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

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informatiques mathématiques

European Research Council

École des Ponts ParisTech

Outline

Numerical approximations of PDEs

Numerical methods

- mathematically-based algorithms evaluated by **computers**
- deliver **approximate solutions**
- conception: more effort $\Rightarrow$ closer to the unknown solution
- example: elastic rod

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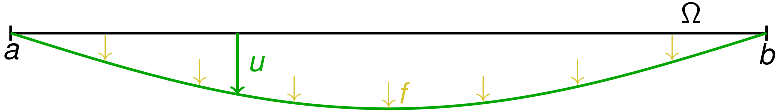

Numerical approximation u_h and its convergence to u

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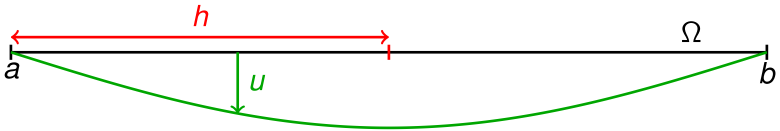

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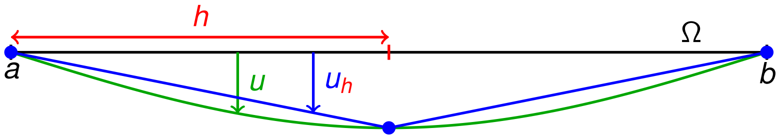

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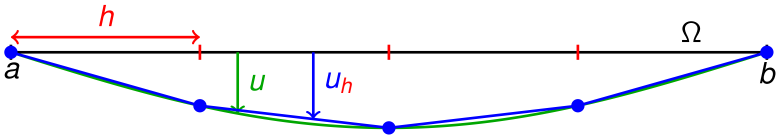

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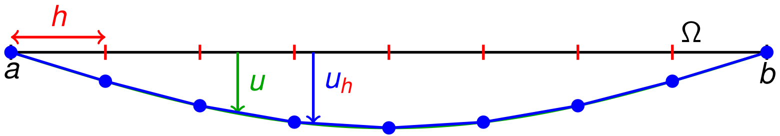

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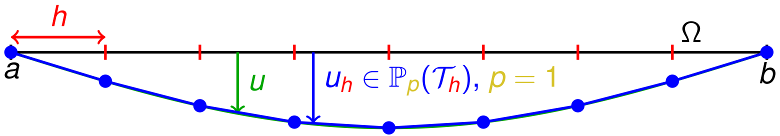

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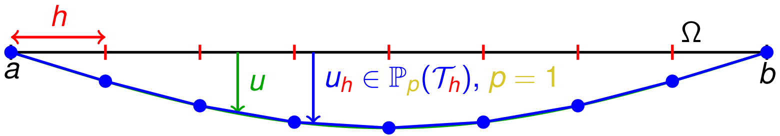

Numerical approximation u_h and its convergence to u

Error

$$\|\nabla(u-u_h)\| = \left\{\int_a^b |(u-u_h)'|^2\right\}^{\frac{1}{2}}$$

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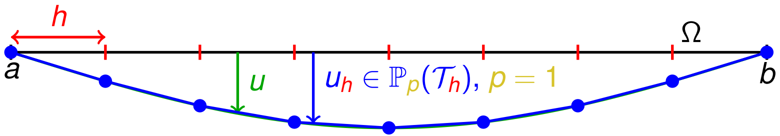

Numerical approximation u_h and its convergence to u

Error

$$\|\nabla(u-u_h)\| = \left\{\int_a^b |(u-u_h)'|^2\right\}^{\frac{1}{2}}$$

Need to solve

$$\mathbb{A}_h \mathrm{U}_h = \mathrm{F}_h$$

3 crucial questions

Crucial questions

1. How **large** is the overall **error**?
2. **Where** (model/space/time/linearization/algebra) is it **localized**?
3. Can we **decrease** it **efficiently**?

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Suggested answers

1. **A posteriori** error **estimates**.

3 crucial questions & suggested answers

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Suggested answers

1. **A posteriori** error **estimates**.
2. Identification of **error components**.
3. **Balancing** error components, **adaptivity** (working where needed).

CDG Terminal 2E collapse in 2004 (opened in 2003)

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Case Studies in Engineering Failure Analysis 3 (2015) 88–95

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Y. El Kamari [a], W. Raphael [a,*], A. Chateauneuf [b,c]

[a] Ecole Supérieure d'Ingénieurs de Beyrouth (ESIB), Université Saint-Joseph, CST Mar Roukos, PO Box 11-514, Riad El Solh Beirut 1107 2050,

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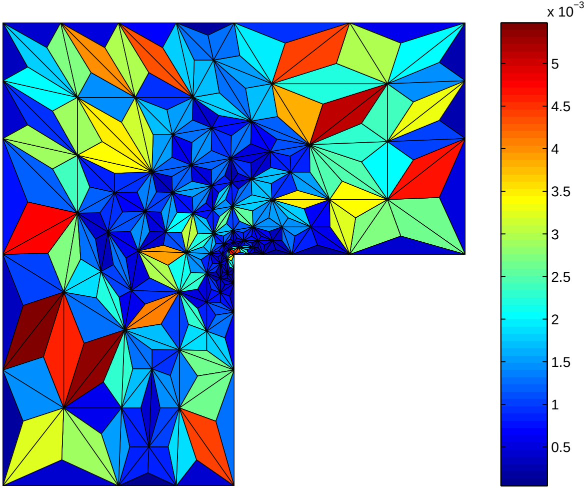
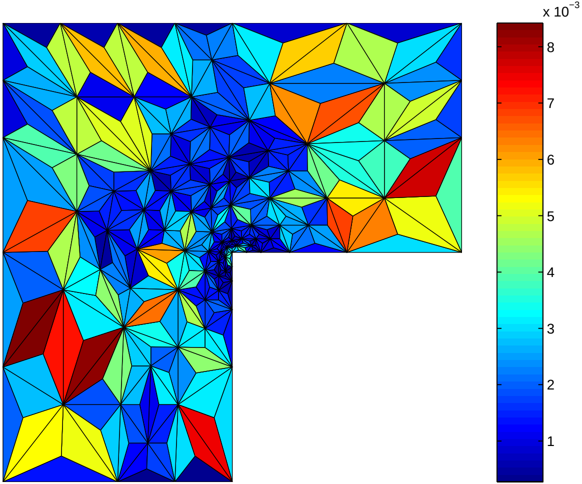
Appetizer: it works! (nonlinear problem with linearization & algebra)



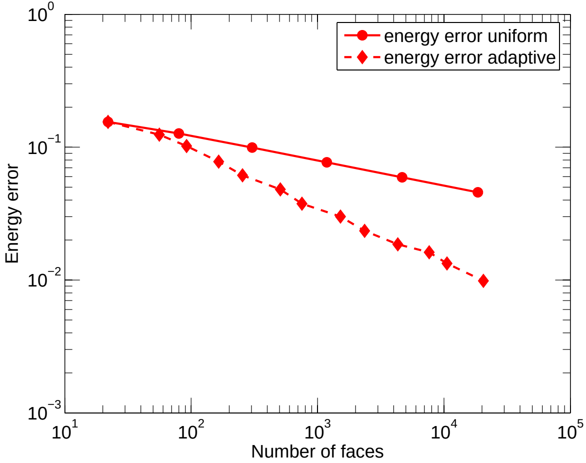
Estimated error distribution



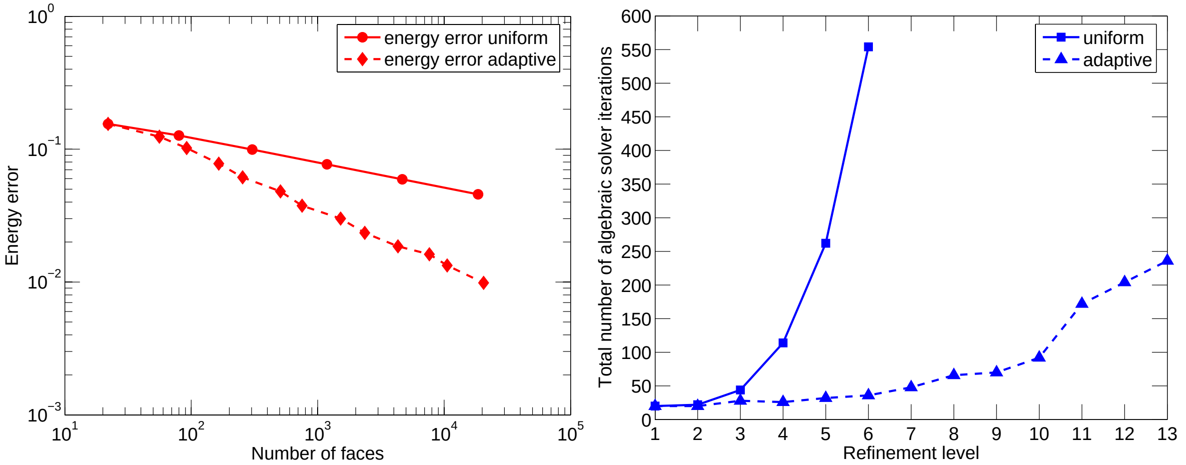
Exact error distribution

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

Commercial: get more



Commercial: get more, pay less! (balancing all error components)



A posteriori error estimates: control the error

Elastic membrane equation

$$-\Delta u = f \quad \text{in} \quad \Omega,$$
$$u = 0 \quad \text{on} \quad \partial\Omega$$

Guaranteed error upper bound (reliability)

$$\underbrace{\|\nabla(u - u_h)\|}_{\text{unknown error}} \leq \underbrace{\eta(u_h)}_{\text{computable estimator}}$$

Error lower bound (efficiency)

$$\eta(u_h) \leq C_{\text{eff}} \|\nabla(u - u_h)\|$$

- C_{eff} independent of Ω, u, u_h, h, p
- computable bound on C_{eff} available, $C_{\text{eff}} \approx 5$
- Prager and Synge (1947), Ladevèze (1975), Babuška & Rheinboldt (1987), Verfürth (1989), Ainsworth & Oden (1993), Destuynder & Métivet (1999), Braess, Pillwein, & Schöberl (2009), Ern & Vohralík (2015)

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How large is the overall error? (model pb, known smooth solution)

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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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$\approx h_0/2$		6.07×10^{-1}	14%	5.56×10^{-1}	13%	**1.09**
$\approx h_0/4$		3.10×10^{-1}	7.0%	2.92×10^{-1}	6.6%	**1.06**
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	**1.04**
$\approx h_0/2$	2	4.23×10^{-2}	9.5×10^{-1}%	4.07×10^{-2}	9.2×10^{-1}%	**1.04**
$\approx h_0/4$	3	2.62×10^{-4}	5.9×10^{-3}%	2.60×10^{-4}	5.9×10^{-3}%	**1.01**
$\approx h_0/8$	4	2.60×10^{-7}	5.9×10^{-6}%	2.58×10^{-7}	5.8×10^{-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)

How large is the overall error? (model pb, known smooth solution)

h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\|\nabla u_h\|}$	$\|\nabla(u-u_h)\|$	rel. error $\frac{\|\nabla(u-u_h)\|}{\|\nabla u_h\|}$	$I^{\mathrm{eff}} = \frac{\eta(u_h)}{\|\nabla(u-u_h)\|}$
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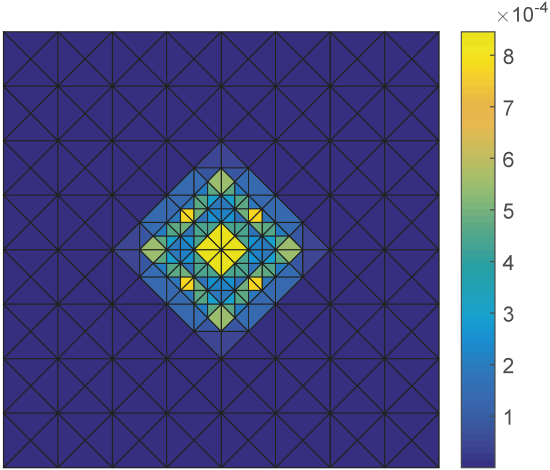
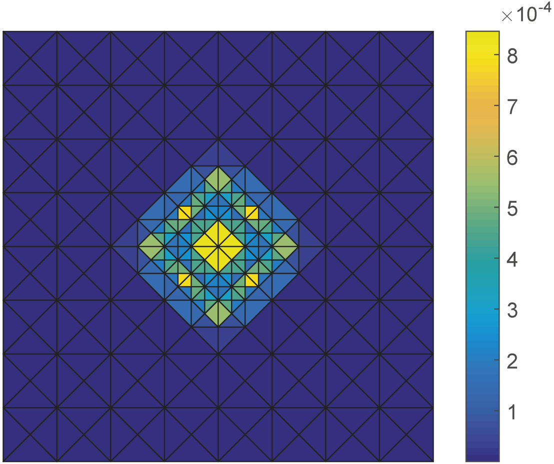
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

Outline

Where (in space) is the error localized?



Estimated error distribution $\eta_K(u_h)$



Exact error distribution $\|\nabla(u - u_h)\|_K$

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

Adaptive mesh refinement (linear problem with exact solvers)

Adaptive mesh refinement

- Dörfler marking: subset $\mathcal{M}_\ell$ containing θ-fraction of the estimates

$$\sum_{K \in \mathcal{M}_\ell} \eta_K(u_\ell)^2 \geq \theta^2 \sum_{K \in \mathcal{T}_\ell} \eta_K(u_\ell)^2$$

Convergence on a sequence of adaptively refined meshes

- $$\|\nabla(u - u_\ell)\| \to 0$$
- some mesh elements may not be refined at all: $h \not\searrow 0$
- Babuška & Miller (1987), Dörfler (1996)

Optimal error decay rate wrt degrees of freedom

- $$\|\nabla(u - u_\ell)\| \lesssim |\mathrm{DoF}_\ell|^{-p/d} \qquad \text{(replaces } h^p\text{)}$$
- same for smooth & singular solutions: ~~higher-order only pay-off for sm. sol.~~
- decays to zero as fast as on a best-possible sequence of meshes
- Morin, Nochetto, Siebert (2000), Stevenson (2005, 2007), Cascón, Kreuzer, Nochetto, Siebert (2008), Canuto, Nochetto, Stevenson, Verani (2017)

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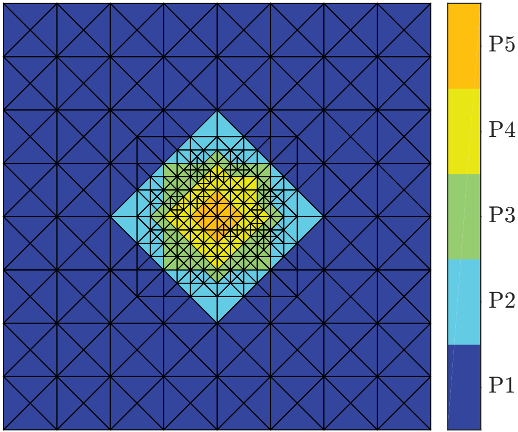
Can we decrease the error efficiently? *hp* adaptivity, (**smooth** solution)



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

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

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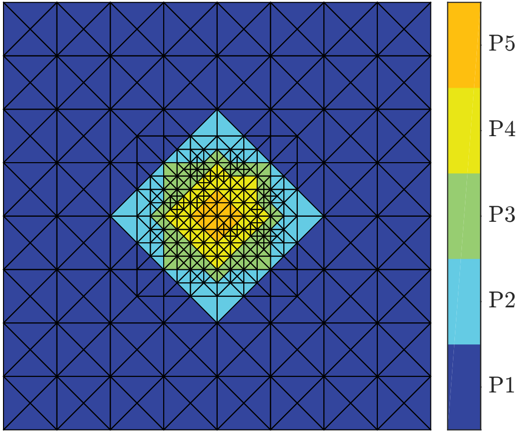

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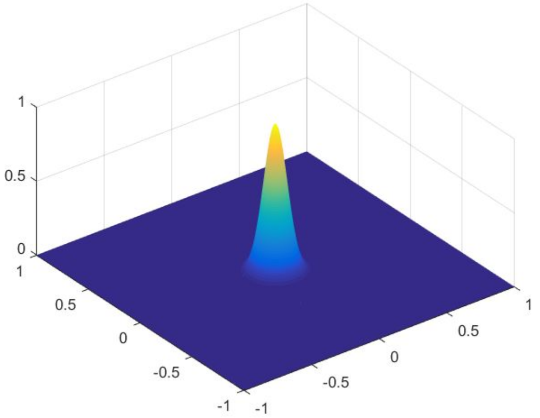
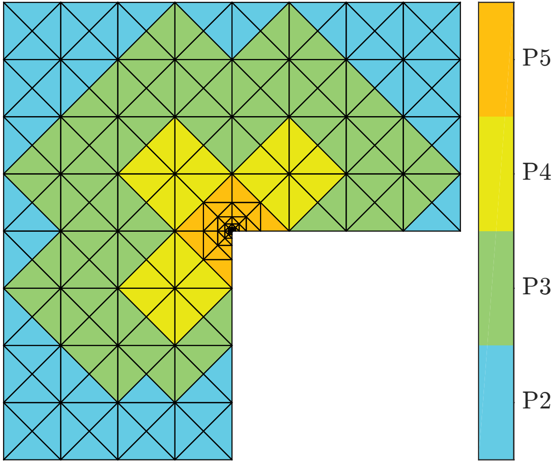


Exact solution

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

Can we decrease the error efficiently? *hp* adaptivity, (**singular** solution)



Mesh $\mathcal{T}_\ell$ and polynomial degrees p_K

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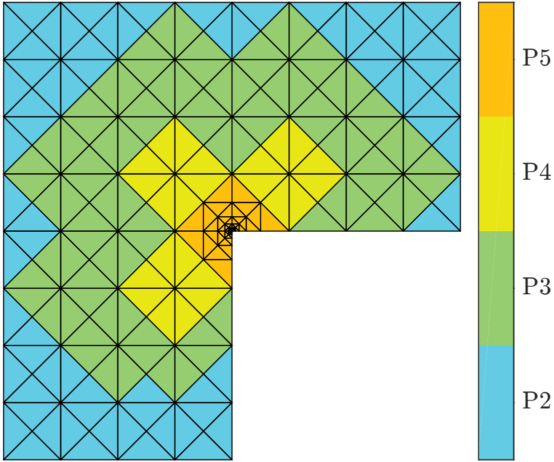

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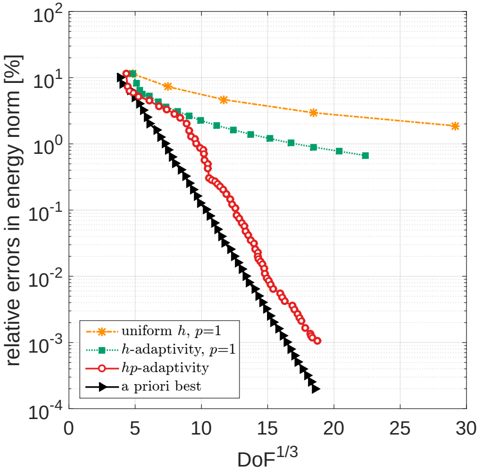

Relative error as a function of DoF

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

Outline

Balancing error components (nonlinear problem with inexact solvers)

Fully adaptive algorithm (adaptive inexact Newton method)

- **total error estimate** on mesh $\mathcal{T}_\ell$, linearization step k, algebraic solver step i

$$\underbrace{\|u - u_\ell^{k,i}\|_*}_{\text{total error}} \leq \underbrace{\eta_{\ell,\mathrm{disc}}^{k,i}}_{\text{discretization estimate}} + \underbrace{\eta_{\ell,\mathrm{lin}}^{k,i}}_{\text{linearization estimate}} + \underbrace{\eta_{\ell,\mathrm{alg}}^{k,i}}_{\text{algebraic estimate}}$$

- **balancing error components**: work where needed

$\eta_{\ell,\mathrm{alg}}^{k,i} \leq \gamma_{\mathrm{alg}} \max\{\eta_{\ell,\mathrm{disc}}^{k,i}, \eta_{\ell,\mathrm{lin}}^{k,i}\}$	stopping criterion linear solver
$\eta_{\ell,\mathrm{lin}}^{k,i} \leq \gamma_{\mathrm{lin}} \eta_{\mathrm{disc}}^{k,i}$	stopping criterion nonlinear solver
$\theta\eta_{\ell,\mathrm{disc}}^{k,i} \leq \eta_{\mathrm{disc},\mathcal{M}_\ell}^{k,i}$	adaptive mesh refinement

- link – inexact Newton method: Bank & Rose (1982), Hackbusch & Reusken (1989), Deuflhard (1991), Eisenstat & Walker (1994)

Convergence, optimal **error decay rate** wrt **DoFs**

- Gantner, Haberl, Praetorius, & Stiftner (2018), Heid & Wihler (2019)

Optimal error decay rate wrt overall computational cost

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Including **algebraic** error: $\mathbb{A}_\ell \mathrm{U}_\ell^i \neq \mathrm{F}_\ell$

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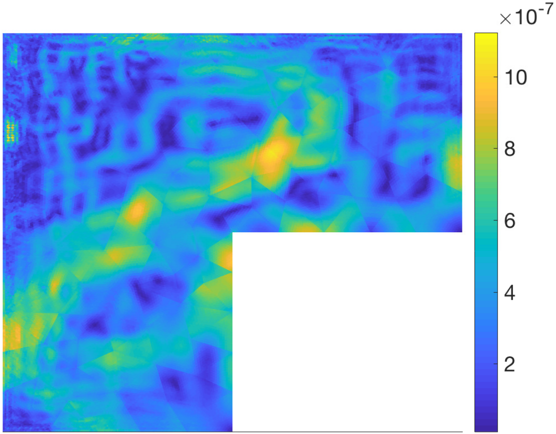
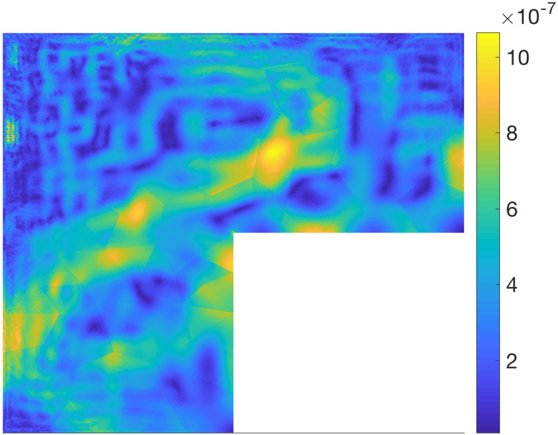


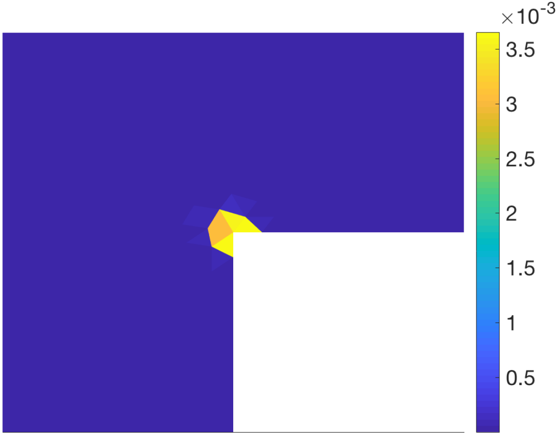
Estimated algebraic errors $\eta_{\mathrm{alg},K}(u_\ell^i)$



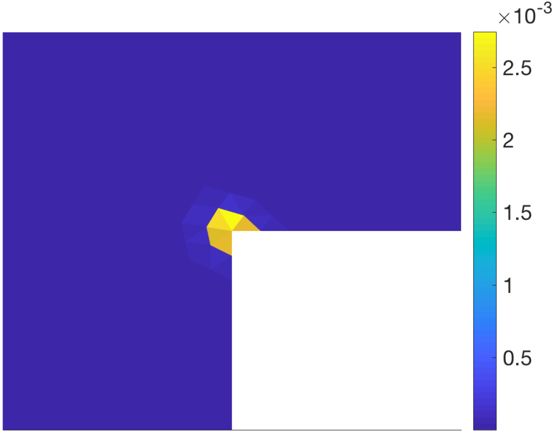
Exact algebraic errors $\|\nabla(u_\ell - u_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, preprint (2020)

Including **algebraic** error: $\mathbb{A}_\ell \mathrm{U}_\ell^i \neq \mathrm{F}_\ell$



Estimated total errors $\eta_K(u_\ell^i)$



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J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, preprint (2020)

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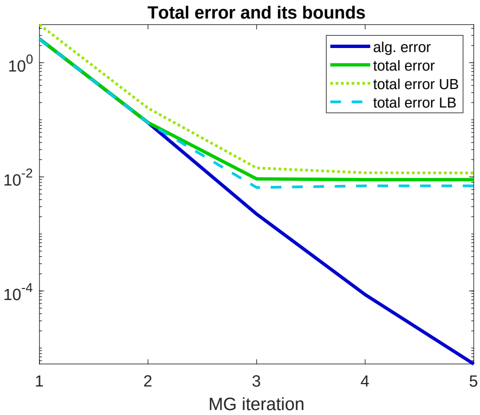
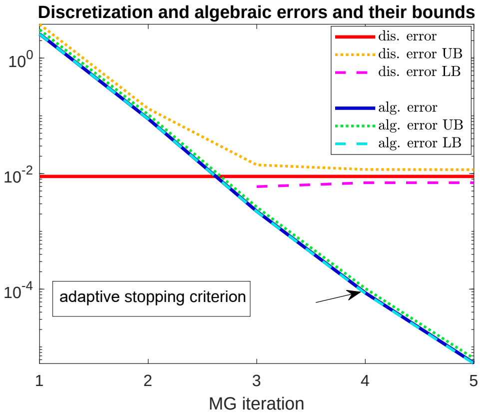


Total error



Error components and adaptive st. crit.

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth (2020)

Nonlinear pb $-\nabla\cdot\sigma(\nabla u) = f$: including **linearization** and **algebraic** error: $\mathcal{A}_\ell(\mathrm{U}_\ell^{k,i}) \neq \mathrm{F}_\ell$, $\mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,i} \neq \mathrm{F}_\ell^{k-1}$

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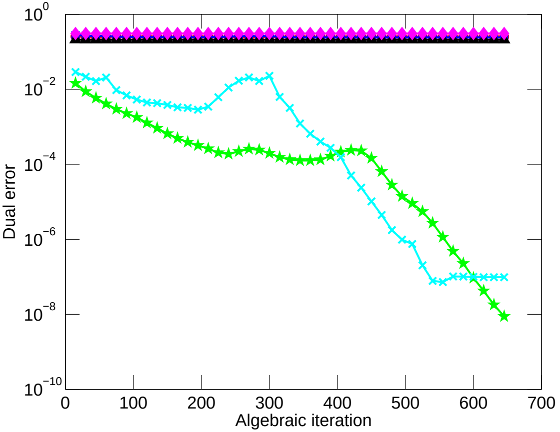

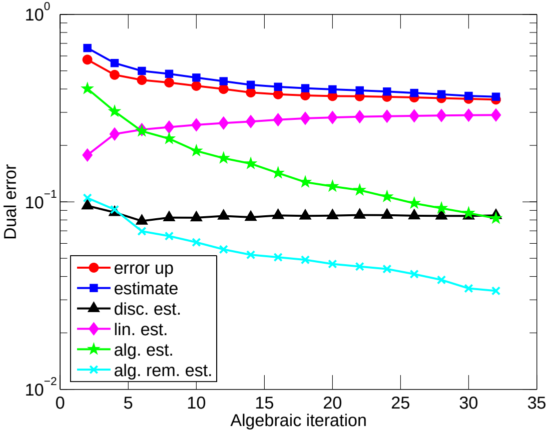

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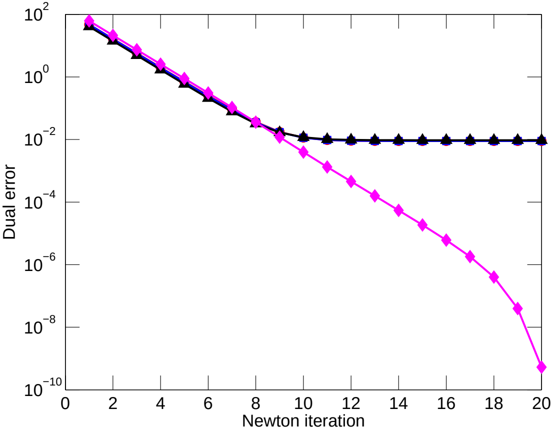

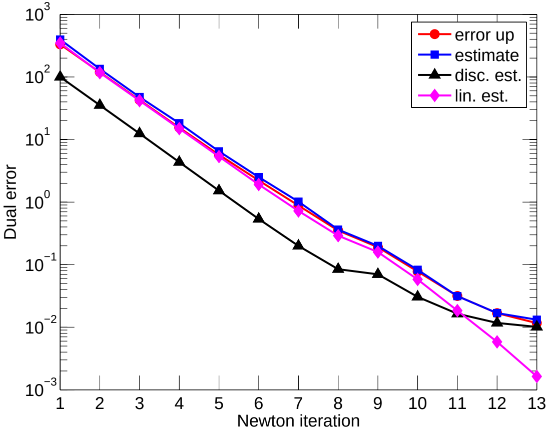

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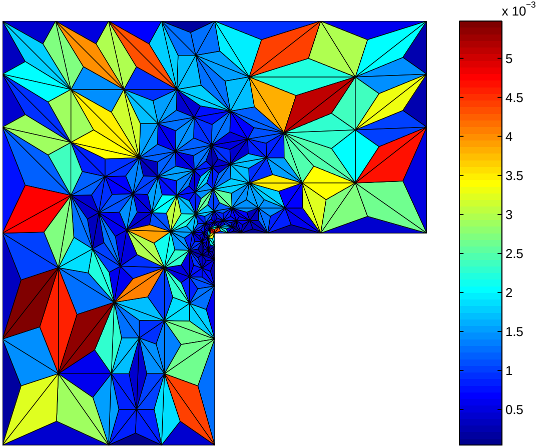
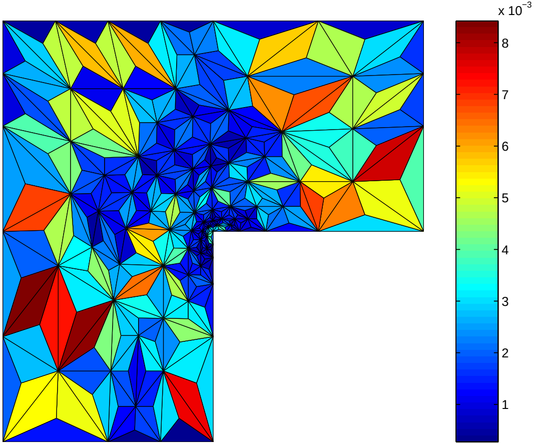


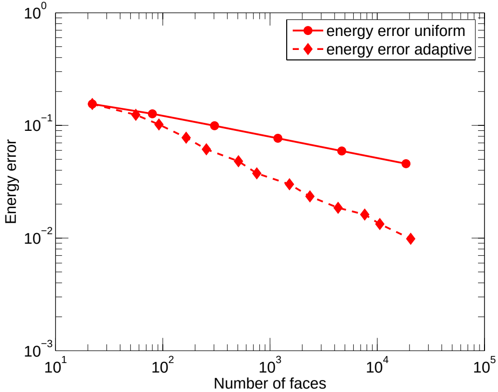
Estimated errors $\eta_K(u_\ell^{k,i})$



Exact errors $\|[\|]\boldsymbol{\sigma}(\nabla u) - \boldsymbol{\sigma}(\nabla u_\ell^{k,i})\|_{q,K}$

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

Convergence and optimal decay rate wrt DoFs & computational cost



Optimal decay rate wrt DoFs

classical		
	alg. solver its last mesh	550
	relative error estimate	4.6%

adaptive		
	alg. solver its last mesh	242
	relative error estimate	1.1%

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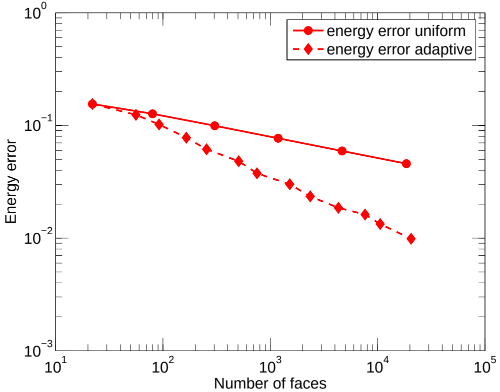

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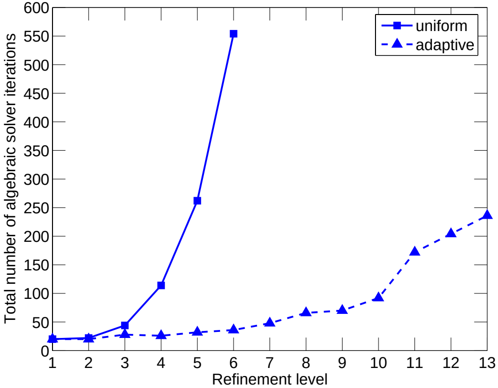

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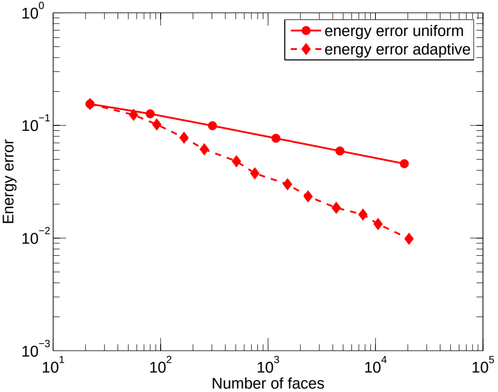

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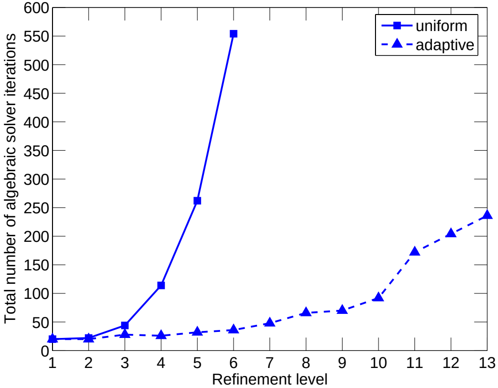

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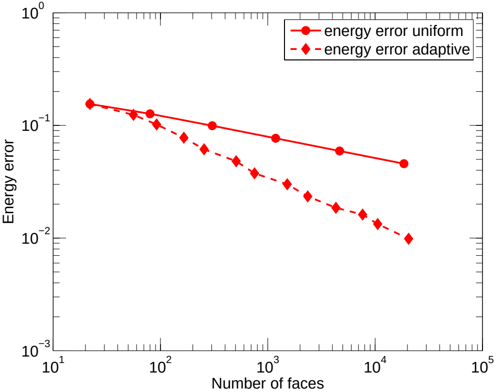

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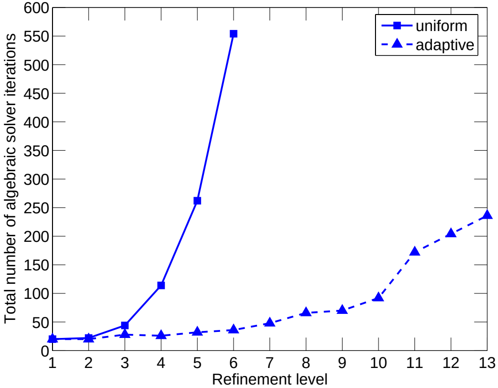

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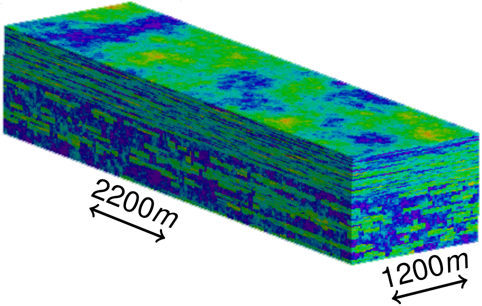
Can we certify error in a practical case $-\nabla\cdot(\mathbf{K}\nabla u) = f$: outflow error $\left|\int_{y=2200} \mathbf{K}\nabla(u-u_\ell)\cdot\mathbf{n}\right|$ (goal functional)

no of unknowns	825	3300	13200
rel. error est.	46%	34%	24%



Underground reservoir,
10th SPE test case

G. Mallik, M. Vohralík, S. Yousef, Journal of Computational and Applied Mathematics (2019)

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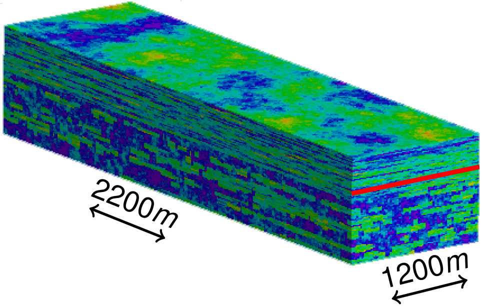

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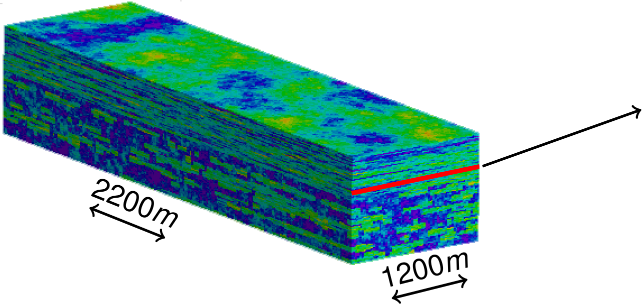

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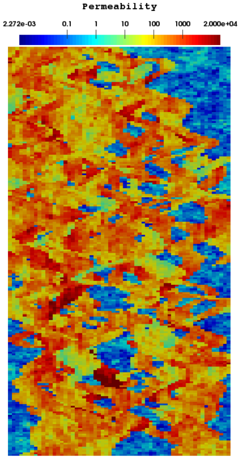

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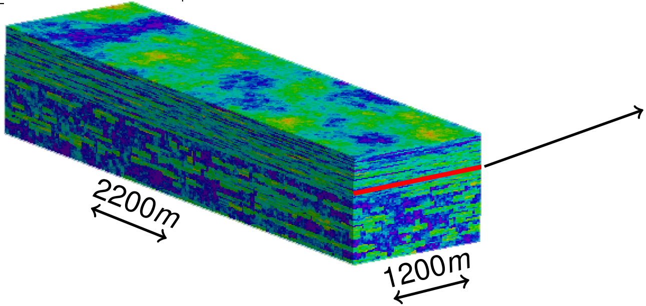

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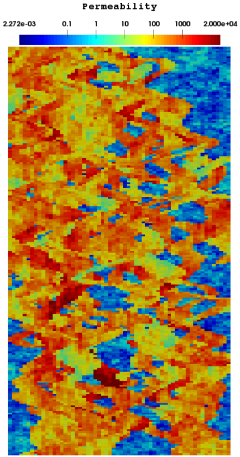

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Outline

The heat equation: $f \in L^2(0,T;L^2(\Omega))$, $u_0 \in L^2(\Omega)$

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

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

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

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An optimal a posteriori estimate for evolutive problems

Guaranteed upper bound

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

Local efficiency

- $\eta_K^n(u_{h\tau}) \leq C_{\rm eff} \|u - u_{h\tau}\|_{?,\text{neighbors of } K\times(t^{n-1},t^n)}$
- 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

- $\sum_{n=1}^{N} \sum_{K\in\mathcal{T}_h^n} \eta_K^n(u_{h\tau})^2 / \|u - u_{h\tau}\|^2_{?,\Omega\times(0,T)} \searrow 1$
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- estimators $\eta_K^n(u_{h\tau})$ can be evaluated cheaply (locally)

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Outline

Equivalence between error and residual

Weak solution

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

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Equivalence between error and residual

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:

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

- 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

$$\|u - u_{h\tau}\|_Y^2 = \|\mathcal{R}(u_{h\tau})\|_{X'}^2 + \|u_0 - u_{h\tau}(0)\|^2$$

Equivalence between error and residual

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:

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

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Proof of the parabolic inf–sup identity: $\varphi \in Y$

Proof.

- let $w_* \in X$ be defined by, a.e. in $(0, T)$,

$$(\nabla w_*, \nabla v) = \langle \partial_t \varphi, v \rangle \quad \forall v \in H_0^1(\Omega) \Rightarrow \|\nabla w_*\|^2 = \|\partial_t \varphi\|^2_{H^{-1}(\Omega)}$$

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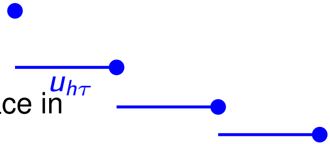
Outline

Approximate solution and Radau reconstruction



Approximate solution

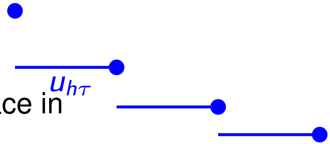
- ✓ $u_{h\tau}(t)$, $t \in I_n$, is a piecewise continuous polynomial in space in $V_h^n := \{v_h \in H_0^1(\Omega),\ v_h|_K \in \mathcal{P}_{p_K}(K) \quad \forall K \in \mathcal{T}^n\}$
- ✗ $u_{h\tau}$ is a piecewise discontinuous polynomial in time
- ✗ $u_{h\tau} \notin Y \Rightarrow$ impossible to estimate $\|u - u_{h\tau}\|_Y$

Radau reconstruction

- ✓ $\mathcal{I}u_{h\tau} \in Y$, $\mathcal{I}u_{h\tau}|_{I_n} \in \mathcal{Q}_{q_n+1}(I_n; \widetilde{V_h^n})$ (Makridakis–Nochetto)

$$\int_{I_n} (\partial_t \mathcal{I}u_{h\tau}, v_{h\tau}) + (\nabla u_{h\tau}, \nabla v_{h\tau})\,\mathrm{d}t = \int_{I_n} (f, v_{h\tau})\,\mathrm{d}t \quad \forall v_{h\tau} \in \mathcal{Q}_{q_n}(I_n; V_h^n)$$

Approximate solution and Radau reconstruction



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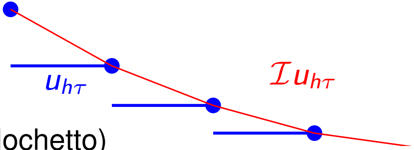

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- ✓ final norm: $\|u - u_{h\tau}\|_{\mathcal{E}_Y}^2 := \|u - \mathcal{I}u_{h\tau}\|_Y^2 + \underbrace{\|u_{h\tau} - \mathcal{I}u_{h\tau}\|_X^2}_{\text{known, computable}}$

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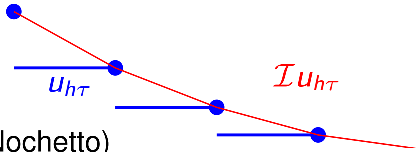

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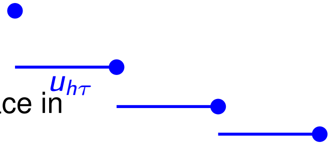

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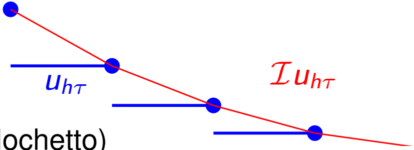

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Outline

Results in the Y norm

Theorem (Reliability in the Y norm)

Suppose no data oscillation for simplicity. Then, for any $\boldsymbol{\sigma}_{h\tau} \in L^2(0,T;\mathbf{H}(\mathrm{div},\Omega))$ *with* $\nabla\cdot\boldsymbol{\sigma}_{h\tau} = f - \partial_t \mathcal{I} u_{h\tau}$*, there holds*

$$\|u - \mathcal{I}u_{h\tau}\|_Y^2 \leq \int_0^T \|\boldsymbol{\sigma}_{h\tau} + \nabla \mathcal{I} u_{h\tau}\|^2 \,\mathrm{d}t.$$

Proof of the upper bound

Proof.

- equivalence error-residual (no error in the initial condition):

$$\|u - \mathcal{I}u_{h\tau}\|_Y = \sup_{v \in X, \|v\|_X = 1} \langle \mathcal{R}(\mathcal{I}u_{h\tau}), v \rangle$$

- Green theorem

$$\int_0^T (\boldsymbol{\sigma}_{h\tau}, \nabla \mathcal{I}u_{h\tau}) + (\nabla \cdot \boldsymbol{\sigma}_{h\tau}, \mathcal{I}u_{h\tau}) \, \mathrm{d}t = 0$$

- residual definition, Cauchy–Schwarz inequality:

$$\begin{aligned} \langle \mathcal{R}(\mathcal{I}u_{h\tau}), v \rangle &= \int_0^T (f, v) - (\partial_t \mathcal{I}u_{h\tau}, v) - (\nabla \mathcal{I}u_{h\tau}, \nabla v) \, \mathrm{d}t \\ &= \int_0^T \underbrace{(f - \partial_t \mathcal{I}u_{h\tau} - \nabla \cdot \boldsymbol{\sigma}_{h\tau}, v)}_{=0} - (\nabla \mathcal{I}u_{h\tau} + \boldsymbol{\sigma}_{h\tau}, \nabla v) \, \mathrm{d}t \\ &\leq \left\{ \int_0^T \|\boldsymbol{\sigma}_{h\tau} + \nabla \mathcal{I}u_{h\tau}\|^2 \, \mathrm{d}t \right\}^{\frac{1}{2}} \|v\|_X \end{aligned}$$

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&\leq \left\{ \int_0^T \|\boldsymbol{\sigma}_{h\tau} + \nabla \mathcal{I}u_{h\tau}\|^2 \,\mathrm{d}t \right\}^{\frac{1}{2}} \|v\|_X
\end{aligned}$$

Equilibrated flux reconstruction

Definition (Equilibrated flux reconstruction)

For each time-step interval I_n and for each vertex $\mathbf{a} \in \mathcal{V}^n$, let

$$\boldsymbol{\sigma}_{h\tau}^{\mathbf{a},n} := \arg \min_{\substack{\mathbf{v}_h \in \mathbf{V}_{h\tau}^{\mathbf{a},n} \\ \nabla\cdot\mathbf{v}_h = \psi_{\mathbf{a}}(f - \partial_t \mathcal{I} u_{h\tau}) - \nabla\psi_{\mathbf{a}}\cdot\nabla u_{h\tau}}} \int_{I_n} \|\mathbf{v}_h + \psi_{\mathbf{a}} \nabla u_{h\tau}\|_{\omega_{\mathbf{a}}}^2 \,\mathrm{d}t.$$

Then set

$$\boldsymbol{\sigma}_{h\tau} := \sum_{n=1}^{N} \sum_{\mathbf{a}\in\mathcal{V}^n} \boldsymbol{\sigma}_{h\tau}^{\mathbf{a},n}.$$

Comments

- ✓ satisfies $\boldsymbol{\sigma}_{h\tau} \in L^2(0,T;\mathbf{H}(\mathrm{div},\Omega))$ with $\nabla\cdot\boldsymbol{\sigma}_{h\tau} = f - \partial_t \mathcal{I} u_{h\tau}$
- works on the common refinement $\widetilde{\mathcal{T}}^{\mathbf{a},n}$ of the patch $\omega_{\mathbf{a}}$
- ✓ uncouples to q_n elliptic problems posed in $\mathbf{V}_h^{\mathbf{a},n}$

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Comments

- ✓ satisfies $\boldsymbol{\sigma}_{h\tau} \in L^2(0,T;\mathbf{H}(\mathrm{div},\Omega))$ with $\nabla\cdot\boldsymbol{\sigma}_{h\tau} = f - \partial_t \mathcal{I} u_{h\tau}$
- works on the common refinement $\widetilde{\mathcal{T}}^{\mathbf{a},n}$ of the patch $\omega_{\mathbf{a}}$
- ✓ uncouples to q_n elliptic problems posed in $\boldsymbol{V}_h^{\mathbf{a},n}$

Equilibrated flux reconstruction

Definition (Equilibrated flux reconstruction)

For each time-step interval I_n and for each vertex $\mathbf{a} \in \mathcal{V}^n$, let

$$\boldsymbol{\sigma}_{h\tau}^{\mathbf{a},n} := \arg \min_{\substack{\boldsymbol{v}_h \in \boldsymbol{V}_{h\tau}^{\mathbf{a},n} \\ \nabla\cdot\boldsymbol{v}_h = \psi_{\mathbf{a}}(f - \partial_t \mathcal{I} u_{h\tau}) - \nabla\psi_{\mathbf{a}}\cdot\nabla u_{h\tau}}} \int_{I_n} \|\boldsymbol{v}_h + \psi_{\mathbf{a}} \nabla u_{h\tau}\|_{\omega_{\mathbf{a}}}^2 \,\mathrm{d}t.$$

Then set

$$\boldsymbol{\sigma}_{h\tau} := \sum_{n=1}^{N} \sum_{\mathbf{a}\in\mathcal{V}^n} \boldsymbol{\sigma}_{h\tau}^{\mathbf{a},n}.$$

Comments

- ✓ satisfies $\boldsymbol{\sigma}_{h\tau} \in L^2(0,T;\mathbf{H}(\mathrm{div},\Omega))$ with $\nabla\cdot\boldsymbol{\sigma}_{h\tau} = f - \partial_t \mathcal{I} u_{h\tau}$
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Guaranteed upper bound

Theorem (Guaranteed upper bound)

In the absence of data oscillation (f and u_0 piecewise polynomial), there holds

$$\|u - u_{h\tau}\|_{\mathcal{E}_Y}^2 \leq \sum_{n=1}^{N} \sum_{K \in \mathcal{T}^n} \int_{I_n} \|\boldsymbol{\sigma}_{h\tau} + \nabla \mathcal{I} u_{h\tau}\|_K^2 + \|\nabla (u_{h\tau} - \mathcal{I} u_{h\tau})\|_K^2 \,\mathrm{d}t.$$

Outline

Local space-time efficiency and robustness

Local error contributions

$$|u - u_{h\tau}|^2_{\mathcal{E}_Y^{\mathbf{a},n}} = \int_{I_n} \|\partial_t(u - \mathcal{I}u_{h\tau})\|^2_{H^{-1}(\omega_{\mathbf{a}})} + \|\nabla(u - \mathcal{I}u_{h\tau})\|^2_{\omega_{\mathbf{a}}}\,\mathrm{d}t + \int_{I_n} \|\nabla(u_{h\tau} - \mathcal{I}u_{h\tau})\|^2_{\omega_{\mathbf{a}}}\,\mathrm{d}t$$

Theorem (Local space-time efficiency and robustness)

For each time-step interval I_n and for each element $K \in \mathcal{T}^n$, there holds, in the absence of data oscillation,

$$\int_{I_n} \|\sigma_{h\tau} + \nabla\mathcal{I}u_{h\tau}\|^2_K + \|\nabla(u_{h\tau} - \mathcal{I}u_{h\tau})\|^2_K \mathrm{d}t \leq C^2_{\mathrm{eff}} \sum_{\mathbf{a}\in\mathcal{V}_K} |u - u_{h\tau}|^2_{\mathcal{E}_Y^{\mathbf{a},n}}.$$

Comments

- ✓ **local** in **space** and **time**
- ✓ C_{eff} only depends on shape regularity $\Rightarrow$ **robustness** w.r.t the final time T and the **polynomial degrees** p and q

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recall

$$\|u - u_{h\tau}\|^2_{\mathcal{E}_Y} = \int_0^T \|\partial_t(u - \mathcal{I}u_{h\tau})\|^2_{H^{-1}(\Omega)} \,\mathrm{d}t + \int_0^T \|\nabla(u - \mathcal{I}u_{h\tau})\|^2 \,\mathrm{d}t + \int_0^T \|\nabla(u_{h\tau} - \mathcal{I}u_{h\tau})\|^2 \,\mathrm{d}t + \|(u - \mathcal{I}u_{h\tau})(T)\|^2$$

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Outline

Multi-phase multi-compositional flows

Unknowns

- reference pressure P
- phase saturations $\boldsymbol{S} := (S_p)_{p\in\mathcal{P}}$
- component molar fractions $\boldsymbol{C}_p := (C_{p,c})_{c\in\mathcal{C}_p}$ of phase $p \in \mathcal{P}$

Constitutive laws

- phase pressure = reference pressure + capillary pressure

$$P_p := P + P_{c_p}(\boldsymbol{S})$$

- Darcy's law

$$\mathbf{u}_p(P_p) := -\underline{\mathbf{K}}(\nabla P_p + \rho_p g \nabla z)$$

- component fluxes

$$\boldsymbol{\theta}_c := \sum_{p\in\mathcal{P}_c} \boldsymbol{\theta}_{p,c}, \qquad \boldsymbol{\theta}_{p,c} := \nu_p C_{p,c} \mathbf{u}_p(P_p)$$

- amount of moles of component c per unit volume

$$l_c = \phi \sum_{p\in\mathcal{P}_c} \zeta_p S_p C_{p,c}$$

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Governing PDEs

- conservation of mass for components

$$\partial_t l_c + \nabla\cdot\boldsymbol{\theta}_c = q_c \qquad \forall c \in \mathcal{C}$$

- + boundary & initial conditions

Closure algebraic equations

- conservation of pore volume: $\sum_{p\in¶} S_p = 1$
- conservation of the quantity of the matter: $\sum_{c\in\mathcal{C}_p} C_{p,c} = 1$ for all $p \in ¶$
- thermodynamic equilibrium

Mathematical issues

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

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A posteriori error estimate

Theorem (Multi-phase multi-compositional Darcy flow)

Under Assumption A, there holds

$$\text{dual residual norm} \le \left\{ \sum_{c\in\mathcal{C}} \left(\eta^{n,k,i}_{\mathrm{sp},c} + \eta^{n,k,i}_{\mathrm{tm},c} + \eta^{n,k,i}_{\mathrm{lin},c} + \eta^{n,k,i}_{\mathrm{alg},c} + \eta^{n,k,i}_{\mathrm{rem},c}\right)^2 \right\}^{\frac{1}{2}}$$

$$\text{with } \eta^{n,k,i}_{\bullet,c} := \left\{ \int_{I_n} \sum_{K\in\mathcal{M}^n} \left(\eta^{n,k,i}_{\bullet,K,c}\right)^2 \mathrm{d}t \right\}^{\frac{1}{2}}, \bullet = \mathrm{sp}, \mathrm{tm}, \mathrm{lin}, \mathrm{alg}, \mathrm{rem}.$$

Comments

- immediate extension of the results of the steady case
- still matrix-vector multiplication on each element
- same element matrices $\mathbb{S}_K$, $\mathbb{M}_K$, and $\mathbb{A}_K$ or $\widetilde{\mathbb{A}}_K$
- input: available normal face fluxes, reference pressure, phase saturations, and component molar fractions
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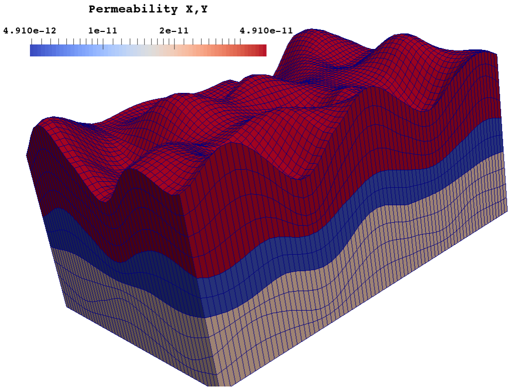
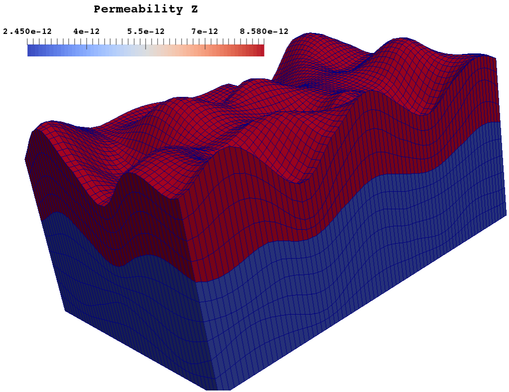
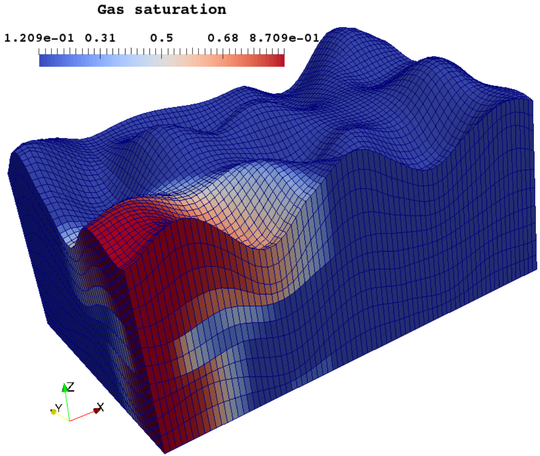
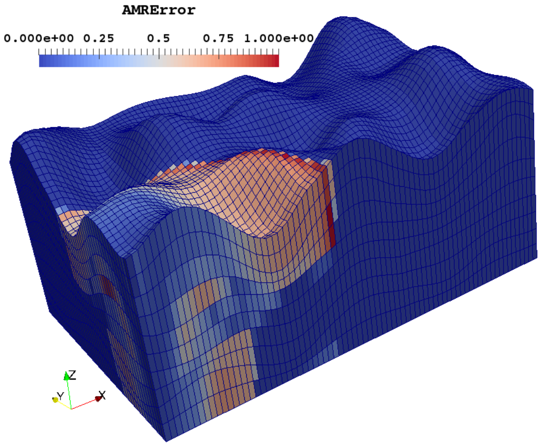
3 phases, 3 components (black-oil) problem: permeability



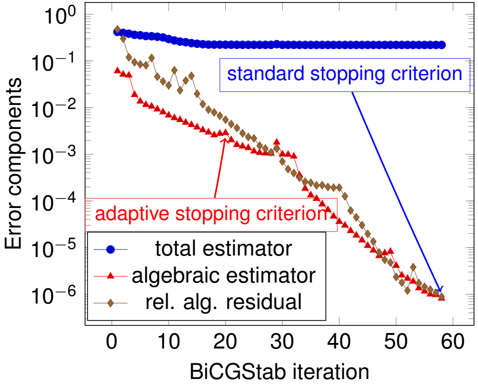


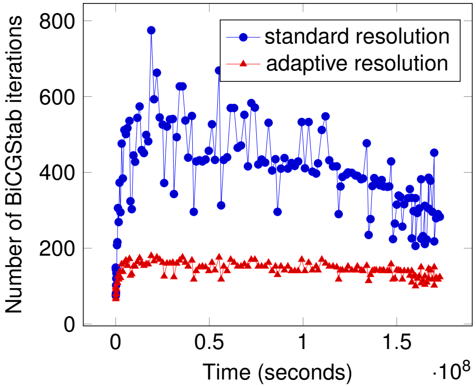
3 phases, 3 components (black-oil) problem: gas saturation and a posteriori estimate





3 phases, 3 components (black-oil): alg. solver & 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

M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2020)

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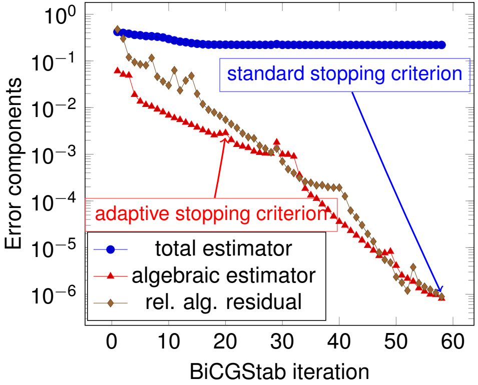

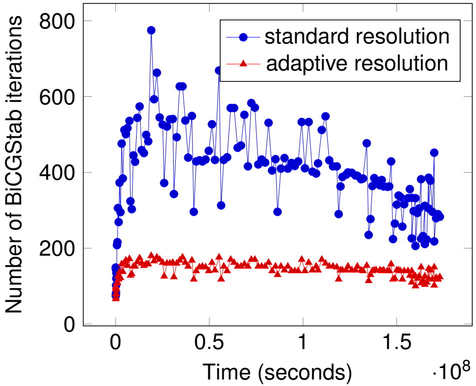

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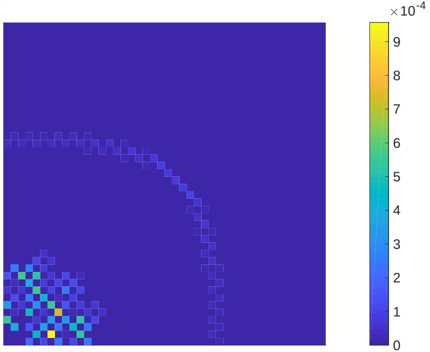
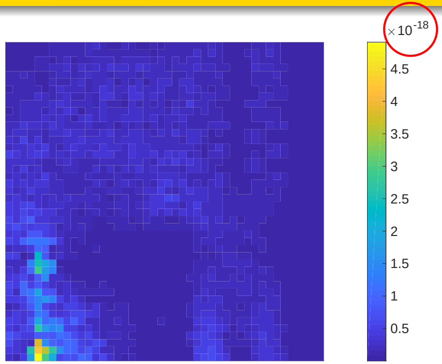
2 phases: recovering water mass balance



original mass balance misfit $(\mathrm{m}^2\mathrm{s}^{-1})$



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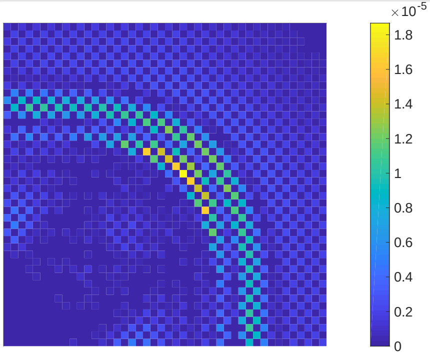

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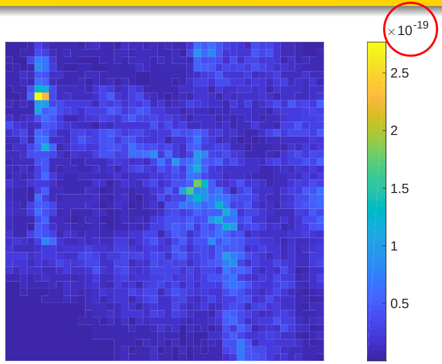

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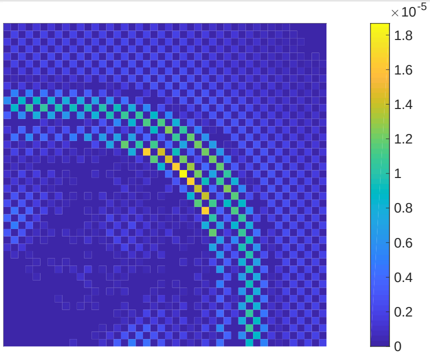

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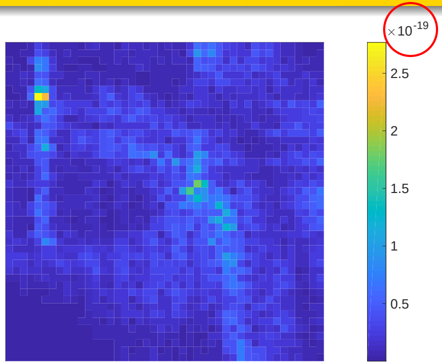

corrected mass balance misfit $(\mathrm{m}^2\mathrm{s}^{-1})$

Setting

- fully implicit discretization
- cell-centered finite volumes on a square mesh
- time step 260 (60 days), 1st Newton linearization, GMRes iteration 195

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, HAL Preprint 01662944 (2020)

Outline

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- a posteriori **error control**
- **simple** estimates on polygonal/polyhedral meshes
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