

Error control and adaptivity in numerical simulations

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Outline

- 1 Introduction: numerical approximation of partial differential equations
- 2 Laplace equation: error control and mesh adaptivity
 - A posteriori error estimates: error control
 - Potential reconstruction
 - Flux reconstruction
 - A posteriori error estimates: mesh adaptivity
- 3 Nonlinear Laplace equation: error control and solver adaptivity
 - A posteriori error estimates: error control
 - A posteriori error estimates: solver adaptivity
- 4 Reaction–diffusion equation: robustness wrt parameters
- 5 Heat equation: robustness wrt final time and space–time localization
- 6 Eigenvalue problems
- 7 Conclusions

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Numerical approximations of PDEs:

Setting

- u : unknown exact PDE solution
- u_h : known numerical approximation on mesh \mathcal{T}_h

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- $u_h^{n,k,i}$: known numerical approximation on mesh \mathcal{T}_h , time step n , linearization step k , and linear solver step i

Numerical approximations of PDEs: 3 crucial questions

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- $u_h^{n,k,i}$: known numerical approximation on mesh \mathcal{T}_h , time step n , linearization step k , and linear solver step i

Crucial questions

- 1 How **large** is the overall **error** between u and $u_h^{n,k,i}$?

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- 1 How **large** is the overall **error** between u and $u_h^{n,k,i}$?
- 2 **Where** (model/space/time/linearization/algebra) is it **localized**?

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- 3 Can we **decrease** it **efficiently**?

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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Suggested answers

- 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: error control

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

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

$$u = 0 \quad \text{on } \partial\Omega$$

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

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

unknown error

$$\underbrace{\eta(u_h)}_{\text{computable estimator}}$$

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 shape regularity of \mathcal{T}_h and thus independent of Ω , u , u_h , h , p

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

$$\eta_K(u_h) \leq C_{\text{eff}} \|\nabla(u - u_h)\|_{L^2(K)} \quad \forall K \in \mathcal{T}_h$$

- C_{eff} a generic constant only dependent on shape regularity of \mathcal{T}_h and thus independent of Ω , u , u_h , h , p
- computable bound on C_{eff} available, $C_{\text{eff}} \approx 5$

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

h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\ \nabla u_h\ }$	$\ \nabla(u - u_h)\ $	rel. error $\frac{\ \nabla(u - u_h)\ }{\ \nabla u_h\ }$	$p^{\text{eff}} = \frac{\eta(u_h)}{\ \nabla(u - u_h)\ }$
h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$	2	0.37	10%	0.37	10%	1.17
$\approx h_0/4$	3	0.10	10%	0.10	10%	1.17
$\approx h_0/8$	4	0.03	10%	0.03	10%	1.17

A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2014)
 V. Daligault, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

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h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$		6.07×10^{-1}		5.58×10^{-1}		
$\approx h_0/4$		3.10×10^{-1}		2.92×10^{-1}		
$\approx h_0/8$		1.45×10^{-1}		1.32×10^{-1}		
$\approx h_0/2$	2	4.23×10^{-2}				
$\approx h_0/4$	3	2.62×10^{-3}				
$\approx h_0/8$	4	2.60×10^{-4}				

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$\approx h_0/4$		3.10×10^{-1}	7.0%	2.92×10^{-1}	6.5%	
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.50×10^{-1}	3.0%	
$\approx h_0/2$	2	4.23×10^{-2}	$9.5 \times 10^{-1}\%$			
$\approx h_0/4$	3	2.62×10^{-3}	$5.9 \times 10^{-2}\%$			
$\approx h_0/8$	4	2.60×10^{-7}	$5.9 \times 10^{-6}\%$			

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$\approx h_0/8$	4	2.60×10^{-7}	$5.9 \times 10^{-6}\%$	2.58×10^{-7}		

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$\approx h_0/4$		3.10×10^{-1}	7.0%	2.92×10^{-1}	6.6%	1.08
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	
$\approx h_0/2$	2	4.23×10^{-2}	$9.5 \times 10^{-1}\%$	4.07×10^{-2}	$9.2 \times 10^{-1}\%$	
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$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	1.04
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$\approx h_0/4$	3	2.62×10^{-3}	$5.9 \times 10^{-3}\%$	2.60×10^{-3}	$5.9 \times 10^{-3}\%$	1.01
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$\approx h_0/8$	4	2.60×10^{-7}	$5.9 \times 10^{-6}\%$	2.58×10^{-7}	$5.8 \times 10^{-6}\%$	1.01

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

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

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

h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\ \nabla u_h\ }$	$\ \nabla(u - u_h)\ $	rel. error $\frac{\ \nabla(u - u_h)\ }{\ \nabla u_h\ }$	$j^{eff} = \frac{\eta(u_h)}{\ \nabla(u - u_h)\ }$
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
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A. Ern, M. Vohralik, SIAM Journal on Numerical Analysis (2015)

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

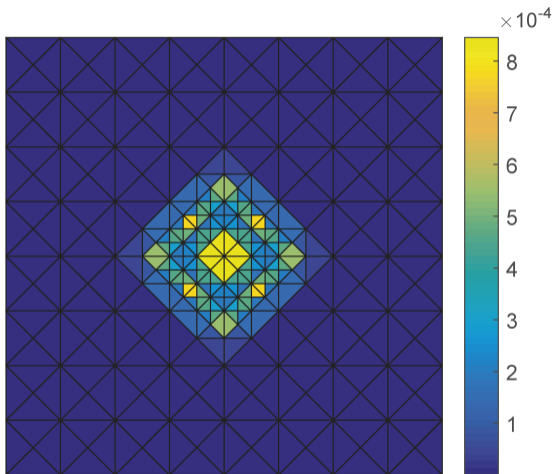
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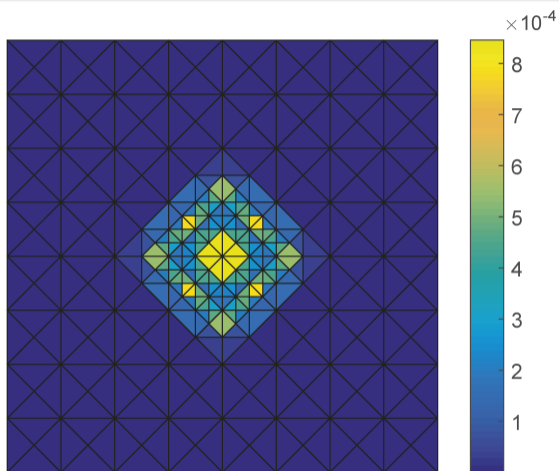
A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)

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

$$\|\nabla(u - u_h)\|^2 = \underbrace{\min_{\substack{\sigma \in \mathbf{H}(\text{div}, \Omega) \\ \nabla \cdot \sigma = f}} \|\nabla u_h + \sigma\|^2}_{= \max_{\substack{\varphi \in H_0^1(\Omega) \\ \|\nabla \varphi\| = 1}} [(f, \varphi) - (\nabla u_h, \nabla \varphi)]^2} + \min_{s \in H_0^1(\Omega)} \|\nabla(u_h - s)\|^2.$$

Comments

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

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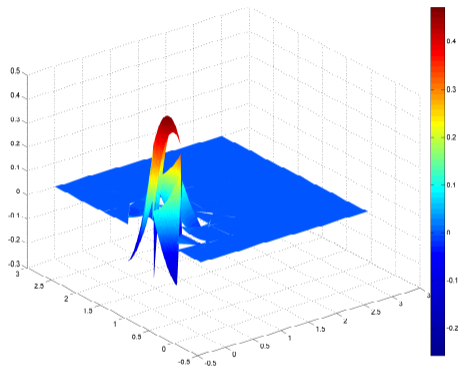
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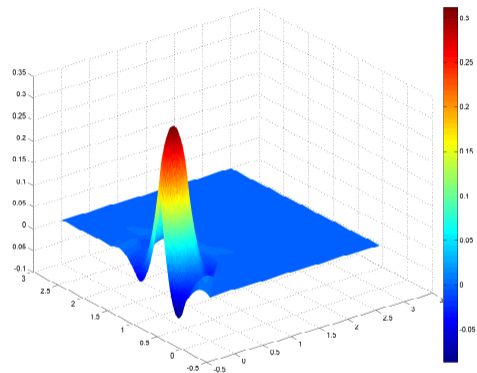
Outline

- 1 Introduction: numerical approximation of partial differential equations
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 - A posteriori error estimates: error control
 - **Potential reconstruction**
 - Flux reconstruction
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- 3 Nonlinear Laplace equation: error control and solver adaptivity
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Potential reconstruction



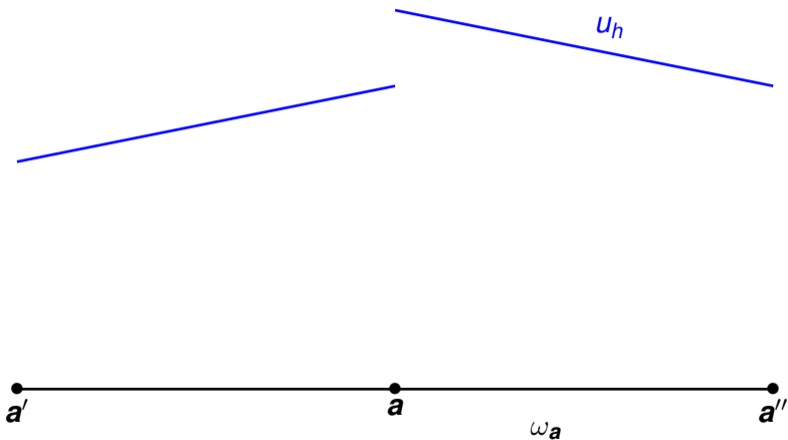
Potential u_h



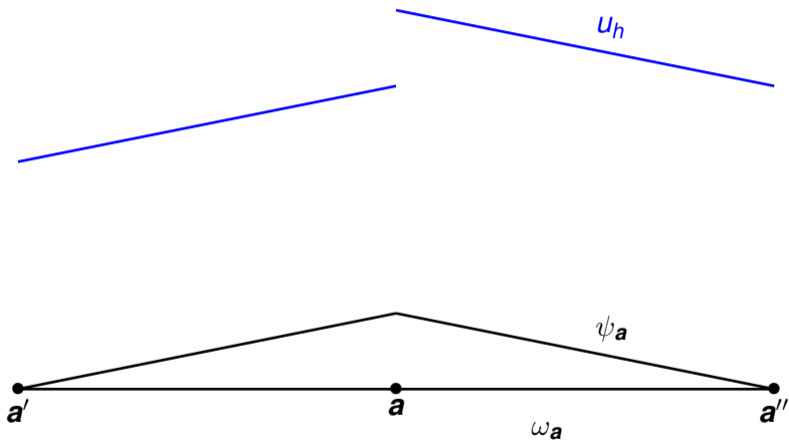
Potential reconstruction s_h

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

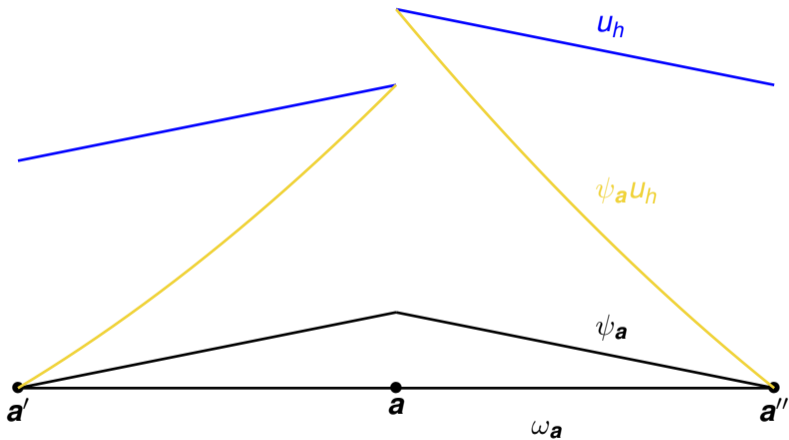
Potential reconstruction in 1D, $p = 1$



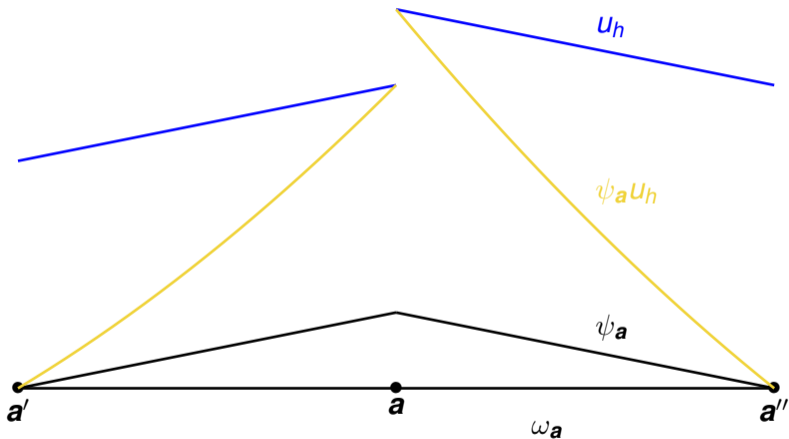
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Potential reconstruction: datum $u_h \in \mathcal{P}_p(\mathcal{T}_h)$, $p \geq 1$

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

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

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

and combine

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

Equivalent form: **conforming FEs**

Find $s_h^a \in V_h^a$ such that

$$(\nabla s_h^a, \nabla v_h)_{\omega_a} = (\nabla(\psi_a u_h), \nabla v_h)_{\omega_a} \quad \forall v_h \in V_h^a.$$

Key points

- localization to patches \mathcal{T}^a
- cut-off by hat basis functions ψ_a
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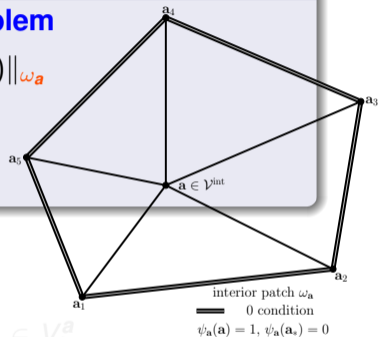
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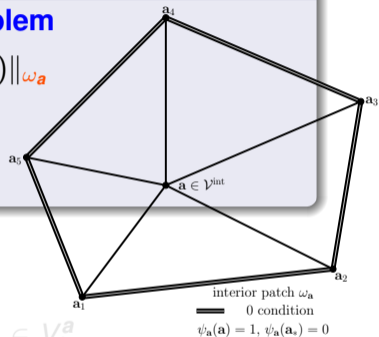
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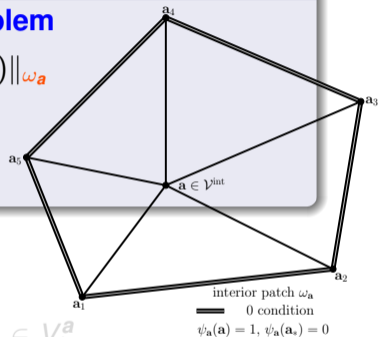
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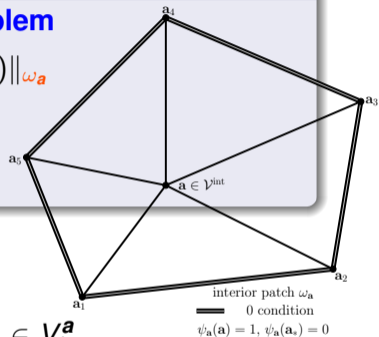
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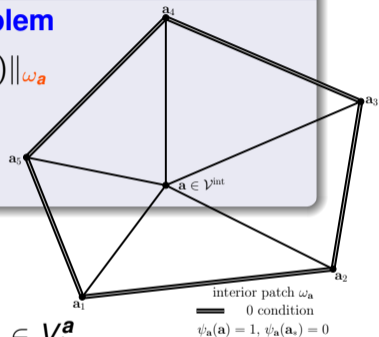
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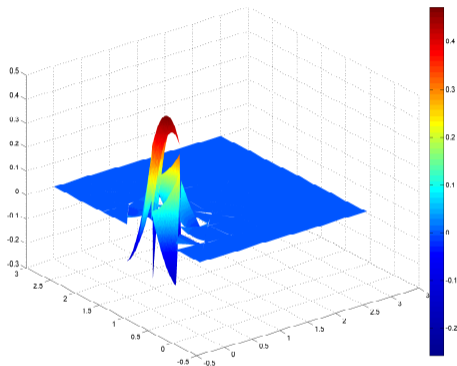
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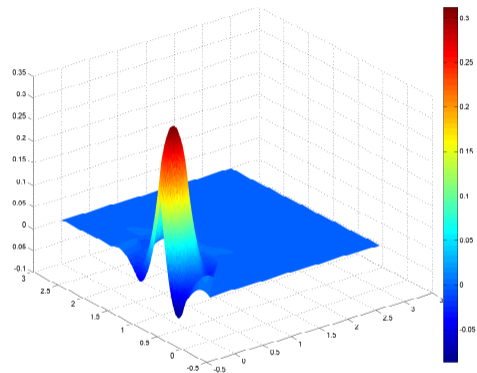
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Potential reconstruction



Potential u_h



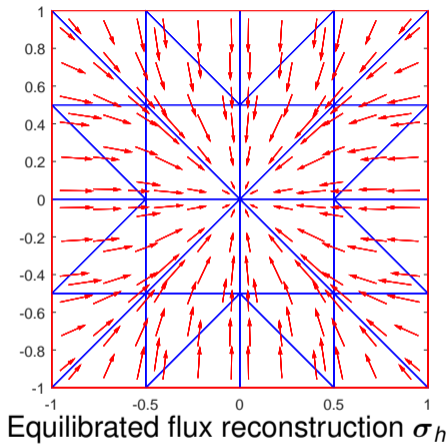
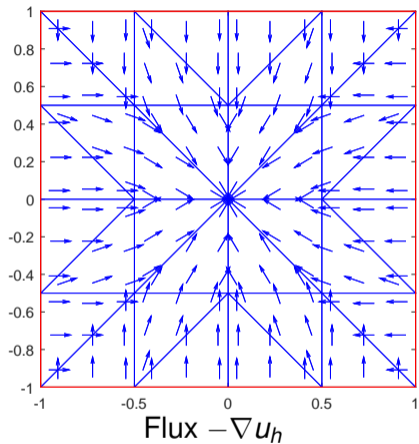
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Outline

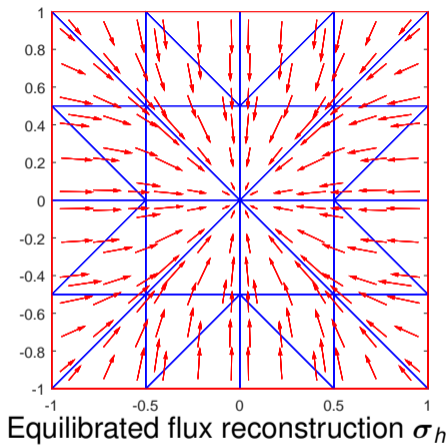
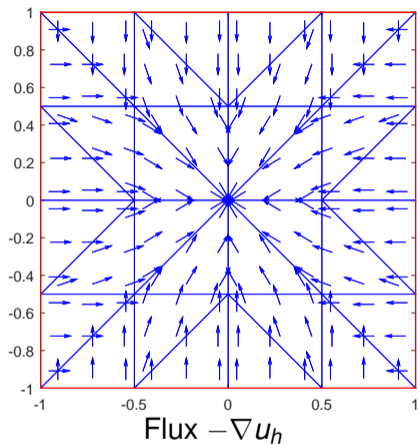
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Equilibrated flux reconstruction



$$\underbrace{-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h), f \in L^2(\Omega)}_{(f, \psi_a)_{\omega_a} - (\nabla u_h, \nabla \psi_a)_{\omega_a} = 0 \quad \forall a \in \mathcal{V}_h^{\text{int}}} \rightarrow \sigma_h \in \mathcal{RT}_p(\mathcal{T}_h) \cap \mathbf{H}(\text{div}, \Omega), \nabla \cdot \sigma_h = \Pi_p f$$

Equilibrated flux reconstruction



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

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For each $a \in \mathcal{V}_h$, solve the **local constrained minimization pb**

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and combine

$$\sigma_h = \sum_{a \in \mathcal{V}_h} \sigma_h^a$$

Key points

- homogeneous Neumann BC on $\partial\omega_a$: $\sigma_h \in \mathcal{RT}_p(\mathcal{T}_h) \cap H(\text{div}, \Omega)$
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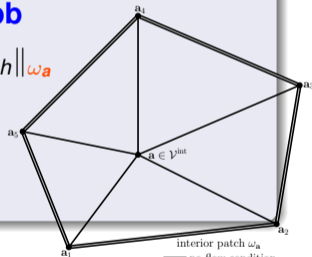
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interior patch ω_a
 — no-flow condition
 $\psi_a(\mathbf{a}) = 1$, $\psi_a(\mathbf{a}_i) = 0$

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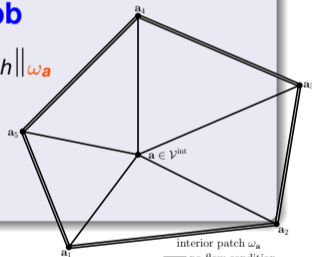
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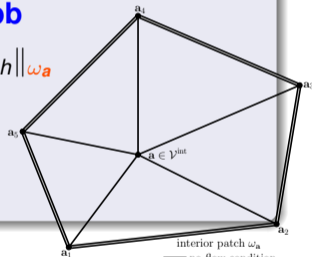
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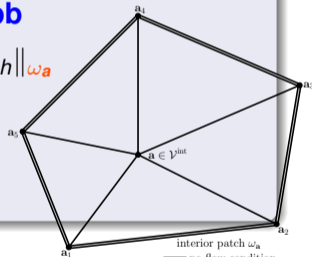
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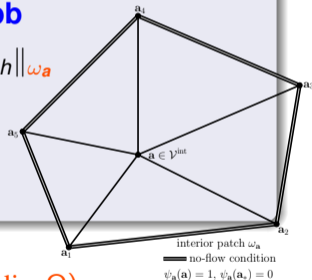
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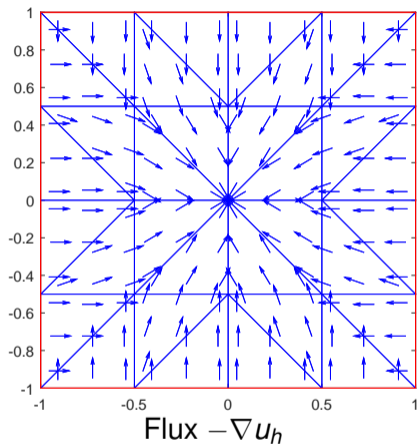
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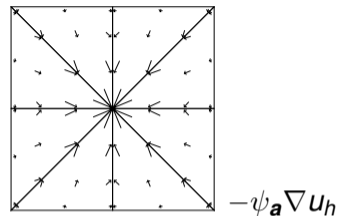
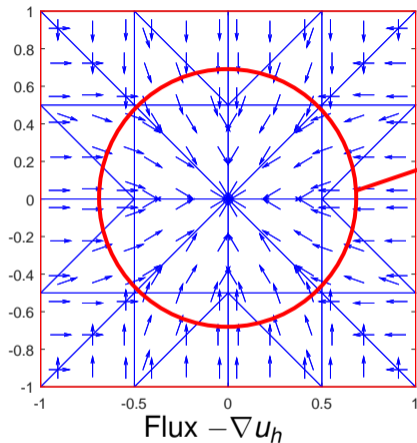
Equilibrated flux reconstruction



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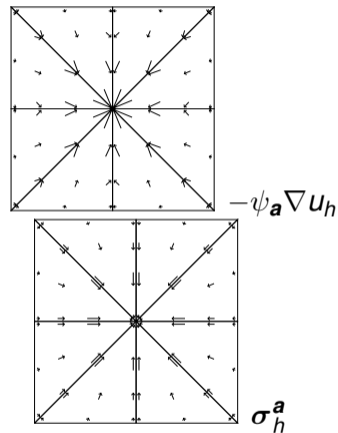
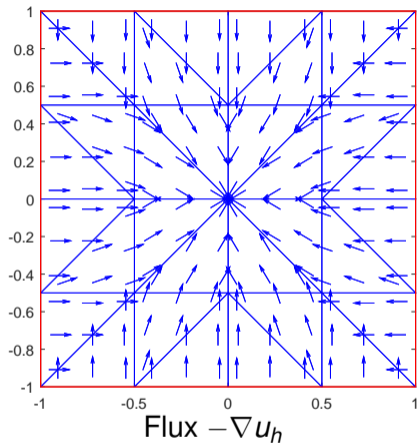
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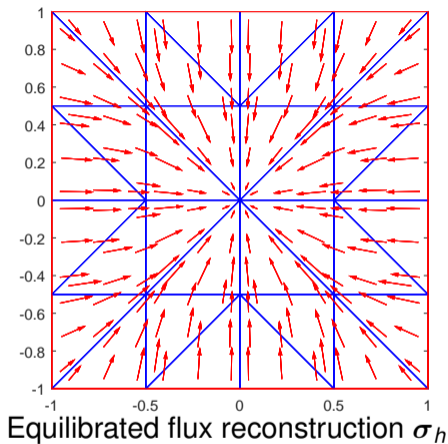
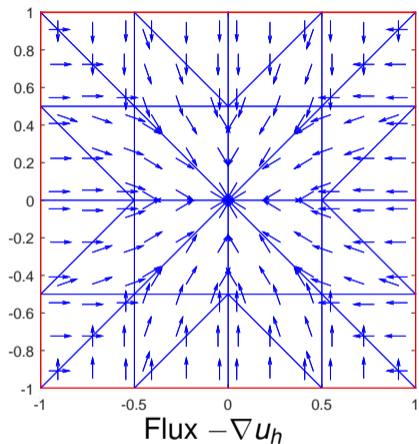
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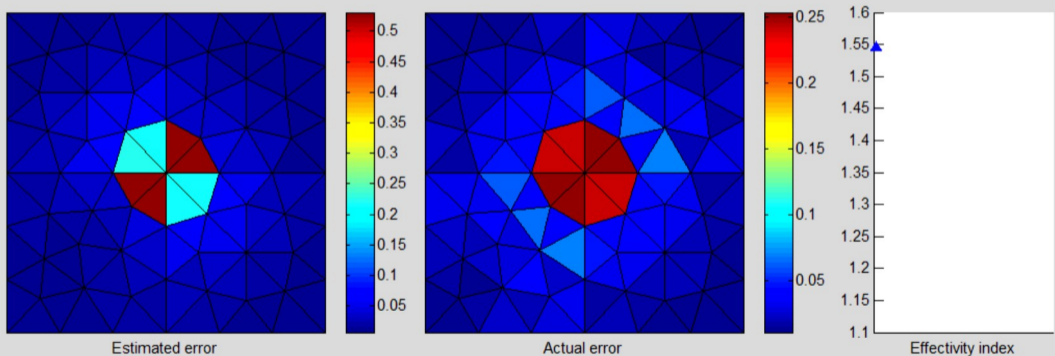


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Outline

- 1 Introduction: numerical approximation of partial differential equations
- 2 Laplace equation: error control and mesh adaptivity
 - A posteriori error estimates: error control
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- 3 Nonlinear Laplace equation: error control and solver adaptivity
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- 5 Heat equation: robustness wrt final time and space–time localization
- 6 Eigenvalue problems
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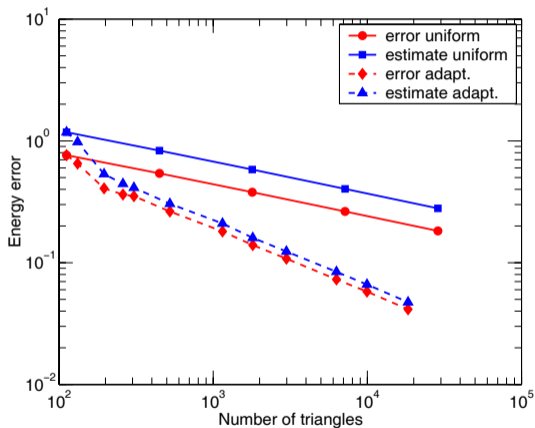
Can we decrease the error efficiently? (adaptive mesh refinement)



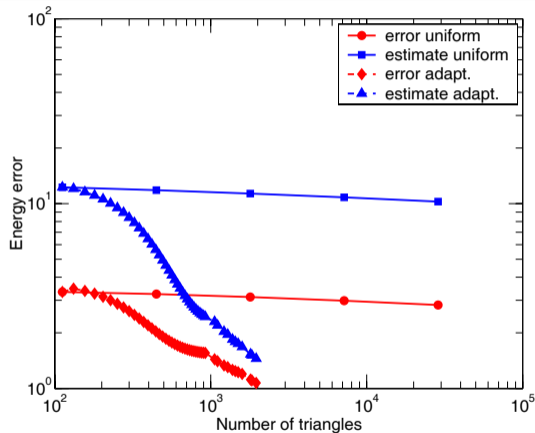
M. Vohralík, SIAM Journal on Numerical Analysis (2007)



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



$H^{1.54}$ singularity



$H^{1.13}$ singularity

Adaptive mesh refinement

Adaptive mesh refinement ↪ Talk by Dirk Praetorius

Adaptive mesh refinement

Adaptive mesh refinement \hookrightarrow Talk by Dirk Praetorius

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

Adaptive mesh refinement

Adaptive mesh refinement \hookrightarrow Talk by Dirk Praetorius

- Dörfler marking: subset \mathcal{M}_ℓ 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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Adaptive mesh refinement \leftrightarrow Talk by Dirk Praetorius

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Convergence on a sequence of adaptively refined meshes

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

Adaptive mesh refinement

Adaptive mesh refinement \leftrightarrow Talk by Dirk Praetorius

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Optimal error decay rate wrt degrees of freedom

- $\|\nabla(u - u_\ell)\| \lesssim |\text{DoF}_\ell|^{-p/d}$ (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)

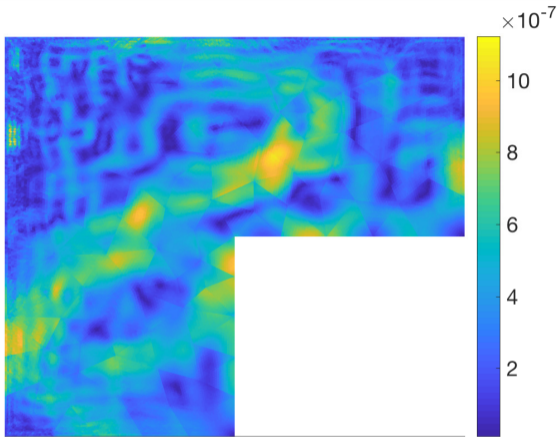
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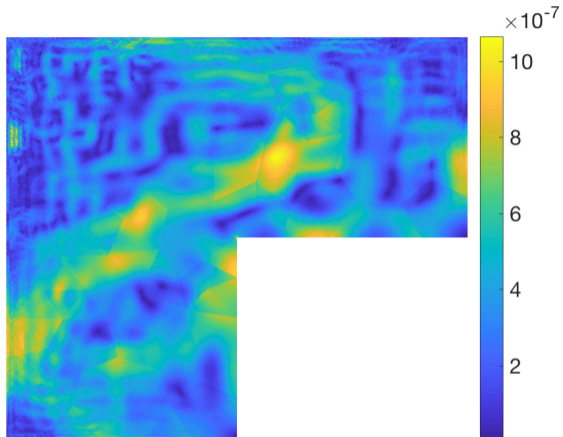
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Including algebraic error: $\mathbb{A}_\ell \mathbf{U}_\ell^i \neq \mathbf{F}_\ell$



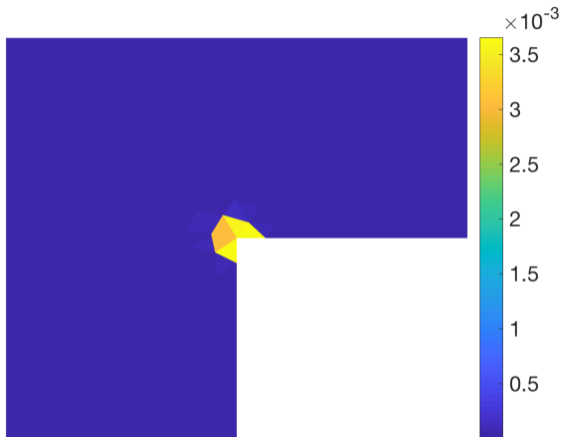
Estimated algebraic errors $\eta_{\text{alg},K}(u_\ell^i)$



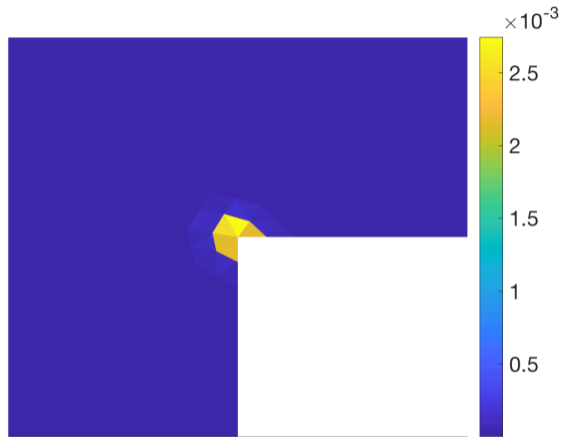
Exact algebraic errors $\|\nabla(u_\ell - u_\ell^i)\|_K$

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

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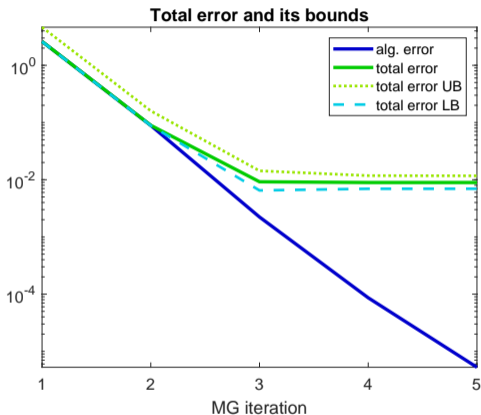
Estimated total errors $\eta_K(u_\ell^i)$



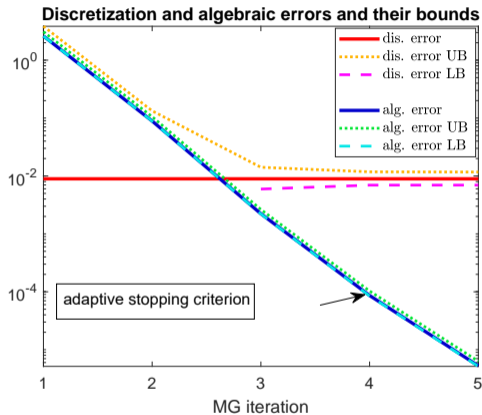
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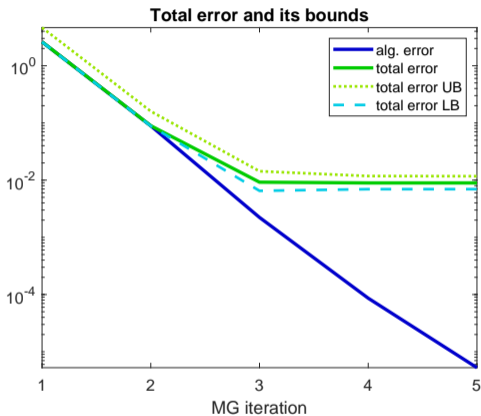
Total error



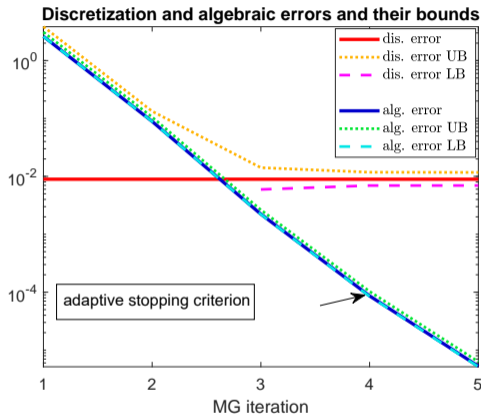
Error components and adaptive st. crit.

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

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

↪ Talk by Ani Miraçi



Nonlinear pb $-\nabla \cdot \sigma(\nabla u) = f$: including **linearization** and **algebraic**

error: $\mathcal{A}_\ell(U_\ell^{k,d}) \neq F_\ell, \mathbb{A}_\ell^{k-1} U_\ell^{k,d} \neq F_\ell^{k-1}$

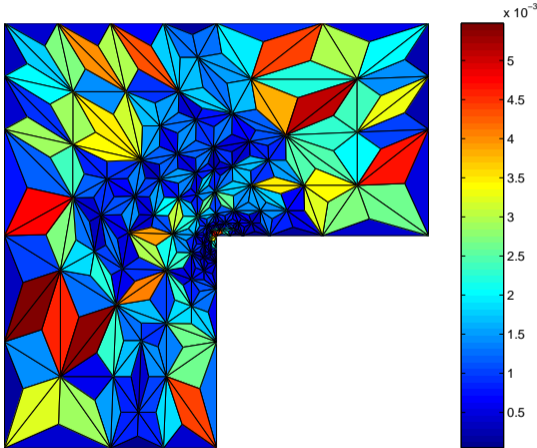
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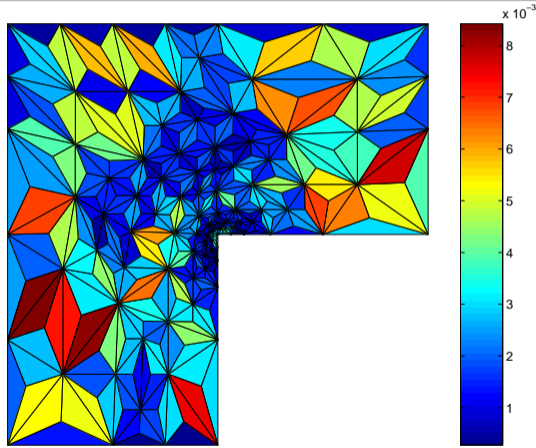
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Estimated errors $\eta_K(u_\ell^{k,i})$

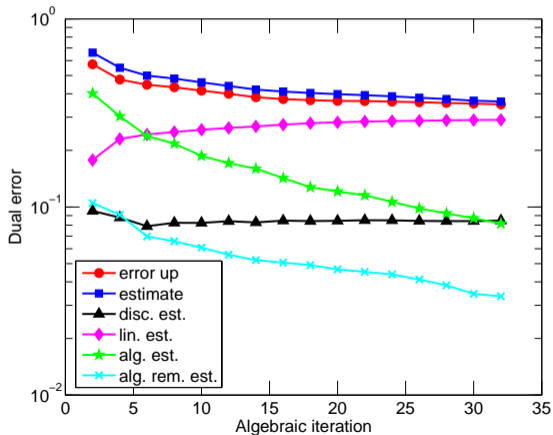
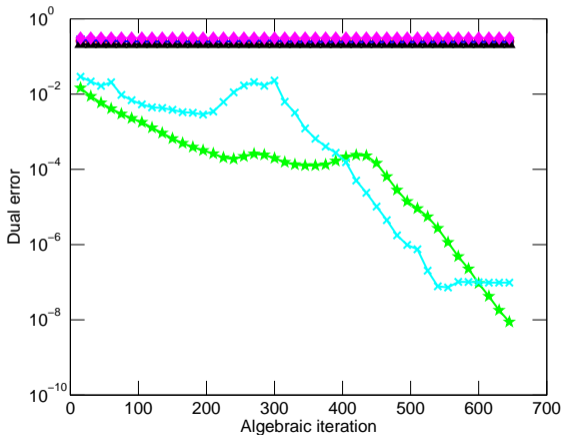


Exact errors $\|\sigma(\nabla u) - \sigma(\nabla u_\ell^{k,i})\|_{q,K}$

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

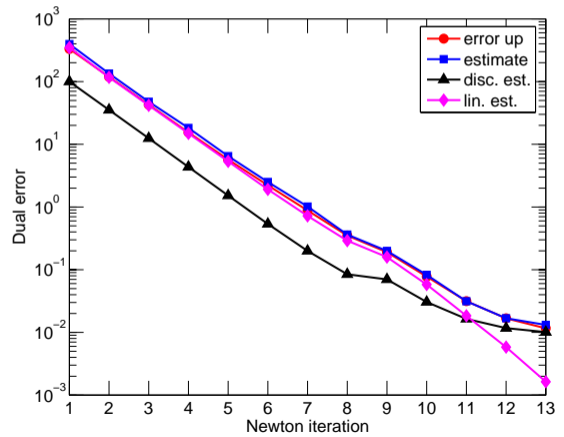
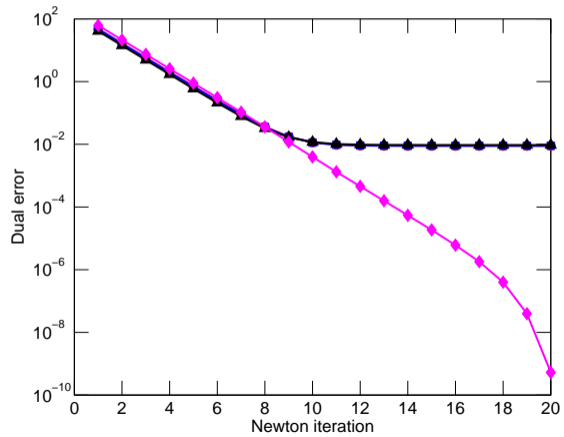
Nonlinear pb $-\nabla \cdot \sigma(\nabla u) = f$: including **linearization** and **algebraic**

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Solver adaptivity (nonlinear problem, inexact solvers)

Fully adaptive algorithm (adaptive inexact Newton method)

- total error estimate on mesh \mathcal{T}_ℓ , linearization step k , algebraic solver step i

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

- balancing error components: work where needed

$\eta_{\ell,\text{alg}}^{k,i} \leq \gamma_{\text{alg}} \eta_{\ell,\text{lin}}^{k,i}$	stopping criterion linear solver
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- link – inexact Newton method: Bank & Rose (1982), Hackbusch & Reusken (1989), Deuffhard (1991), Eisenstat & Walker (1994)

Convergence, optimal error decay rate wrt DoFs

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

Optimal error decay rate wrt overall computational cost

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

Find $u : \Omega \rightarrow \mathbb{R}$ 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)

$$\|u - u_h\|$$

unknown error

$$\eta(u_h)$$

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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$$\eta_{\kappa}(u_h) \leq C_{\text{eff}} \|u - u_h\|_{\omega_{\kappa}} \quad \forall K \in \mathcal{T}_h$$

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Equilibrated flux and potential reconstructions

Definition (Flux σ_h and potential ϕ_h)

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

$$(\sigma_h^{\mathbf{a}}, \phi_h^{\mathbf{a}}) := \arg \min_{(\mathbf{v}_h, q_h) \in \mathcal{RT}_p(T^{\mathbf{a}}) \times \mathcal{P}_p(T^{\mathbf{a}}) \subset \mathbf{H}_0(\text{div}, \omega_{\mathbf{a}}) \times L^2(\omega_{\mathbf{a}})}$$

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- **local discrete** constrained minimization problems
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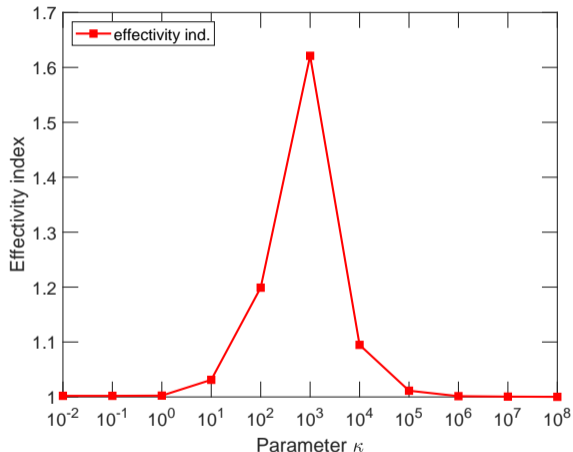
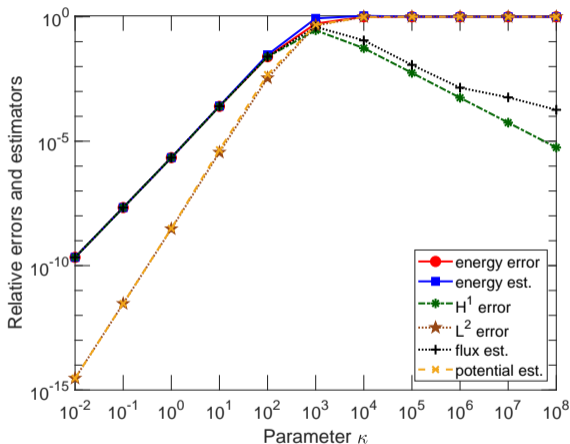
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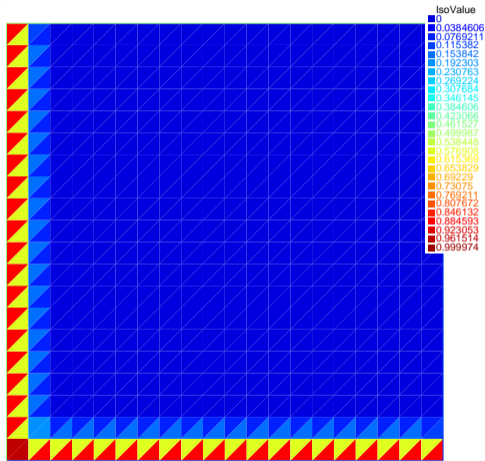


Relative energy errors and estimates

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

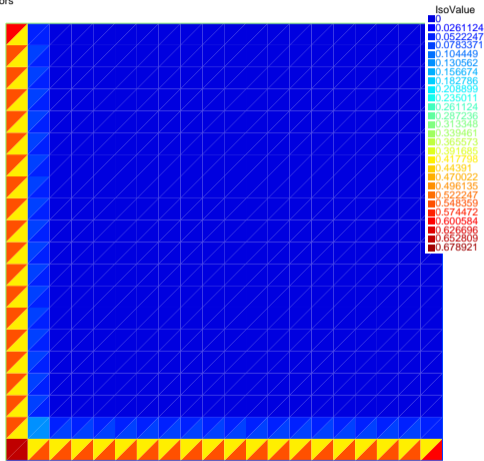
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estimators



Estimated error distribution $\eta_K(u_h)$

energy errors



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

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

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

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

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Eigenvalue problems

↪ Talks by Tomáš Vejchodský and Philip Lederer

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- **full adaptivity**: space mesh, time step, linear solver, nonlinear solver, polynomial degree
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Thank you for your attention!

Outline

- Motivation
- Polynomial-degree (p) adaptivity

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 2 (2015) 88–95



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

Y. El Kamari^a, W. Raphael^{a,*}, A. Chateaufeuf^{b,c}

^a Ecole Supérieure d'Ingenieurs de Bayonne (ESIB), Université de Bordeaux, 107 Rue de l'Université, 64000 Bayonne, France



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probably **numerical simulations done with insufficient precision**,
I believe **without error control**

Case Studies in Engineering Failure Analysis 2 (2015) 88–95



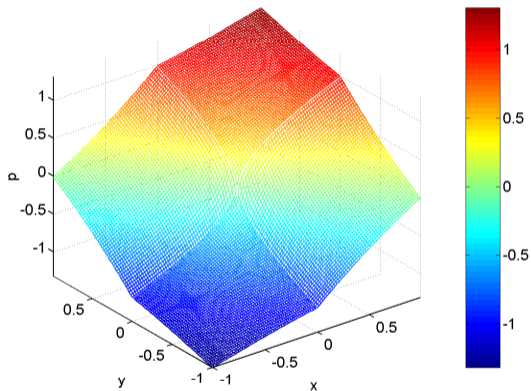
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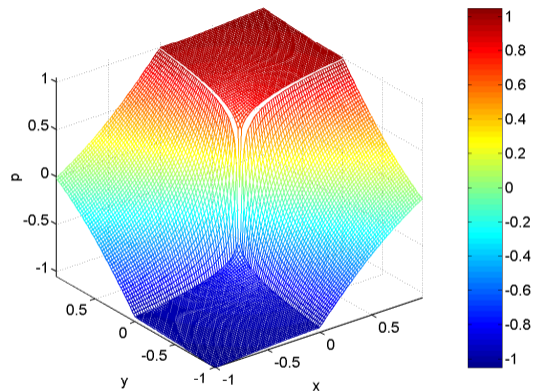
Y. El Kamari^a, W. Raphael^{a,*}, A. Chateaufeuf^{b,c}

^a Ecole Supérieure d'Ingenieurs de Brynmouth (ESIB), Université de Caen, CSF Mar Roules, PO Box 11-534, Road El Sakh Batain 13072050.

Singular solutions



$H^{1.54}$ singularity

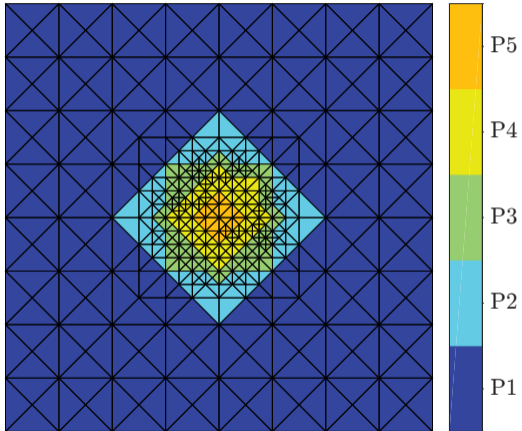


$H^{1.13}$ singularity

Outline

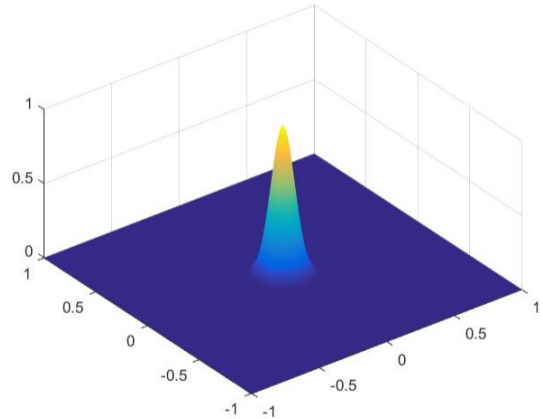
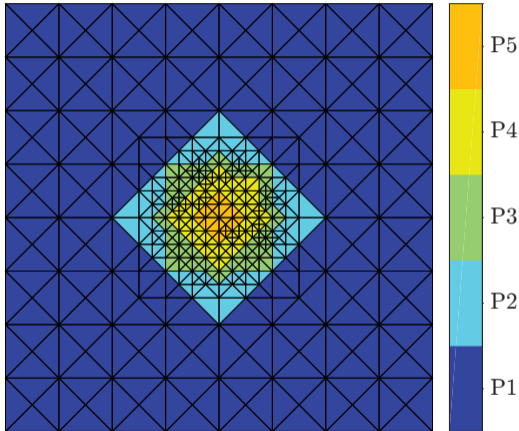
- Motivation
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Best-possible error decrease: *hp* adaptivity, (smooth solution)



Mesh \mathcal{T}_ℓ and pol. degrees p_K

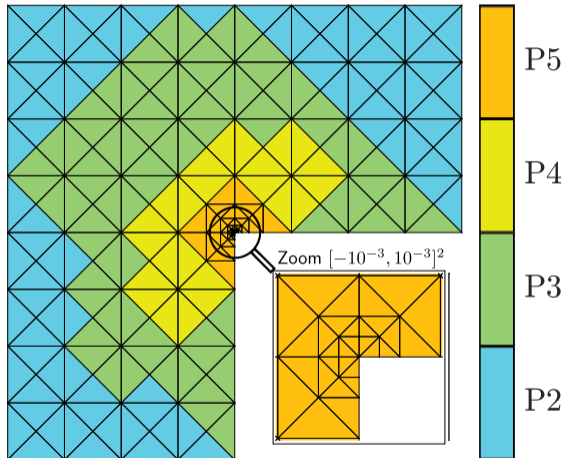
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Mesh \mathcal{T}_ℓ and pol. degrees p_K

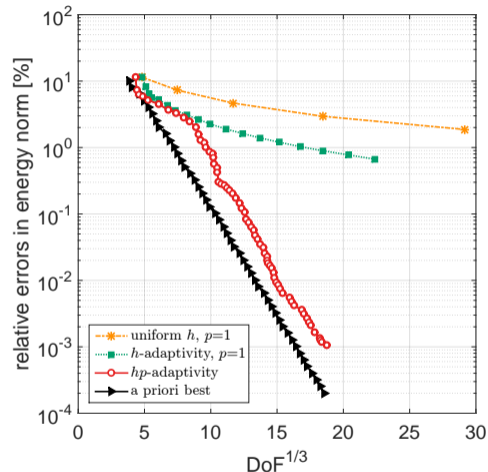
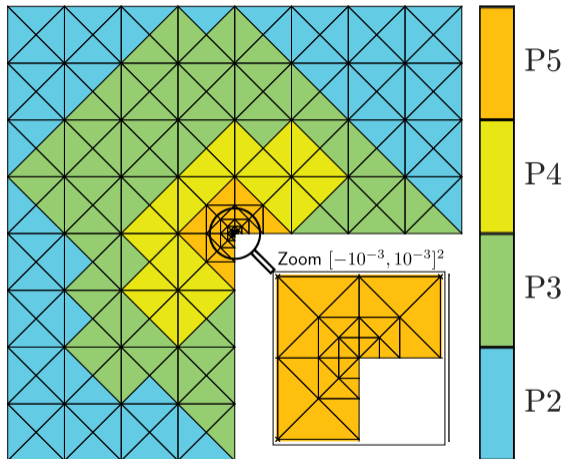
Exact solution

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



Mesh \mathcal{T}_ℓ and polynomial degrees p_K

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



Relative error as a function of DoF