A posteriori error estimates and adaptivity: principles and applications

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Inria Paris & Charles University Prague

11 November 2026, Liberec

Inria



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 & wave equation: robustness wrt final time & space–time error localization
6. Multiphase multicompositional flows: environmental application
   - Error control and adaptivity of error components
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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Reliability study and simulation of the progressive collapse of Roissy Charles de Gaulle Airport

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

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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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Crucial questions

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

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

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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) ($u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H^1_0(\Omega)$, $p \geq 1$, 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 $\frac{\|\nabla(u-u_h)\|}{\|\nabla u\|}$	$I^{\text{eff}} = \frac{\eta(u_h)}{\|\nabla(u-u_h)\|}$
h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$	1	$\approx 6.0 \times 10^{-1}$				
$\approx h_0/4$	1	$\approx 3.0 \times 10^{-1}$				
$\approx h_0/8$	1	$\approx 1.5 \times 10^{-1}$				
$\approx h_0/2$	2	$\approx 2.1 \times 10^{-1}$				
$\approx h_0/4$	2	$\approx 5.2 \times 10^{-2}$				
$\approx h_0/8$	2	$\approx 1.3 \times 10^{-2}$				

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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$\approx h_0/2$	2	4.23×10^{-2}				
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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}	3.5%	1.39×10^{-1}	3.1%	1.04
$\approx h_0/2$	2	4.23×10^{-2}	9.5×10^{-3}%	4.07×10^{-2}	9.2×10^{-3}%	1.04
$\approx h_0/4$	3	2.62×10^{-4}	5.8×10^{-5}%	2.60×10^{-4}	5.8×10^{-5}%	1.01
$\approx h_0/8$	4	2.60×10^{-7}	5.9×10^{-8}%	2.58×10^{-7}	5.8×10^{-8}%	1.01

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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**
$\approx h_0/2$		6.07×10^{-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
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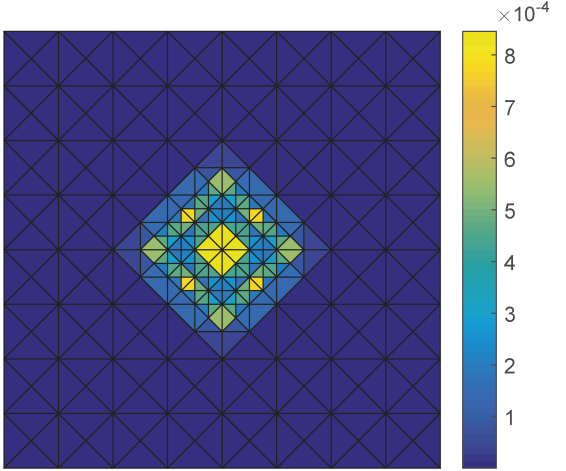
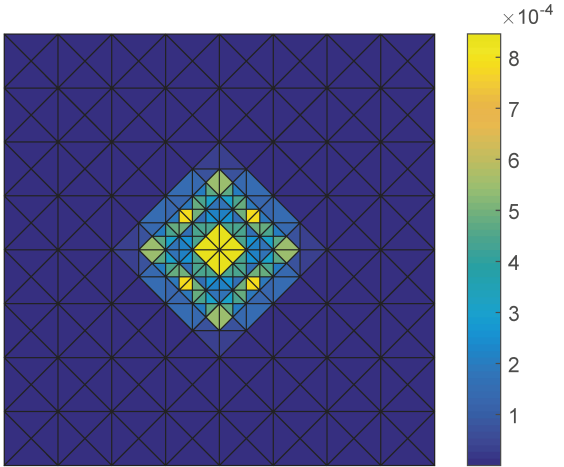
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)



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 $u \in H_0^1(\Omega)$ be the weak solution and let $u_h \in H^1(\mathcal{T}_h)$ be arbitrary. Then

$$\|\nabla(u-u_h)\|^2 = \underbrace{\min_{\substack{\boldsymbol{v}\in\boldsymbol{H}(\mathrm{div},\Omega)\\ \nabla\cdot\boldsymbol{v}=f}} \|\nabla u_h + \boldsymbol{v}\|^2}_{\text{constrained distance to } \boldsymbol{H}(\mathrm{div},\Omega)} + \underbrace{\min_{v\in H_0^1(\Omega)} \|\nabla(u_h - v)\|^2}_{\text{distance to } H_0^1(\Omega)}.$$

$$= \max_{\substack{v\in H_0^1(\Omega)\\ \|\nabla v\|=1}} [(f,v)-(\nabla u_h,\nabla v)]^2$$

dual norm of the residual

Comments

- It is enough to choose suitable (discrete, piecewise polynomial) $\sigma_h \in \boldsymbol{H}(\mathrm{div},\Omega)$ with $\nabla\cdot\sigma_h = f$ and $s_h \in H_0^1(\Omega)$ to get a guaranteed upper bound.

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- Local evaluation of the error and h, p

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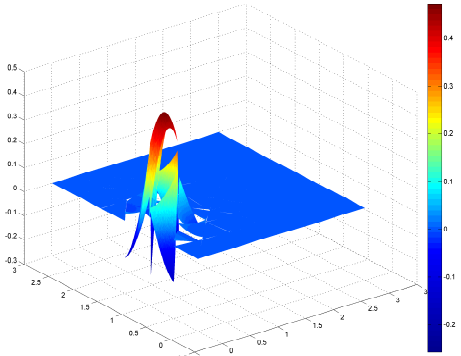
Outline

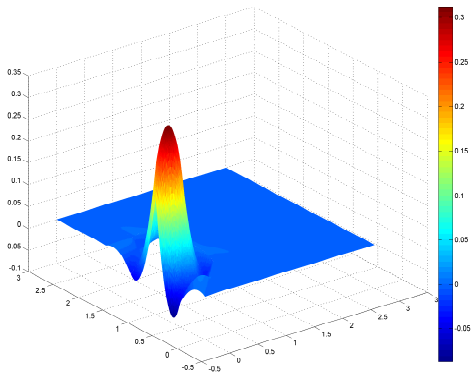
1. Introduction: a posteriori error control and adaptivity
2. Laplace equation: discretization error, mesh and polynomial degree adaptivity
   - A posteriori error control
   - Potential reconstruction
   - Flux reconstruction
   - Balancing error components: mesh adaptivity
   - Balancing error components: 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 & wave equation: robustness wrt final time & space–time error localization
6. Multiphase multicompositional flows: environmental application
   - Error control and adaptivity of error components
7. Conclusions



Potential reconstruction



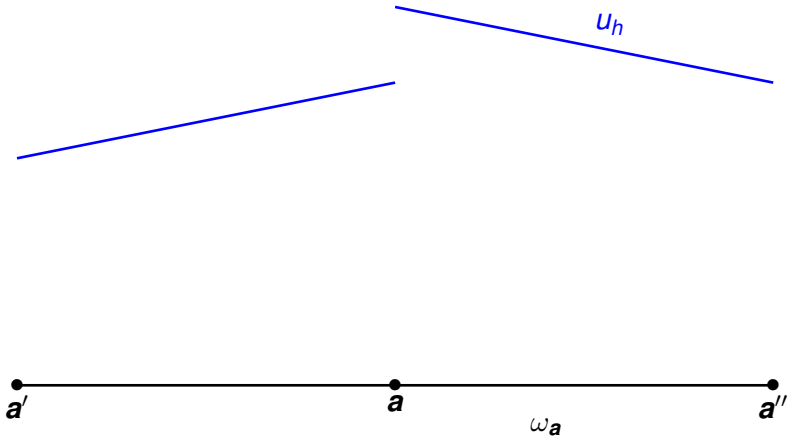
Potential u_h



Potential reconstruction s_h

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

Potential reconstruction in 1D, $p = 1$



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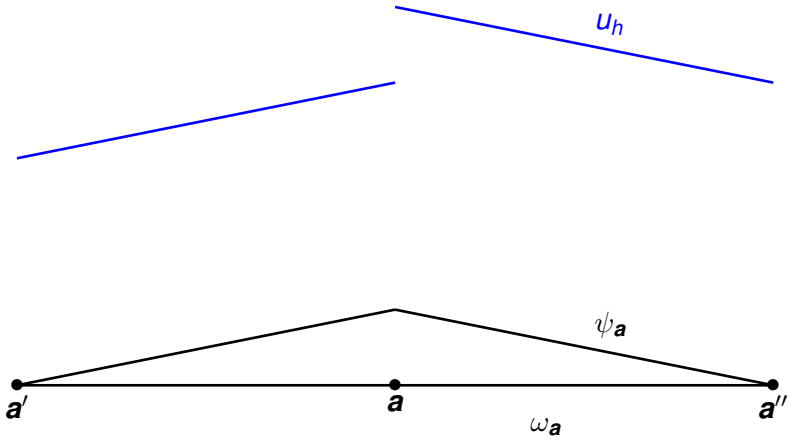

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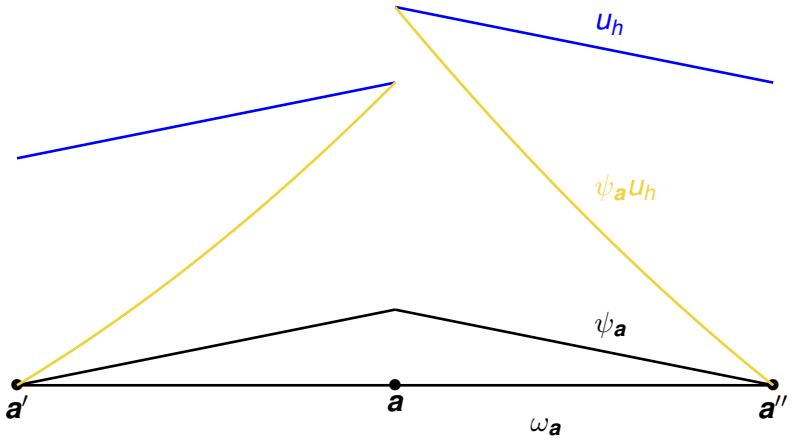

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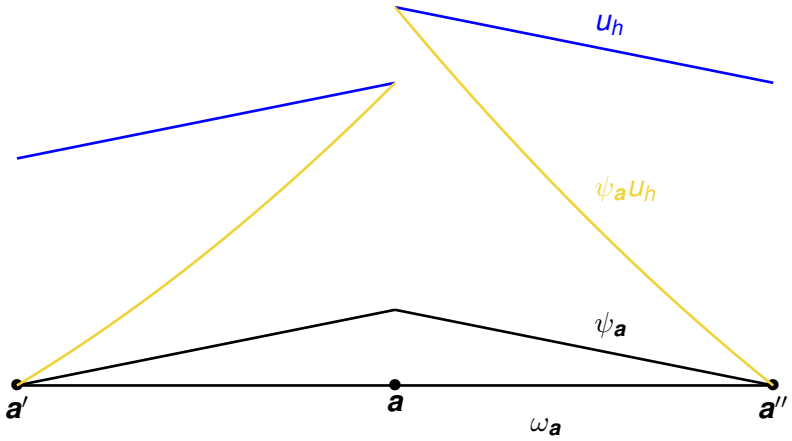

Potential reconstruction: datum $u_h \in \mathcal{P}_p(\mathcal{T}_h)$, $p \geq 1$

Definition (Construction of s_h Ern & V. (2015), $\approx$ Carstensen and Merdon (2013)**)**

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

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

and continue

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

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
- homogeneous Dirichlet BC on $\partial\omega_{\boldsymbol{a}}$: $s_h \in \mathcal{P}_{p+1}(\mathcal{T}_h) \cap H_0^1(\Omega)$

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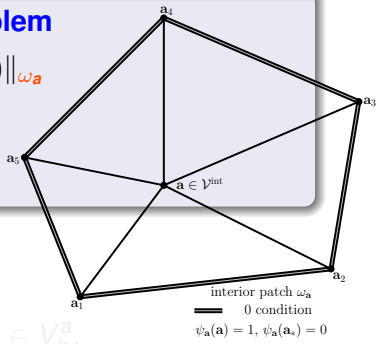

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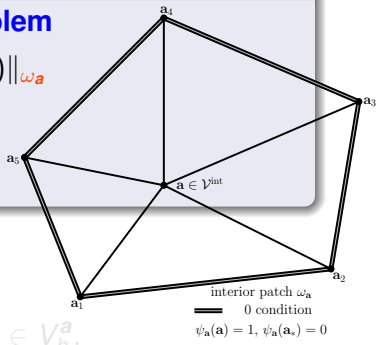

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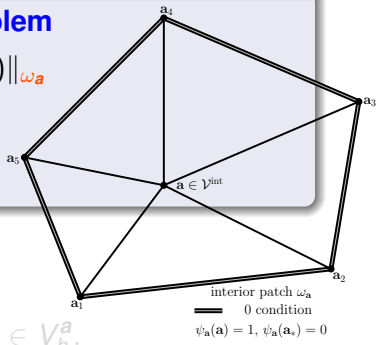

Equivalent form: conforming FEs

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
- homogeneous Dirichlet BC on $\partial\omega_{\boldsymbol{a}}$: $s_h \in \mathcal{P}_{p+1}(\mathcal{T}_h) \cap H_0^1(\Omega)$

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

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

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

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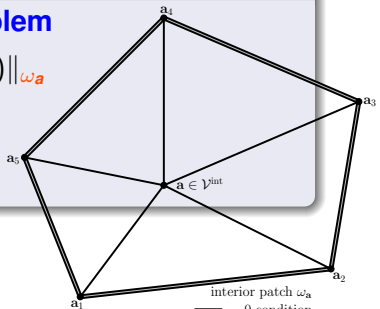

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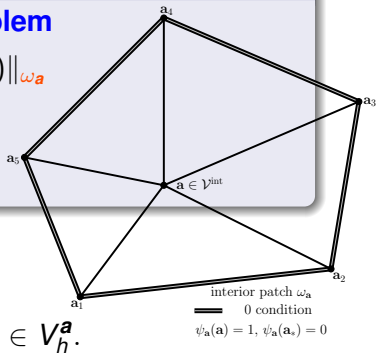

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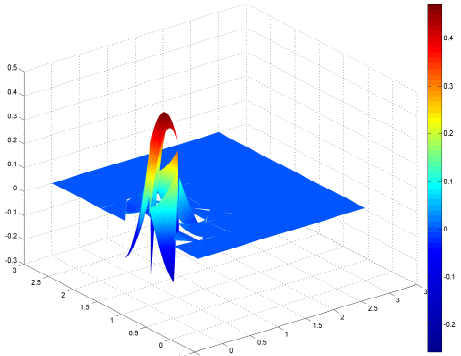
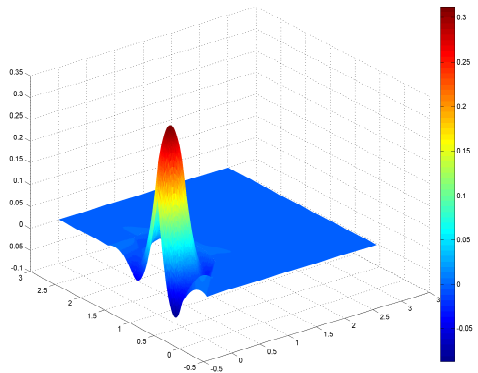
Potential reconstruction



Potential u_h



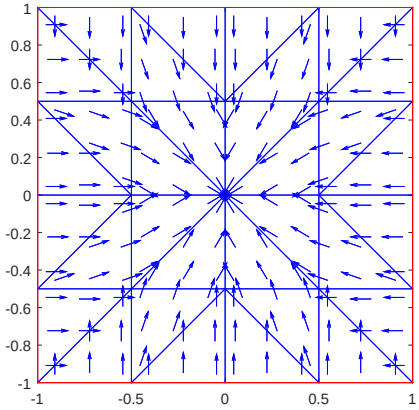
Potential reconstruction s_h

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

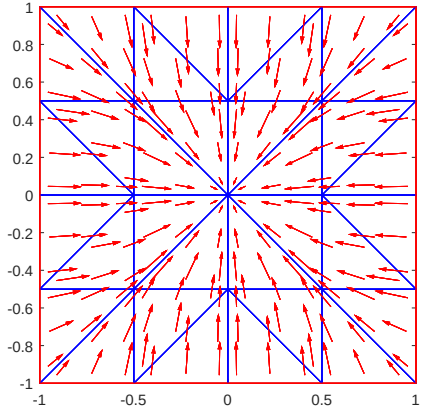
Outline

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 & wave equation: robustness wrt final time & space–time error localization
6. Multiphase multicompositional flows: environmental application
   - Error control and adaptivity of error components
7. Conclusions

Equilibrated flux reconstruction



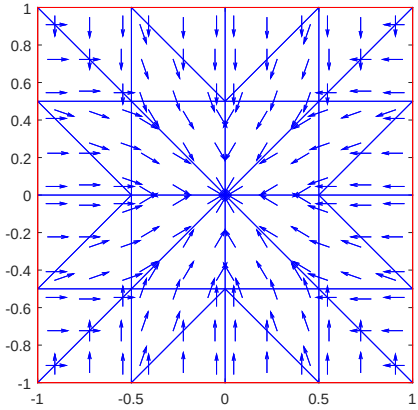
Flux $-\nabla u_h$



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

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

Equilibrated flux reconstruction



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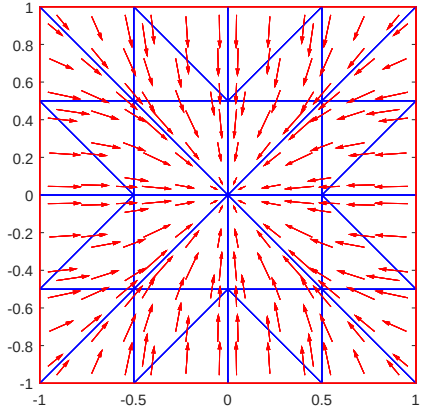

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and sum over $\boldsymbol{a} \in \mathcal{V}_h$: $\boldsymbol{\sigma}_h = \sum_{\boldsymbol{a} \in \mathcal{V}_h} \boldsymbol{\sigma}_h^{\boldsymbol{a}}$

Key points

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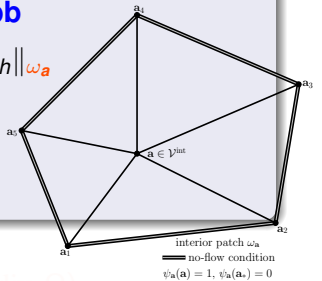

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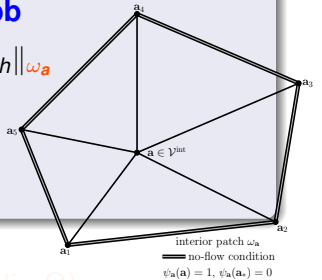

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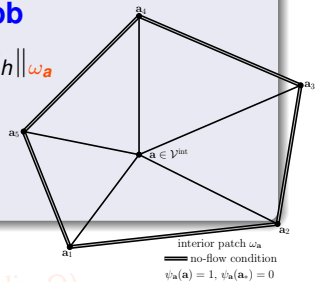

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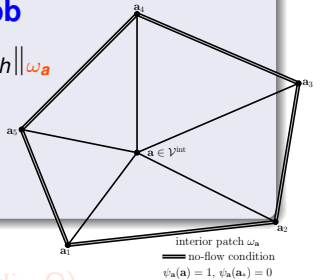

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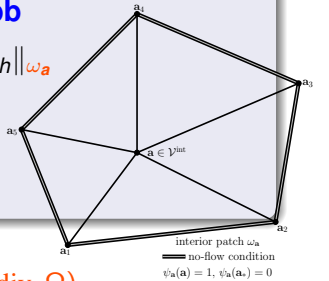

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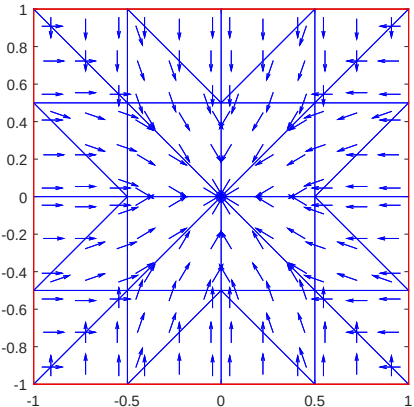
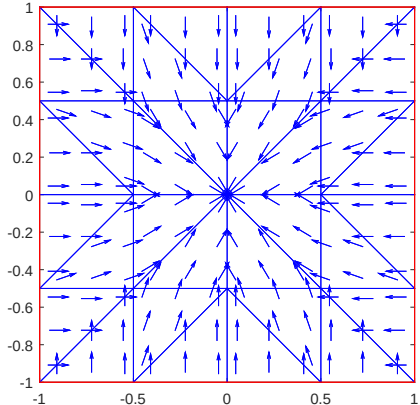


Flux $-\nabla u_h \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla \cdot (-\nabla u_h) \neq f$

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



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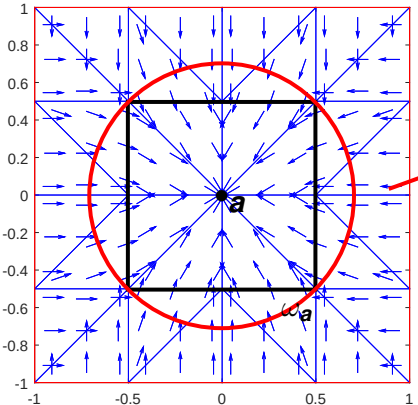
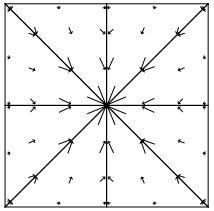


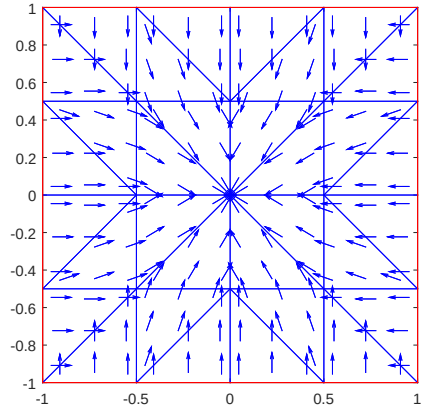


$-\psi_a \nabla u_h$

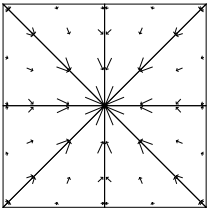
Flux $-\nabla u_h \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla \cdot (-\nabla u_h) \neq f$

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

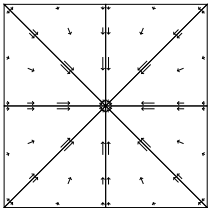
Equilibrated flux reconstruction: $-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h)$, $p \geq 1$, $f \in L^2(\Omega)$



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



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



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

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

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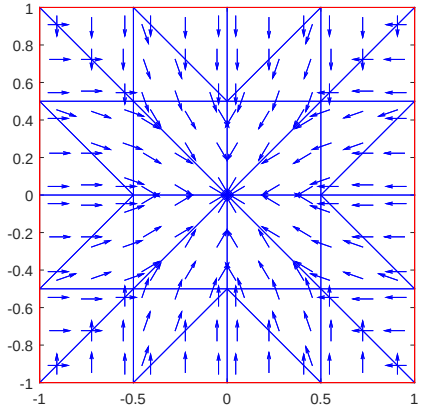
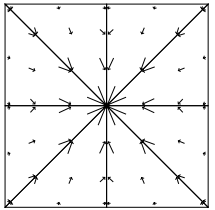


Flux $-\nabla u_h \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot(-\nabla u_h) \neq f$



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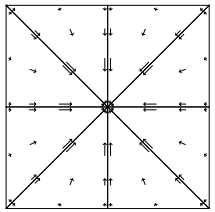
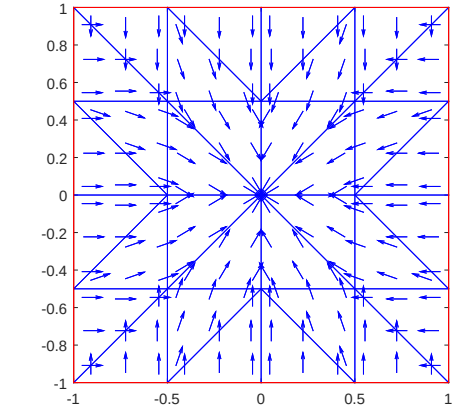


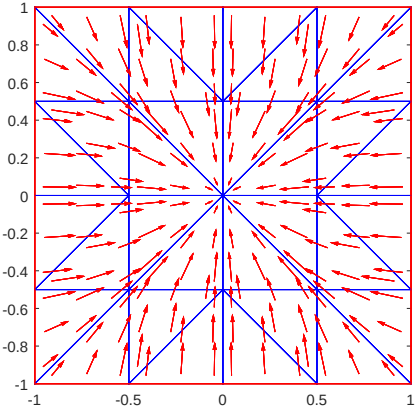
$\boldsymbol{\sigma}_h^{\boldsymbol{a}}$

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

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. $\boldsymbol{\sigma}_h$

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

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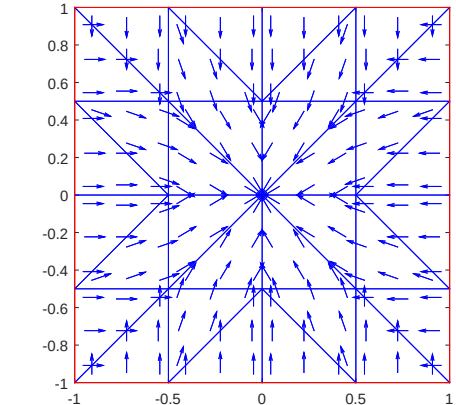
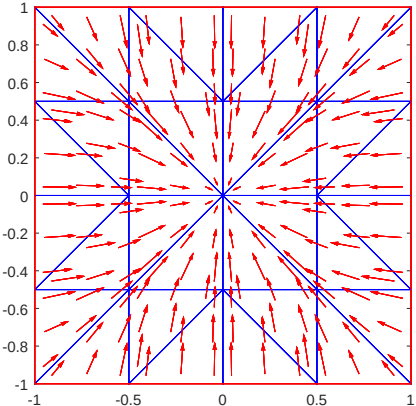


Flux $-\nabla u_h \notin \boldsymbol{H}(\mathrm{div},\Omega)$, $\nabla\cdot(-\nabla u_h) \neq f$



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

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

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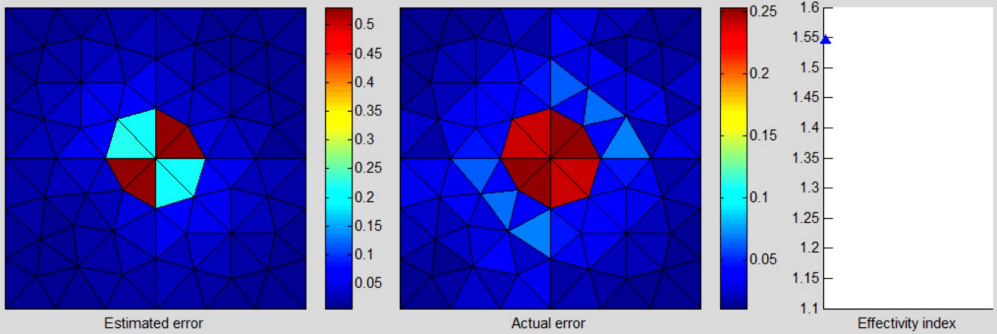
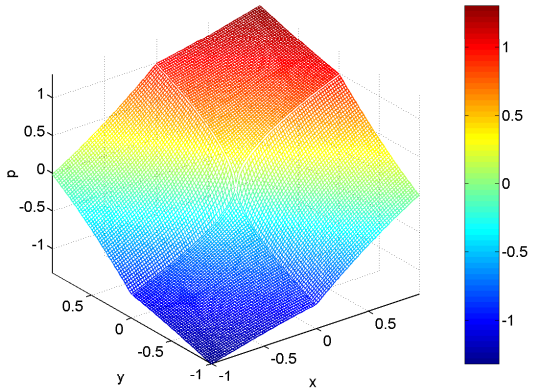
Can we **decrease the error efficiently**? (adaptive mesh refinement)

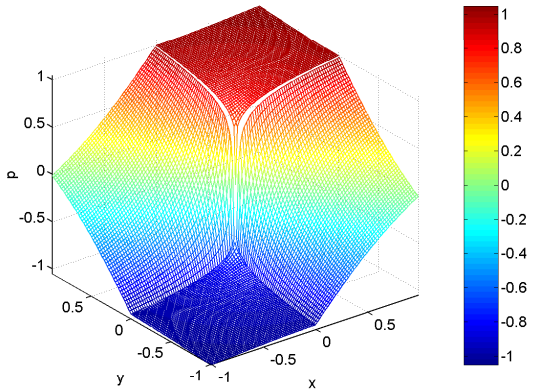


M. Vohralík, SIAM Journal on Numerical Analysis (2007)

Singular solutions

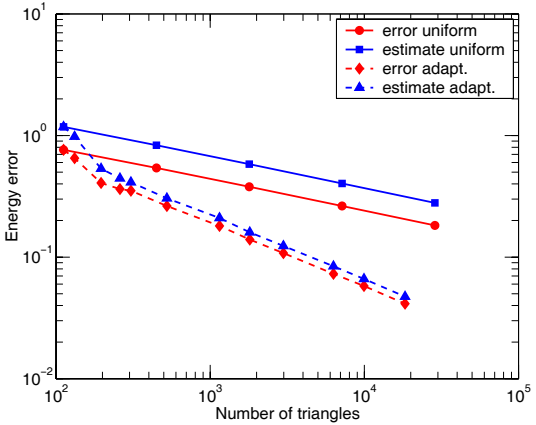


$H^{1.54}$ singularity



$H^{1.13}$ singularity

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



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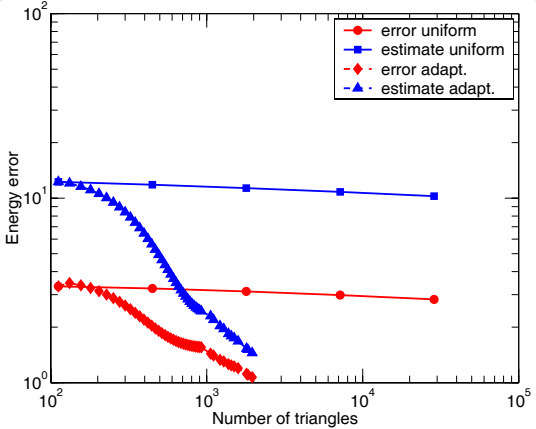

$H^{1.13}$ singularity

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

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

Adaptive mesh refinement

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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: ~~$h \searrow 0$~~
- Babuška & Miller (1987), Dörfler (1996)



Adaptive mesh refinement

Adaptive mesh refinement

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

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

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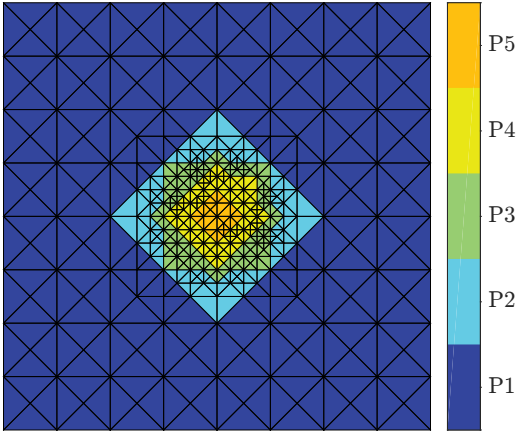
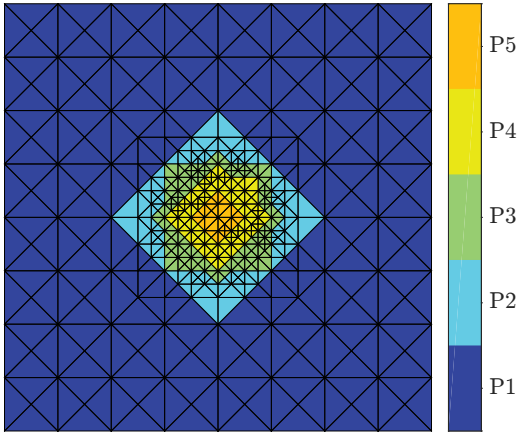
Best-possible error decrease: *hp* **adaptivity**, (**smooth** solution)



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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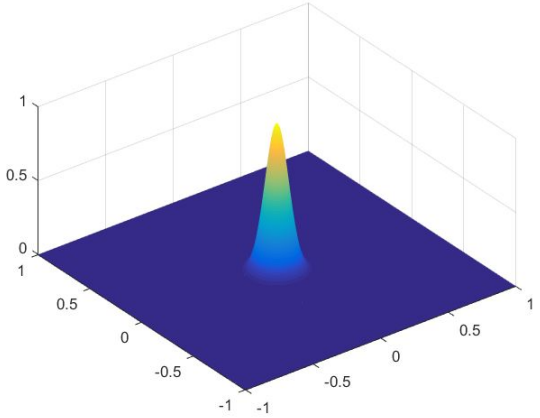
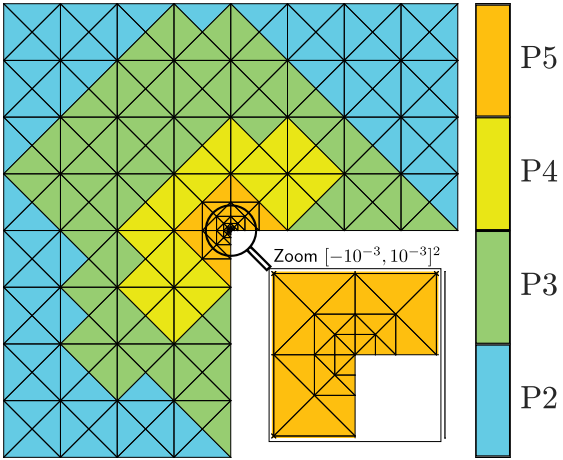


Exact solution

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

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



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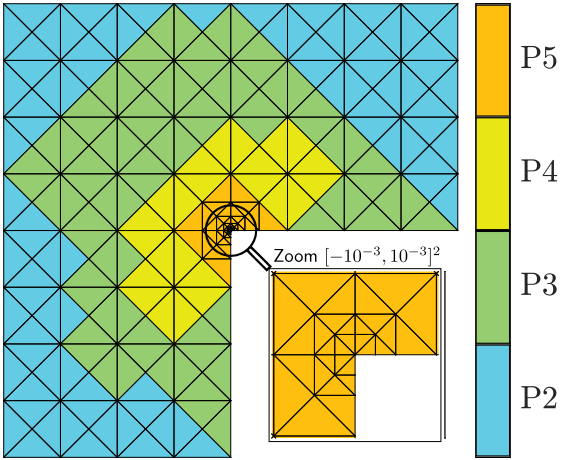

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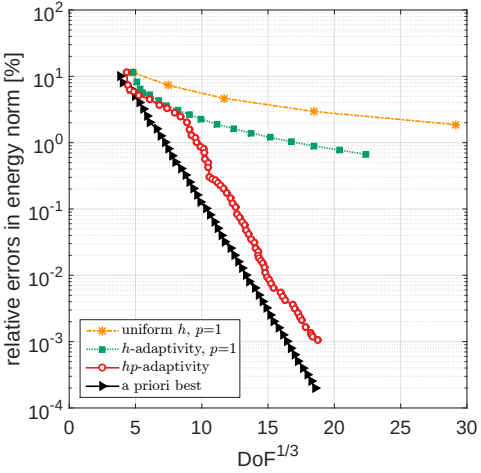

Relative error as a function of DoF

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

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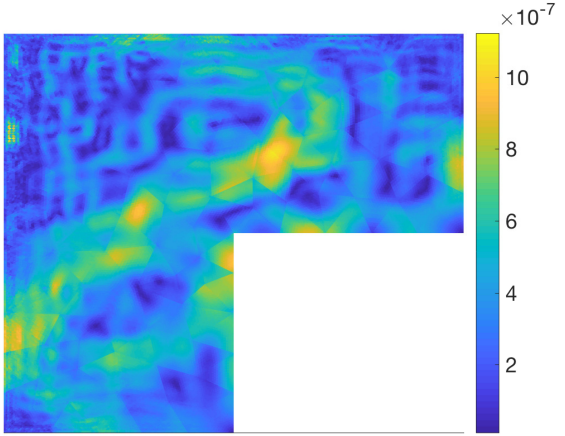
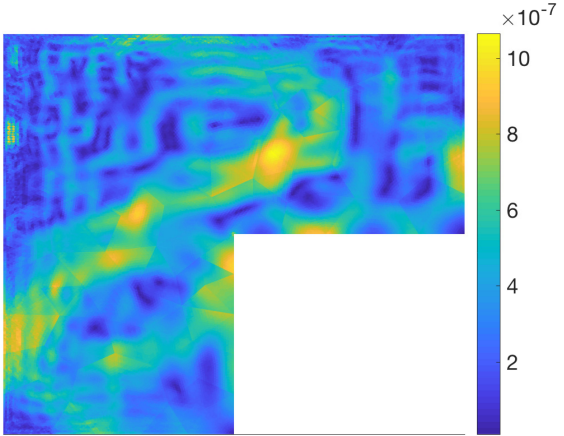
Including **algebraic error**: $\mathbb{A}_\ell \mathbf{U}_\ell^i \neq \mathbf{F}_\ell$



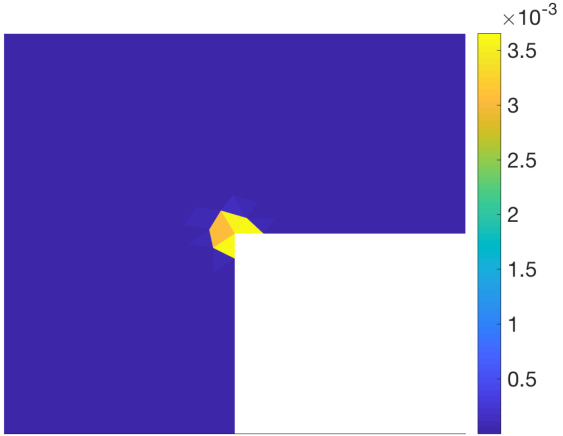
Estimated algebraic errors $\eta_{\mathrm{alg},K}(u_\ell^i)$



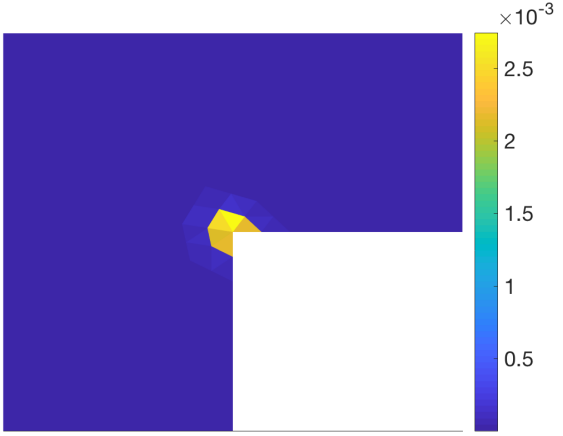
Exact algebraic errors $\|\nabla(u_\ell - u_\ell^i)\|_K$

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

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



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



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

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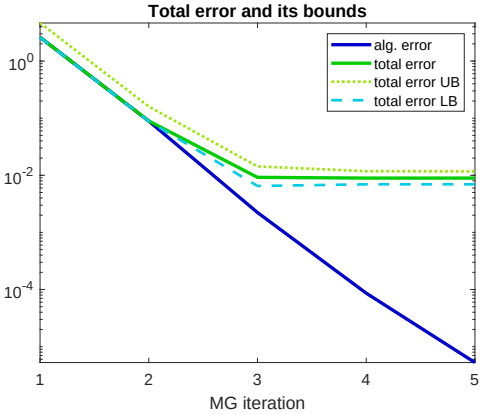
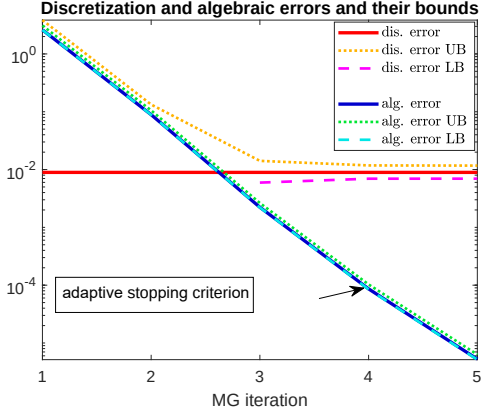
Including **algebraic error**: $\mathbb{A}_\ell \mathrm{U}_\ell^i \neq \mathrm{F}_\ell$



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 $-\nabla\cdot\boldsymbol{\sigma}(\nabla u) = f$: 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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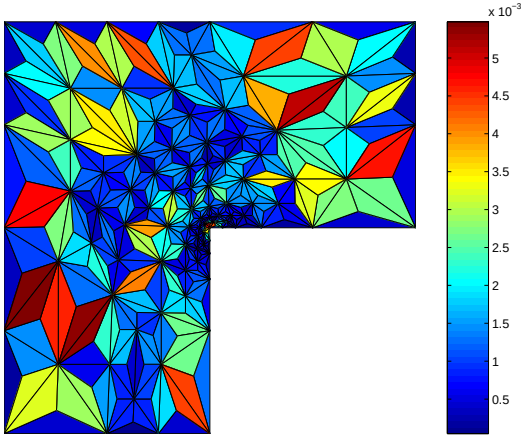
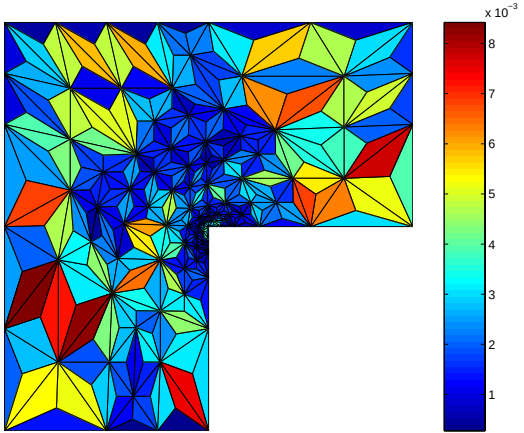


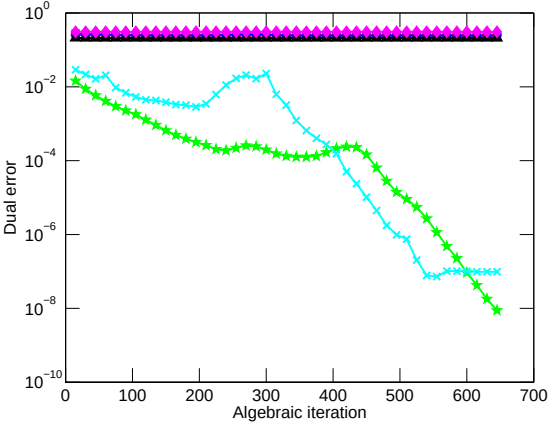
Estimated errors $\eta_K(u_\ell^{k,i})$



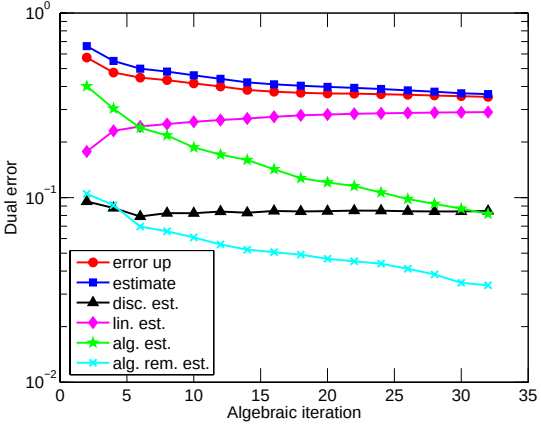
Exact errors $\|\boldsymbol{\sigma}(\nabla u) - \boldsymbol{\sigma}(\nabla u_\ell^{k,i})\|_{q,K}$

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

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



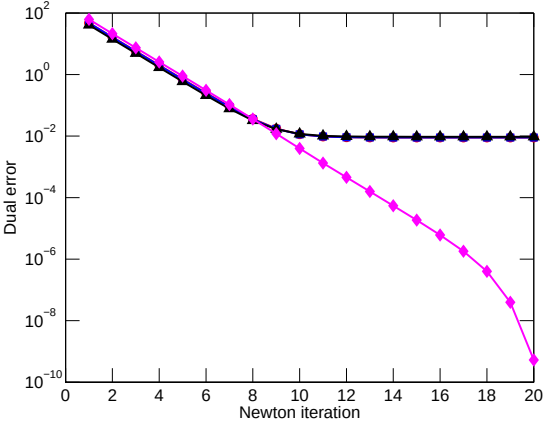
Newton



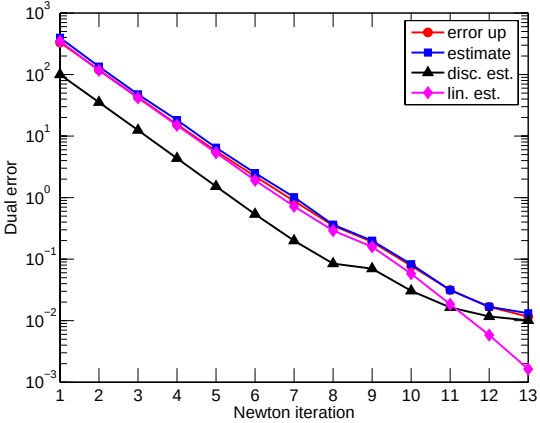
adaptive inexact Newton

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

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



Newton



adaptive inexact Newton

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

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
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7. Conclusions

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

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

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

$$\eta_{\ell,\mathrm{disc}}^{k,i} \leq \eta_{\mathrm{disc},\mathcal{N}_\ell} \quad \text{adaptive mesh refinement}$$

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

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

Optimal error decay rate wrt overall computational cost

$$\|u - u_\ell^{k,i}\|_* \lesssim \left\{ \sum_{\ell=0}^{J} \sum_{k=0}^{\bar{k}} \sum_{i=0}^{\bar{J}} |V_\ell^k|^{p} \right\}^{-p/d} \quad \text{(replaces traditional a priori } h^p\text{)}$$

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

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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**)

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

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

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

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

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

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

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

Verfürth (1998), Ainsworth & Babuška (1999), Cheddadi (2006), Chaumont-Frelet, Ern, Vohralík (2020), Ainsworth & Vejchodský (2011), Kopteva (2014), Kopteva (2021), Smears & Vohralík (2021)

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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

$$(\boldsymbol{\sigma}_h^{\boldsymbol{a}}, \phi_h^{\boldsymbol{a}}) := \arg \min_{(\boldsymbol{v}_h, q_h) \in \mathcal{RT}_p(\mathcal{T}^{\boldsymbol{a}}) \times \mathcal{P}_p(\mathcal{T}^{\boldsymbol{a}}) \subset \boldsymbol{H}_0(\mathrm{div}, \omega_{\boldsymbol{a}}) \times L^2(\omega_{\boldsymbol{a}})} J_{\mu}^{\boldsymbol{a}}(\boldsymbol{v}_h, q_h)$$

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Comments

- **local discrete** constrained minimization problems
- choose the locally best-possible estimators
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with the weight $w_{\boldsymbol{a}} := \min\left\{1, C_* \sqrt{\frac{\varepsilon}{\kappa h_{\omega_{\boldsymbol{a}}}}}\right\}$. Combine

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

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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

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with the weight $w_{\boldsymbol{a}} := \min \left\{1, C_* \sqrt{\frac{\varepsilon}{\kappa h_{\omega_{\boldsymbol{a}}}}}\right\}$. Combine

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

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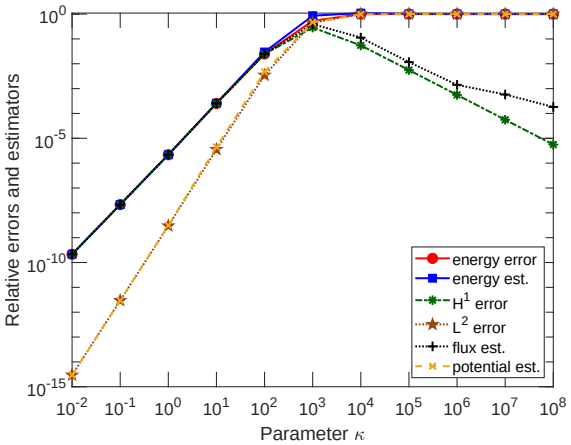
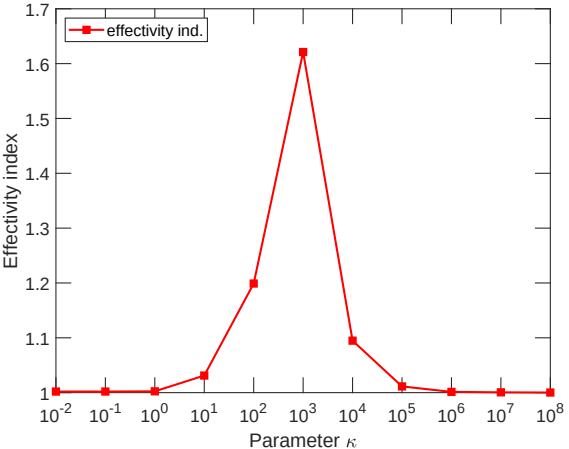
Boundary layer, solution $u(x,y) = e^{-\frac{\kappa}{\varepsilon}x} + e^{-\frac{\kappa}{\varepsilon}y}$, $p = 2$



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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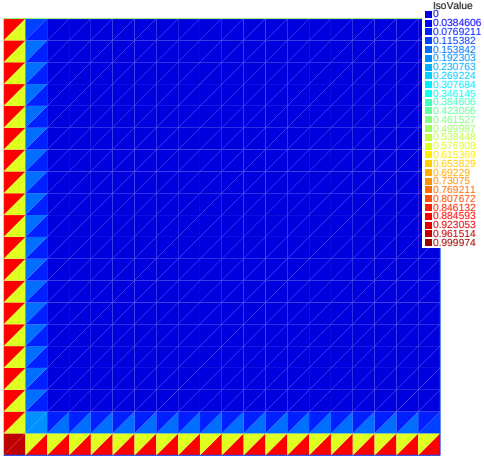
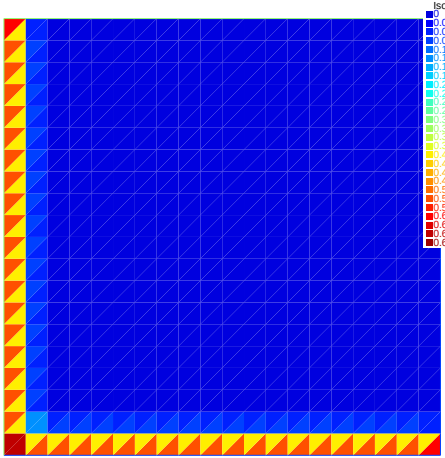
estimators



Estimated error distribution $\eta_K(u_h)$

energy errors



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

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

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 & wave equation: robustness wrt final time & space–time error localization
6. Multiphase multicompositional flows: environmental application
   - Error control and adaptivity of error components
7. Conclusions

The heat & wave equations

The heat equation

Find $u : \Omega \times (0,T) \to \mathbb{R}$ such that

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

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Continuous setting

- T: final time
- Ω: space domain (Lipschitz bounded polytope)
- $Q := \Omega \times (0,T)$: space-time domain
- f: source term, pw polynomial

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Discrete setting

- discrete times $\{t^n\}_{0 \le n \le N}$
- time intervals $I_n := (t^{n-1}, t^n]$, $\tau^n := t^n - t^{n-1}$
- simplicial/affine cuboidal mesh $\mathcal{T}_h$ of Ω
- hat functions $\psi_{\boldsymbol{a}}$ for vertices $\mathcal{V}_h$, support $\omega_{\boldsymbol{a}}$
- conforming finite element space $V_h := \mathcal{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega)$, $p \ge 1$

Reliable and locally space-time efficient a posteriori error estimates

Theorem (A posteriori error estimates)

Let $u_{h\tau} \in H^1_{0,}(Q)$ (heat) or $u_{h\tau} \in H^1_{0,}(Q) \cap H^2(0,T;L^2(\Omega))$ (wave) be piecewise polynomials (order p in space, order q in time).

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$$(f, \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}} \times I_n} - (\partial_t u_{h\tau}, \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}} \times I_n} - (\nabla u_{h\tau}, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}} \times I_n} = 0 \quad \forall 1 \leq n \leq N, \forall \boldsymbol{a} \in \mathcal{V}_h.$$

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Let $\mathcal{R}(u_{h\tau}) \in (H^1_{,T}(Q))'$ be the heat or the wave residual.

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$$\|\mathcal{R}(u_{h\tau})\|^2_{(H^1_{,T}(Q))'} \lesssim \sum_{n=1}^{N} \sum_{K \in \mathcal{T}_h^n} \eta_K^n(u_{h\tau})^2 \lesssim \|\mathcal{R}(u_{h\tau})\|^2_{(H^1_{,T}(Q))'}$$

$$\eta_K^n(u_{h\tau}) \lesssim \|\mathcal{R}(u_{h\tau})\|_{(H^1_0(\omega_K \times I_n))'}$$

where the hidden constants only depend on the space dimension d, shape-regularity of the space and time meshes, and p and q.

Reliable and locally space-time efficient a posteriori error estimates

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$$\eta_K^n(u_{h\tau}) \lesssim \|\mathcal{R}(u_{h\tau})\|_{(H^1_0(\omega_K \times I_n))'} \le \left(\|\partial_t(u - u_{h\tau})\|^2_{\omega_K \times I_n} + \|\nabla(u - u_{h\tau})\|^2_{\omega_K \times I_n}\right)^{1/2},$$

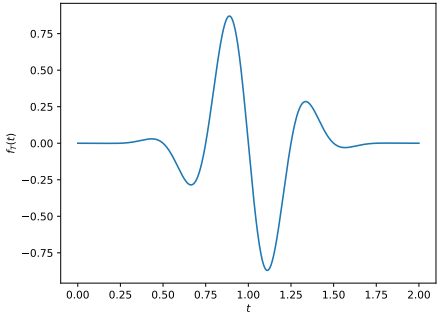
where the hidden constants only depend on the space dimension d, shape-regularity of the space and time meshes, and p and q.

Data and solution

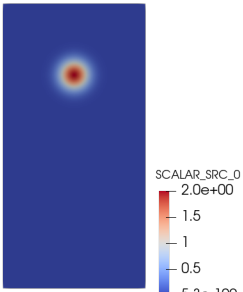
$$\Omega = (0,1) \times (0,2)$$

$$f_T(t) = -\sin(4\pi(t-1)) \times e^{-\left(\frac{t-1}{0.1}\right)^2}$$

$$f_X(x,y) = \exp\left(-\frac{(x-0.5)^2 + (y-1.5)^2}{0.1^2}\right)$$

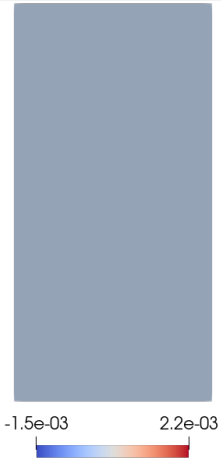


f_T



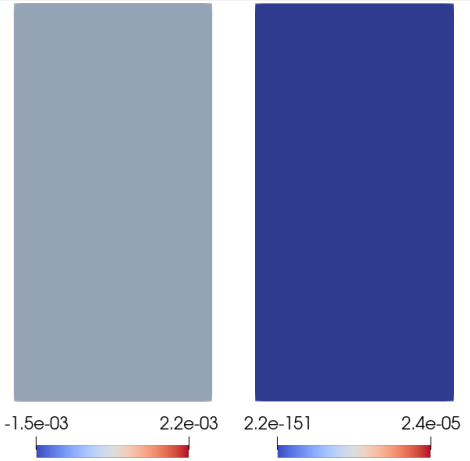
f_X

Approximation, error, and estimators



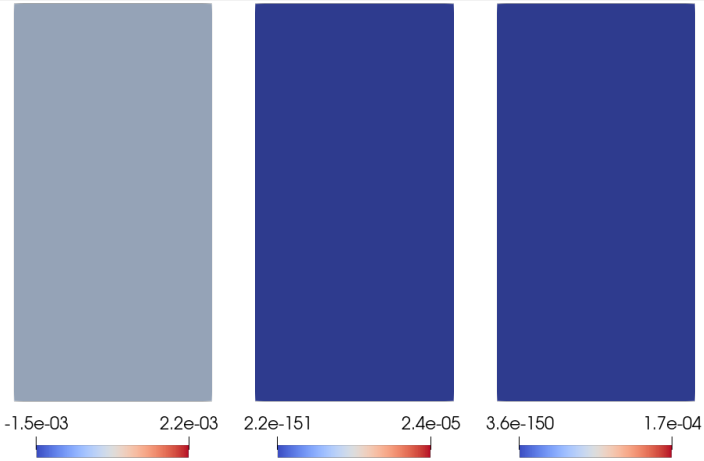
Approximation u_h^n

Approximation, error, and estimators



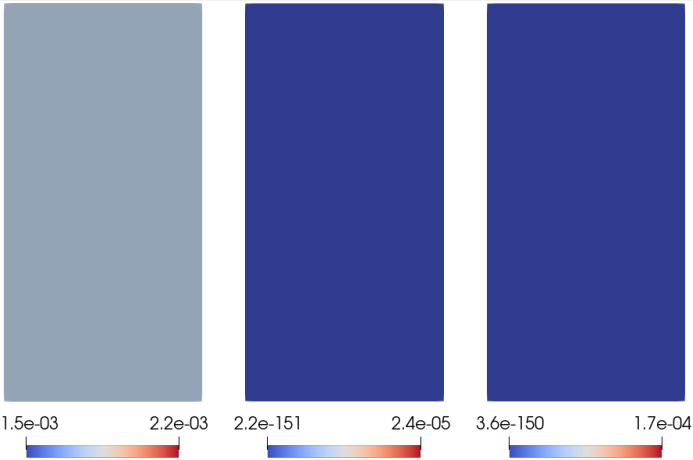
Approximation u_h^n, error $|u - u_{h\tau}|_{H^1(K\times I_n)}$

Approximation, error, and estimators



Approximation u_h^n, error $|u - u_{h\tau}|_{H^1(K\times I_n)}$, estimators $\eta_K^n(u_{h\tau})$

Approximation, error, and estimators



Remarks:

- equilibrated fluxes estimators
- local H^1 norms in place of the dual local norms:

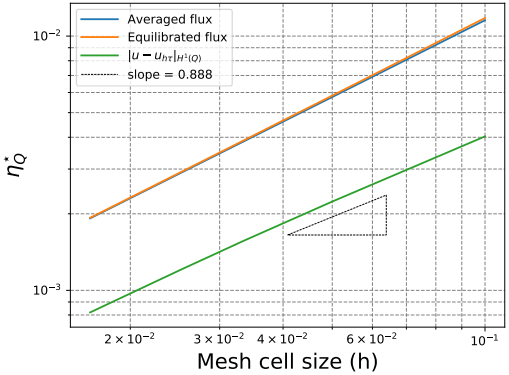
$$\|\mathcal{R}(u_{h\tau})\|_{(H_0^1(\omega_K\times I_n))'} \leq |v|^2_{H^1(\omega_K\times I_n)}$$

- quadrature error ignored

N. Hugot, A. Imperiale, M. Vohralík, preprint (2026).

Approximation u_h^n, error $|u - u_{h\tau}|_{H^1(K\times I_n)}$, estimators $\eta_K^n(u_{h\tau})$

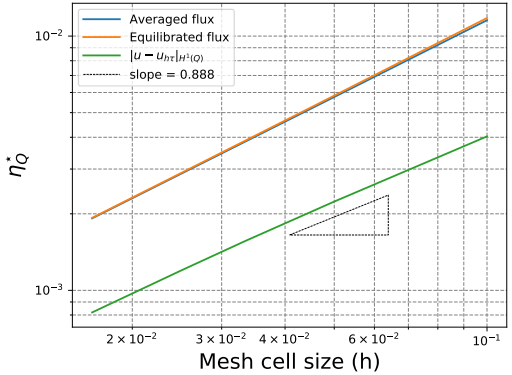
Convergence rates and effectivity indices



Estimators and error

N. Hugot, A. Imperiale, M. Vohralík, preprint (2026).

Convergence rates and effectivity indices



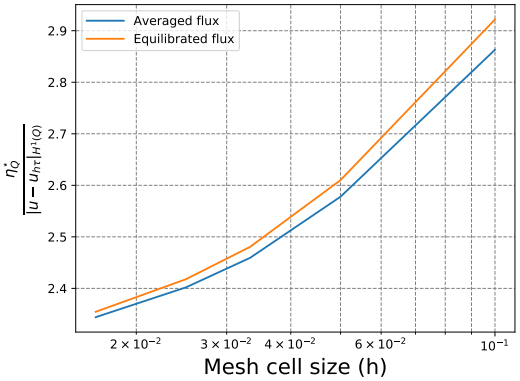
Estimators and error

Remarks:

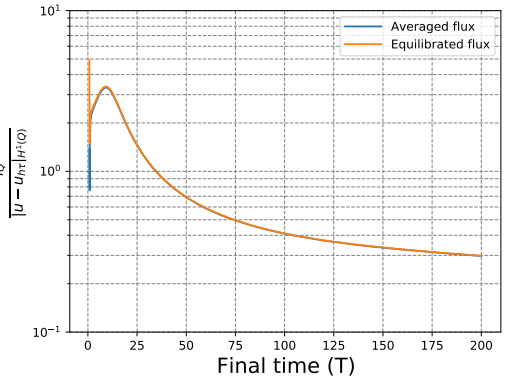
- estimators are **superior to the error**
- estimators and error are of **same order of magnitude**
- estimators and error have the **same order of convergence**

N. Hugot, A. Imperiale, M. Vohralík, preprint (2026).

Robustness wrt h and T



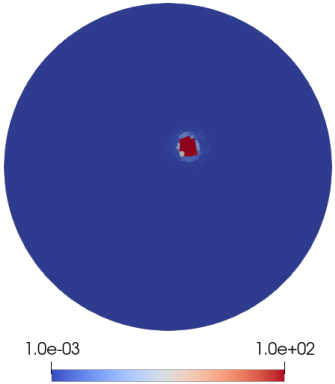
Dependence on h with $T = 5$



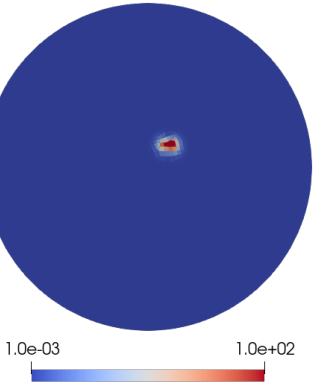
Dependence on T with $h = 0.1$

N. Hugot, A. Imperiale, M. Vohralík, preprint (2026).

Extension to elastic waves (stress tensor $\boldsymbol{\sigma} := 2\mu\boldsymbol{\varepsilon}(u) + \lambda\,\mathrm{tr}(\boldsymbol{\varepsilon}(u))\boldsymbol{I}$, Lamé parameters $\lambda = \mu = 0.4$)



$\eta_K^n(u_{h\tau})$



$|u - u_{h\tau}|_{H^1(K\times I_n)}$

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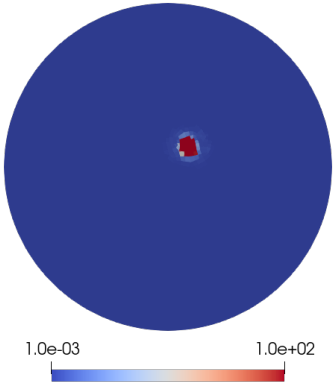

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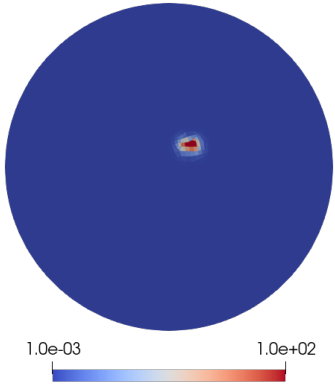

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Two-phase flow

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
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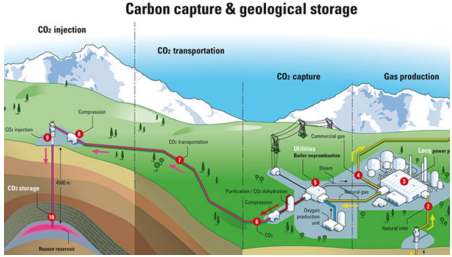

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Multi-phase multi-compositional flow

Theorem (Multi-phase multi-compositional Darcy flow with phase (dis)appearance, I. Ben Gharbia, J. Dabaghi, V. Martin, M. Vohralík (2020)**)**

There holds

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

Error components

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Error control

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

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- **same physical units** of all component estimators
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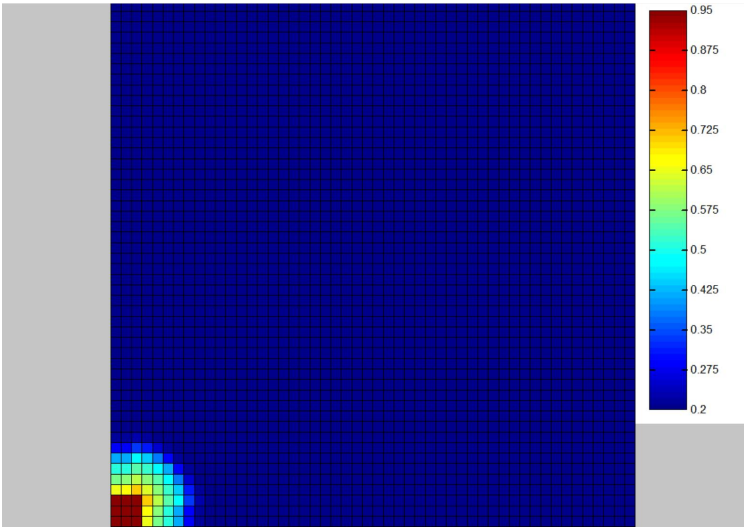
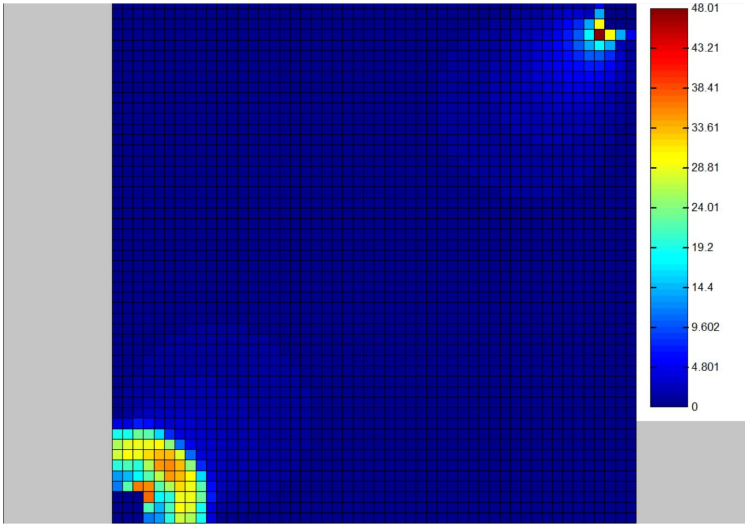
Academic example of oil recovery



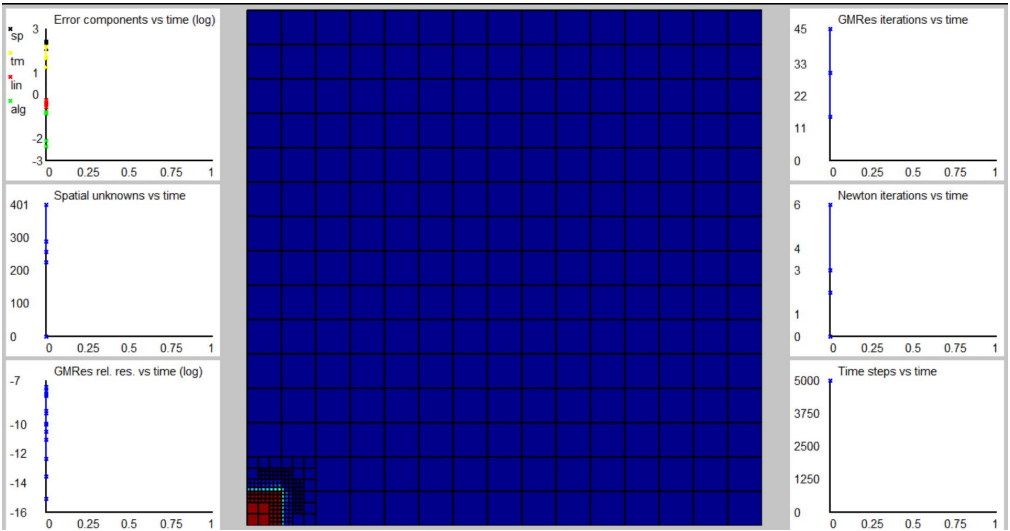
M. Vohralík, M. F. Wheeler, Computational Geosciences (2013)

Academic example of oil recovery, **overall a posteriori estimate**



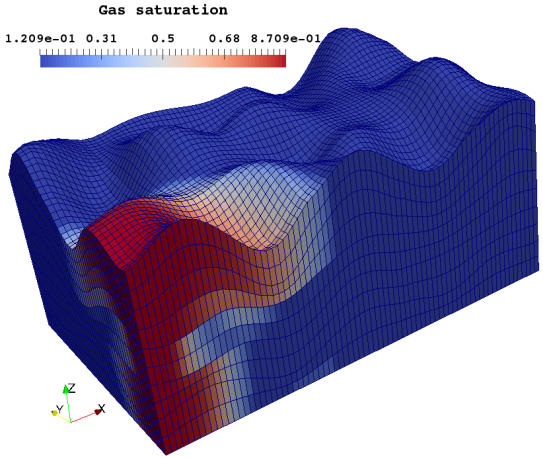
M. Vohralík, M. Wheeler, Computational Geosciences (2013)

Academic example of oil recovery, **adaptivity of error components**

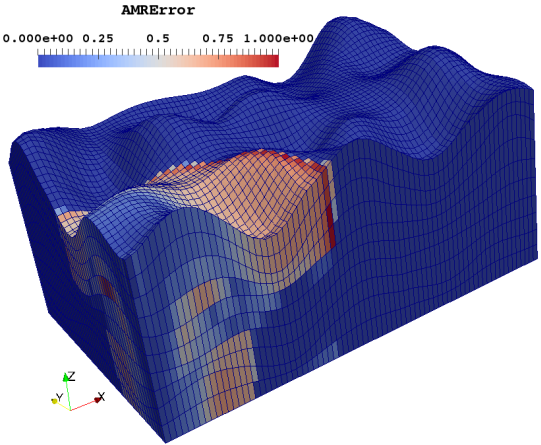


M. Vohralík, M. Wheeler, Computational Geosciences (2013)

Real-world example: 3 phases, 3 components (black-oil) problem



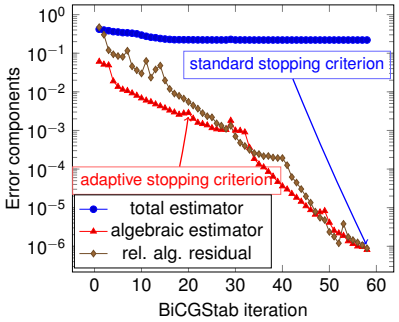
Gas saturation

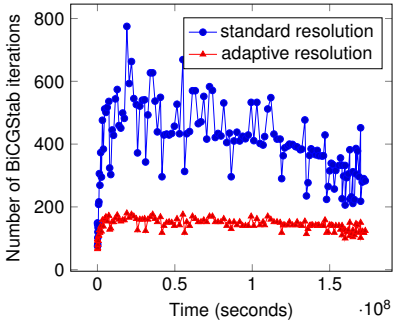


A posteriori error estimate

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

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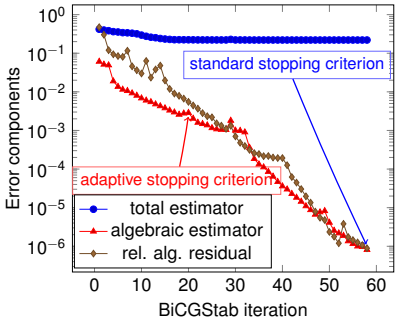

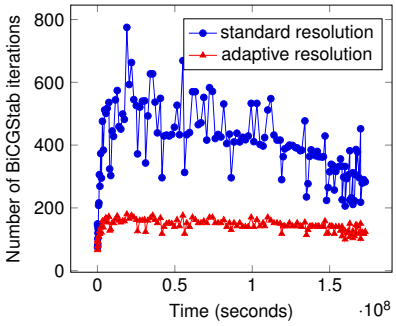

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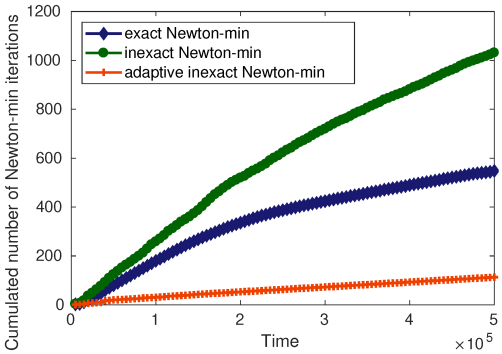
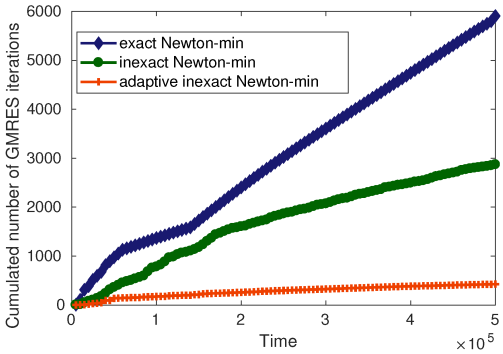
Phase (dis)appearance: Couplex-gas benchmark

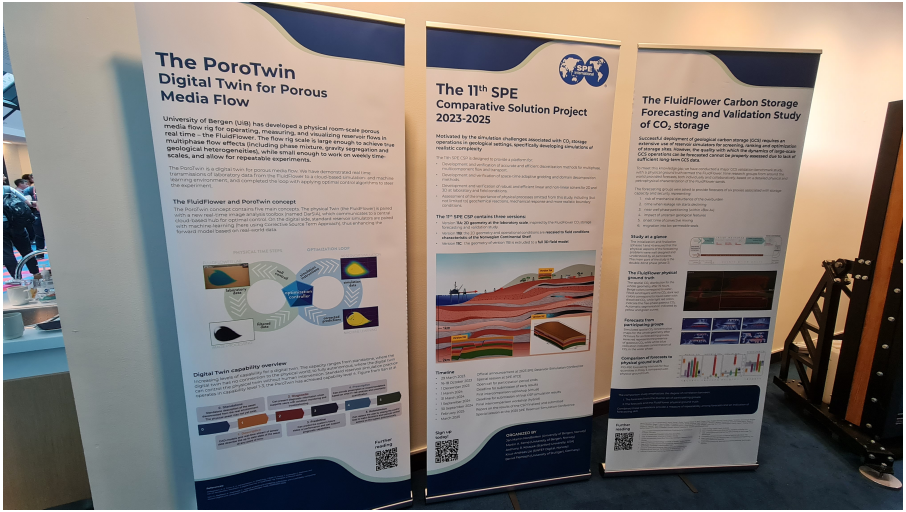




Adaptive linear and nonlinear solvers

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

SIAM Conference on Mathematical & Computational Issues in the Geosciences, Bergen, June 2023: the FluidFlower experiment



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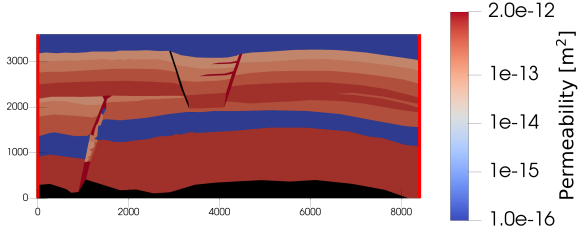
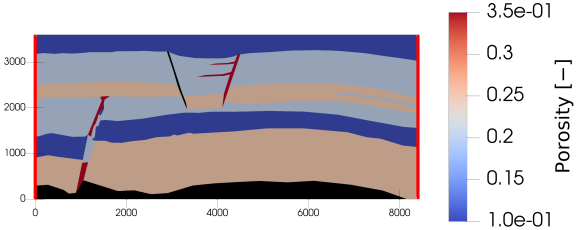
Geological sequestration of CO_2



FluidFlower permeability



FluidFlower porosity

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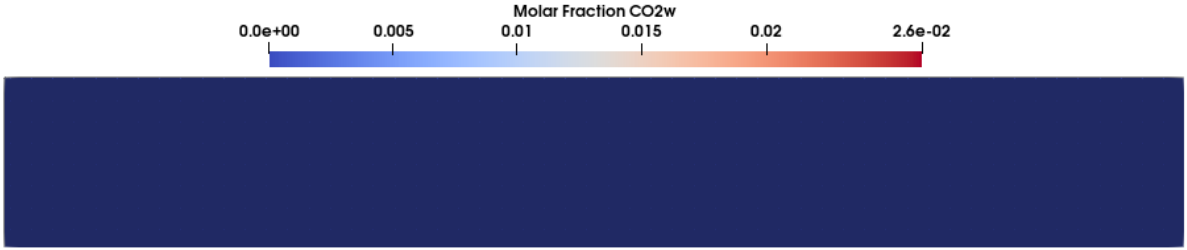
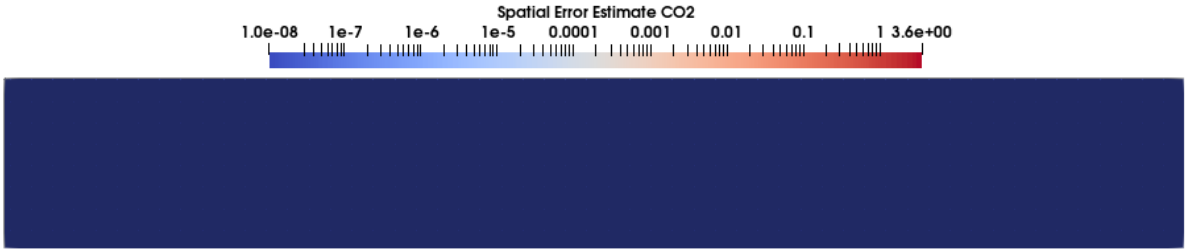


CO_2 molar fraction

E. Flauraud, I. Lannabi, M. Vohralík, S. Yousef, in preparation (2026)

Geological sequestration of CO_2: a posteriori error estimates



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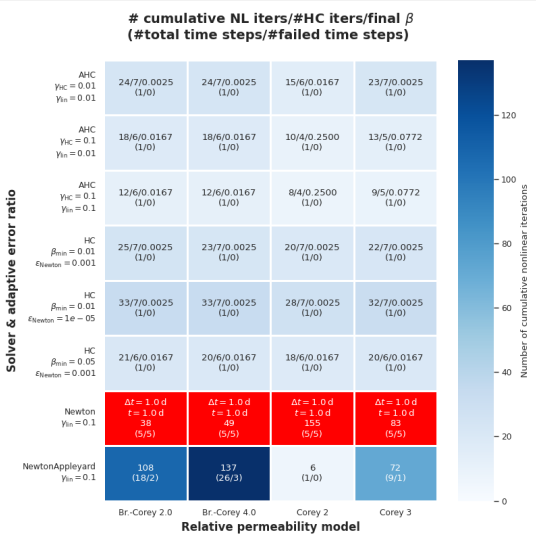

P. von Schultzendorff, J. W. Both, J. M. Nordbotten, T. H. Sandve, M. Vohralík, submitted (2026)

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References


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ERN A., VOHRALÍK M., Adaptive inexact Newton methods with a posteriori stopping criteria for nonlinear diffusion PDEs, *SIAM J. Sci. Comput.* **35** (2013), A1761–A1791.


SMEARS I., VOHRALÍK M., Simple and robust equilibrated flux a posteriori estimates for singularly perturbed reaction–diffusion problems, *ESAIM Math. Model. Numer. Anal.* **54** (2020), 1951–1973.


ERN A., SMEARS I., VOHRALÍK M., Guaranteed, locally space-time efficient, and polynomial-degree robust a posteriori error estimates for high-order discretizations of parabolic problems, *SIAM J. Numer. Anal.* **55** (2017), 2811–2834.


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Thank you for your attention!