A posteriori error estimates and adaptivity: principles and applications

Martin Vohralík

Inria Paris & Ecole nationale des ponts et chaussées

Journées scientifiques du RT Terre et Energies
6 novembre 2024, Nouan-le-Fuzelier

Outline

1. Introduction: a posteriori error control and adaptivity
2. Laplace equation: discretization error, mesh and polynomial degree adaptivity
    - A posteriori error control
    - Potential reconstruction
    - Flux reconstruction
    - Balancing error components: mesh adaptivity
    - Balancing error components: polynomial-degree adaptivity
3. Nonlinear Laplace equation: overall error and solvers adaptivity
    - A posteriori error control (overall and components)
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4. Reaction–diffusion equation: robustness wrt parameters
5. Heat equation: robustness wrt final time and space–time error localization
6. Multiphase multicompositional flows: environmental application
7. Conclusions

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

- no earthquake, flooding, tsunami, heavy rain, extreme temperature
- deterministic, steady problem, PDE known, data known, implementation OK

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

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Reliability study and simulation of the progressive collapse of Roissy Charles de Gaulle Airport

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

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Numerical approximations of PDEs:

Setting

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- u_h : known numerical approximation on mesh $\mathcal{T}_h$

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Numerical approximations of PDEs: **3 crucial questions & suggested answers**

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Suggested answers

1. Computable **a posteriori** error **estimates**.

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1. Computable **a posteriori error estimates**.
2. Identification of **error components**.

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Suggested answers

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

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A posteriori error estimates: discretization error control

Laplace equation in $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, $f \in L^2(\Omega)$

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

Guaranteed error upper bound (reliability) ($u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega)$, $p \geq 1$, FEs)

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

error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h)$)

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

- C_{eff} a generic constant only dependent on d and shape regularity of $\mathcal{T}_h$ and thus independent of Ω, u, u_h, h, p

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How **large** is the discretization 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 $\frac{\|\nabla(u-u_h)\|}{\|\nabla u_h\|}$	$I^{\text{eff}} = \frac{\eta(u_h)}{\|\nabla(u-u_h)\|}$
h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$		$6.07 \times 10^{[illegible]}$				
$\approx h_0/4$		$3.10 \times 10^{[illegible]}$				
$\approx h_0/8$		$1.45 \times 10^{[illegible]}$				
$\approx h_0/2$	2	$4.23 \times 10^{[illegible]}$				
$\approx h_0/4$	3	$2.62 \times 10^{[illegible]}$				
$\approx h_0/8$	4	$2.60 \times 10^{[illegible]}$				

A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)

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h_0	1	1.25	28%	1.07	24%	**1.17**
$\approx h_0/2$		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}	$9.5 \times 10^{-1}\%$	4.07×10^{-2}	$9.2 \times 10^{-1}\%$	**1.04**
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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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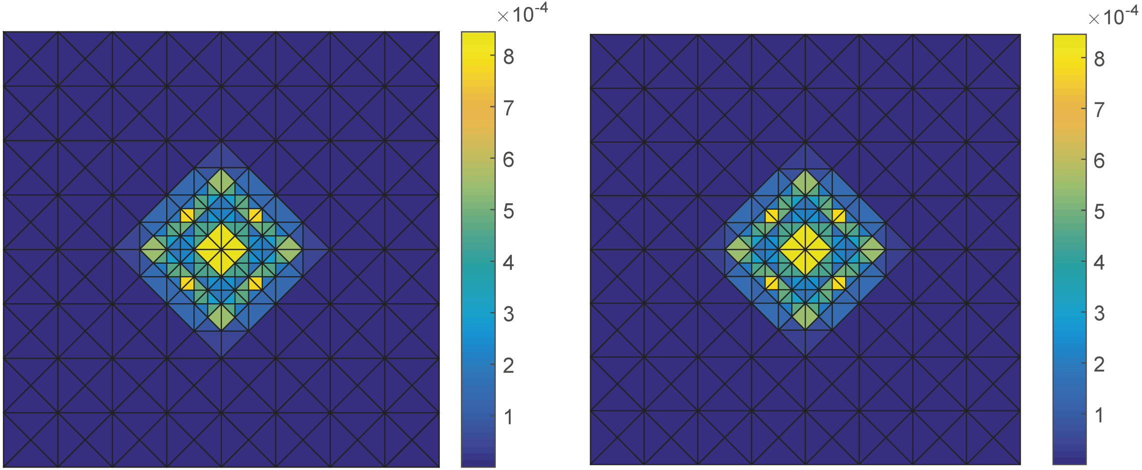
A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)

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

Where (in space) is the error **localized**? (known smooth solution)



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)

Error characterization

Theorem (Error characterization)

Let $u \in H^1_0(\Omega)$ be the weak solution and let $u_h \in H^1(\mathcal{T}_h)$ be arbitrary. Then

$$\|\nabla(u-u_h)\|^2 = \underbrace{\min_{\substack{\mathbf{v}\in\mathbf{H}(\mathrm{div},\Omega)\\ \nabla\cdot\mathbf{v}=f}} \|\nabla u_h + \mathbf{v}\|^2}_{\substack{\text{constrained distance to } \mathbf{H}(\mathrm{div},\Omega)\\ =\max_{\substack{v\in H^1_0(\Omega)\\ \|\nabla v\|=1}}[(f,v)-(\nabla u_h,\nabla v)]^2\\ \text{dual norm of the residual}}} + \underbrace{\min_{v\in H^1_0(\Omega)} \|\nabla(u_h - v)\|^2}_{\text{distance to } H^1_0(\Omega)}.$$

Comments

- It is enough to choose suitable (discrete, piecewise polynomial) $\sigma_h \in \mathbf{H}(\mathrm{div},\Omega)$ with $\nabla\cdot\sigma_h = f$ and $s_h \in H^1_0(\Omega)$ to get a guaranteed upper bound.

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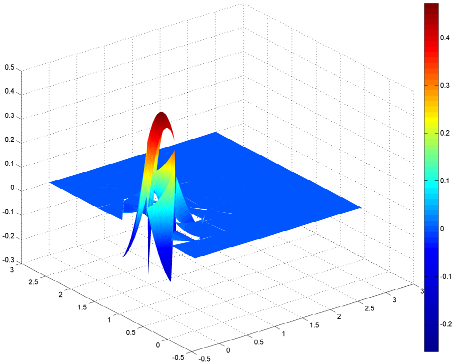
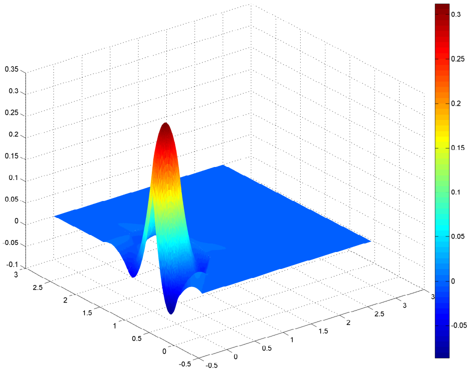
Outline

1. Introduction: a posteriori error control and adaptivity
2. Laplace equation: discretization error, mesh and polynomial degree adaptivity
    - A posteriori error control
    - Potential reconstruction
    - Flux reconstruction
    - Balancing error components: mesh adaptivity
    - Balancing error components: polynomial-degree adaptivity
3. Nonlinear Laplace equation: overall error and solvers adaptivity
    - A posteriori error control (overall and components)
    - Balancing error components: solvers adaptivity
4. Reaction–diffusion equation: robustness wrt parameters
5. Heat equation: robustness wrt final time and space–time error localization
6. Multiphase multicompositional flows: environmental application
7. Conclusions

Potential reconstruction



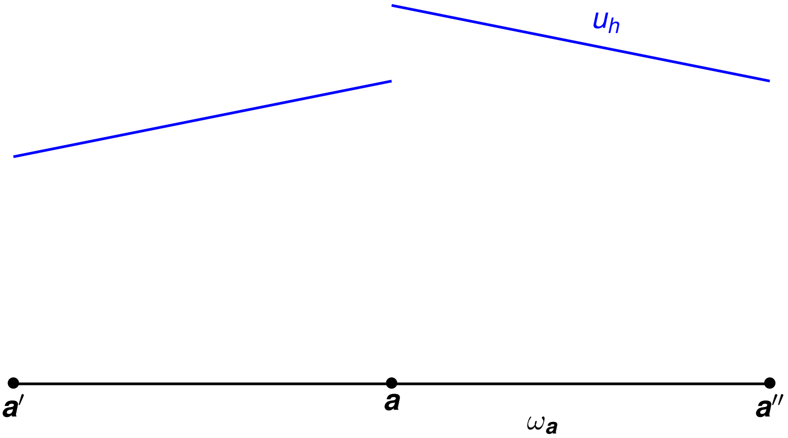
Potential u_h



Potential reconstruction s_h

$$\boxed{u_h \in \mathcal{P}_p(\mathcal{T}_h) \to s_h \in \mathcal{P}_{p+1}(\mathcal{T}_h) \cap H_0^1(\Omega)}$$

Potential reconstruction in 1D, $p = 1$



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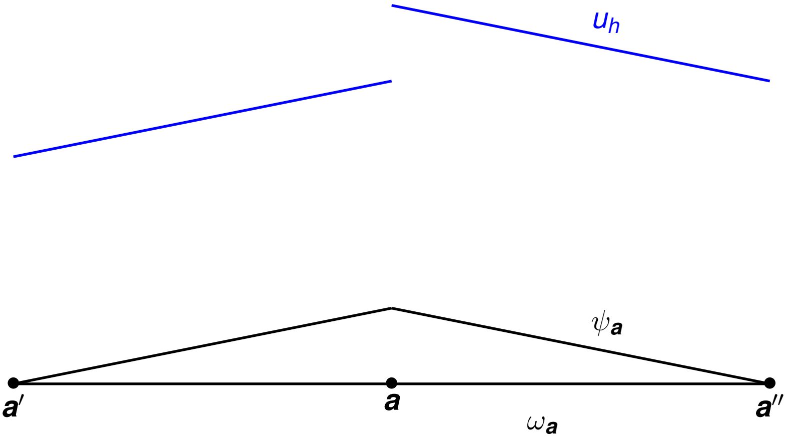

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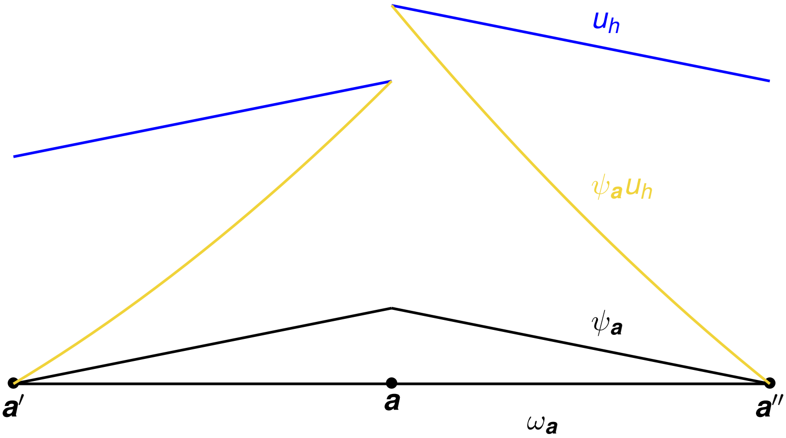

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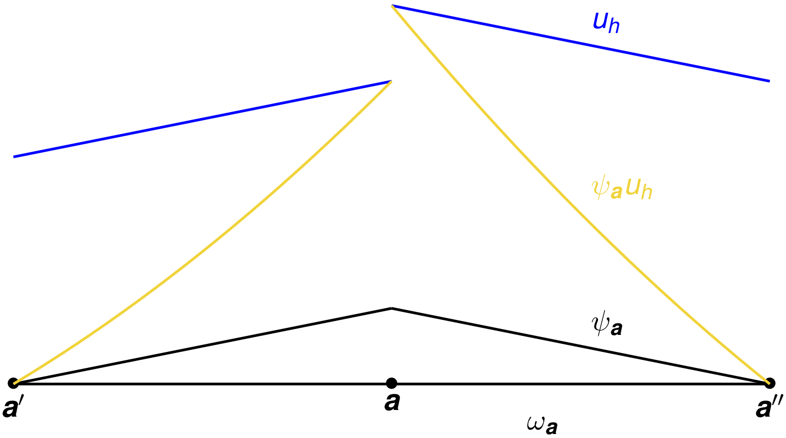

Potential reconstruction: datum $u_h \in \mathcal{P}_p(\mathcal{T}_h)$, $p \geq 1$

Definition (Construction of s_h Ern & V. (2015), ≈ Carstensen and Merdon (2013))

For each vertex $\boldsymbol{a} \in \mathcal{V}_h$, solve the **local minimization problem**

$$s_h^{\boldsymbol{a}} := \arg \min_{v_h \in V_h^{\boldsymbol{a}} := \mathcal{P}_{p+1}(\mathcal{T}^{\boldsymbol{a}}) \cap H_0^1(\omega_{\boldsymbol{a}})} \|\nabla(\psi_{\boldsymbol{a}} u_h - v_h)\|_{\omega_{\boldsymbol{a}}}$$

and combine

$$s_h := \sum_{\boldsymbol{a} \in \mathcal{V}_h} s_h^{\boldsymbol{a}}.$$

Equivalent form: conforming FEs

Find $s_h^{\boldsymbol{a}} \in V_h^{\boldsymbol{a}}$ such that

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Key points

- localization to patches $\mathcal{T}^{\boldsymbol{a}}$
- cut-off by hat basis functions $\psi_{\boldsymbol{a}}$
- projection of the discontinuous $\psi_{\boldsymbol{a}} u_h$ to a conforming space
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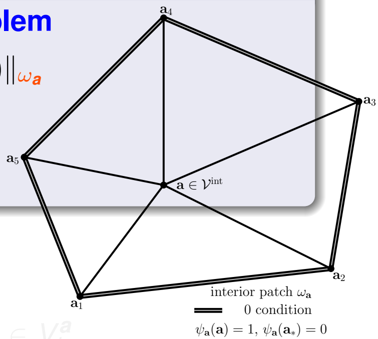

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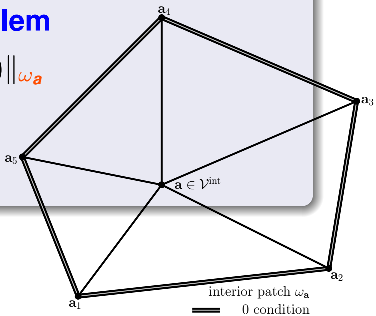

interior patch $\omega_{\mathbf{a}}$

0 condition

$\psi_{\mathbf{a}}(\mathbf{a}) = 1,\ \psi_{\mathbf{a}}(\mathbf{a}_*) = 0$

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Potential reconstruction: datum $u_h \in \mathcal{P}_p(\mathcal{T}_h)$, $p \geq 1$

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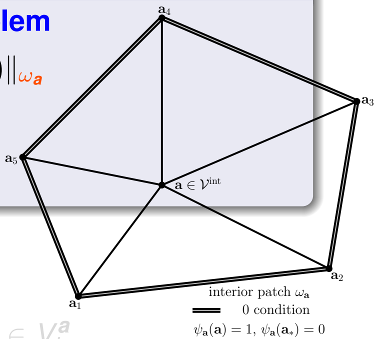

Equivalent form: conforming FEs

Find $s_h^{\boldsymbol{a}} \in V_h^{\boldsymbol{a}}$ such that

$$(\nabla s_h^{\boldsymbol{a}}, \nabla v_h)_{\omega_{\boldsymbol{a}}} = (\nabla(\psi_{\boldsymbol{a}} u_h), \nabla v_h)_{\omega_{\boldsymbol{a}}} \qquad \forall v_h \in V_h^{\boldsymbol{a}}.$$

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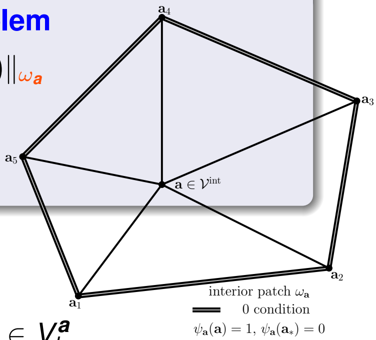

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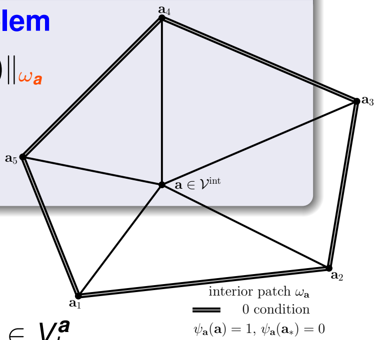

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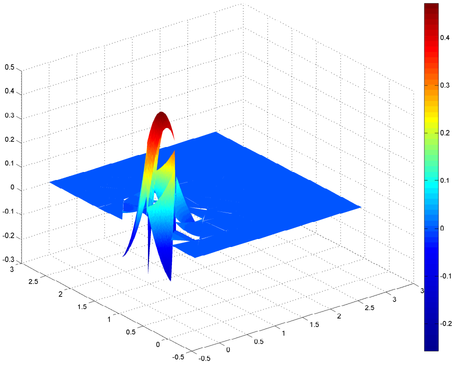
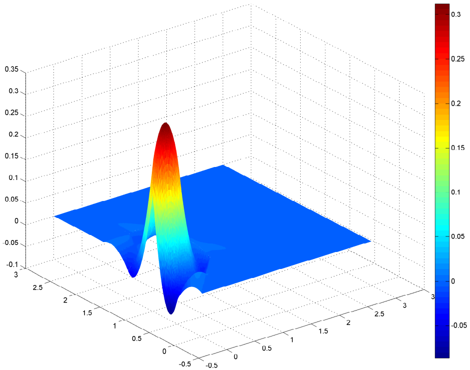


Potential u_h

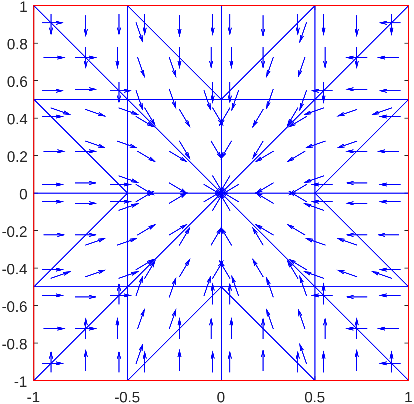


Potential reconstruction s_h

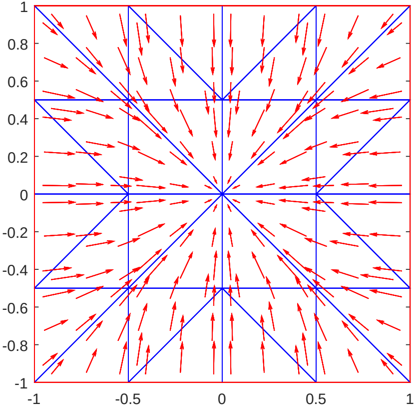
$$\boxed{u_h \in \mathcal{P}_p(\mathcal{T}_h) \to s_h \in \mathcal{P}_{p+1}(\mathcal{T}_h) \cap H_0^1(\Omega)}$$

Outline

Equilibrated flux reconstruction



Flux $-\nabla u_h$



Equilibrated flux reconstruction $\boldsymbol{\sigma}_h$

$$\underbrace{-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}}-(\nabla u_h,\nabla\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}}=0 \ \forall \boldsymbol{a}\in\mathcal{V}_h^{\mathrm{int}}} \to \boldsymbol{\sigma}_h \in \mathcal{RT}_p(\mathcal{T}_h) \cap \boldsymbol{H}(\mathrm{div},\Omega), \nabla\cdot\boldsymbol{\sigma}_h = \Pi_p f$$

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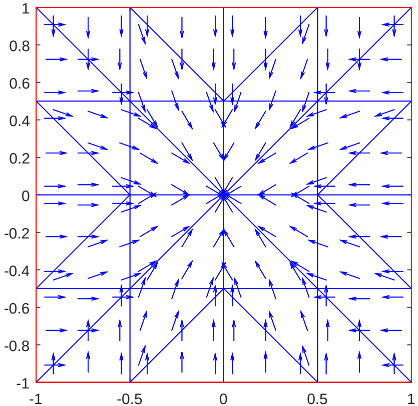

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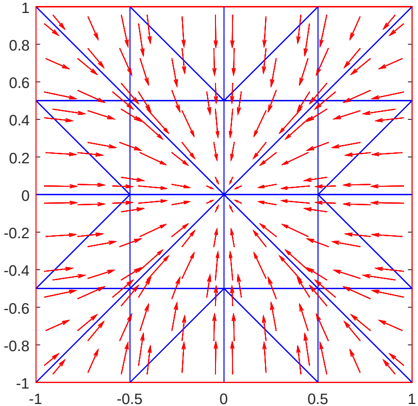

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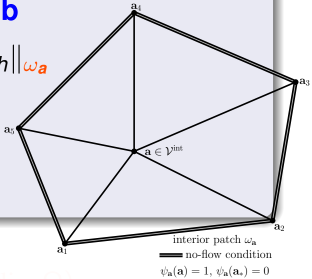

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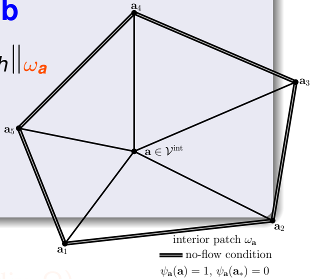

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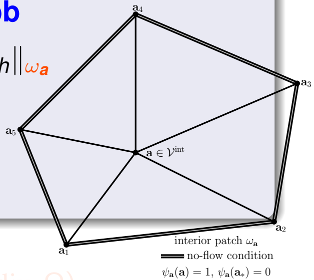

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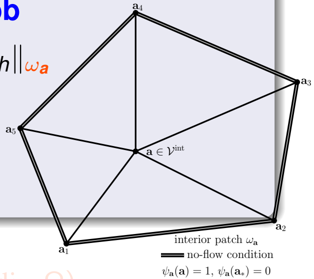

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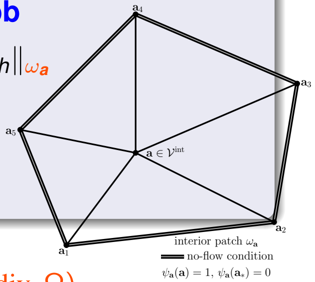

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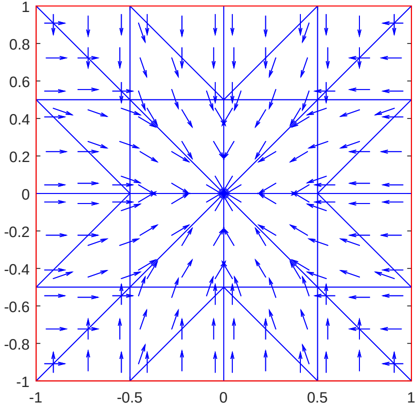

Flux $-\nabla u_h \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot(-\nabla u_h) \neq f$

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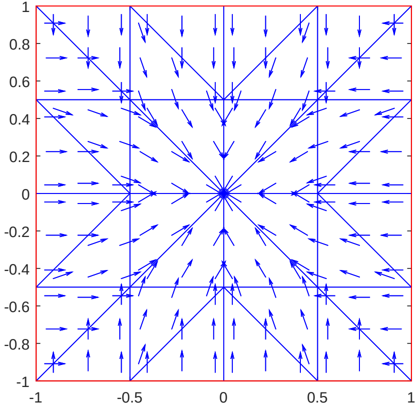

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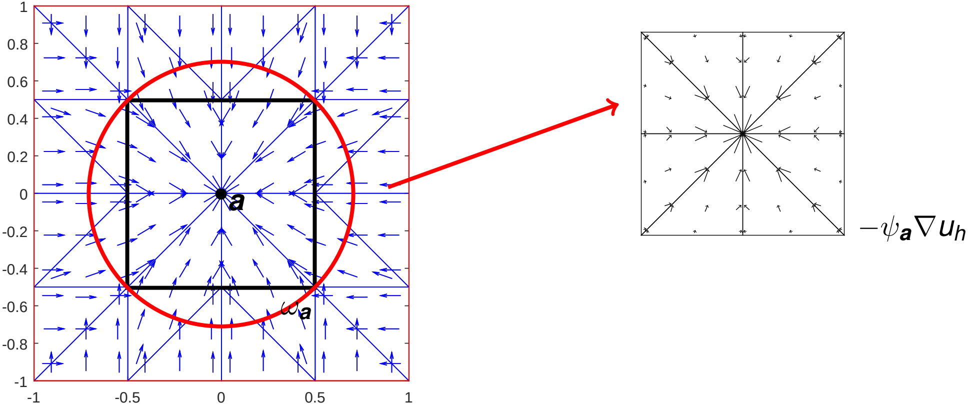

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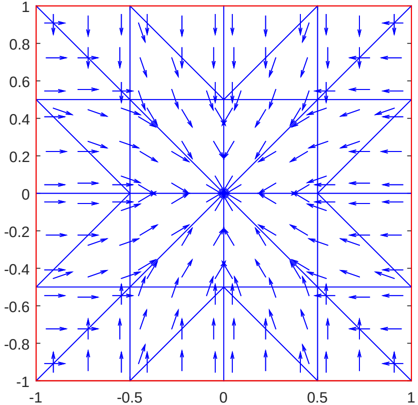
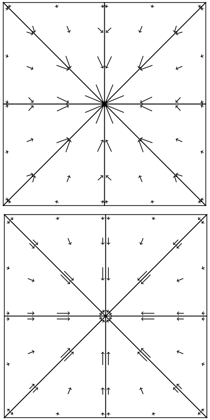




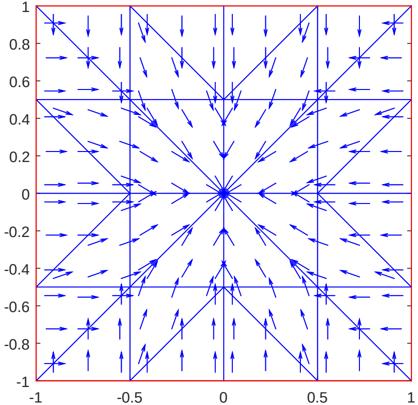
$-\psi_{\boldsymbol{a}}\nabla u_h$

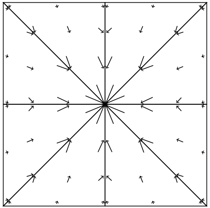
$\boldsymbol{\sigma}_h^{\boldsymbol{a}}$

Flux $-\nabla u_h \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot(-\nabla u_h) \neq f$

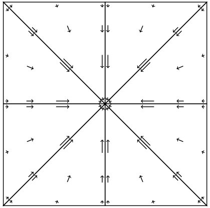
$$\underbrace{-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}}-(\nabla u_h,\nabla\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}}=0\ \forall \boldsymbol{a}\in\mathcal{V}_h^{\mathrm{int}}}$$

Equilibrated flux reconstruction: $-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h)$, $p \geq 1$, $f \in L^2(\Omega)$





$-\psi_{\boldsymbol{a}} \nabla u_h$

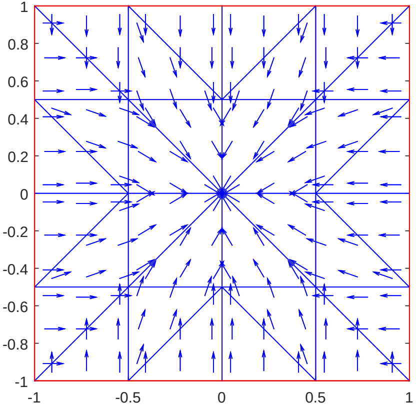


$\boldsymbol{\sigma}_h^{\boldsymbol{a}}$

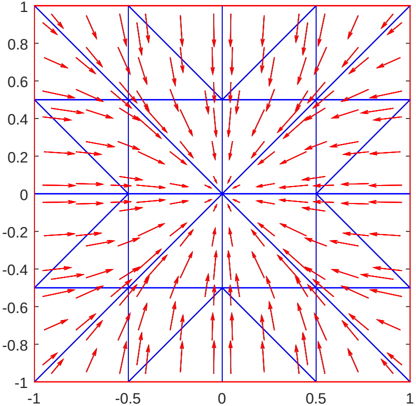
Flux $-\nabla u_h \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla \cdot (-\nabla u_h) \neq f$

$$\underbrace{-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h),\ f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} - (\nabla u_h, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = 0\ \forall \boldsymbol{a} \in \mathcal{V}_h^{\mathrm{int}}} \qquad \boldsymbol{\sigma}_h^{\boldsymbol{a}} := \arg \min_{\substack{\boldsymbol{v}_h \in \mathcal{RT}_p(\mathcal{T}^{\boldsymbol{a}}) \cap \boldsymbol{H}_0(\mathrm{div}, \omega_{\boldsymbol{a}}) \\ \nabla \cdot \boldsymbol{v}_h = \Pi_p(f\psi_{\boldsymbol{a}} - \nabla u_h \cdot \nabla \psi_{\boldsymbol{a}})}} \|\psi_{\boldsymbol{a}} \nabla u_h + \boldsymbol{v}_h\|_{\omega_{\boldsymbol{a}}}$$

Equilibrated flux reconstruction: $-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h)$, $p \geq 1$, $f \in L^2(\Omega)$



Flux $-\nabla u_h \notin \boldsymbol{H}(\mathrm{div},\Omega)$, $\nabla\cdot(-\nabla u_h) \neq f$



Equilibrated flux rec. $\boldsymbol{\sigma}_h$

$$\boxed{\underbrace{-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}}-(\nabla u_h,\nabla\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}}=0\ \forall \boldsymbol{a}\in\mathcal{V}_h^{\mathrm{int}}} \to \boldsymbol{\sigma}_h := \sum_{\boldsymbol{a}\in\mathcal{V}_h} \boldsymbol{\sigma}_h^{\boldsymbol{a}} \in \mathcal{RT}_p(\mathcal{T}_h) \cap \boldsymbol{H}(\mathrm{div},\Omega), \nabla\cdot\boldsymbol{\sigma}_h = \Pi_p f}$$

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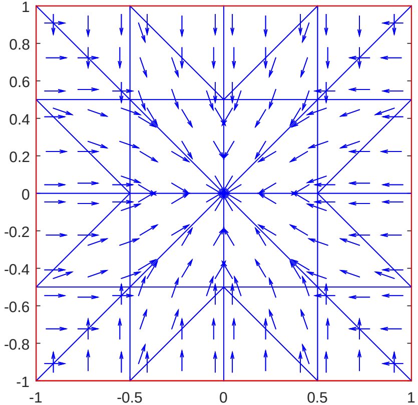

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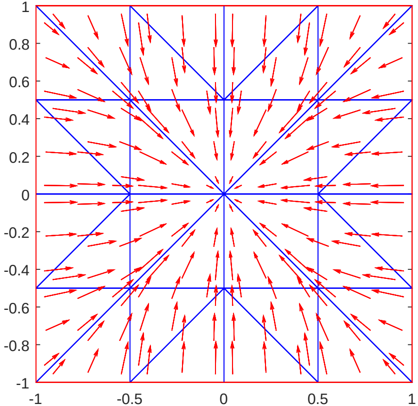

Equilibrated flux rec. $\boldsymbol{\sigma}_h \in \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot\boldsymbol{\sigma}_h = f$

$$\boxed{\underbrace{-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}}-(\nabla u_h,\nabla\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}}=0\ \forall \boldsymbol{a}\in\mathcal{V}_h^{\mathrm{int}}} \to \boldsymbol{\sigma}_h := \sum_{\boldsymbol{a}\in\mathcal{V}_h} \boldsymbol{\sigma}_h^{\boldsymbol{a}} \in \mathcal{RT}_p(\mathcal{T}_h) \cap \boldsymbol{H}(\mathrm{div}, \Omega), \nabla\cdot\boldsymbol{\sigma}_h = \Pi_p f}$$

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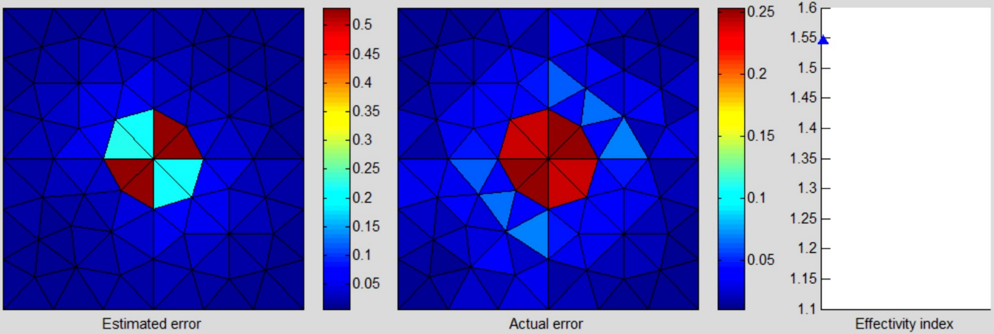
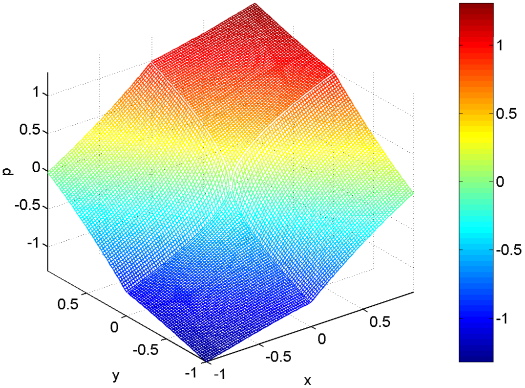
Can we **decrease the error efficiently**? (adaptive mesh refinement)

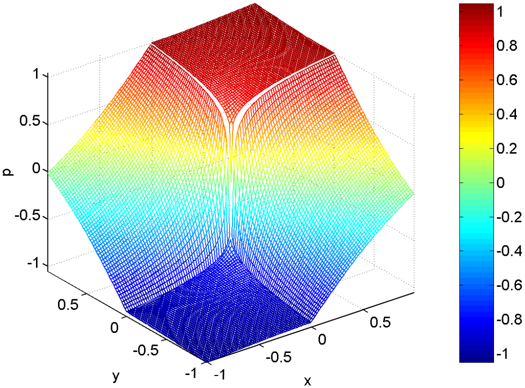


M. Vohralík, SIAM Journal on Numerical Analysis (2007)

Singular solutions

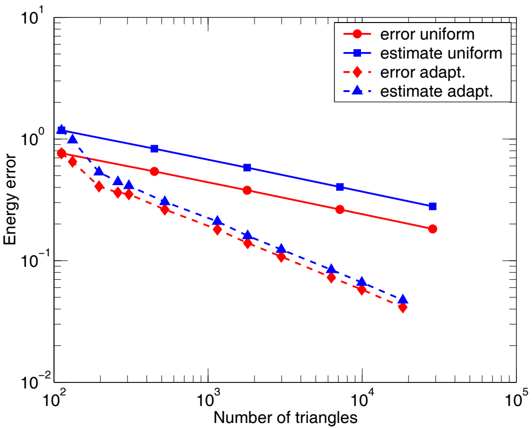


$H^{1.54}$ singularity



$H^{1.13}$ singularity

Estimated and actual error against the number of elements in uniformly/adaptively refined meshes (singular solutions)



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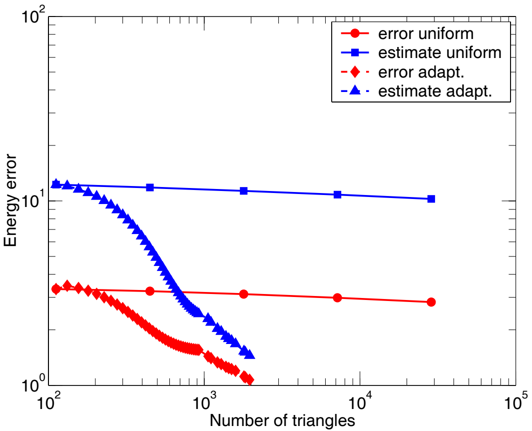

$H^{1.13}$ singularity

M. Vohralík, SIAM Journal on Numerical Analysis (2007)

Adaptive mesh refinement

Adaptive mesh refinement

Adaptive mesh refinement

Adaptive mesh refinement

$$\sum_{K\in\mathcal{T}_\ell} \eta_K(u_\ell)^2 = \quad \eta(u_\ell)^2$$

Adaptive mesh refinement

Adaptive mesh refinement

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

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

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Convergence on a sequence of adaptively refined meshes

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

Adaptive mesh refinement

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

Optimal error decay rate wrt degrees of freedom

- $\|\nabla(u-u_\ell)\| \lesssim |\mathrm{DoF}_\ell|^{-p/d}$ (replaces h^p)
- 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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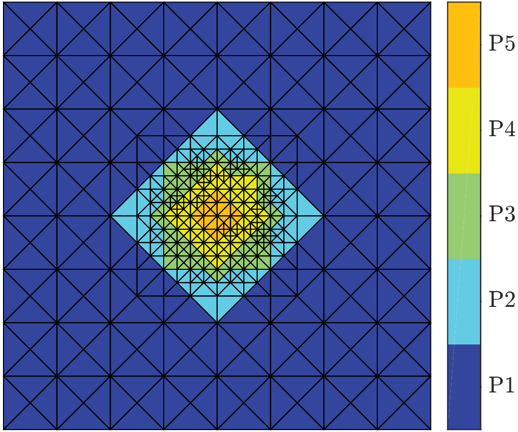
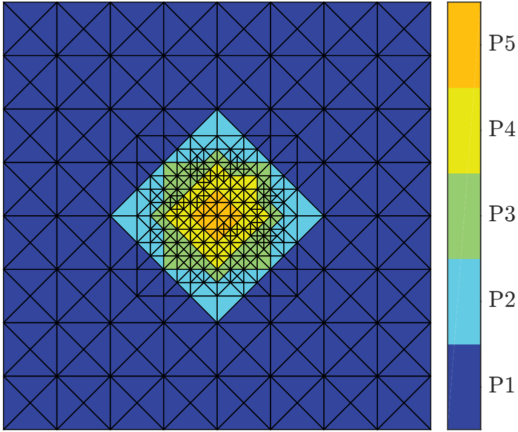
Best-possible error decrease: *hp* **adaptivity**, (**smooth** solution)



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

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

Best-possible error decrease: *hp* **adaptivity**, (**smooth** solution)



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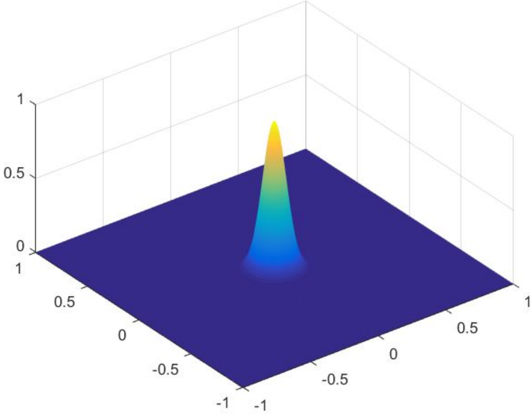
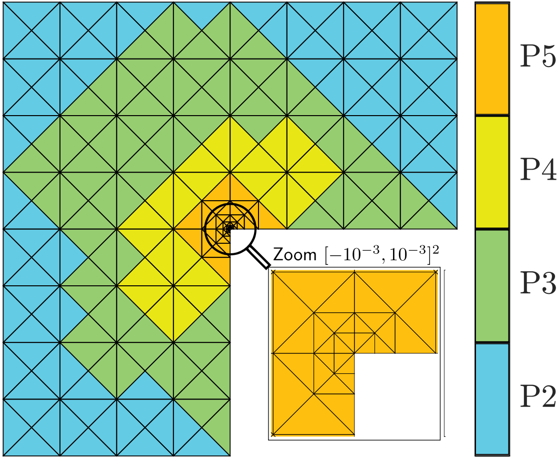


Exact solution

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

Best-possible error decrease: *hp* **adaptivity**, (**singular** solution)



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

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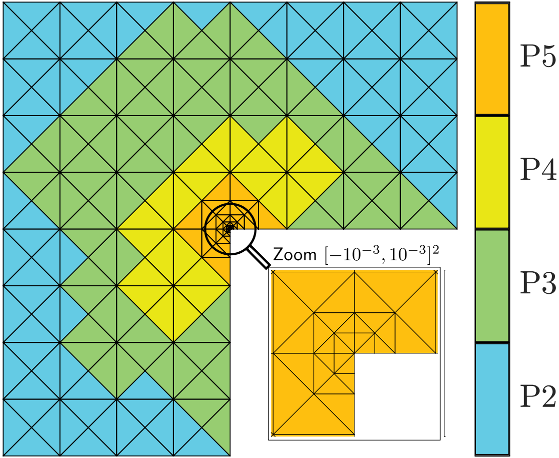
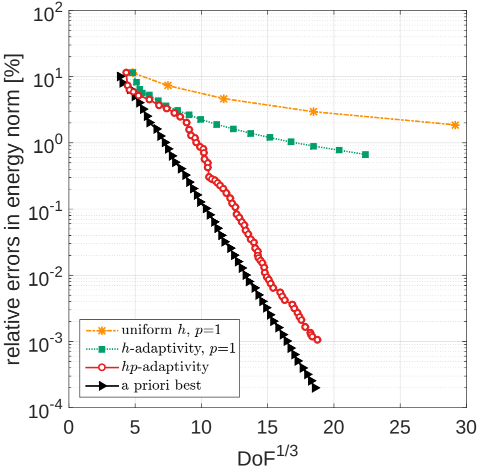


Mesh $\mathcal{T}_\ell$ and polynomial degrees p_K



Relative error as a function of DoF

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

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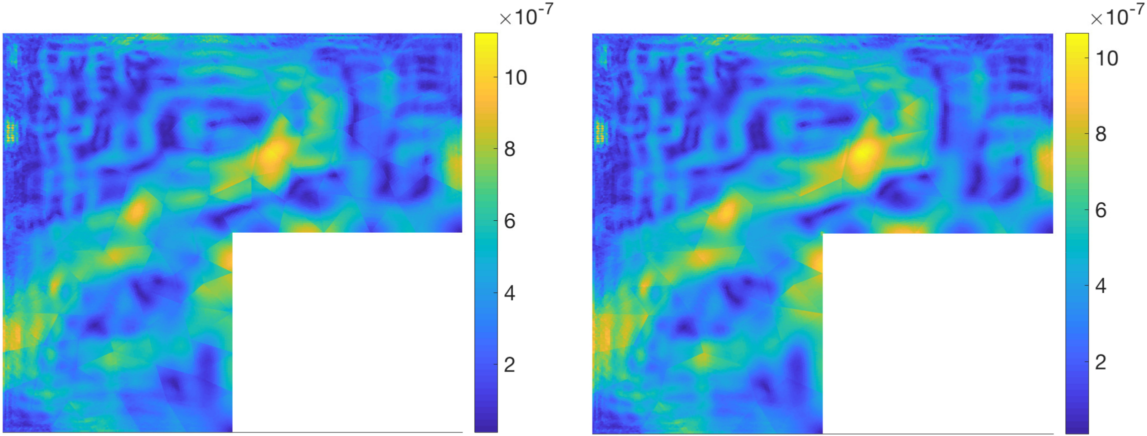
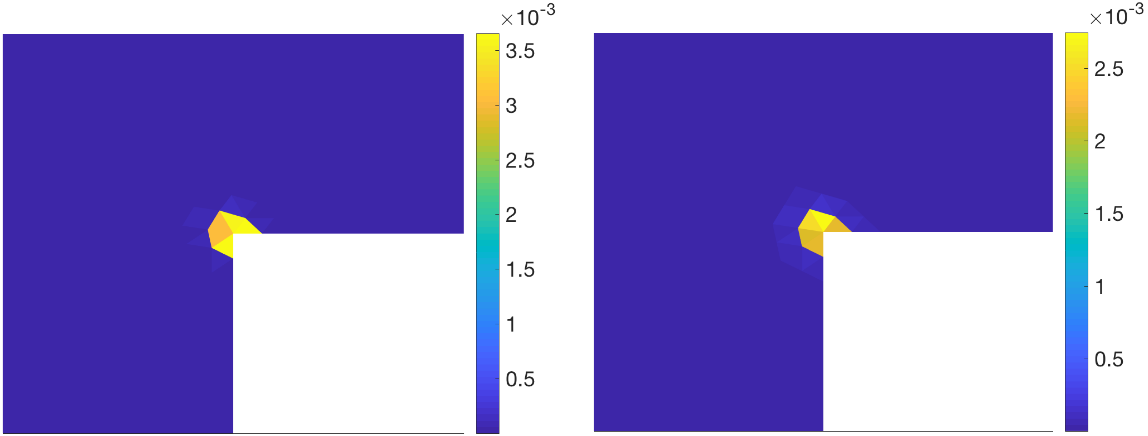
Including **algebraic error:** $\mathbb{A}_\ell \mathsf{U}_\ell^i \neq \mathsf{F}_\ell$



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, Computer Methods in Applied Mechanics and Engineering (2020)

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



Estimated total errors $\eta_K(u_\ell^i)$ Exact total errors $\|\nabla(u - u_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

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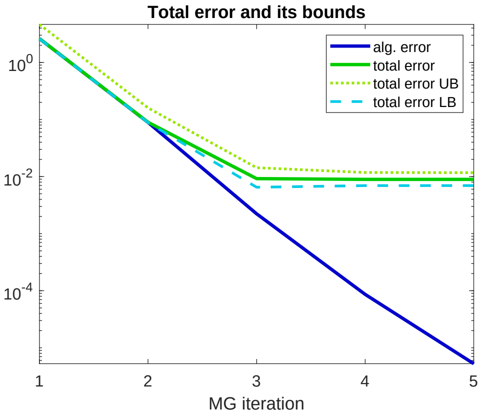
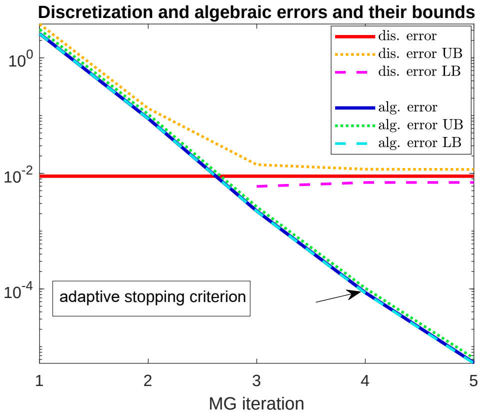


Total error



Error components and adaptive st. crit.

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (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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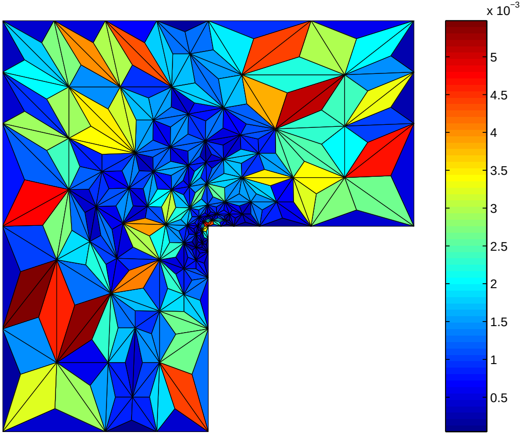
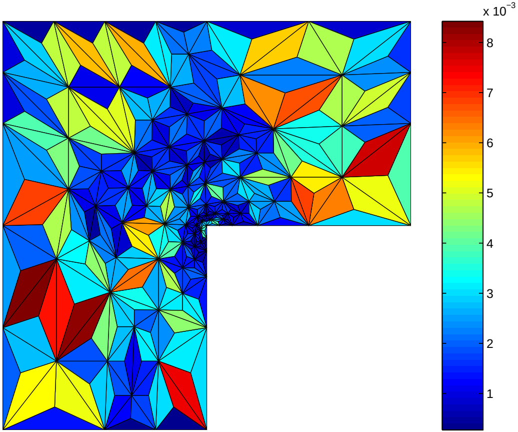


Estimated errors $\eta_K(u_\ell^{k,i})$



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)

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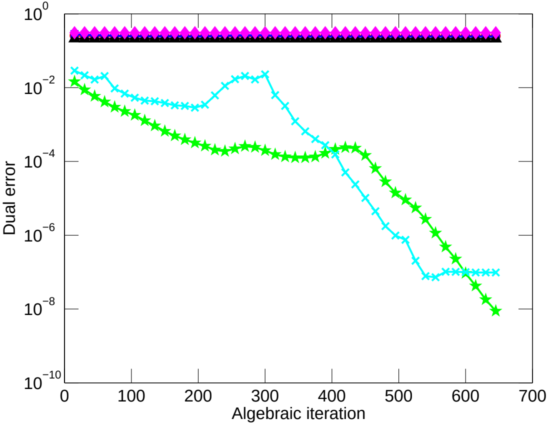
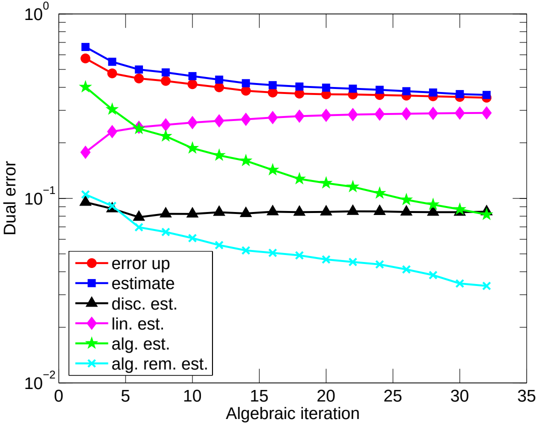


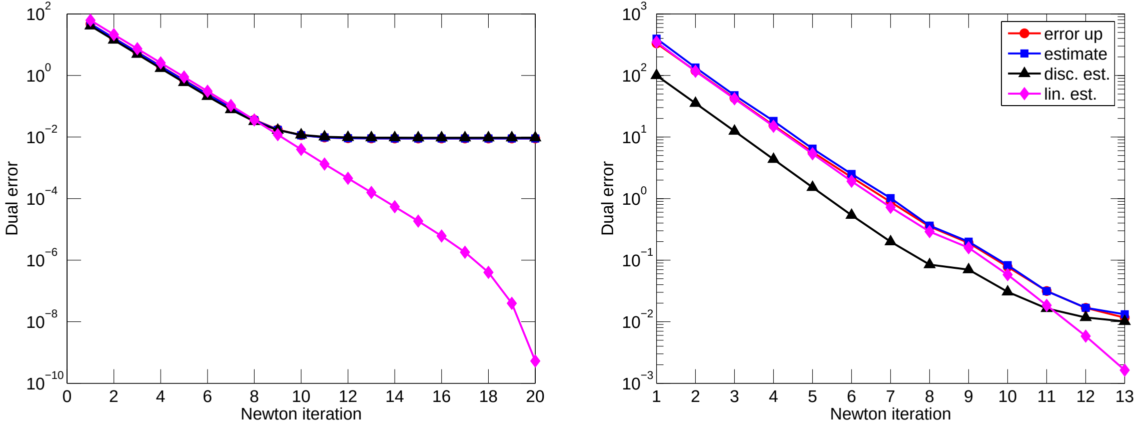
Newton



adaptive inexact Newton

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

Nonlinear pb $-\nabla\cdot\boldsymbol{\sigma}(\nabla u) = f$: 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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Solver adaptivity (nonlinear problem, 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

$$\eta_{\ell,\mathrm{alg}}^{k,i} \leq \gamma_{\mathrm{alg}} \eta_{\ell,\mathrm{lin}}^{k,i} \qquad \text{stopping criterion linear solver}$$

$$\eta_{\ell,\mathrm{lin}}^{k,i} \leq \gamma_{\mathrm{lin}} \eta_{\mathrm{disc}}^{k,i} \qquad \text{stopping criterion nonlinear solver}$$

$$\theta \eta_{\ell,\mathrm{disc}}^{k,i} \leq \eta_{\mathrm{disc},\mathcal{M}_\ell}^{k,i} \qquad \text{adaptive mesh refinement}$$

- 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

- Haberl, Praetorius, Schimanko, & Vohralík (2021)

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

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

$$\boxed{\begin{array}{ll} \eta_{\ell,\mathrm{alg}}^{k,i} \le \gamma_{\mathrm{alg}} \eta_{\ell,\mathrm{lin}}^{k,i} & \text{stopping criterion linear solver} \\ \eta_{\ell,\mathrm{lin}}^{k,i} \le \gamma_{\mathrm{lin}} \eta_{\mathrm{disc}}^{k,i} & \text{stopping criterion nonlinear solver} \\ \theta \eta_{\ell,\mathrm{disc}}^{k,i} \le \eta_{\mathrm{disc},\mathcal{M}_\ell}^{k,i} & \text{adaptive mesh refinement} \end{array}}$$

- 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)

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Outline

1. Introduction: a posteriori error control and adaptivity
2. Laplace equation: discretization error, mesh and polynomial degree adaptivity
    - A posteriori error control
    - Potential reconstruction
    - Flux reconstruction
    - Balancing error components: mesh adaptivity
    - Balancing error components: polynomial-degree adaptivity
3. Nonlinear Laplace equation: overall error and solvers adaptivity
    - A posteriori error control (overall and components)
    - Balancing error components: solvers adaptivity
4. Reaction–diffusion equation: robustness wrt parameters
5. Heat equation: robustness wrt final time and space–time error localization
6. Multiphase multicompositional flows: environmental application
7. Conclusions

The reaction–diffusion equation: $f \in L^2(\Omega)$, $\varepsilon > 0$, $\kappa \geq 0$ parameters

Find $u : \Omega \to \mathbb{R}$ such that ($\varepsilon \ll \kappa$ **singular perturbation**)

$$\begin{aligned} -\varepsilon^2 \Delta u + \kappa^2 u = f \quad & \text{in } \Omega, \\ u = 0 \quad & \text{on } \partial\Omega \end{aligned}$$

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

error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h)$)

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

- C_{eff} a generic constant independent of Ω, u, u_h, h,

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Equilibrated flux and potential reconstructions

Definition (Flux $\boldsymbol{\sigma}_h$ and potential ϕ_h)

For each vertex $\boldsymbol{a} \in \mathcal{V}$, let

$$(\boldsymbol{\sigma}_h^{\boldsymbol{a}}, \phi_h^{\boldsymbol{a}}) := \arg \min_{\substack{(\boldsymbol{v}_h, q_h) \in \mathcal{RT}_p(\mathcal{T}^{\boldsymbol{a}}) \times \mathcal{P}_p(\mathcal{T}^{\boldsymbol{a}}) \subset \boldsymbol{H}_0(\mathrm{div}, \omega_{\boldsymbol{a}}) \times L^2(\omega_{\boldsymbol{a}}) \\ \nabla\cdot\boldsymbol{v}_h + \kappa^2 q_h = \Pi_h(f\psi_{\boldsymbol{a}}) - \varepsilon^2 \nabla u_h \cdot \nabla \psi_{\boldsymbol{a}}}}$$

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$$\boldsymbol{\sigma}_h := \sum_{\mathbf{a}\in\mathcal{V}} \boldsymbol{\sigma}_h^{\mathbf{a}} \in \mathcal{RT}_p \cap \mathbf{H}(\mathrm{div},\Omega), \quad \phi_h := \sum_{\mathbf{a}\in\mathcal{V}} \phi_h^{\mathbf{a}} \in \mathcal{P}_p(\mathcal{T}_h).$$

Comments

- **local discrete** constrained minimization problems
- choose the locally **best-possible** estimators
- yields $\nabla\cdot\boldsymbol{\sigma}_h + \kappa^2\phi_h = \Pi_h f$

Equilibrated flux and potential reconstructions

Definition (Flux $\boldsymbol{\sigma}_h$ and potential ϕ_h)

For each vertex $\boldsymbol{a} \in \mathcal{V}$, let

$$(\boldsymbol{\sigma}_h^{\boldsymbol{a}}, \phi_h^{\boldsymbol{a}}) := \arg \min_{\substack{(\boldsymbol{v}_h, q_h) \in \mathcal{RT}_p(\mathcal{T}^{\boldsymbol{a}}) \times \mathcal{P}_p(\mathcal{T}^{\boldsymbol{a}}) \subset \boldsymbol{H}_0(\mathrm{div}, \omega_{\boldsymbol{a}}) \times L^2(\omega_{\boldsymbol{a}}) \\ \nabla \cdot \boldsymbol{v}_h + \kappa^2 q_h = \Pi_h(f \psi_{\boldsymbol{a}}) - \varepsilon^2 \nabla u_h \cdot \nabla \psi_{\boldsymbol{a}}}} J_{u_h}^{\boldsymbol{a}}(\boldsymbol{v}_h, q_h)$$

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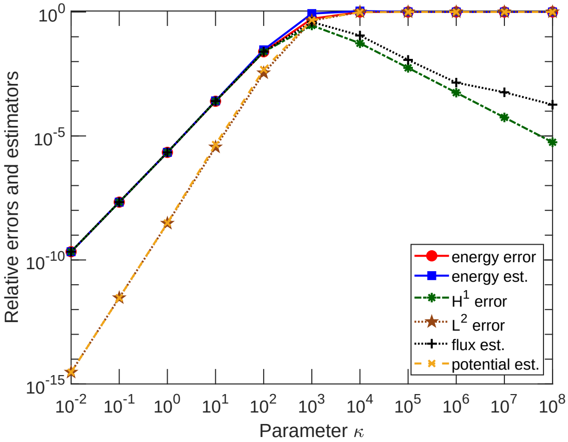
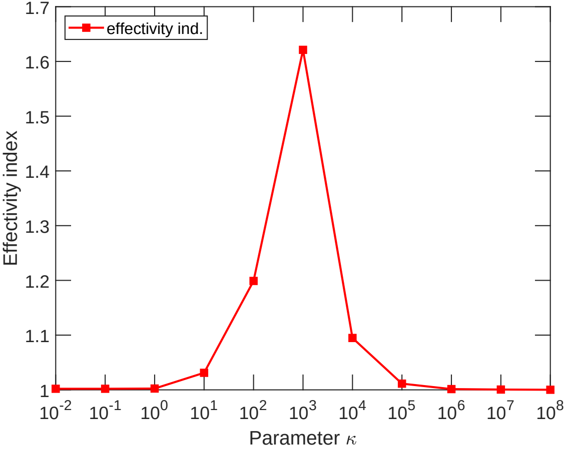
Boundary layer, solution $u(x,y) = e^{-\frac{\kappa}{\varepsilon}x} + e^{-\frac{\kappa}{\varepsilon}y}$, $p = 2$



Relative energy errors and estimates



Effectivity indices $\eta(u_h)/|||u - u_h|||$

I. Smears, M. Vohralík, ESAIM Math. Model. Numer. Anal. (2020)

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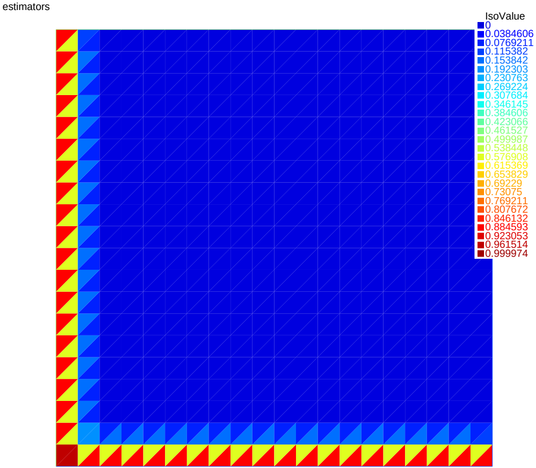
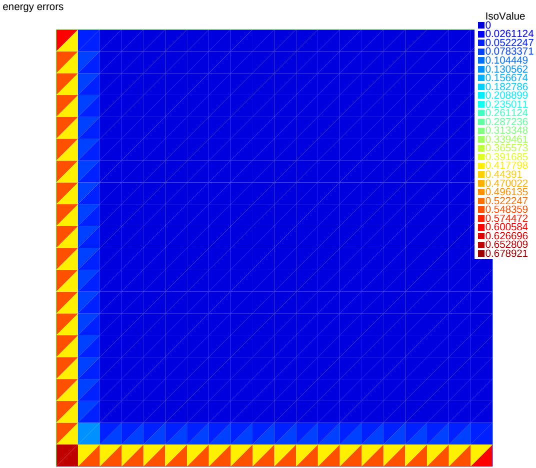


Estimated error distribution $\eta_K(u_h)$



Exact error distribution $|||u - u_h|||_K$

I. Smears, M. Vohralík, ESAIM Math. Model. Numer. Anal. (2020)

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

The heat equation

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$$X := L^2(0,T;H_0^1(\Omega)), \|v\|_X^2 := \int_0^T \|\nabla v\|^2 \,\mathrm{d}t,$$

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Y norm error is the dual X norm of the residual + initial condition error

$$\|u - u_{h\tau}\|_Y^2 = \sup_{v \in X, \|v\|_X = 1} \left[\int_0^T (f, v) - \langle \partial_t u_{h\tau}, v \rangle - (\nabla u_{h\tau}, \nabla v) \,\mathrm{d}t \right]^2 + \|u_0 - u_{h\tau}(0)\|^2$$

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▸ Laplace setting

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$$\underbrace{|||u - u_{h\tau}|||}_{\text{unknown error}} \leq \underbrace{\eta(u_{h\tau})}_{\text{computable estimator}}$$

- C_{eff} a generic constant independent of Ω, u, $u_{h\tau}$, h, p, τ, q,

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

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Two-phase flow

Incompressible two-phase flow in porous media

Find *saturations* s_α and *pressures* p_α, $\alpha \in \{\mathrm{g}, \mathrm{w}\}$, such that

$$\begin{aligned}\partial_t(\phi s_\alpha) - \nabla\cdot\left(\frac{k_{\mathrm{r},\alpha}(s_\mathrm{w})}{\mu_\alpha}\boldsymbol{K}(\nabla p_\alpha + \rho_\alpha g \nabla z)\right) &= q_\alpha, \qquad \alpha \in \{\mathrm{g}, \mathrm{w}\},\\ s_\mathrm{g} + s_\mathrm{w} &= 1,\\ p_\mathrm{g} - p_\mathrm{w} &= p_\mathrm{c}(s_\mathrm{w})\end{aligned}$$

- unsteady, nonlinear, and degenerate problem
- coupled system of PDEs & algebraic constraints

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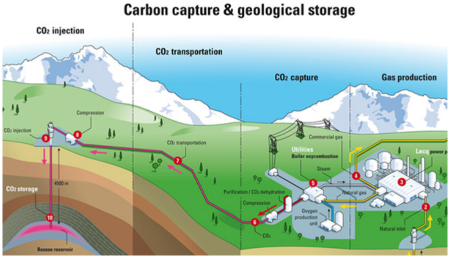
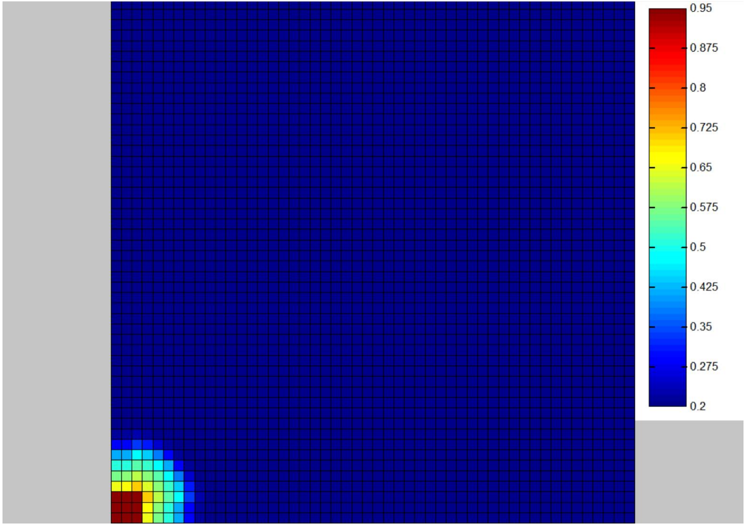
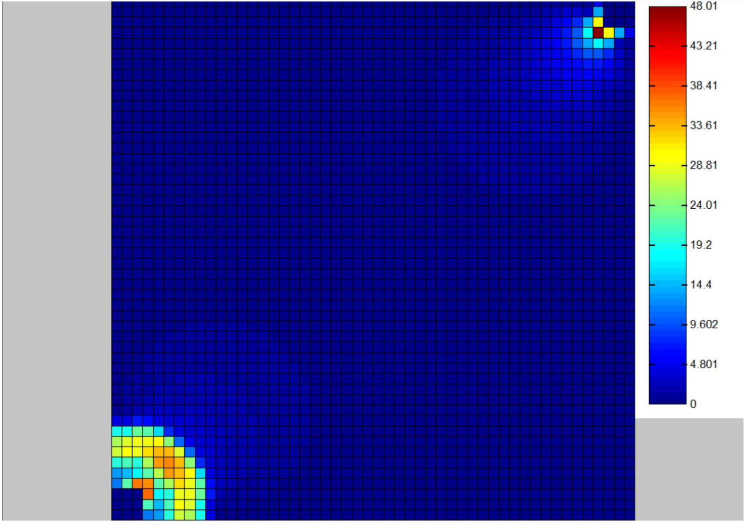


Geological sequestration of CO_2, CO_2 saturation



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

Geological sequestration of CO_2, **overall a posteriori estimate**



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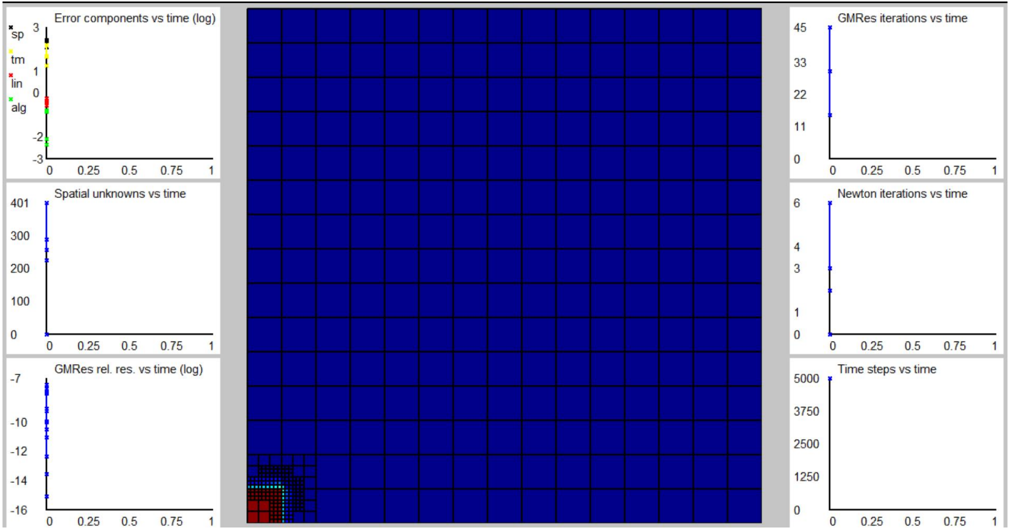
Geological sequestration of CO_2, **full adaptivity**



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Multi-phase multi-compositional flow

Theorem (Multi-phase multi-compositional Darcy flow with phase (dis)appearance)

There holds

$$\textit{error on time interval } I_n \leq \left\{ \sum_{c \in \mathcal{C}} \left(\eta_{\mathrm{mod},c}^{n,j,k,i} + \eta_{\mathrm{sp},c}^{n,j,k,i} + \eta_{\mathrm{tm},c}^{n,j,k,i} + \eta_{\mathrm{reg},c}^{n,j,k,i} + \eta_{\mathrm{lin},c}^{n,j,k,i} + \eta_{\mathrm{alg},c}^{n,j,k,i} \right)^2 \right\}^{1/2}.$$

Error components

- $\eta_{\mathrm{mod},c}^{n,j,k,i}$: modeling
- $\eta_{\mathrm{sp},c}^{n,j,k,i}$: spatial discretization
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- $\eta_{\mathrm{lin},c}^{n,j,k,i}$: linearization
- $\eta_{\mathrm{alg},c}^{n,j,k,i}$: algebraic solver

Error control

- at **any moment** during the simulation
- price: sparse **matrix-vector** multiplication

Full adaptivity

- **same physical units** of all component estimators
- **balance** all component estimators
- **online steering**

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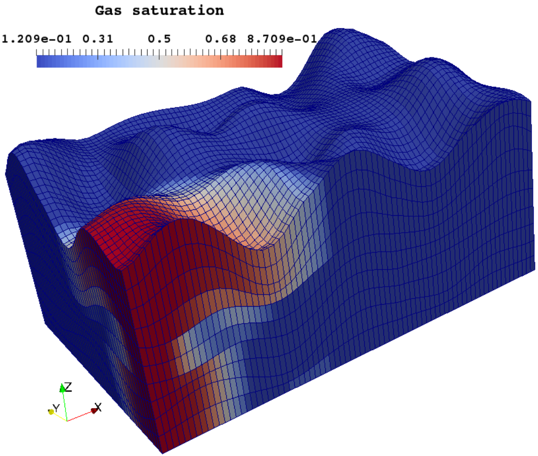
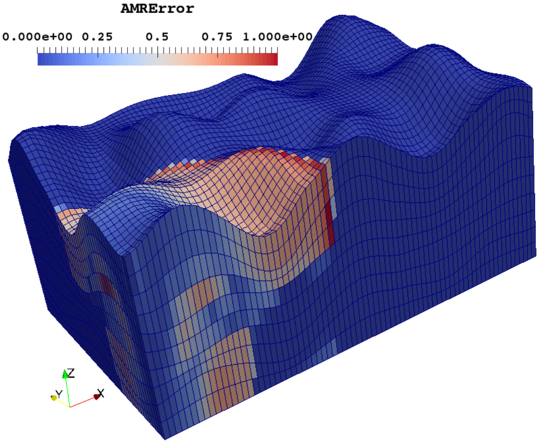
Adaptivity: 3 phases, 3 components (black-oil) problem



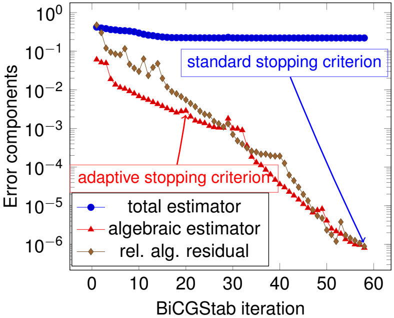
Gas saturation

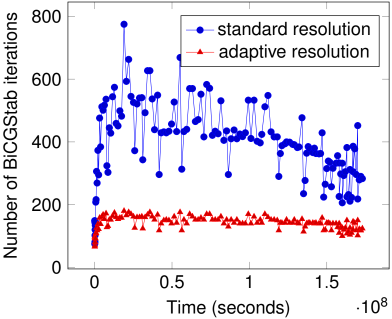


A posteriori error estimate

M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2018)

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

M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2018)

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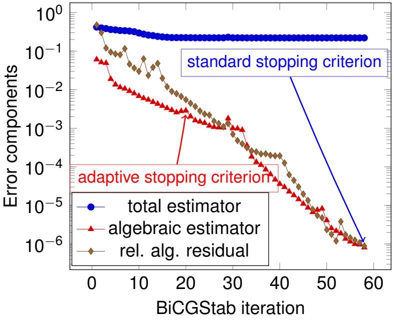

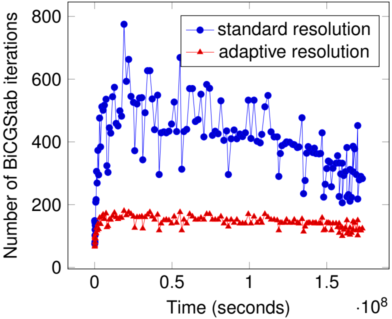

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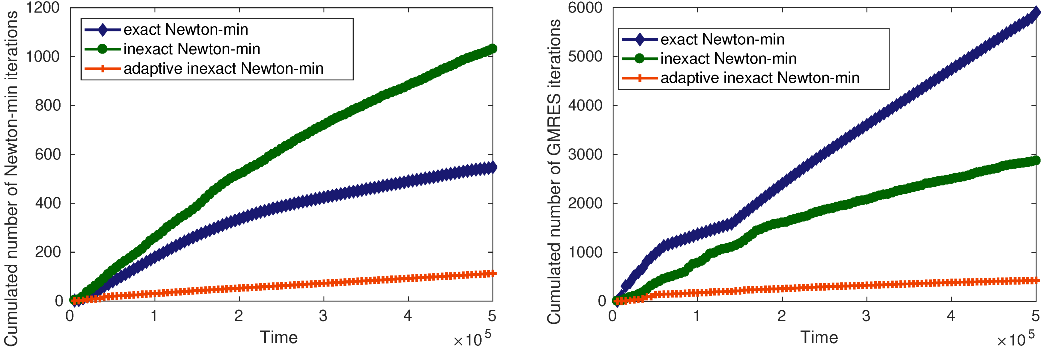
M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2018)

Phase (dis)appearance: Couplex-gas benchmark



Adaptive linear and nonlinear solvers

I. Ben Gharbia, J. Dabaghi, V. Martin, M. Vohralík, Computational Geosciences (2020)

Outline

Conclusions

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  adaptivity: space mesh, time step,

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Thank you for your attention!