4. Generalization to an arbitrary residual functional in $[W_0^{1,\alpha}(\Omega)]'$
5. Application to the Stokes flow
6. Application to a multi-phase multi-compositional porous media Darcy flow
7. Conclusions and outlook

Setting: $-\Delta u = f$ in Ω, $u = 0$ on $\partial\Omega$, $\Omega \subset \mathbb{R}^d$, $d \geq 1$

Exact solution

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

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

Finite element approximation

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Linear algebraic system

Find $U_h \in \mathbb{R}^N$, $N = |V_h|$, such that

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

Algebraic solver (iterative)

On each iteration $i \geq 1$: $U_h^i \in \mathbb{R}^N \Leftrightarrow$ **inexact FE approximation** $u_h^i \in V_h$

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

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Total error

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

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Discretization error

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Algebraic error

$$\|\nabla(u_h - u_h^i)\| = \|U_h - U_h^i\|_{\mathbb{A}_h} = \|R_h^i\|_{\mathbb{A}_h^{-1}}$$

Discretization error

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

Context & goals: **a posteriori estimates** for **any** $i \geq 1$

Total error

$$\underline{\eta}^i_{\mathrm{tot}} \leq \|\nabla(u - u^i_h)\| \leq \eta^i_{\mathrm{tot}}$$

Algebraic error

$$\underline{\eta}^i_{\mathrm{alg}} \leq \|\nabla(u_h - u^i_h)\| = \|U_h - U^i_h\|_{\mathbb{A}_h} = \|R^i_h\|_{\mathbb{A}_h^{-1}} \leq \eta^i_{\mathrm{alg}}$$

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Further goals

- prove (local) **efficiency** & p-**robustness**
- design safe (local) **stopping criteria**
- estimate the **distribution** of the errors
- design adaptive algorithms
- study convergence and cost

The pathway

Algebraic residual representer

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- gives **equivalent form** of the **residual equation**: $u_h^i \in V_h$ s.t.

$$(\nabla u_h^i, \nabla v_h) = (f, v_h) - (r_h^i, v_h) \qquad \forall v_h \in V_h \quad \Leftarrow \quad \mathbb{A}_h U_h^i = F_h - R_h^i$$

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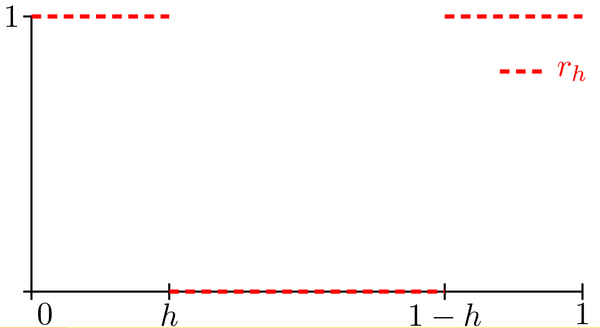

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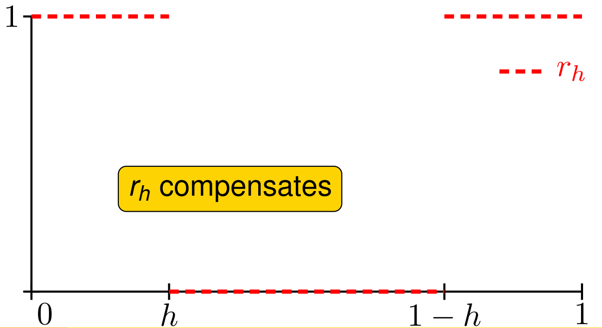
$\Rightarrow \|R_h\|_2$ explodes



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Tools

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Tools

- flux and potential reconstructions, $\boxed{\nabla \cdot \boldsymbol{\sigma}_{h,\mathrm{alg}} = r_h^i}$
- local Neumann MFE & local Dirichlet FE problems
- separate components for algebraic & discretization errors
- multilevel hierarchy (algebraic components)

Previous contributions

Linear problems

- Becker, Johnson, and Rannacher (1995), multigrid stopping criteria
- Repin (since 1997), guaranteed bounds including algebraic error
- Arioli (2000's), general stopping criteria
- Stevenson (2005) / Becker and Mao (2008), convergence and optimal rate
- Burstedde and Kunoth (2008), wavelets & inexact CG
- Meidner, Rannacher, Vihharev (2009), goal-oriented error control
- Silvester and Simoncini (2011), inexact mixed approximations
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Nonlinear problems

- Hackbusch and Reusken (1989) / Deuflhard (1990), adaptive Newton damping
- Ern and Vohralík (2013) / Congreve and Wihler (2017), adaptive inexact Newton methods
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Algebraic error upper bound

Theorem (Upper bound via algebraic error flux reconstruction)

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

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

Proof.

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

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

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Previous cheap constructions of $\boldsymbol{\sigma}_{h,\mathrm{alg}}^i$

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

Algebraic error flux reconstruction, two-level setting

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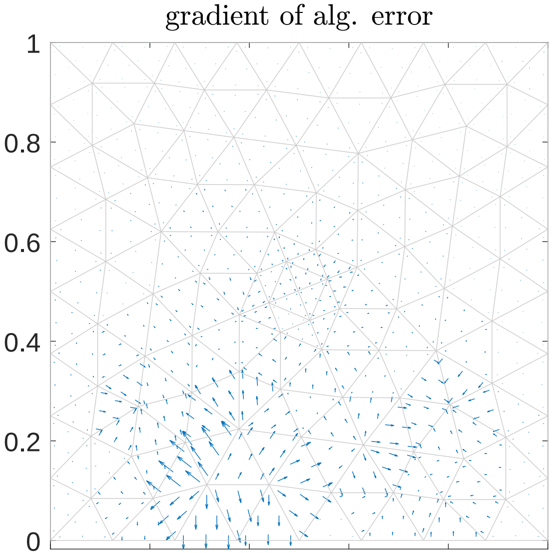

Algebraic error flux reconstruction, two-level setting

Definition (Coarse grid solve)

Find $\rho^i_{H,\mathrm{alg}} \in V_H := \mathbb{P}_1(\mathcal{T}_H) \cap H^1_0(\Omega)$ s.t.

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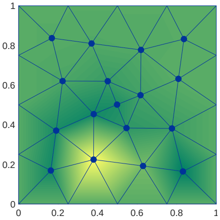
- $\mathbb{P}_1$ FE solve on coarse mesh $\mathcal{T}_H$



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- local homogeneous MFE Neumann pbs
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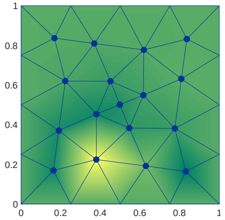

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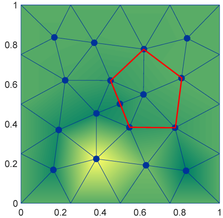

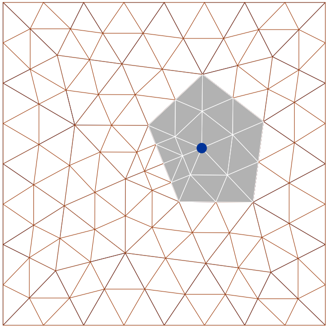

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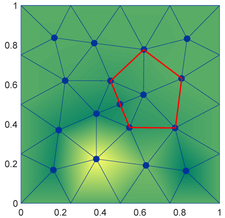
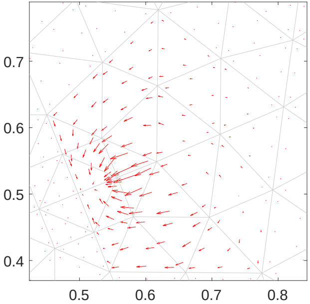


local alg. error flux reconstruction, $\sigma^{\mathrm{a},i}_{h,\mathrm{alg}}$



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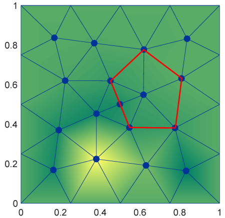

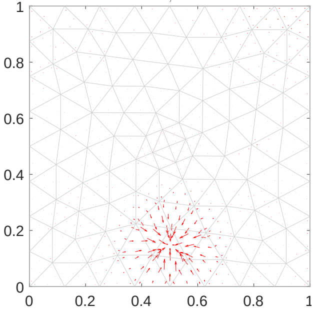

Discretization flux reconstruction

Definition (Discretization flux reconstruction, Destuynder & Métivet (1999), Braess & Schöberl (2008), EV (2013))

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

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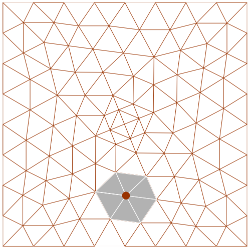
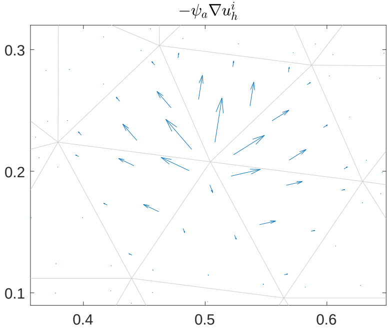
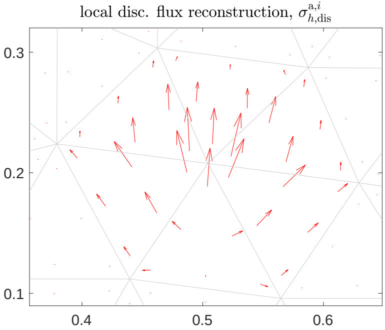
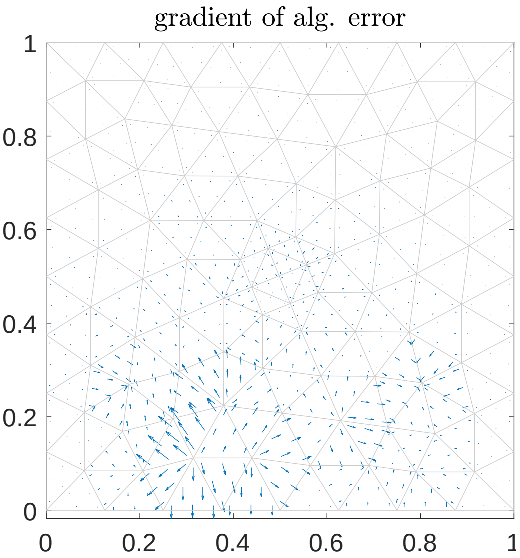
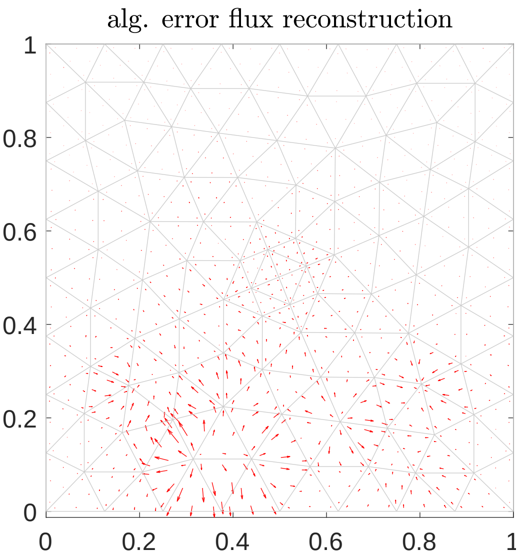






Reconstructions





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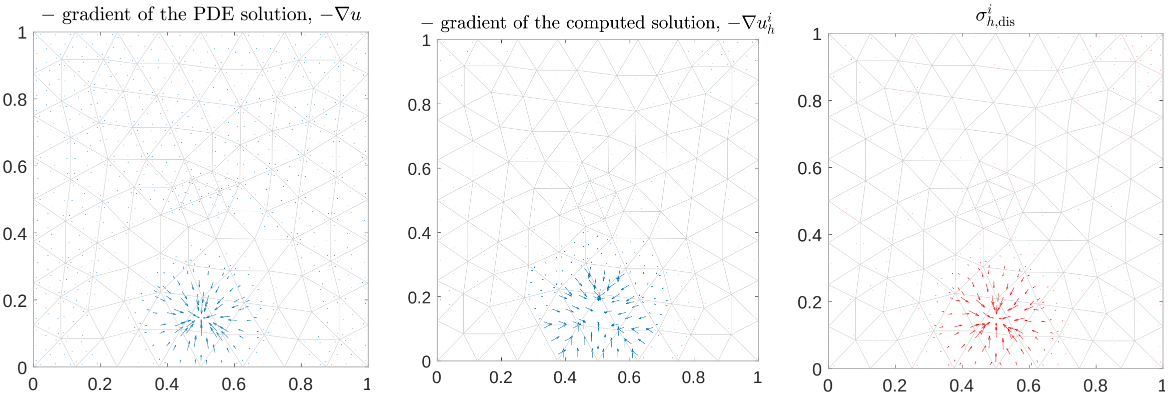

Upper bound on the total error

Theorem (Total error upper bound)

On each iteration $i \geq 1$, there holds

$$\underbrace{\|\nabla(u-u_h^i)\|}_{\text{total error}} \leq \underbrace{\|\nabla u_h^i + \boldsymbol{\sigma}_{h,\mathrm{dis}}^i\|}_{\text{discretization est.}} + \underbrace{\|\boldsymbol{\sigma}_{h,\mathrm{alg}}^i\|}_{\text{algebraic est.}} + \underbrace{\left\{\sum_{K\in\mathcal{T}_h} \frac{h_K^2}{\pi^2}\|f-\Pi_{Q_h} f\|_K^2\right\}^{1/2}}_{\text{data osc. est.}}.$$

Proof.

$$\|\nabla(u-u_h^i)\| = \sup_{v\in H_0^1(\Omega),\, \|\nabla v\|=1} (\nabla(u-u_h^i), \nabla v)$$

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Outline

Stopping criteria

Galerkin orthogonality

$$\underbrace{\|\nabla(u - u_h^i)\|^2}_{\text{total error}} = \underbrace{\|\nabla(u - u_h)\|^2}_{\text{discretization error}} + \underbrace{\|\nabla(u_h - u_h^i)\|^2}_{\text{algebraic error}}$$

Discretization error upper and lower bounds

- lower bound on total error & upper bound on algebraic error $\Rightarrow$ lower bound on the discretization error
- upper bound on total error & lower bound on algebraic error $\Rightarrow$ upper bound on the discretization error

Safe stopping criterion ($\gamma_{\text{alg}} \approx 0.1$)

$$\text{algebraic error} \leq \gamma_{\text{alg}}\ \text{discretization error}$$

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upper algebraic **estimate** $\leq \gamma_{\text{alg}}$ lower discretization **estimate**

Efficiency and polynomial-degree-robustness

Theorem (Efficiency & p-robustness, Braess, Pillwein, & Schöberl (2009), EV (2016))

Let the algebraic estimate be below the discretization estimate. Let $f \in \mathbb{P}_p(\mathcal{T}_h)$. Then

$$\underbrace{\|\nabla u_h^i + \boldsymbol{\sigma}_{h,\mathrm{dis}}^i\| + \|\boldsymbol{\sigma}_{h,\mathrm{alg}}^i\|}_{\text{total estimate}} \lesssim \underbrace{\|\nabla(u - u_h^i)\|}_{\text{total error}}.$$

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local stopping criterion ⇒ local efficiency & p-robustness

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local stopping criterion $\Rightarrow$ local efficiency & p-robustness

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Outline

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, $p = 1, \ldots, 4$
- 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

Numerical illustration

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

Discretization

- conforming finite elements, $p = 1, \ldots, 4$
- 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

Numerical illustration

Peak

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

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PCG

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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

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	—
	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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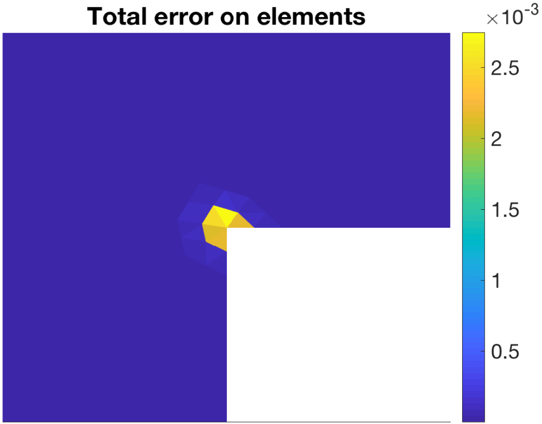
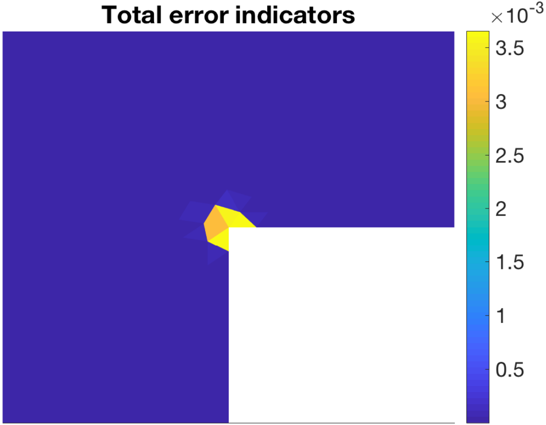
L-shape problem, $p = 3$, total error, 28th PCG iteration





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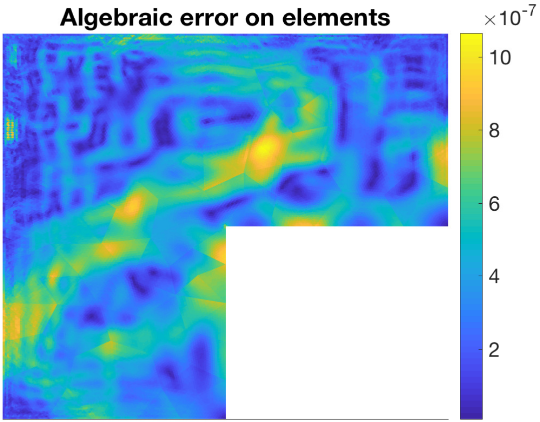
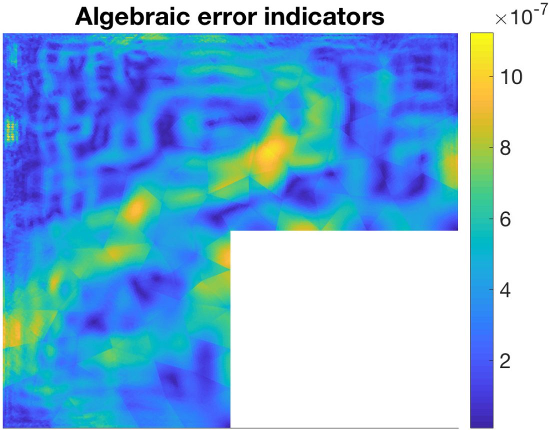
L-shape problem, $p = 3$, alg. error, 28th PCG iteration





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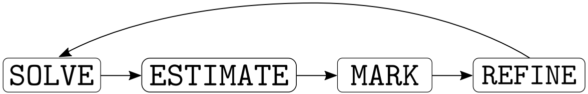
Outline

hp-refinement with inexact algebraic solvers

Goal

- avoid the *unrealistic* exact solution of $\mathbb{A}_\ell U_\ell^{\mathrm{ex}} = F_\ell$



- only *approximate* solution $\mathbb{A}_\ell U_\ell \approx F_\ell$ (corresponding $u_\ell \approx u_\ell^{\mathrm{ex}}$)

Theorem (Guaranteed contraction under realistic stopping criteria)

For the safe stopping criteria with $\gamma_{\mathrm{alg}} \approx 0.1$ and the hp-refinement decision, there are fully computable numbers $C_{\ell,\mathrm{red}}$, $0 \le C_{\ell,\mathrm{red}} \le C_{\theta,d,\kappa_\mathcal{T},p_{\max}}$, where $C_{\theta,d,\kappa_\mathcal{T},p_{\max}} < 1$ is generic constant, such that

$$\|\nabla(u - u_{\ell+1})\| \le C_{\ell,\mathrm{red}} \|\nabla(u - u_\ell)\|.$$

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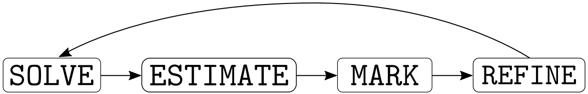

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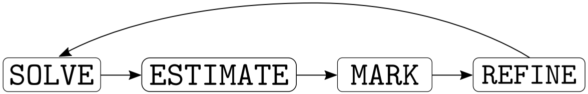

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Errors and estimates for *hp* refinement

L-shape domain in 2D: $\Omega := (-1,1) \times (-1,1) \setminus [0,1] \times [-1,0]$, $f = 0$

- singular exact solution: $u(r,\varphi) = r^{\frac{2}{3}} \sin \frac{2\varphi}{3}$

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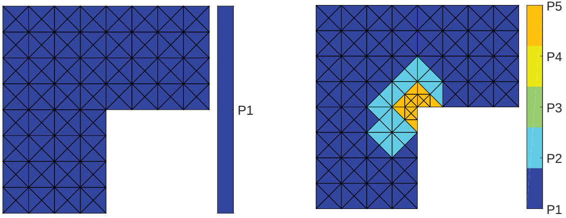
Inexact setting: V-cycle multigrid with Gauss–Seidel as a smoother



$(\mathcal{T}_1, \mathbf{p}_1)$ $(\mathcal{T}_7, \mathbf{p}_7)$

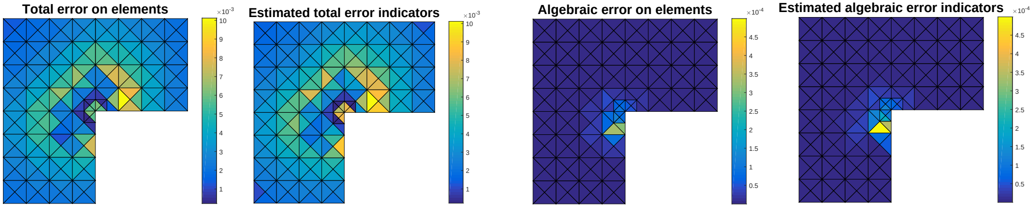
Errors and estimates for *hp* refinement

L-shape domain in 2D: $\Omega := (-1,1) \times (-1,1) \setminus [0,1] \times [-1,0]$, $f = 0$

- singular exact solution: $u(r,\varphi) = r^{\frac{2}{3}} \sin \frac{2\varphi}{3}$

Inexact setting: V-cycle multigrid with Gauss–Seidel as a smoother

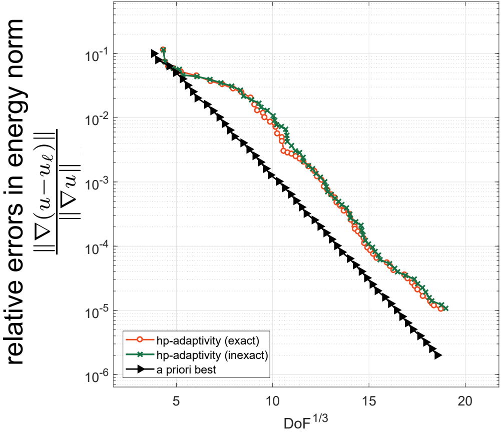
$I_{\mathrm{eff}}^{\mathrm{tot}} = 1.096$ $\quad$ $I_{\mathrm{eff}}^{\mathrm{alg}} = 1.365$

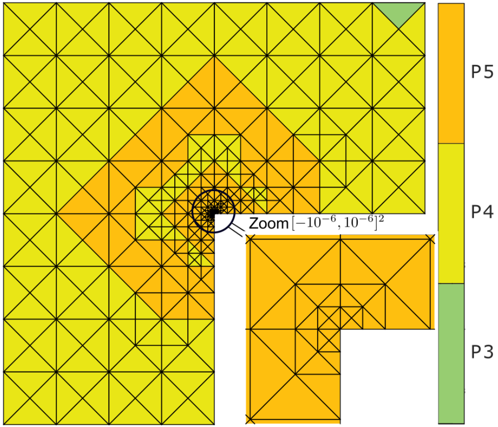


$\|\nabla(u - u_7)\|_K$ $\quad$ $\eta_K(u_7)$ $\quad$ $\|\nabla(u_7^{\mathrm{ex}} - u_7)\|_K$ $\quad$ $\eta_{\mathrm{alg},K}(u_7)$

P. Daniel, A. Ern, M. Vohralík, Computer Methods in Applied Mechanics and Engineering (2018)

Numerical exponential convergence with inexact solvers





P. Daniel, A. Ern, M. Vohralík, Computer Methods in Applied Mechanics and Engineering (2019)

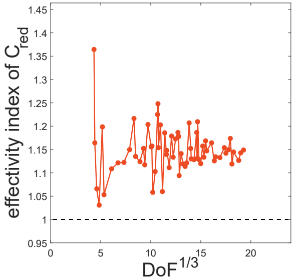
Effectivity indices

Effectivity indices of the estimated error reduction factor $C_{\ell,\mathrm{red}}$ and $\underline{\eta}_{\mathcal{M}_\ell^\theta}$

$$I_{\mathrm{red}}^{\mathrm{eff}} = \frac{C_{\ell,\mathrm{red}}}{\|\nabla(u-u_{\ell+1})\| \,/\, \|\nabla(u-u_\ell)\|}$$

$\gamma_{\mathrm{alg},\ell}$

$$I_{\mathrm{LB}}^{\mathrm{eff}} = \frac{\|\nabla(u_{\ell+1}^{\mathrm{ex}} - u_\ell)\|_{\omega_\ell}}{\underline{\eta}_{\mathcal{M}_\ell^\theta}}$$



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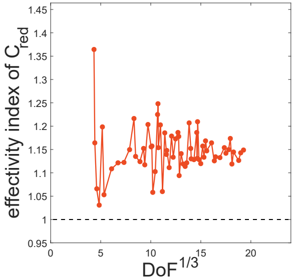

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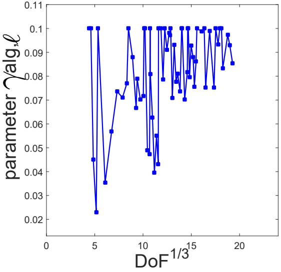

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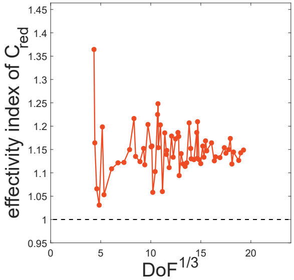
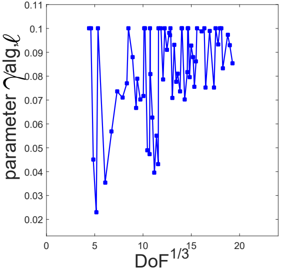
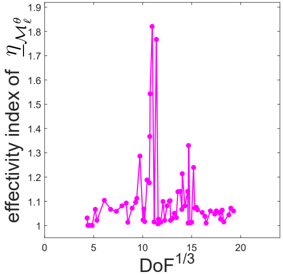


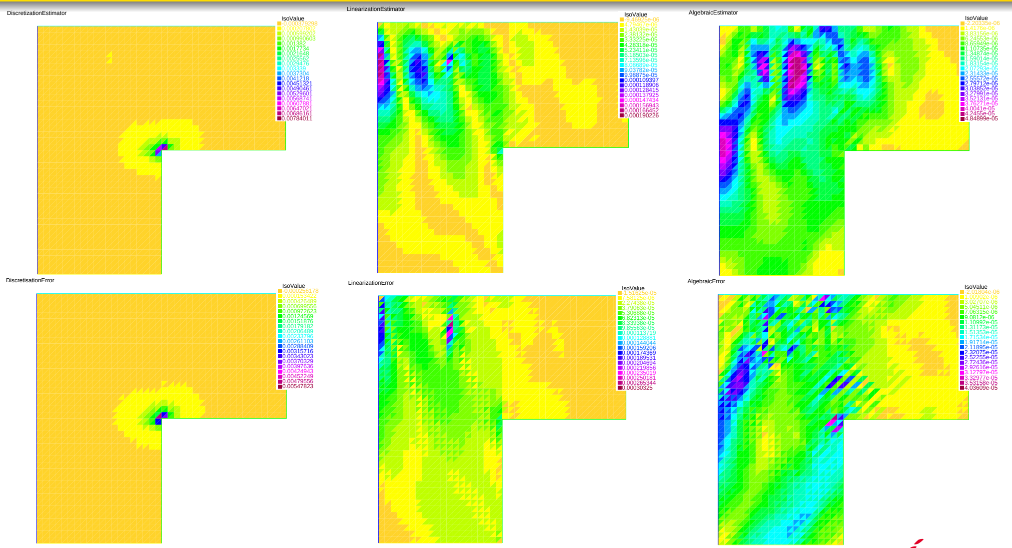




P. Daniel, A. Ern, M. Vohralík, Computer Methods in Applied Mechanics and Engineering (2019)

Outline

A steady nonlinear problem (FreeFem++ implementation Z. Tang)



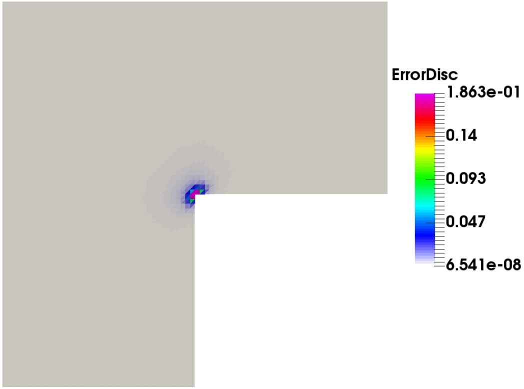
Estimate

Error

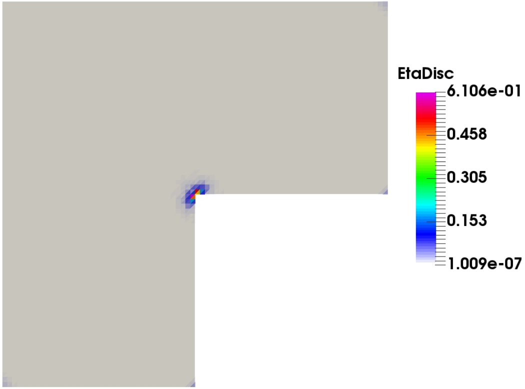
Discretization Linearization Algebraic

Outline

Adaptive inexact MinRes algorithm

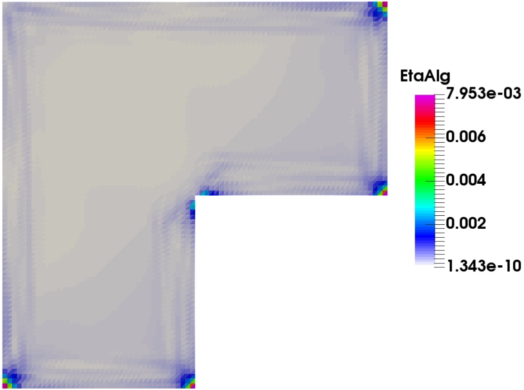


Discretization error

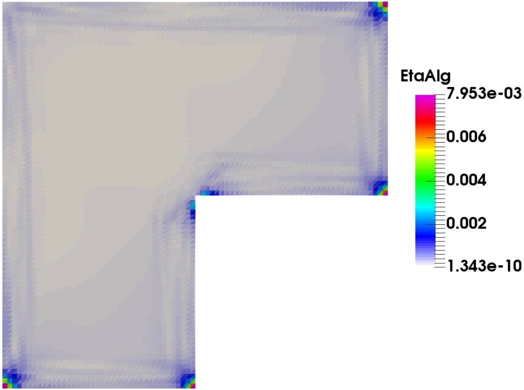


Discretization estimator

Adaptive inexact MinRes algorithm



Algebraic error



Algebraic estimator

M. Čermák, F. Hecht, Z. Tang, M. Vohralík, Numerische Mathematik (2018)

Outline

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})
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+ boundary & initial conditions

Mathematical issues

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

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Distinguishing the error components

Theorem (Distinguishing the error components)

Let

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

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

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

Error components

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

- only a **necessary number** of all **solver iterations**
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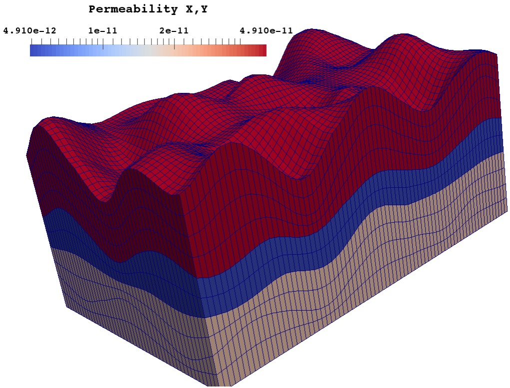
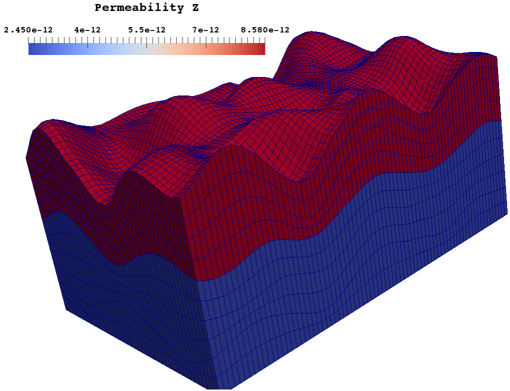
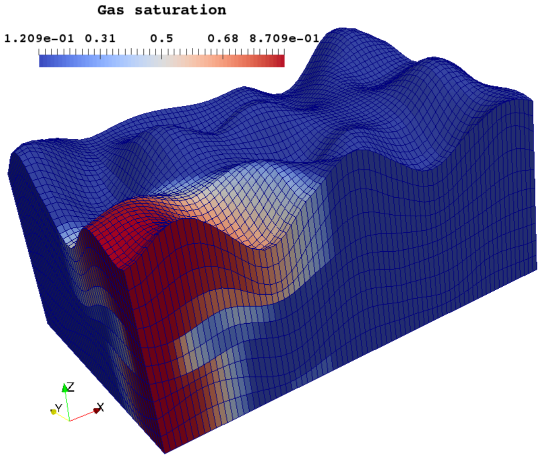
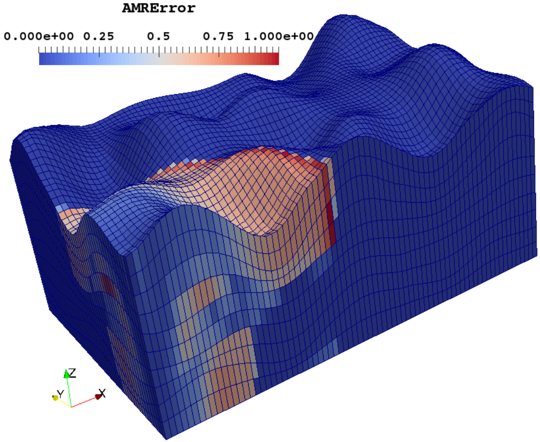
Three-phases, three-components (black-oil) problem: permeability



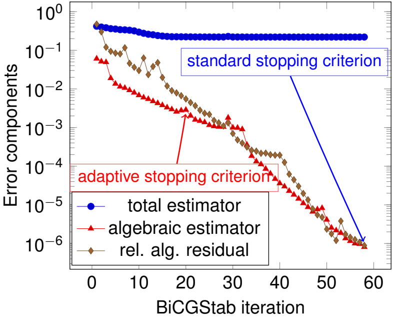


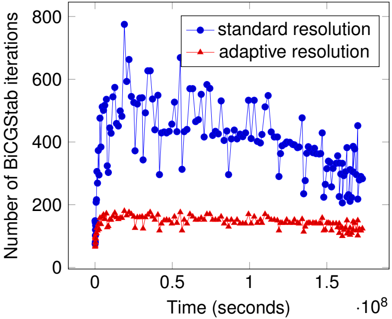
Three-phases, three-components (black-oil) problem: gas saturation and a posteriori estimate





Three-phases, three-components (black-oil) problem: algebraic solver & spatial mesh adaptivity





	Linear solver steps	Resolution time	AMR time	Estimators evaluation	Gain factor
Standard resolution	66386	1023s	-	-	-
Adaptive resolution	20184	201s	42s	26s	3.8

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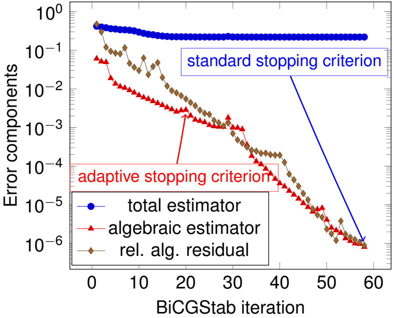

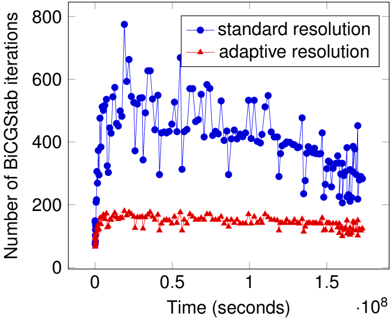

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Conclusions and outlook

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- **hierarchical construction** of the algebraic error estimate
- **local efficiency** and **robustness** wrt polynomial degree for model problems
- fully adaptive algorithms
- applications to complex problems

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References

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- A. Miraçi, J. Papež, M. Vohralík, *A multilevel algebraic error estimator and the corresponding iterative solver with p-robust behavior*, HAL Preprint 02070981, 2019.
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Thank you for your attention!

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Thank you for your attention!

Interplay of discretization and algebraic solvers: *a posteriori error estimates and adaptivity*

Monday, March 30 – Wednesday, April 1, 2020

Inria Paris

Confirmed speakers:

Mark Ainsworth
Randolph Bank
Roland Becker
Xiao-Chuan Cai
Long Chen
Emmanuil Georgoulis
Jay Gopalakrishnan
Ralf Hiptmair
Guido Kanschat
Volker Mehrmann
Gérard Meurant
Frédéric Nataf
Peter Oswald
Dirk Praetorius
Ulrich Rüde
Joachim Schöberl
David Silvester
Iain Smears
Rob Stevenson
Zdeněk Strakoš
Daniel Szyld
Marco Verani
Thomas Wihler
Barbara Wohlmuth
Ludmil Zikatanov

registration is free but mandatory

Webpage: *project.inria.fr/gatipor/*

Organizers:

Alexandre Ern
Kenan Kergrene
Ani Miraçi
Jan Papež
Martin Vohralík

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informatics mathematics