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. 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

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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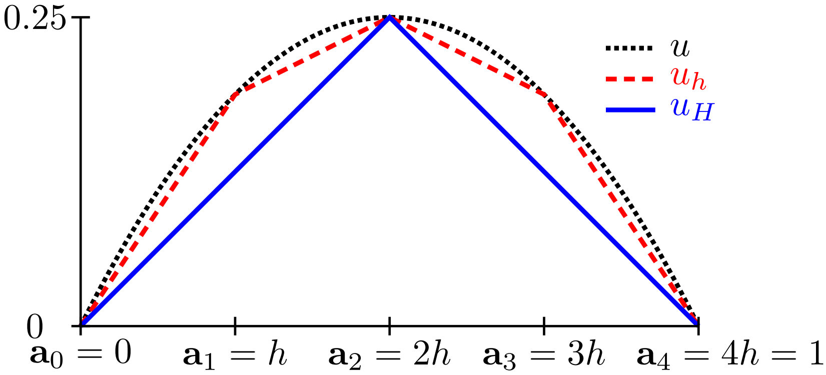
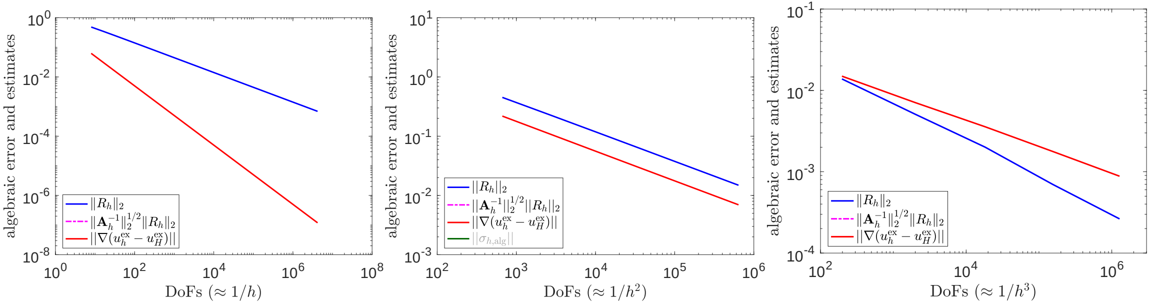


Euclidean norm of the algebraic residual vector is highly misleading



$d = 1$ $d = 2$ $d = 3$

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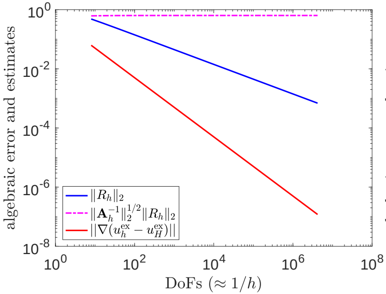

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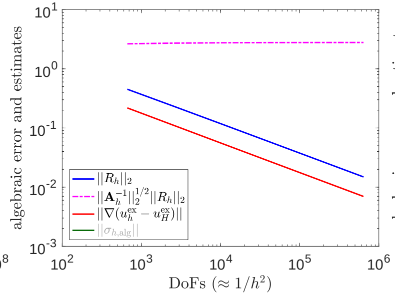

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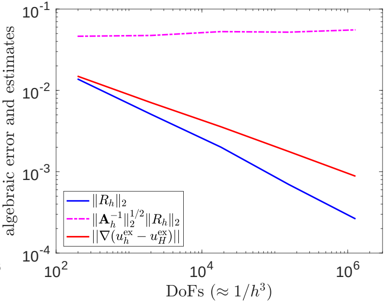

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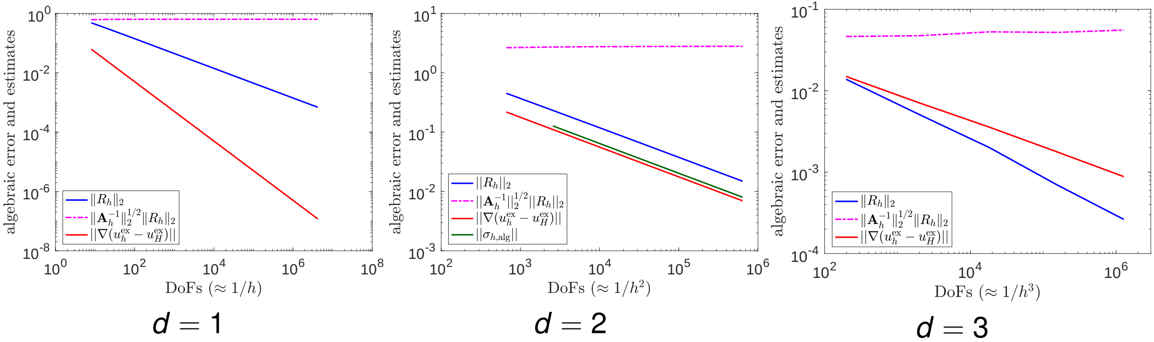


J. Papež, M. Vohralík, *Numerical Algorithms* (2020), DOI 10.1007/s11075-021-01118-5

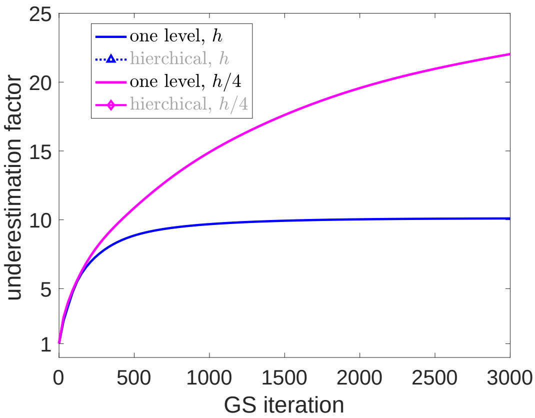
2. Slowly-converging Gauss–Seidel solver

Setting

- L-shape problem, $d = 2$
- regular triangular mesh
- random initial guess
- an algebraic estimate based on local Dirichlet FE problems
  - on the finest level
  - on a mesh hierarchy
- effectivity index

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

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



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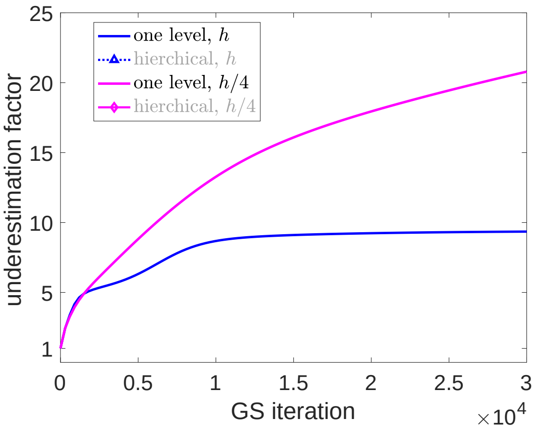

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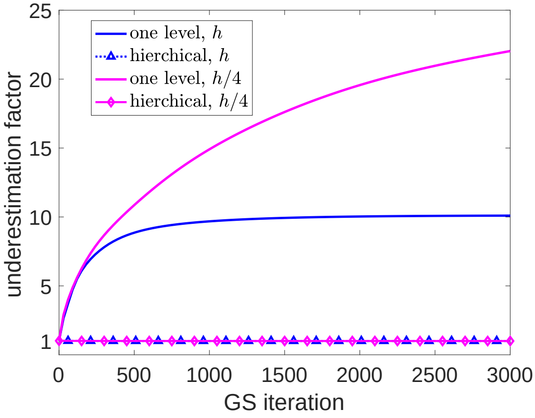

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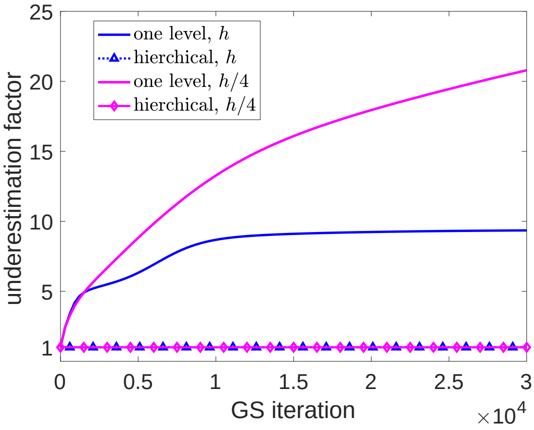

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J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, *Comput. Methods Appl. Mech. Engrg.* **371** (2020), 113243

Outline

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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

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 $U_h \in \mathbb{R}^N$, $N = |V_h|$, 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** $u_h^i \in V_h$

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Context

Total error

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

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Discretization error

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

Context

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

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

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

Algebraic error

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

Discretization error

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

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Discretization error

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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

- $r_h^i \in \mathbb{P}_p(\mathcal{T}_h)$ **discontinuous** piecewise polynomial $\leftarrow - -$ R_h^i

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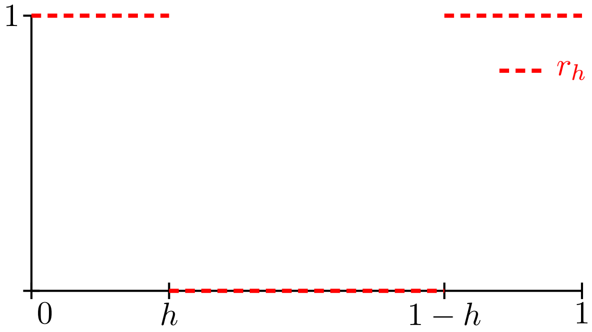
$$R_h := F_h - \mathbb{A}_h U_H = \begin{pmatrix} 2h \\ -2h \\ 2h \\ -2h \\ \vdots \\ 2h \end{pmatrix}$$



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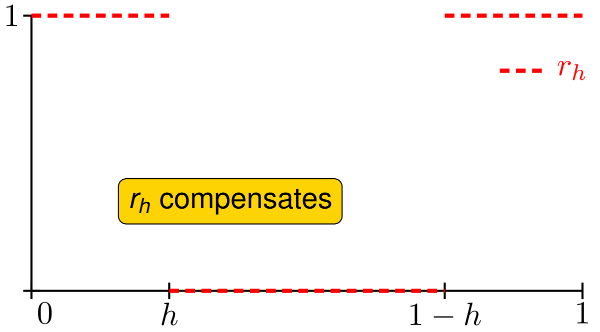
$\Rightarrow \|R_h\|_2$ explodes



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Tools

- flux and potential reconstructions, $\boxed{\nabla \cdot \boldsymbol{\sigma}_{h,\mathrm{alg}} = r_h^i}$

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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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Upper bound on the **algebraic error**

Theorem (Upper bound via algebraic error flux reconstruction)

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

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

Proof.

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

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

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Algebraic error flux reconstruction, 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.

$$(\nabla \rho^i_{H,\mathrm{alg}}, \nabla \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} = (r^i_h, \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} \quad \forall \mathbf{a} \in \mathcal{V}_H$$

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

Definition (Algebraic error flux reconstruction)

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

$$\boldsymbol{\sigma}^i_{h,\mathrm{alg}} := \sum_{\mathbf{a}\in\mathcal{V}_H} \boldsymbol{\sigma}^{\mathbf{a},i}_{h,\mathrm{alg}} \in \mathbf{V}_h \subset \mathbf{H}(\mathrm{div},\Omega)$$

- local homogeneous MFE Neumann pbs
- fine meshes of coarse patches $\omega_{\mathbf{a}}$
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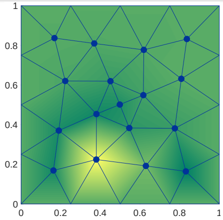

Algebraic error flux reconstruction, two-level setting

Definition (Coarse grid solve)

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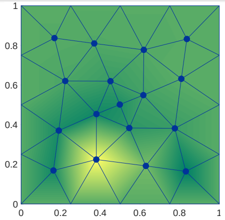

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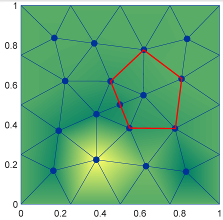

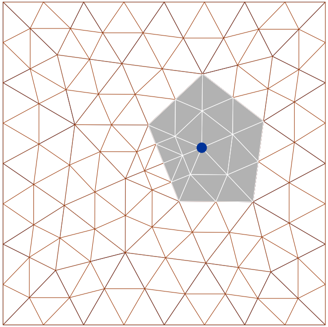

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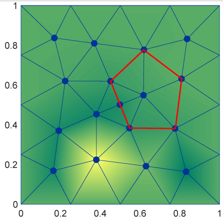
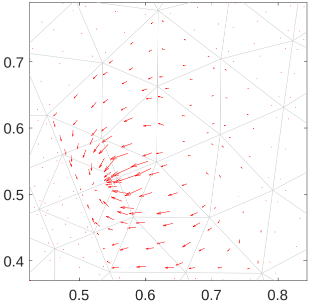


local alg. error flux reconstruction, $\sigma^{\mathrm{a},i}_{h,\mathrm{alg}}$



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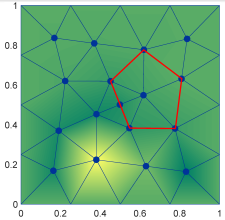
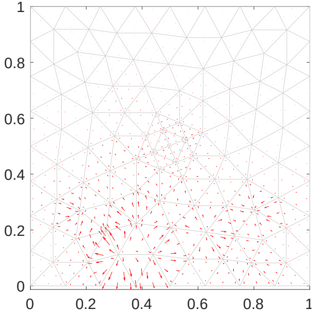


alg. error flux reconstruction



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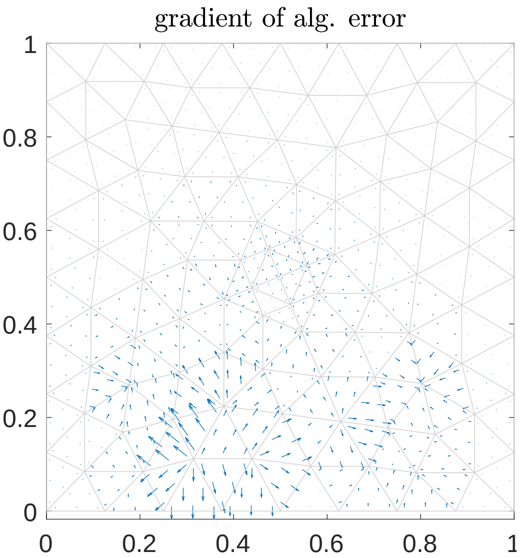

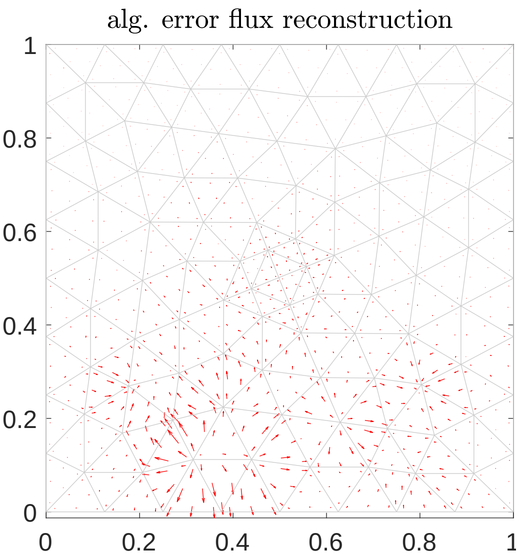

Discretization flux reconstruction

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

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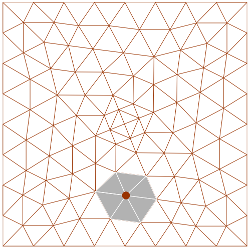

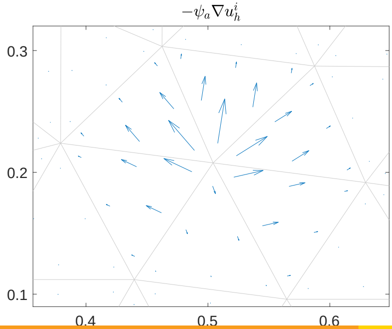

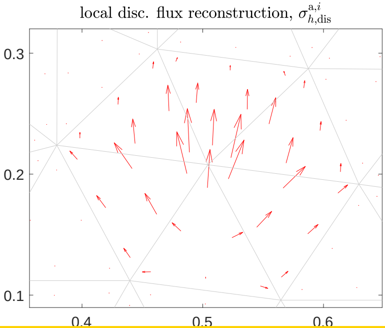

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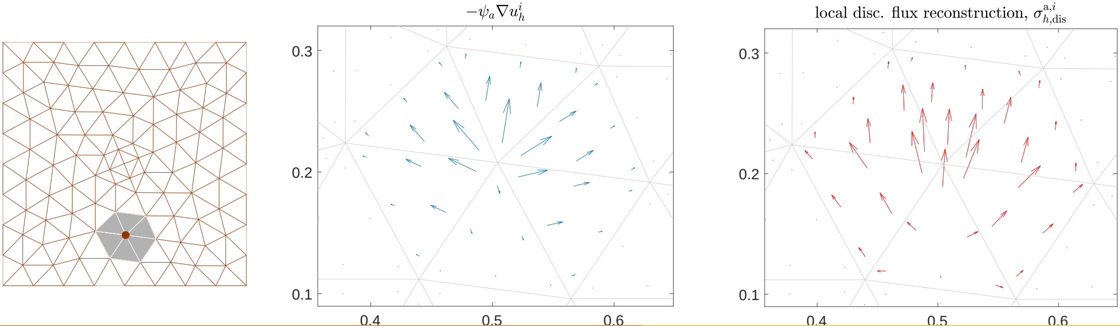
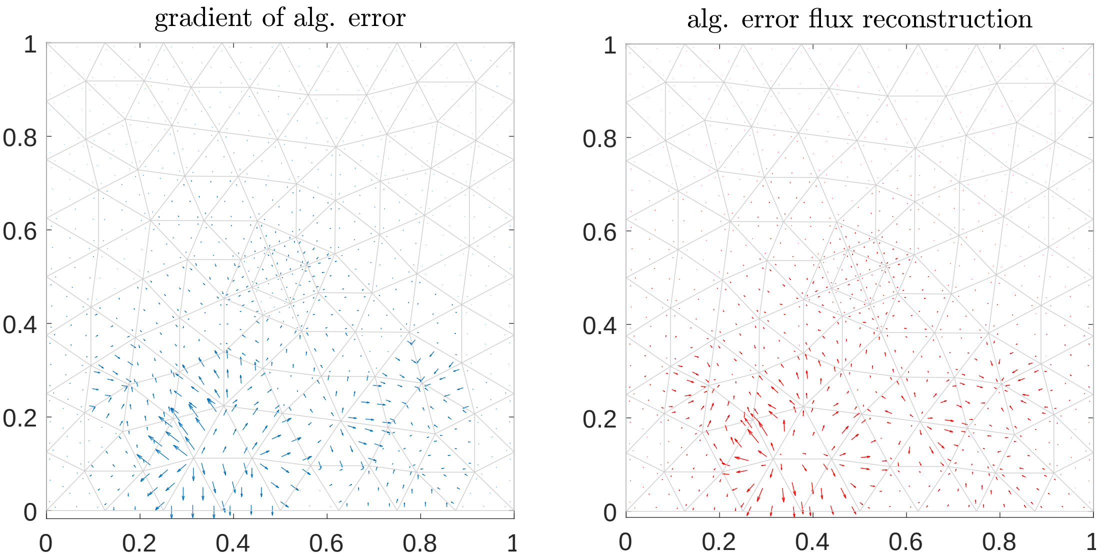


Reconstructions



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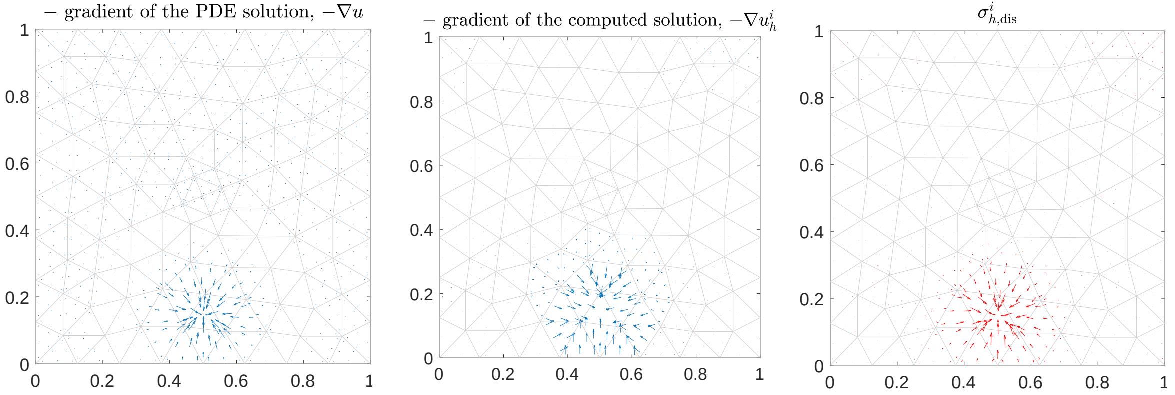

Upper bound on the **total error**

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

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Galerkin orthogonality

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

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- 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 ($\gamma_{\mathrm{alg}} \approx 0.1$)

$$\text{algebraic error} \le \gamma_{\mathrm{alg}} \, \text{discretization error}$$

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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

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

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$$\underbrace{\|\nabla u_h^i + \boldsymbol{\sigma}_{h,\mathrm{dis}}^i\|_K + \|\boldsymbol{\sigma}_{h,\mathrm{alg}}^i\|_K}_{\text{element total estimate}} \lesssim \underbrace{\sum_{\mathbf{a}\in\mathcal{V}_h,\, \mathbf{a}\subset\partial K} \|\nabla(u - u_h^i)\|_{\omega_{\mathbf{a}}}}_{\text{patch total error}} \quad \forall K \in \mathcal{T}_h.$$

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

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

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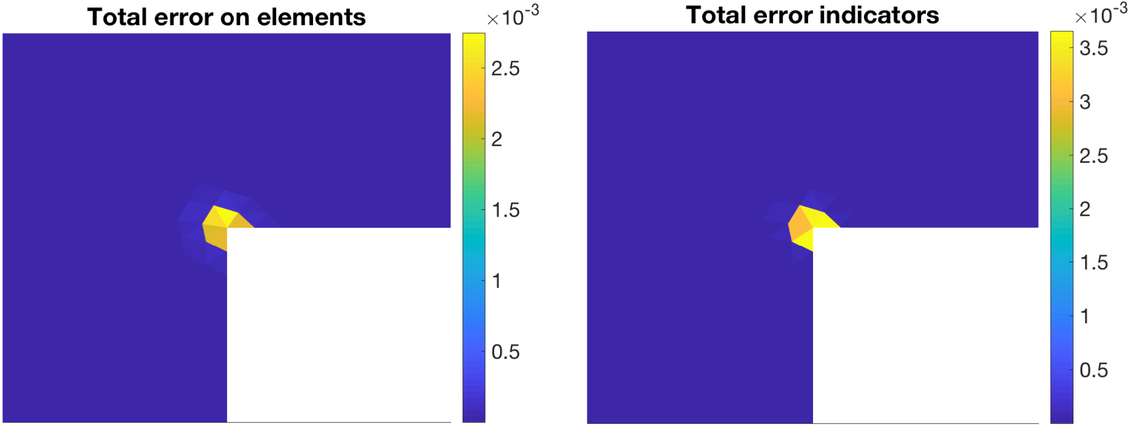
L-shape problem, $p = 3$, total error, 28th PCG iteration



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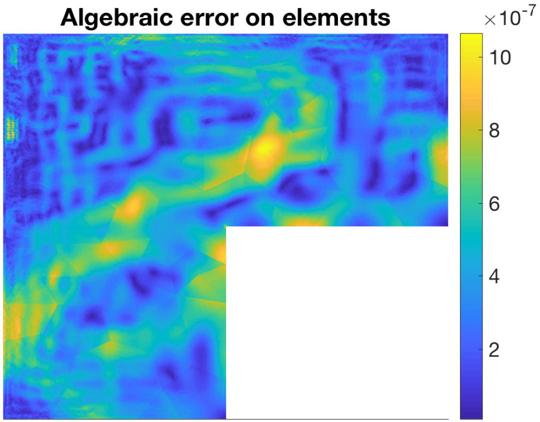

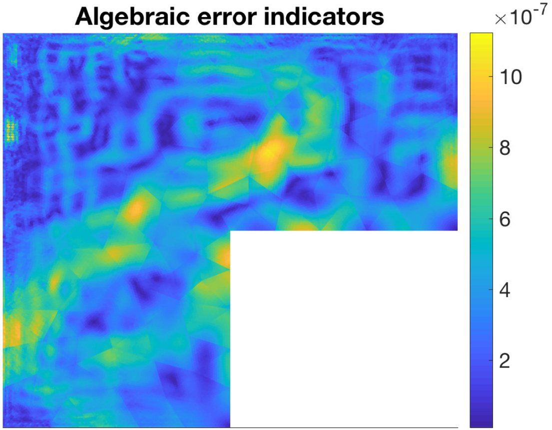

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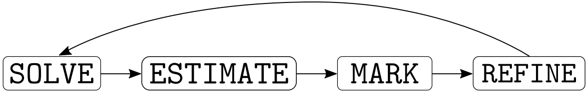
Outline

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

hp-refinement with inexact algebraic solvers

Goal

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



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

Theorem (Guaranteed contraction under realistic stopping criteria)

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

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

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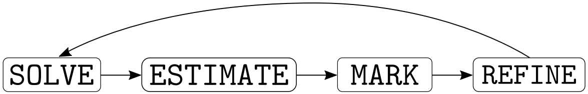

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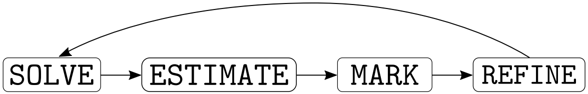

- only *approximate* solution $\mathbb{A}_\ell U_\ell \approx F_\ell$ (corresponding $u_\ell \approx u_\ell^{\text{ex}}$)

Theorem (Guaranteed contraction under realistic stopping criteria)

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

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

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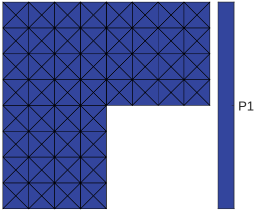
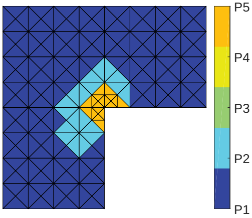
Inexact setting: V-cycle multigrid with Gauss–Seidel as a smoother



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



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

Errors and estimates for *hp* refinement

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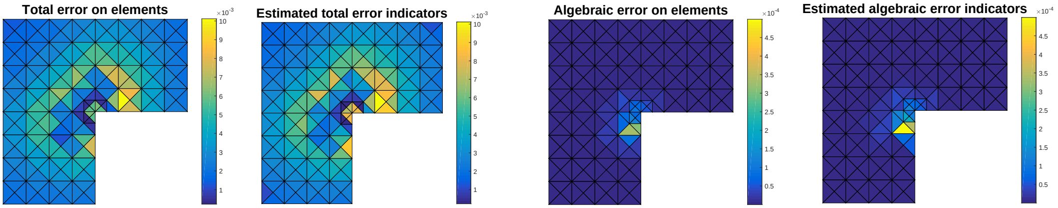
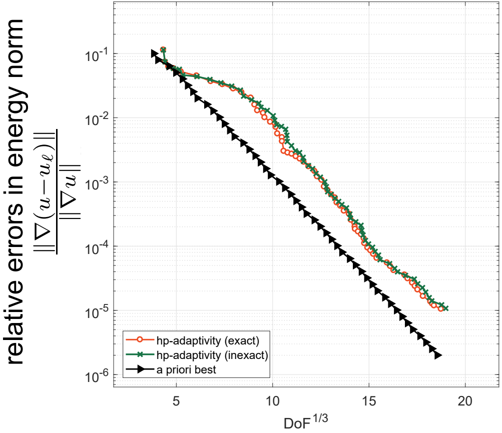
$I_{\mathrm{eff}}^{\mathrm{tot}} = 1.096$ $I_{\mathrm{eff}}^{\mathrm{alg}} = 1.365$

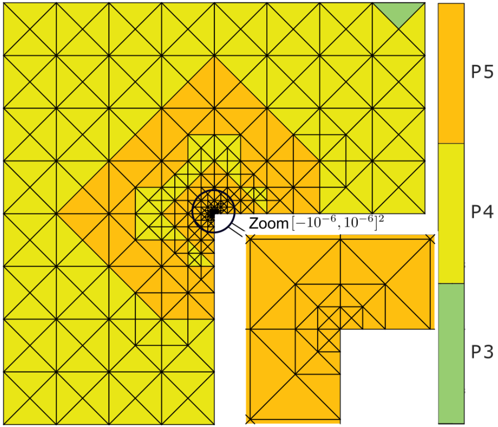


$\|\nabla(u - u_7)\|_K$ $\eta_K(u_7)$ $\|\nabla(u_7^{\mathrm{ex}} - u_7)\|_K$ $\eta_{\mathrm{alg},K}(u_7)$

P. Daniel, A. Ern, M. Vohralík, Computer Methods in Applied Mechanics and Engineering (2020)

Numerical exponential convergence with inexact solvers





P. Daniel, A. Ern, M. Vohralík, Computer Methods in Applied Mechanics and Engineering (2020)

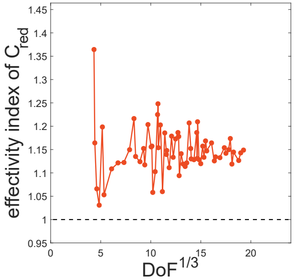
Effectivity indices

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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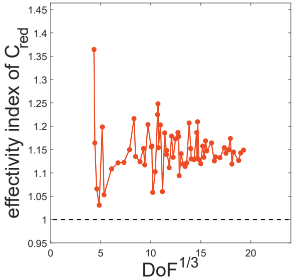

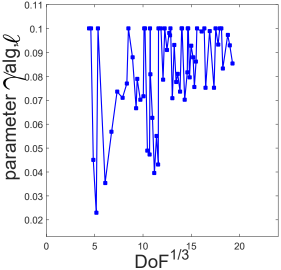

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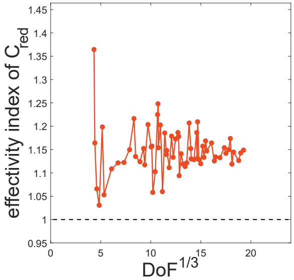
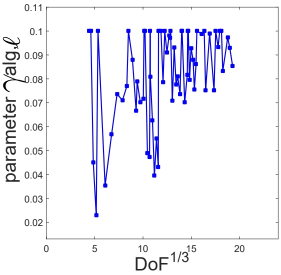
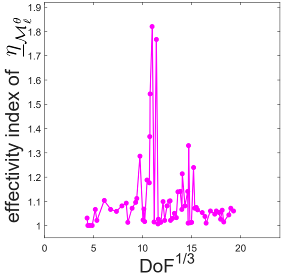


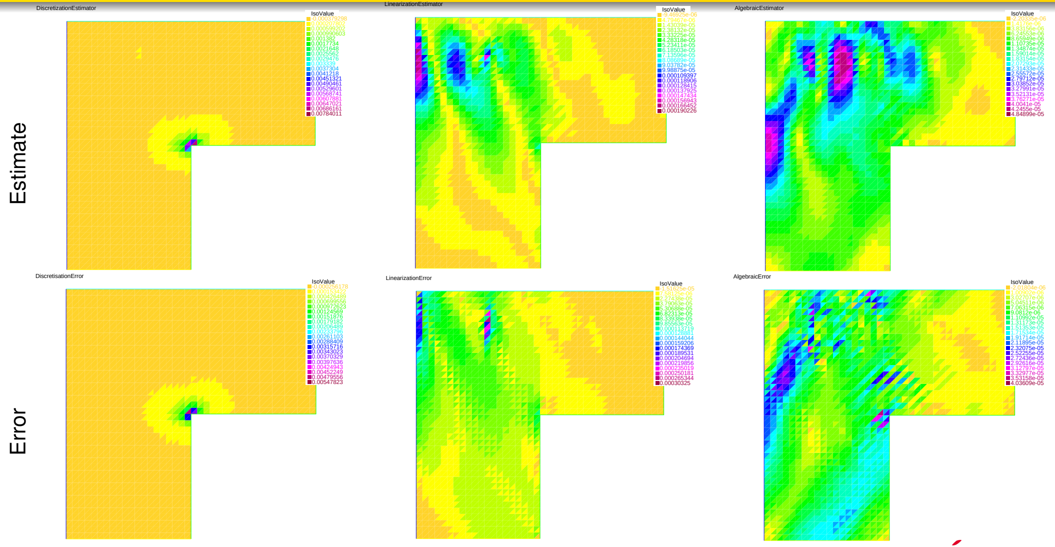




P. Daniel, A. Ern, M. Vohralík, Computer Methods in Applied Mechanics and Engineering (2020)

Outline

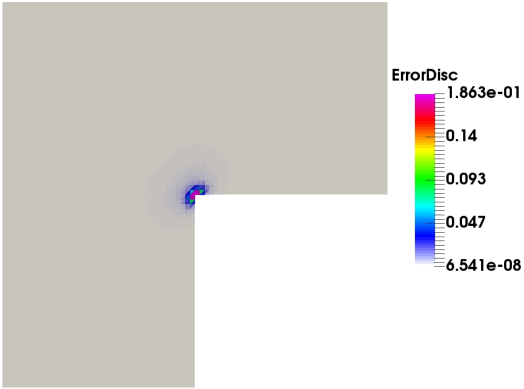
A steady nonlinear problem (FreeFem++ implementation Z. Tang)



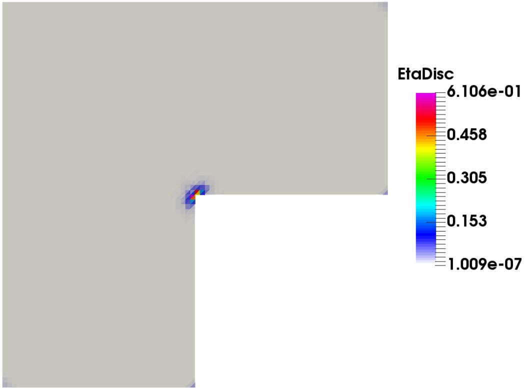
Discretization Linearization Algebraic

Outline

Adaptive inexact MinRes algorithm

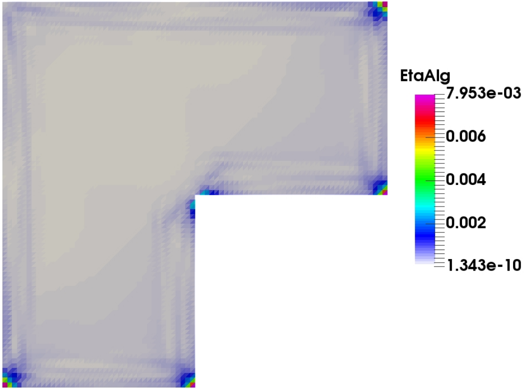


Discretization error

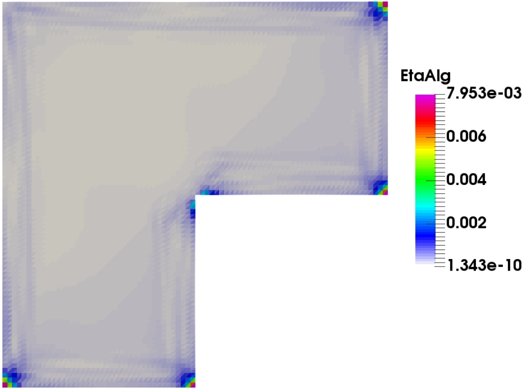


Discretization estimator

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}\},\\
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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*

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- $\eta_{\mathrm{sp}}^{n,k,i}$: spatial discretization
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- only a **necessary number** of all **solver iterations**
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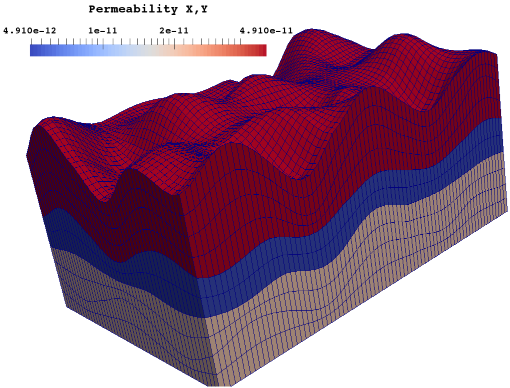
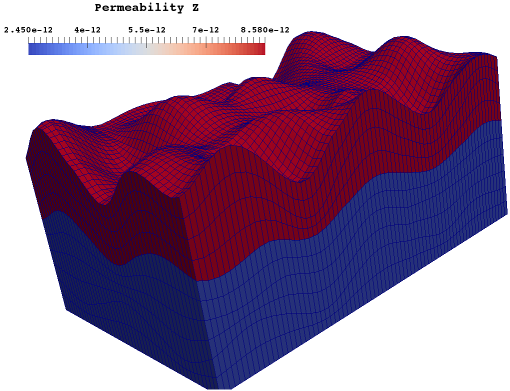
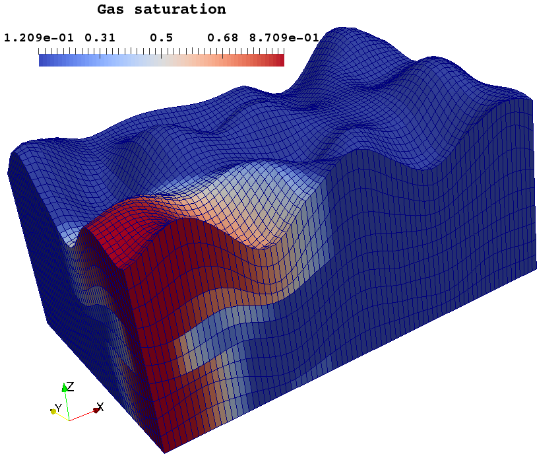
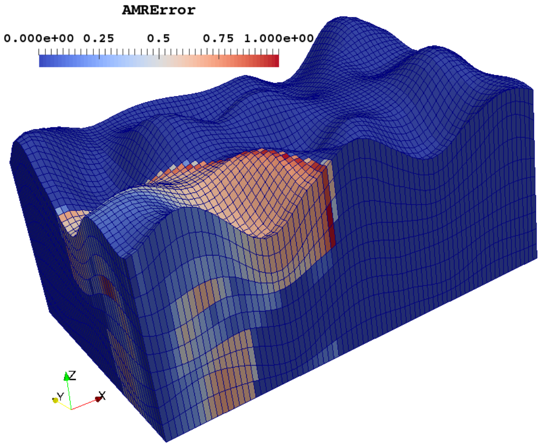
Three-phases, three-components (black-oil) problem: permeability



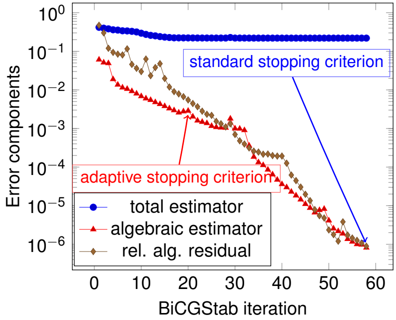


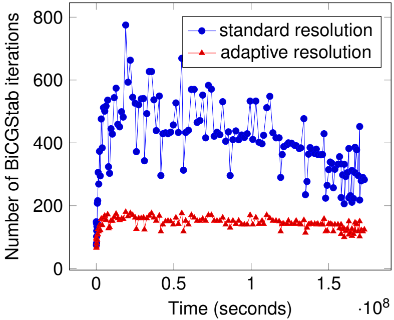
Three-phases, three-components (black-oil) problem: gas saturation and a posteriori estimate





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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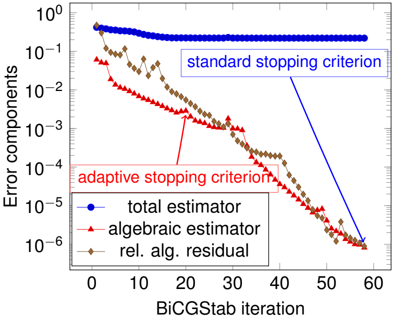

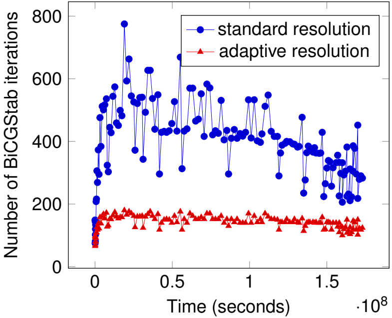

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- **hierarchical construction** of the algebraic error estimate
- **local efficiency** and **robustness** wrt polynomial degree for model problems
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- applications to complex problems

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- use of the reconstructions to **design novel algorithms**

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References

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