Adaptive iterative approximation in nonlinear PDEs I

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in collaboration with

Patrik Daniel, Vít Dolejší, Alexandre Ern, Alexander Haberl, Koondanibha Mitra, Jan Papež, Dirk Praetorius, Ulrich Rüde, Stefan Schimanko, & Barbara Wohlmuth

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Outline

1. Introduction: adaptive iterative approximation
   - A posteriori error estimates and adaptivity
   - Achievements and example results
   - Real life comparison
2. Linear diffusion: discretization error, mesh and polynomial degree adaptivity
   - A posteriori error estimates
   - Potential reconstruction
   - Flux reconstruction
   - A posteriori error control
   - Balancing error components: mesh adaptivity
   - Balancing error components: polynomial-degree adaptivity
3. Nonlinear diffusion: overall error and solvers adaptivity
   - A posteriori error estimates (overall and components)
   - Balancing error components: solvers adaptivity
4. Conclusions

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Numerical methods for PDEs: example $-\Delta u = f$ in Ω, $u = 0$ on $\partial\Omega$

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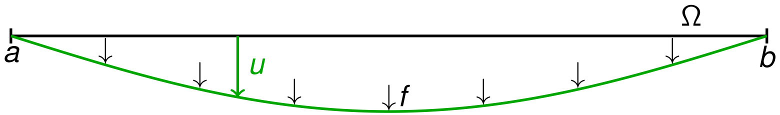
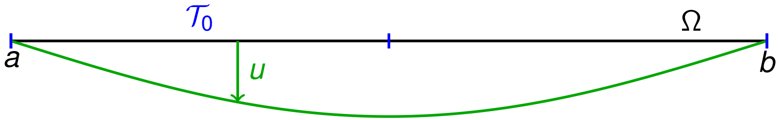
- unknown exact solution u



Numerical methods for PDEs: example $-\Delta u = f$ in Ω, $u = 0$ on $\partial\Omega$

- unknown exact solution u
- computational mesh $\mathcal{T}_0$



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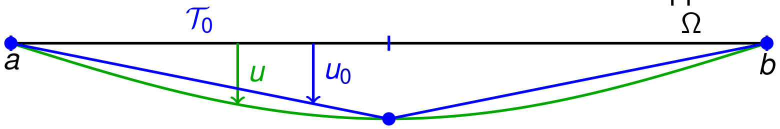
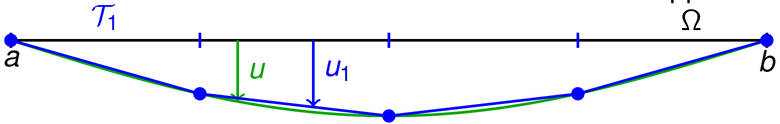
numerical approximation u_0



Numerical methods for PDEs: example $-\Delta u = f$ in Ω, $u = 0$ on $\partial\Omega$

- unknown exact solution u
- computational mesh $\mathcal{T}_1$

numerical approximation u_1



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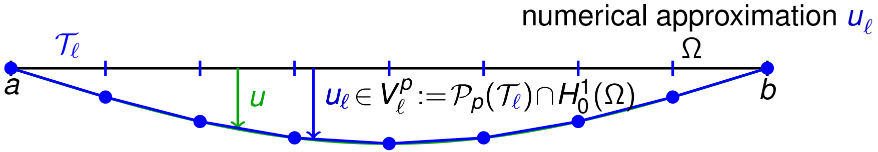

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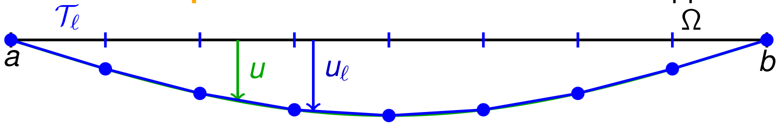
- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



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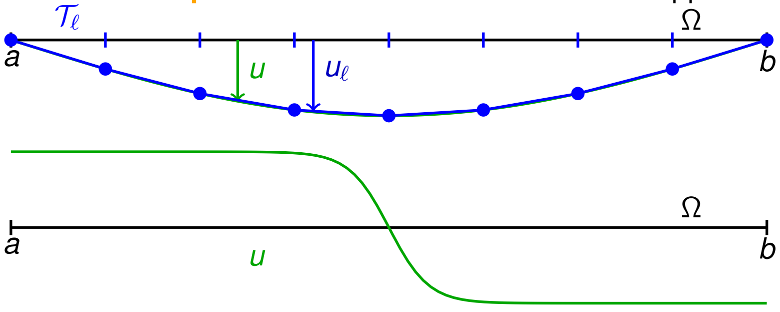

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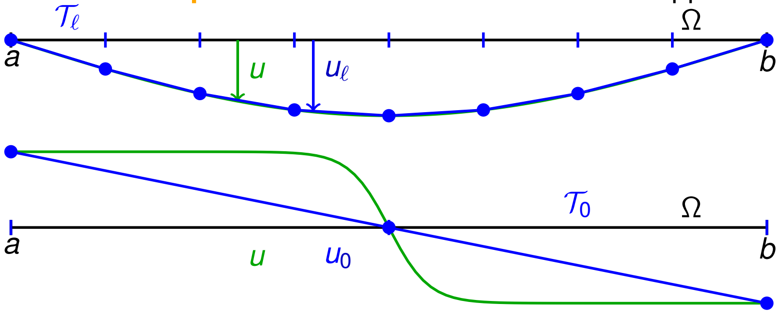

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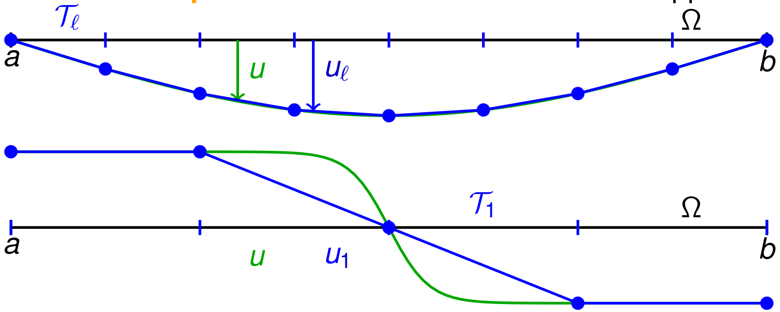

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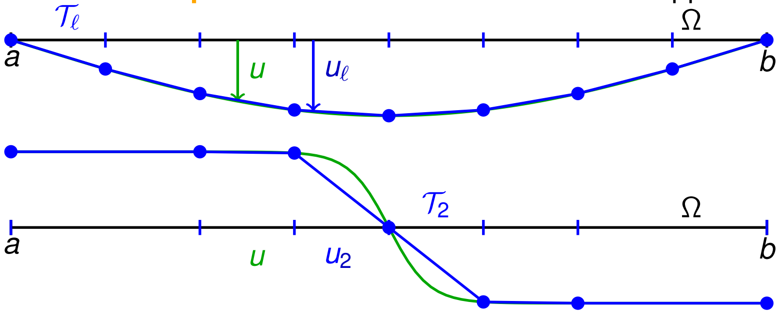

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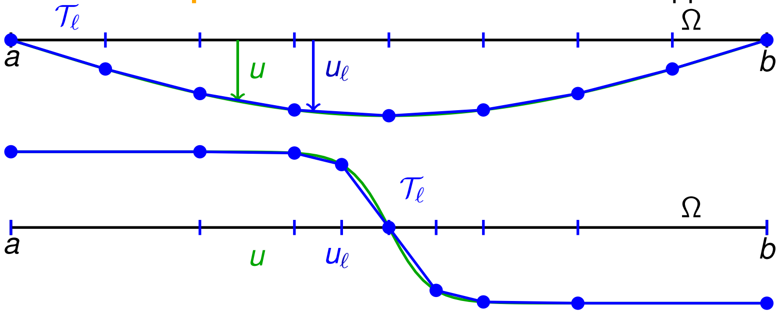

Numerical methods for PDEs: example $-\Delta u = f$ in Ω, $u = 0$ on $\partial\Omega$

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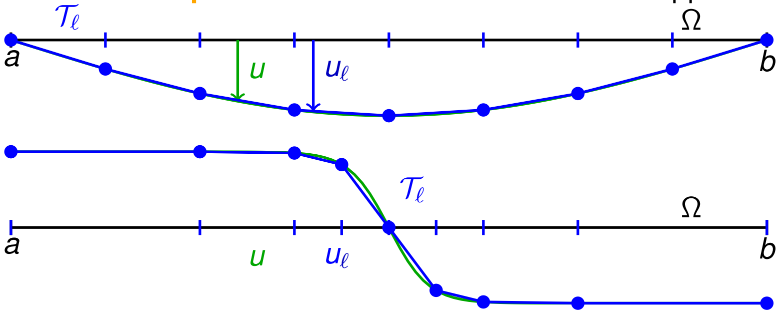

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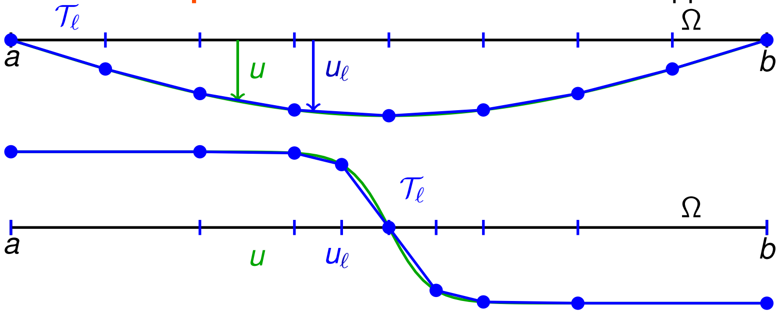

Need to solve

$\mathbb{A}_\ell \mathrm{U}_\ell = \mathrm{F}_\ell$

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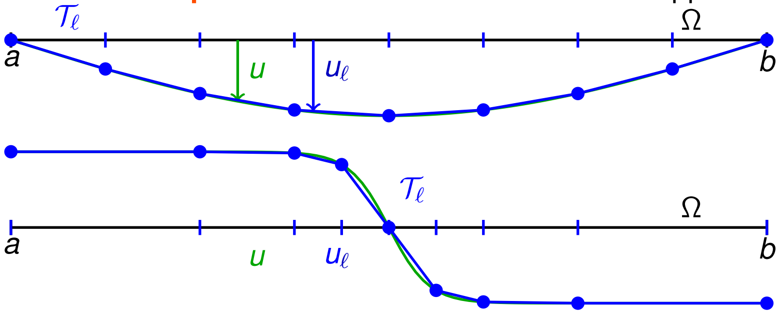

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$$\mathbb{A}_\ell \mathrm{U}_\ell = \mathrm{F}_\ell$$

Algebraic error (on iteration $i \geq 0$)

$$\|\nabla(u_\ell - u_\ell^i)\| = \left\{ \int_a^b |(u_\ell - u_\ell^i)'|^2 \right\}^{\frac{1}{2}}$$

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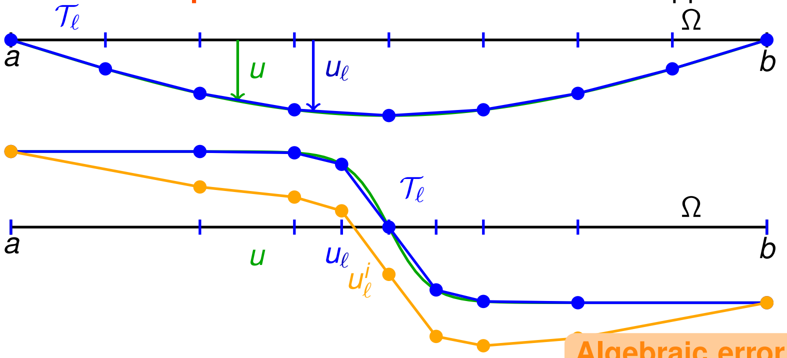

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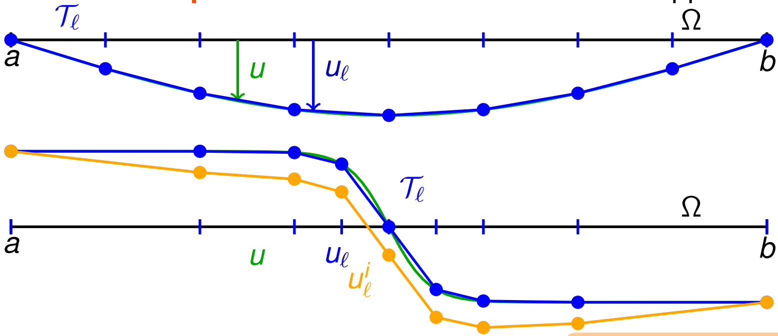

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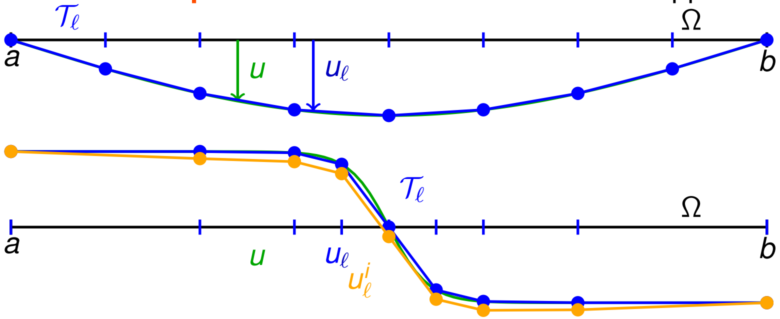

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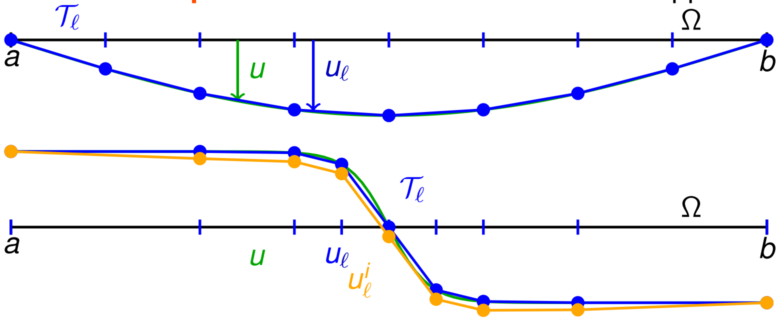


Need to solve

$\mathbb{A}_\ell \mathrm{U}_\ell = \mathrm{F}_\ell$

Total error

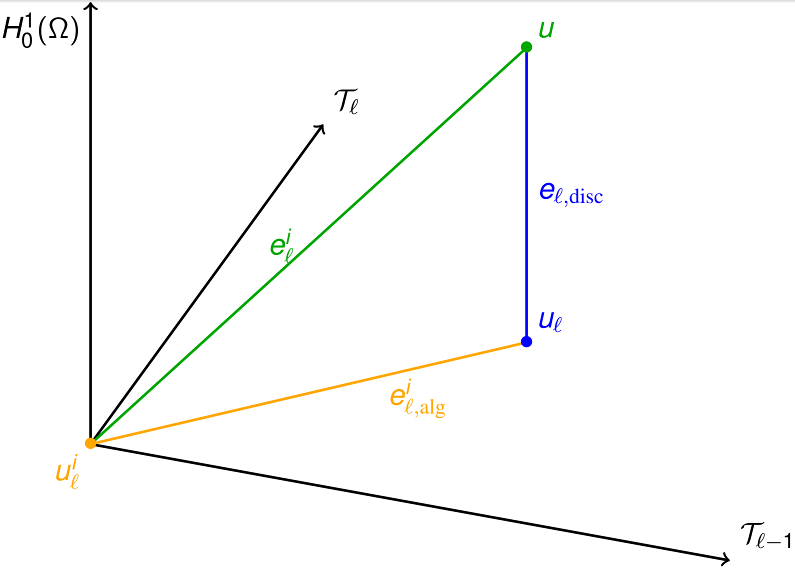
$$\|\nabla(u - u_\ell^i)\| = \left\{ \int_a^b |(u - u_\ell^i)'|^2 \right\}^{\frac{1}{2}}$$

Algebraic error (on iteration $i \geq 0$)

$$\|\nabla(u_\ell - u_\ell^i)\| = \left\{ \int_a^b |(u_\ell - u_\ell^i)'|^2 \right\}^{\frac{1}{2}}$$

Outline

Adaptive iterative approximation



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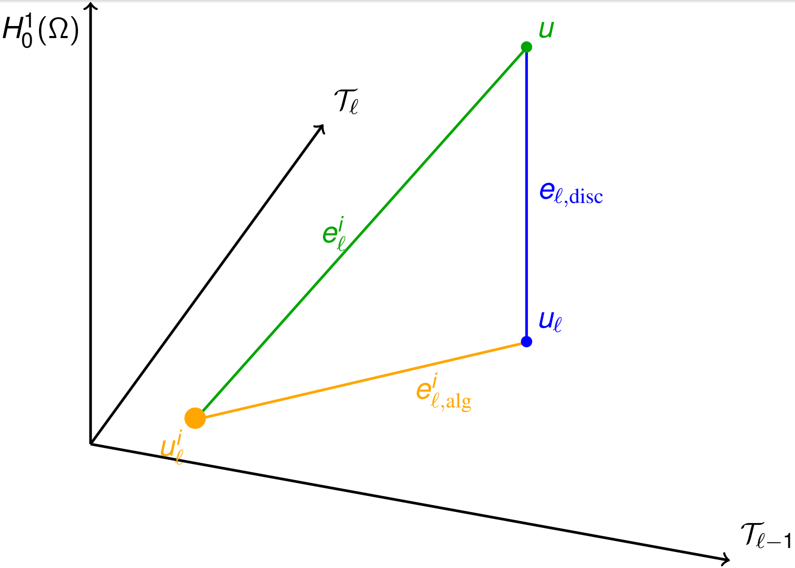

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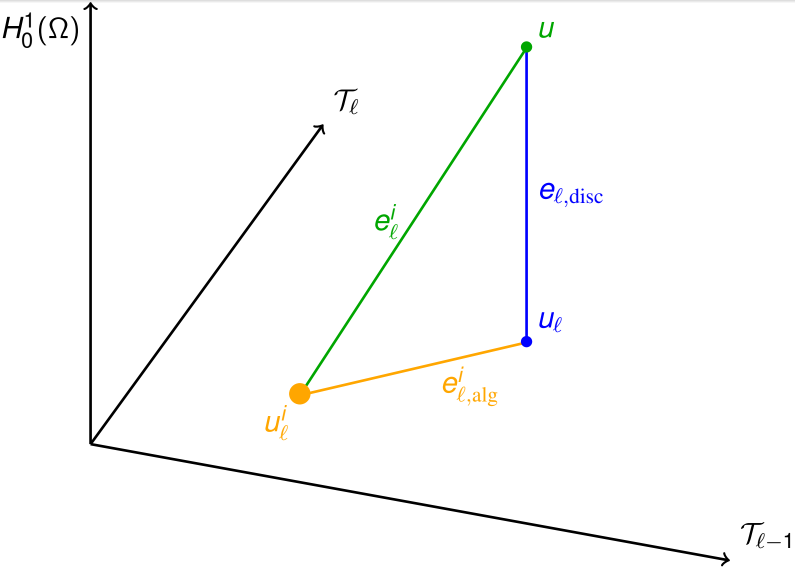

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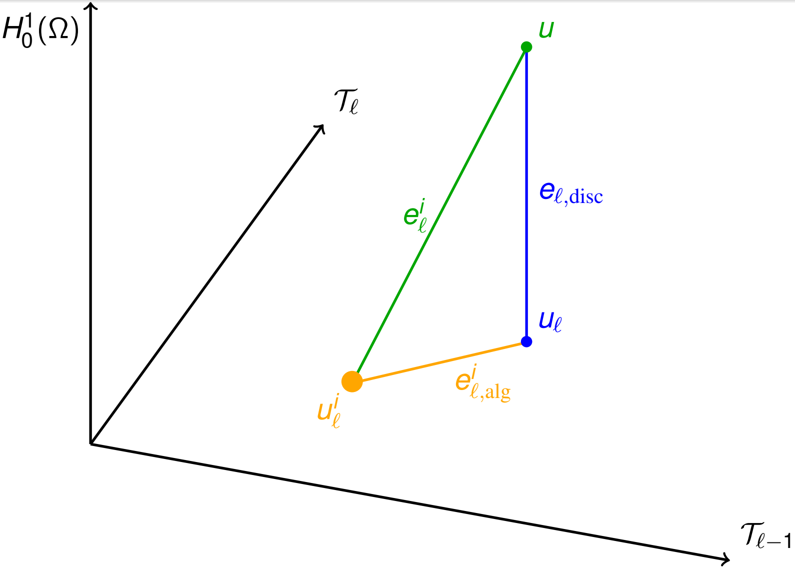

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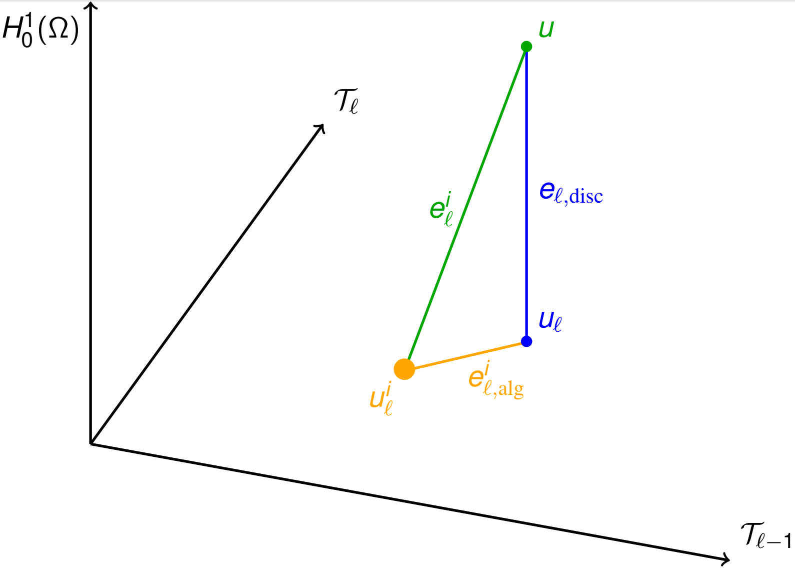

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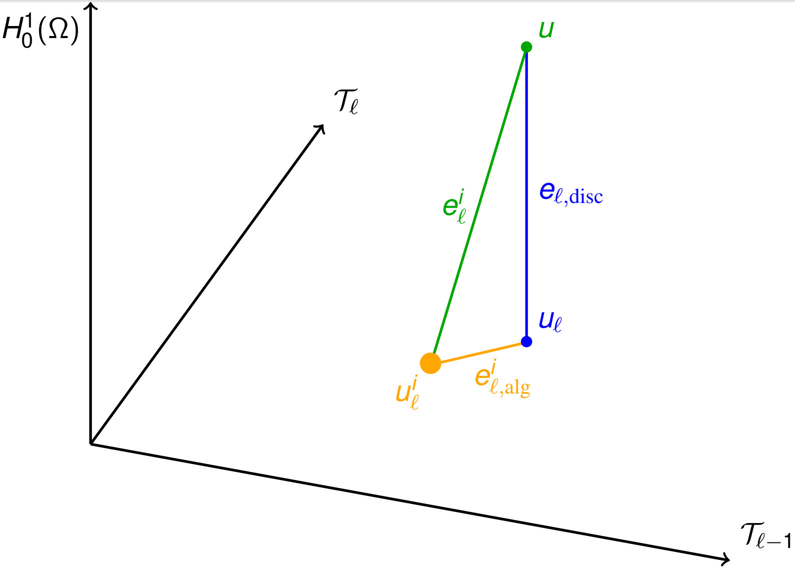

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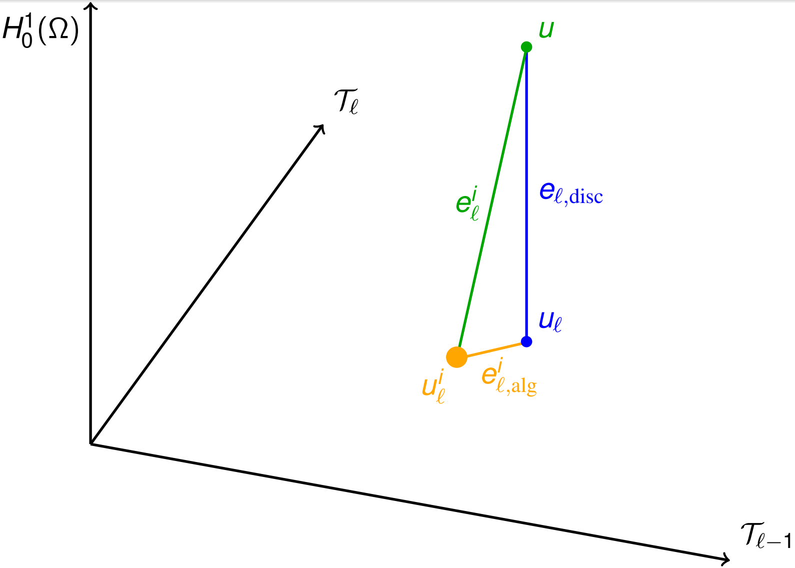

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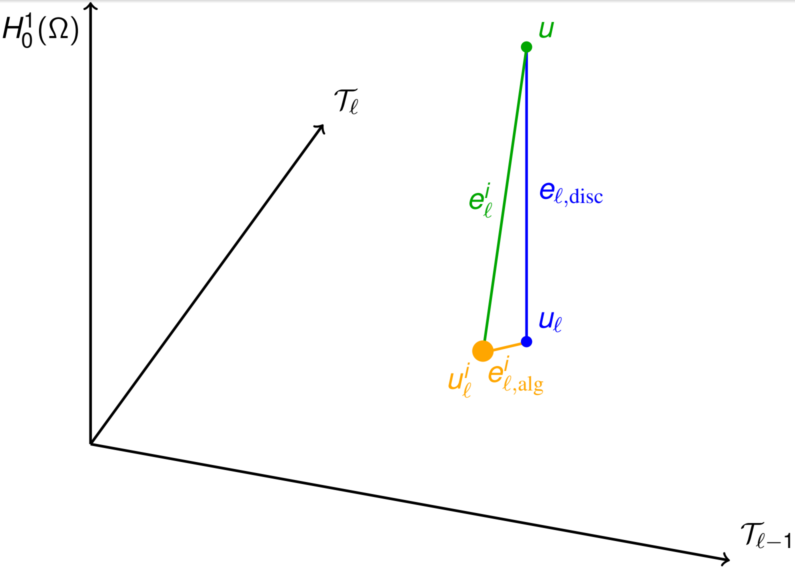

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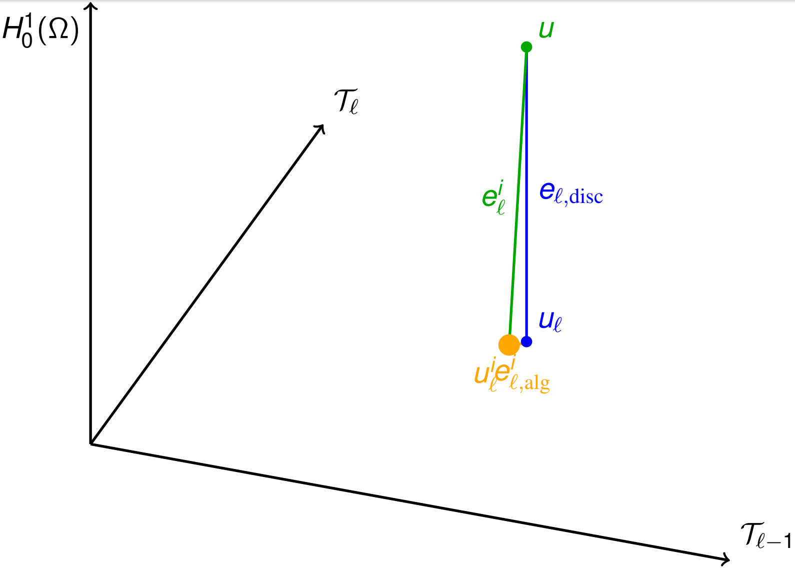

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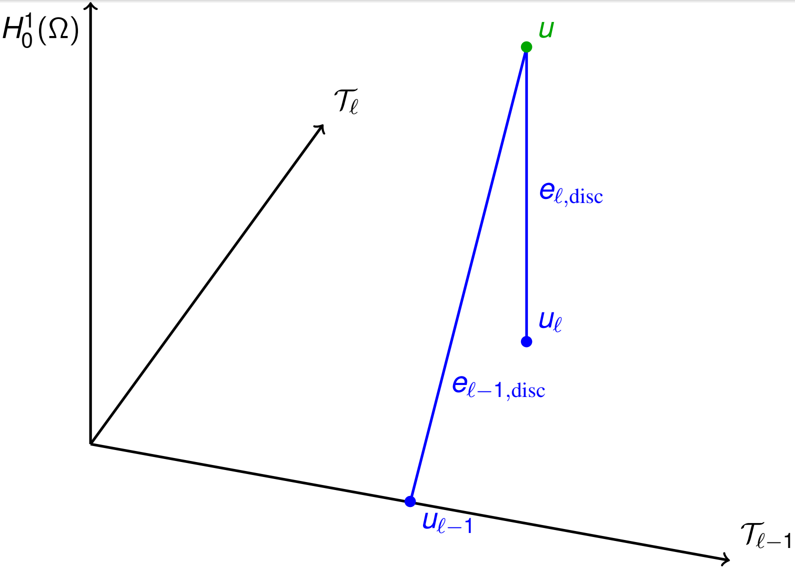

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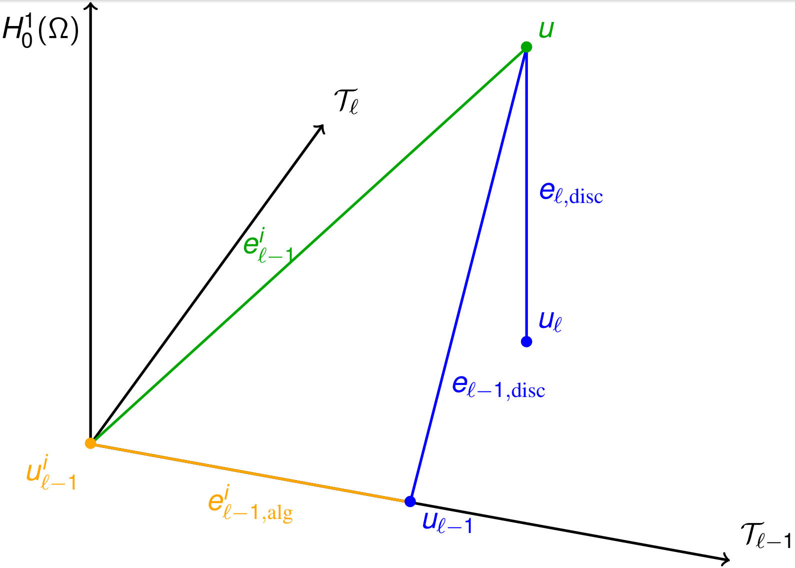

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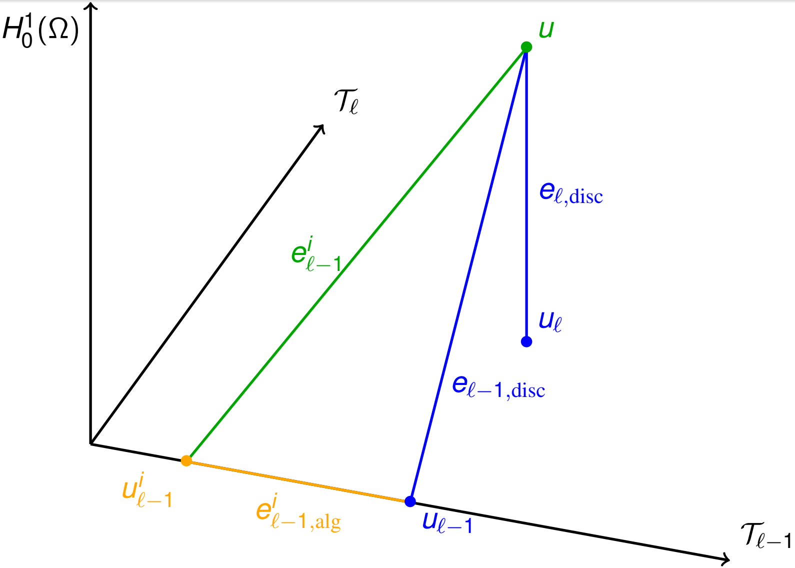

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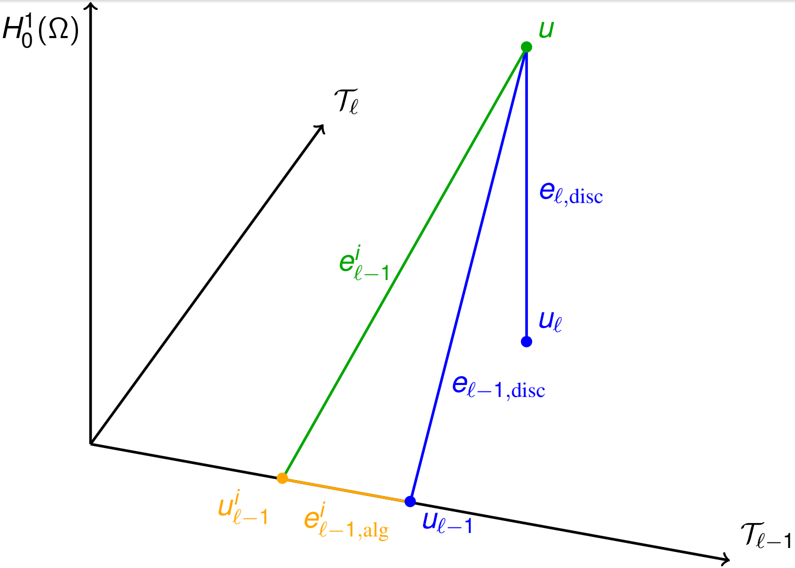

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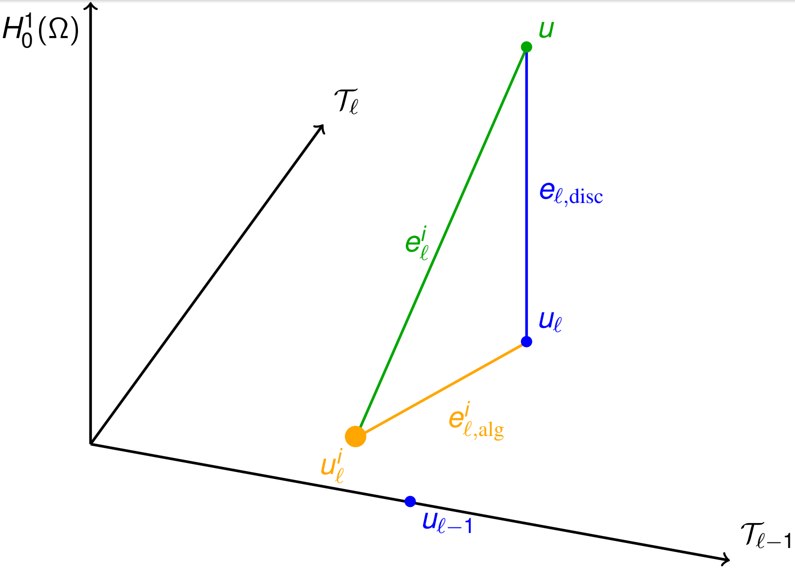

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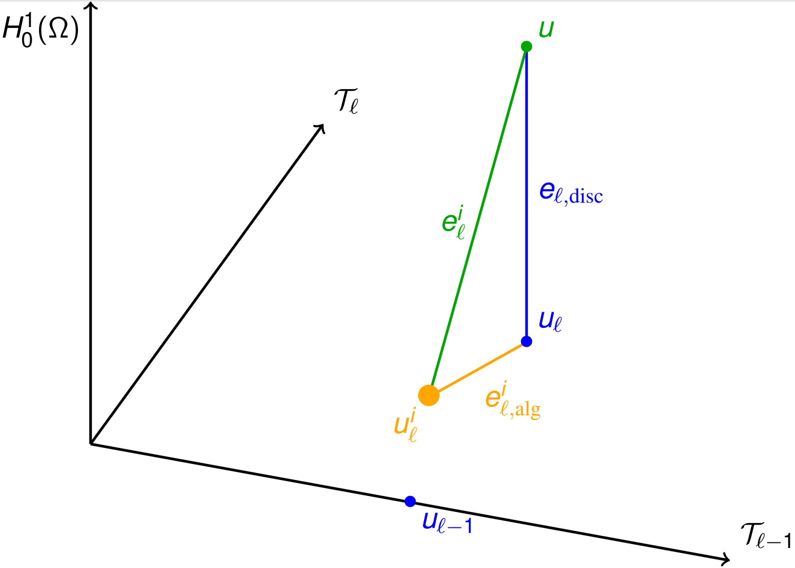

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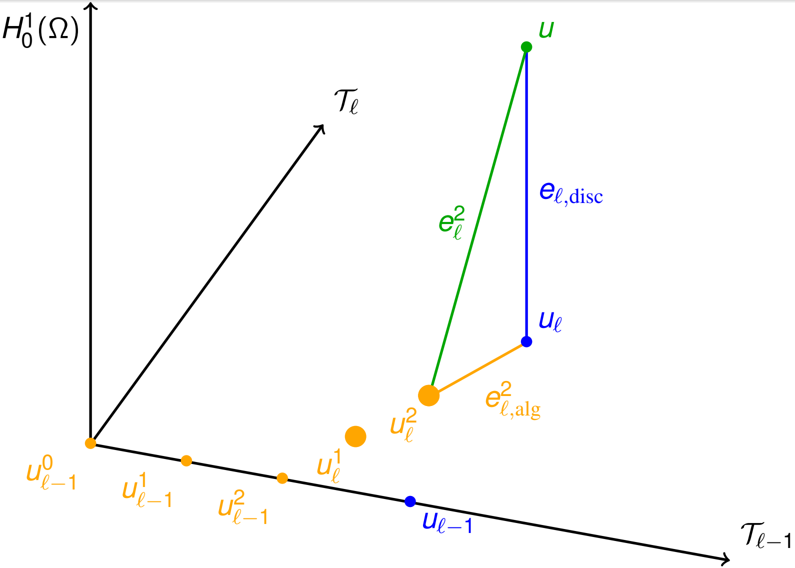

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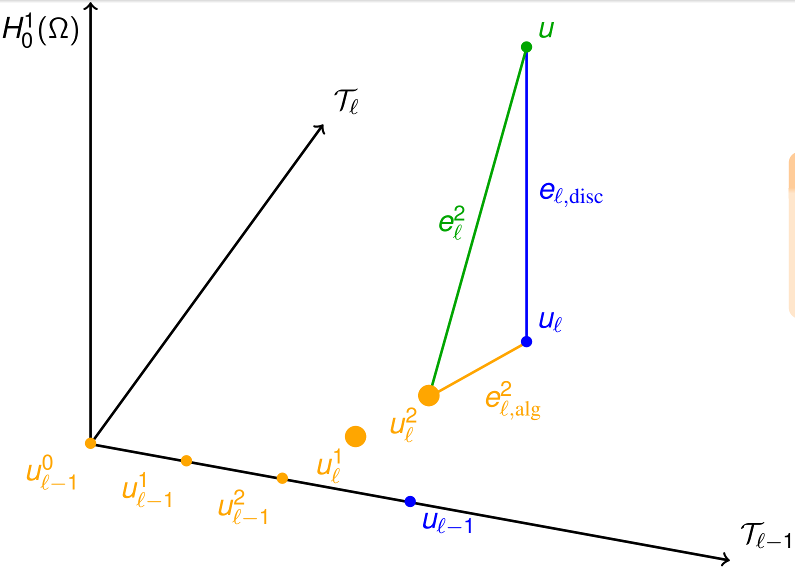
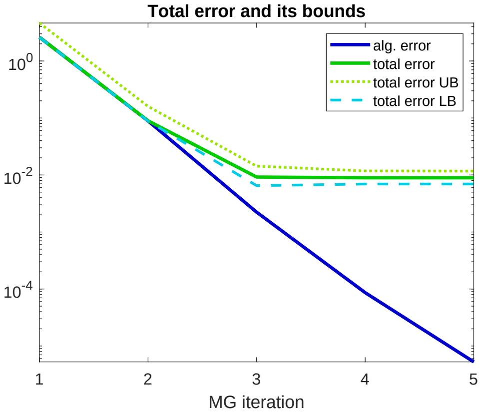


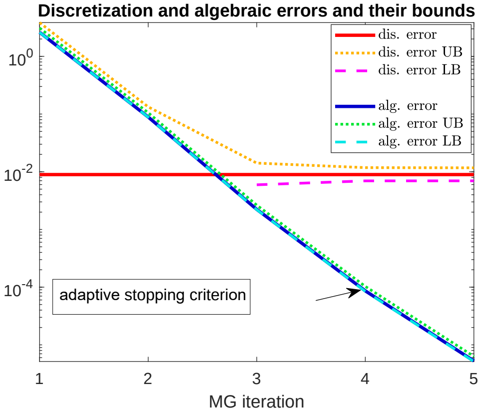
Cost

$$\sum_{\ell=0}^{\bar{\ell}} \sum_{i(\ell)=0}^{\bar{i}(\ell)} |V_\ell^p|$$

A posteriori estimates of total and algebraic errors: $\mathbb{A}_\ell \mathrm{U}_\ell^i \neq \mathrm{F}_\ell$



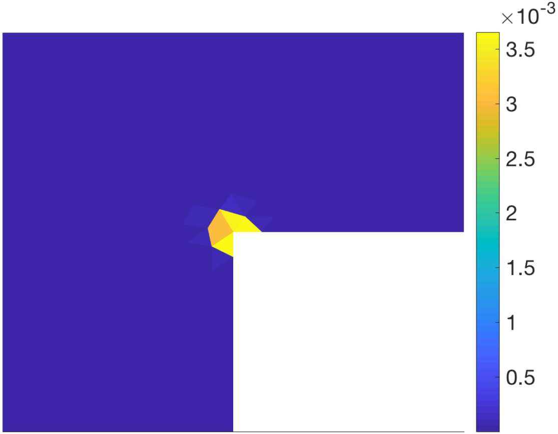
Total error



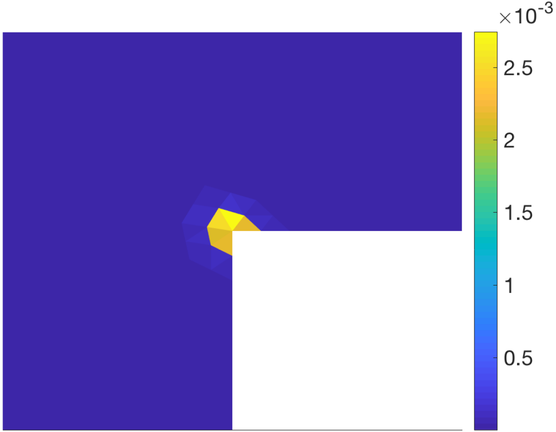
Error components and adaptive st. crit.

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

A posteriori estimates of **total** and **algebraic errors**: $\mathbb{A}_\ell \mathrm{U}_\ell^i \neq \mathrm{F}_\ell$



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



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

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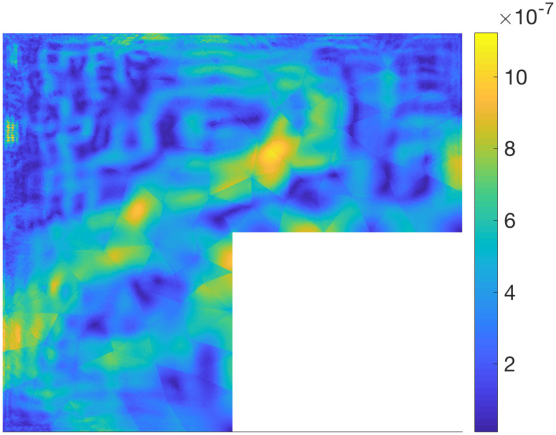
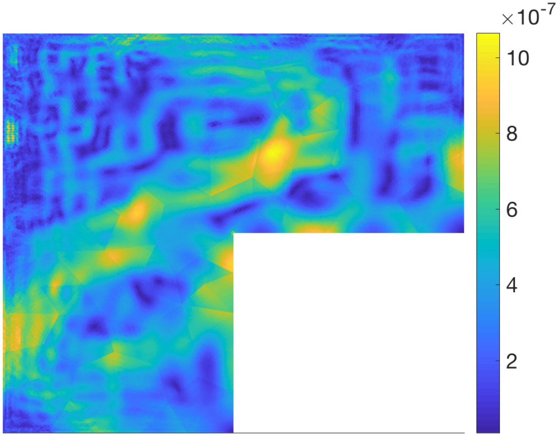


Estimated algebraic errors $\eta_{\mathrm{alg},K}(u_\ell^i)$



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Numerical approximations of nonlinear PDEs:

Setting

- u: unknown exact PDE solution
- u_ℓ : known numerical approximation on mesh $\mathcal{T}_\ell$

Numerical approximations of nonlinear PDEs:

Setting

- u: unknown exact PDE solution
- $u_\ell^{k,i}$: known numerical approximation on mesh $\mathcal{T}_\ell$, linearization step k, and linear solver step i

Numerical approximations of nonlinear PDEs: **3 crucial questions**

Setting

- u: unknown exact PDE solution
- $u_\ell^{k,i}$: known numerical approximation on mesh $\mathcal{T}_\ell$, linearization step k, and linear solver step i

Crucial questions

1. How **large** is the overall **error** between u and $u_\ell^{k,i}$?

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Numerical approximations of nonlinear 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**.
3. **Balancing** error components, **adaptivity** (working where needed).

Main achievements

A posteriori error estimates

a posteriori error estimates

$$|||u - u_\ell^{k,i}||| \leq \eta(u_\ell^{k,i})$$

Main achievements

A posteriori error estimates

Guaranteed a posteriori error estimates

$$|||u - u_\ell^{k,i}||| \leq \eta(u_\ell^{k,i})$$

Main achievements

A posteriori error estimates

Guaranteed a posteriori error estimates **efficient**

$$|||u - u_\ell^{k,i}||| \leq \eta(u_\ell^{k,i}) \leq C_{\text{eff}}|||u - u_\ell^{k,i}|||,$$

Main achievements

A posteriori error estimates

Guaranteed a posteriori error estimates **efficient**, **robust** with respect to **strength of nonlinearities**

$$|||u - u_\ell^{k,i}||| \le \eta(u_\ell^{k,i}) \le C_{\rm eff} |||u - u_\ell^{k,i}|||, \qquad C_{\rm eff} \text{ independent of nonlinearities}$$

Main achievements

A posteriori error estimates

Guaranteed a posteriori error estimates **efficient**, **robust** with respect to **strength of nonlinearities**

$$|||u - u_\ell^{k,i}||| \leq \left\{ \sum_{K \in \mathcal{T}_\ell} \eta_K (u_\ell^{k,i})^2 \right\}^{1/2} \leq C_{\text{eff}} |||u - u_\ell^{k,i}|||,$$

Main achievements

A posteriori error estimates

Guaranteed a posteriori error estimates, **locally efficient**, **robust** with respect to **strength of nonlinearities**

$$\left\{ \sum_{K \in \mathcal{T}_\ell} \eta_K (u_\ell^{k,i})^2 \right\}^{1/2} \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||,$$

$$\eta_K (u_\ell^{k,i}) \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||_{\omega_K} \text{ for all } K \in \mathcal{T}_\ell,$$

Main achievements

A posteriori error estimates

Guaranteed a posteriori error estimates, **locally** **efficient**, **robust** with respect to **strength of nonlinearities**, and identifying **error components**.

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$$\eta_K (u_\ell^{k,i}) = \eta_{\text{disc},K} (u_\ell^{k,i}) + \eta_{\text{lin},K} (u_\ell^{k,i}) + \eta_{\text{alg},K} (u_\ell^{k,i}).$$

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Optimal decay rate of error wrt computational cost

Adaptive iterative approximation allows to achieve

$$|||u - u_\ell^{k,i}||| \lesssim \left\{ \sum_{\ell=0}^{\bar\ell} \sum_{k(\ell)=0}^{\bar k(\ell)} \sum_{i(\ell,k)=0}^{\bar i(\ell,k)} |V_\ell^p| \right\}^{-p/d}.$$

Main achievements

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$$|||u-u_\ell^{k,i}|||\lesssim\left\{\sum_{\ell=0}^{\overline{\ell}}\sum_{k(\ell)=0}^{\overline{k}(\ell)}\sum_{i(\ell,k)=0}^{\overline{i}(\ell,k)}|\mathcal{V}_\ell^p|\right\}^{-p/d}.$$ (replaces traditional a priori h^p)

Holistic approach: interplay PDE–numerics–linearization–algebra

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Algorithm

Algorithm 1 **Adaptive iterative approximation**

while $\frac{\eta(u_\ell^{k,i})}{|||u_\ell^{k,i}|||} > \gamma_{\text{tot}}$ **do** ▷ while user-specified relative precision is not reached
  assemble the finite element space V_ℓ^p
  assemble the nonlinear problem
  while $\eta_{\text{lin},K}(u_\ell^{k,i}) > \gamma_{\text{lin}}\eta_{\text{disc},K}(u_\ell^{k,i})\ \forall K \in \mathcal{T}_\ell$ **do** ▷ while linearization dominates discretization
    assemble the linearized problem
    while $\eta_{\text{alg},K}(u_\ell^{k,i}) > \gamma_{\text{alg}}\eta_{\text{lin},K}(u_\ell^{k,i})\ \forall K \in \mathcal{T}_\ell$ **do** ▷ while algebra dominates linearization
      one step of iterative algebraic solver, $i++$
    end while (iterative algebraic solver)
    $k++$
  end while (iterative linearization)
  refine $K \in \mathcal{T}_\ell$ with big $\eta_{\text{disc},K}(u_\ell^{k,i})$, $\ell++$
end while (adaptive mesh refinement)

Implementation and observations

Error components

- $\eta_{\mathrm{disc},K}(u_\ell^{k,i})$: discretization
- $\eta_{\mathrm{lin},K}(u_\ell^{k,i})$: linearization
- $\eta_{\mathrm{alg},K}(u_\ell^{k,i})$: algebraic solver

Implementation and observations

Error control

- at **any moment** during the simulation
- price: local finite element quadrature/sparse **matrix-vector** multiplication

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Adaptive iterative approximation

- **same physical units** of all component estimators
- **balance** all component estimators
- **online steering** (work where needed)

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- not a novel scheme, rather an **efficient use** of existing **building blocks**
- **easy implementation** into existing codes

Optimal decay rate wrt degrees of freedom & computational cost

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

Optimal decay rate wrt degrees of freedom & computational cost

classical

estimated error	**4.6%**

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

Optimal decay rate wrt degrees of freedom & computational cost

classical	tot. algebraic solver iter.	**10890**
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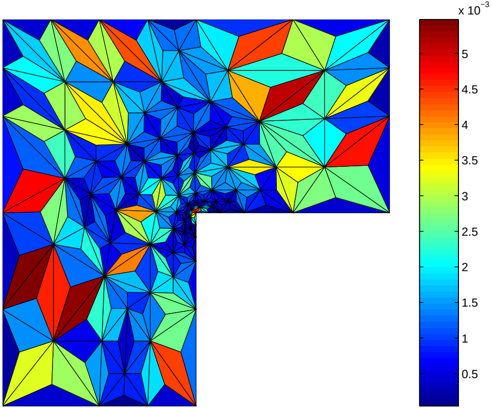
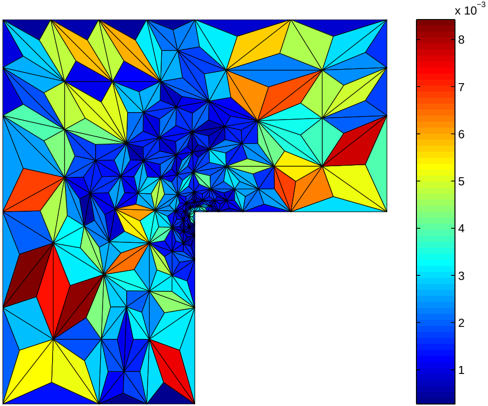
Optimal decay rate wrt degrees of freedom & computational cost



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



Exact local total errors

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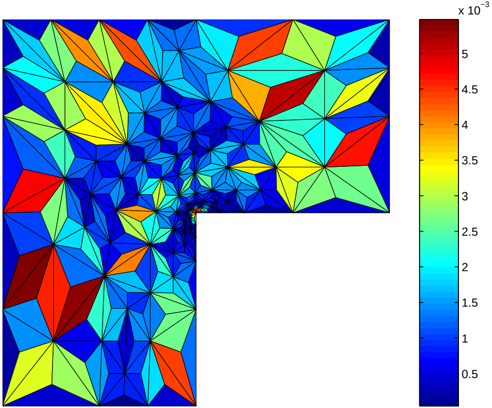

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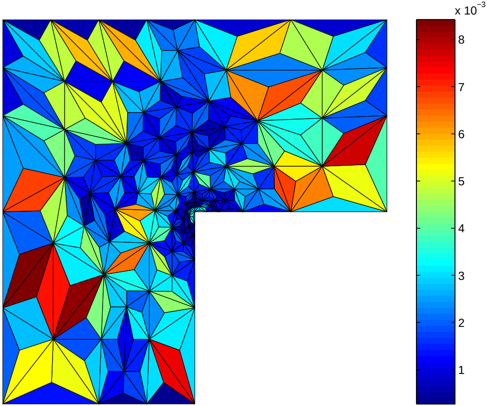


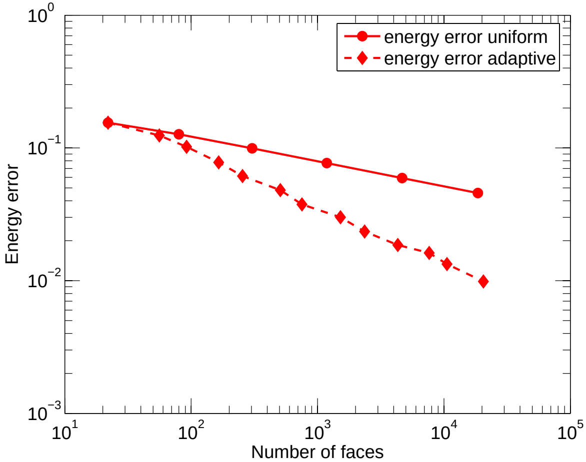
Exact local total errors

classical	tot. algebraic solver iter.	**10890**
	estimated error	**4.6%**

adaptive	tot. algebraic solver iter.	**242**
	estimated error	**1.1%**

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

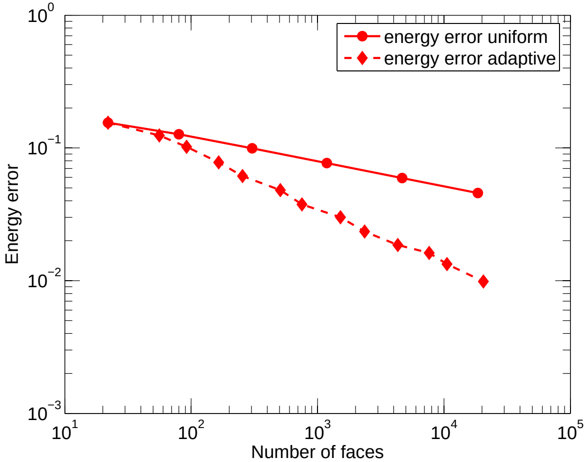
Optimal decay rate wrt degrees of freedom & computational cost



Optimal decay rate wrt DoFs

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

Optimal decay rate wrt degrees of freedom & computational cost



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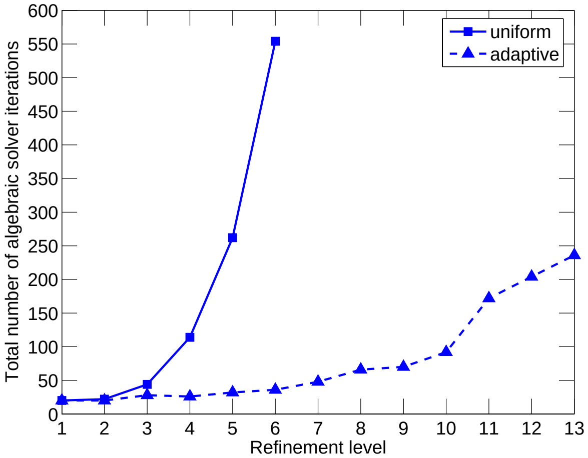
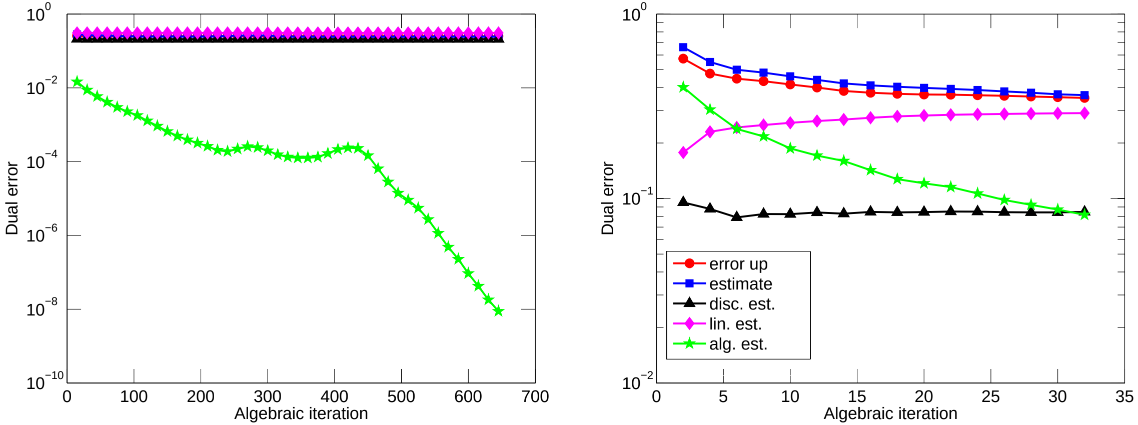


Optimal computational cost

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

Total, linearization, & alg. errors: $(\mathcal{A}_\ell(\mathrm{U}_\ell^{k,i}) \neq \mathrm{F}_\ell,\ \mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,i} \neq \mathrm{F}_\ell^{k-1})$



Newton

adaptive inexact Newton

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

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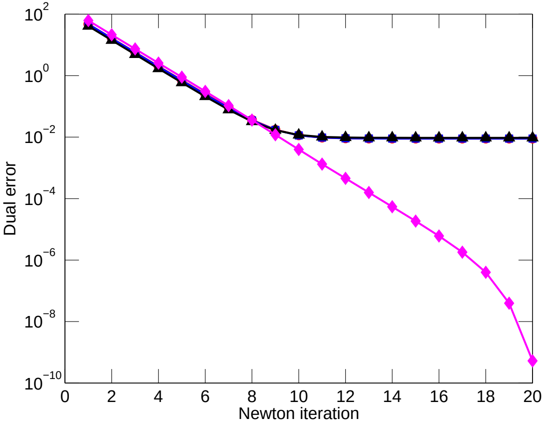
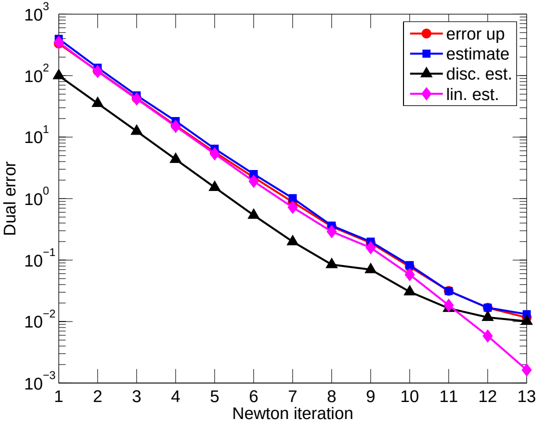


Newton



adaptive inexact Newton

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

Outline

1. Introduction: adaptive iterative approximation
   - A posteriori error estimates and adaptivity
   - Achievements and example results
   - Real life comparison
2. Linear diffusion: discretization error, mesh and polynomial degree adaptivity
   - A posteriori error estimates
   - Potential reconstruction
   - Flux reconstruction
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   - Balancing error components: mesh adaptivity
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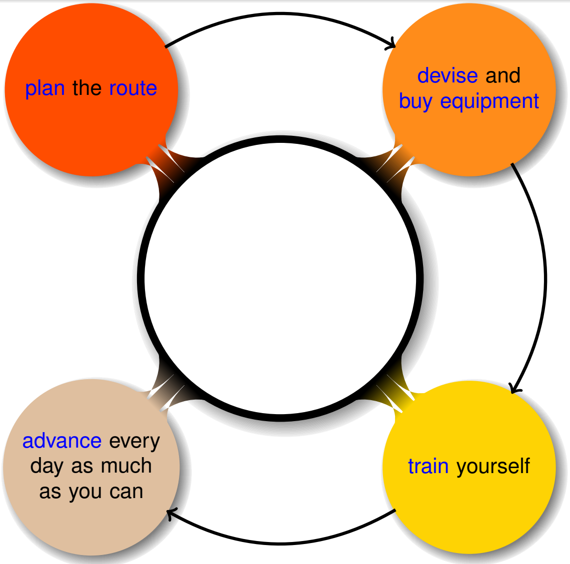
4. Conclusions

Control the error and act adaptively: real life

Control the error and act adaptively: real life

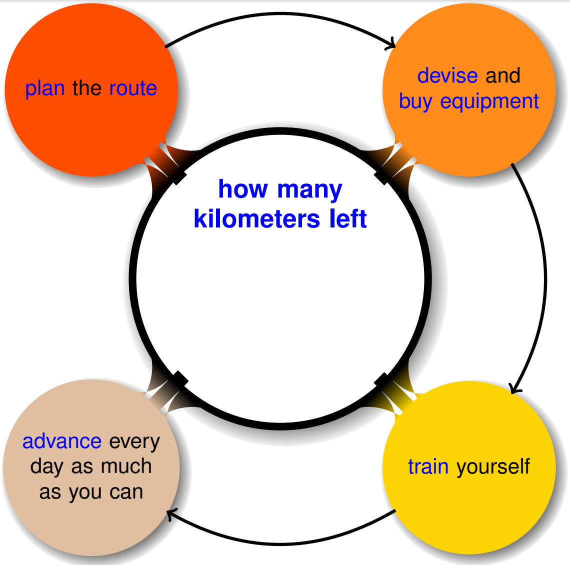
wandering Paris–Santiago de Compostela

Control the error and act adaptively: real life



wandering Paris–Santiago de Compostela

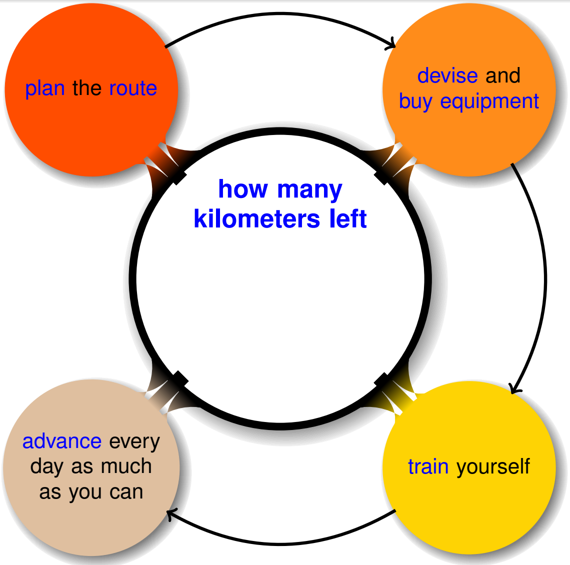
Control the error and act adaptively: real life



wandering Paris–Santiago de Compostela

$\Longleftarrow$ **control the error**

Control the error and act adaptively: real life



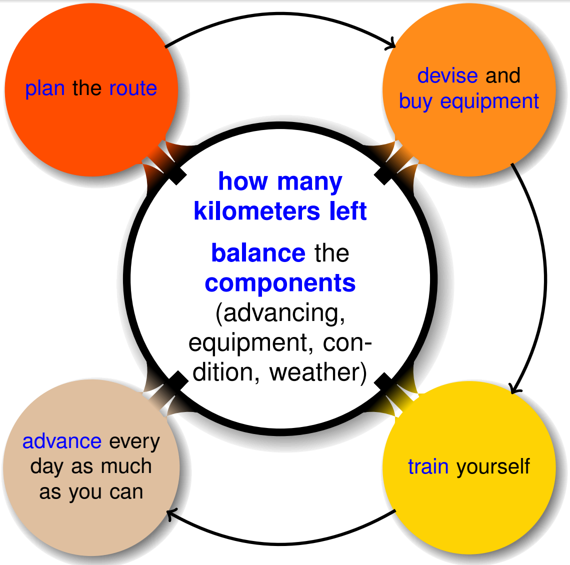
wandering Paris–Santiago de Compostela

$\Longleftarrow$ **control the error**

possible since

- **target known**
-

Control the error and act adaptively: real life



wandering Paris–Santiago de Compostela

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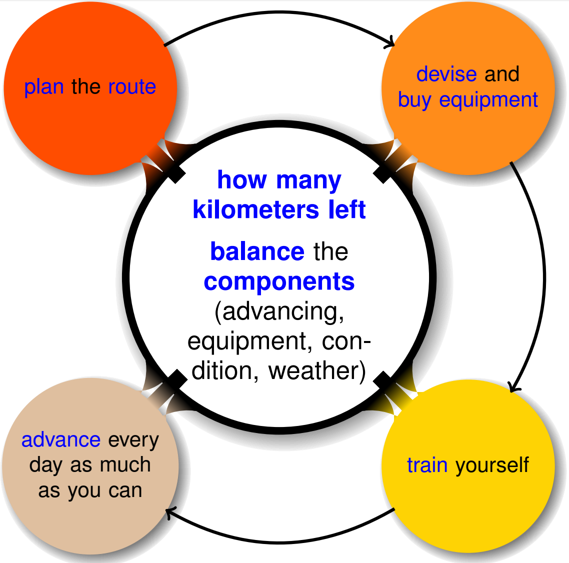


wandering Paris–Santiago de Compostela

⟸ **control the error**

⟸ **act adaptively**

possible since

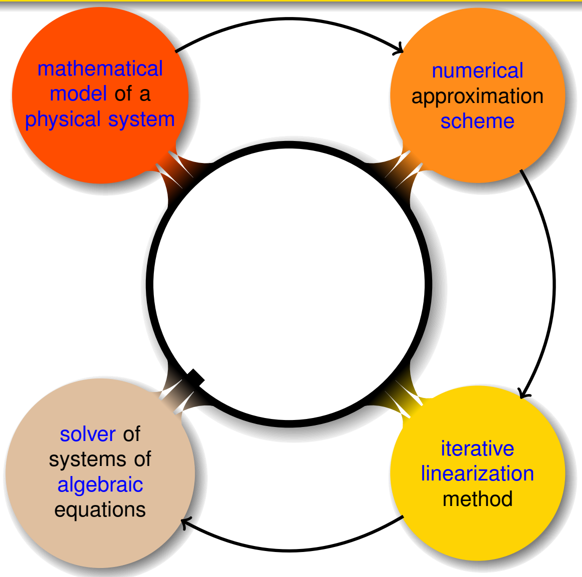
- **target known**
- **components known**

Control the error and act adaptively: numerical simulations

Control the error and act adaptively: numerical simulations

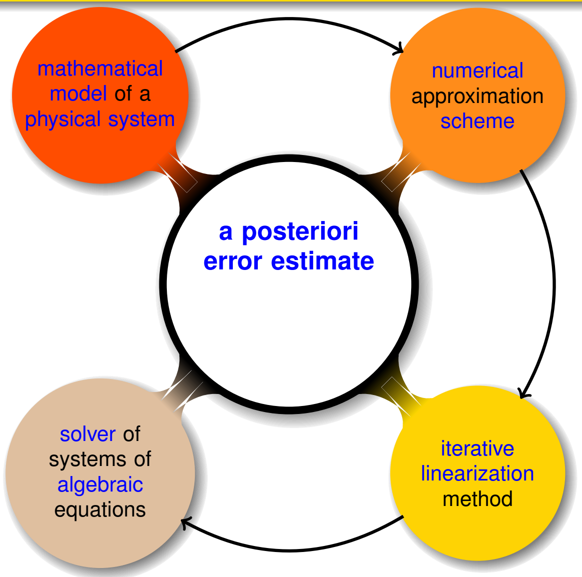
numerical simulation

Control the error and act adaptively: numerical simulations



numerical simulation

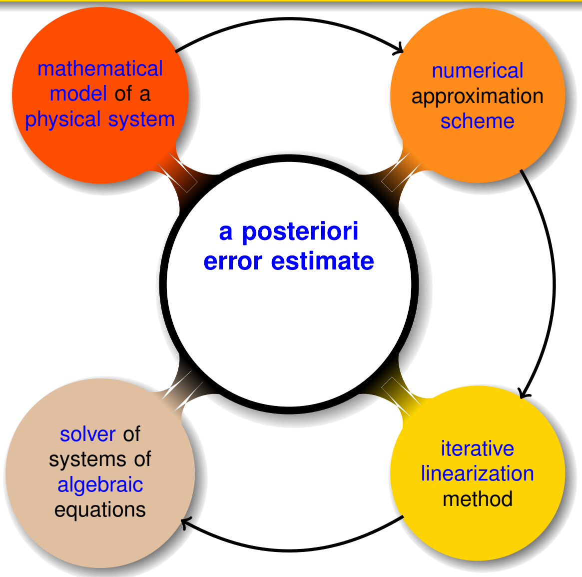
Control the error and act adaptively: numerical simulations



numerical simulation

$\Longleftarrow$ control the error (a posteriori estimates)

Control the error and act adaptively: numerical simulations



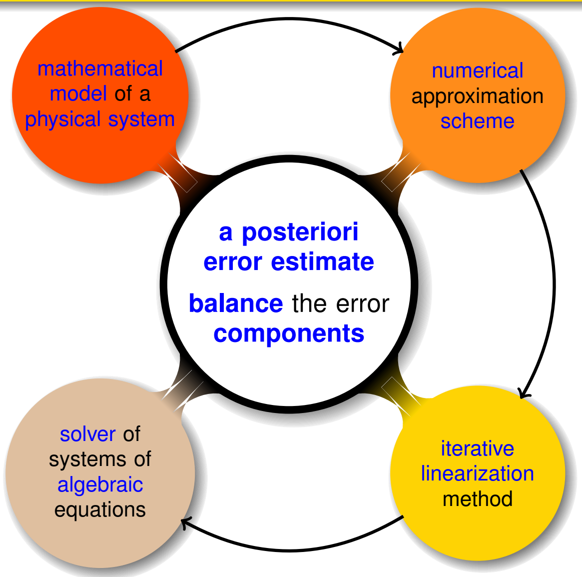
numerical simulation

$\Longleftarrow$ **control the error**
(a posteriori estimates)

hard since

- **target unknown**
-

Control the error and act adaptively: numerical simulations



numerical simulation

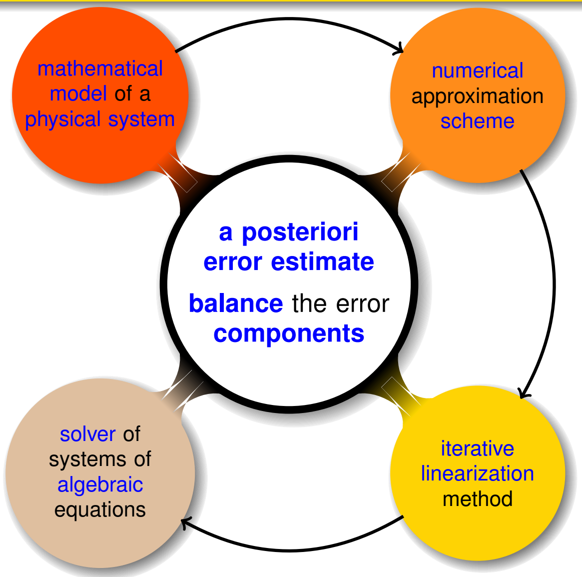
⟸ **control the error (a posteriori estimates)**

⟸ **act adaptively (adaptivity)**

hard since

- **target unknown**
-

Control the error and act adaptively: numerical simulations



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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) ($u_\ell \in \mathcal{P}_p(\mathcal{T}_\ell) \cap H^1_0(\Omega)$, $p \geq 1$, FEs)

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

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

$$
\eta \quad (u_\ell) \leq C_{\mathrm{eff}} \|\nabla(u - u_\ell)\|
$$

- C_{eff} a generic constant only dependent on d and shape regularity of $\mathcal{T}_\ell$ and thus independent of Ω, u, u_ℓ, ℓ, p

A posteriori error estimates: discretization error control

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

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

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

$$\eta_K(u_\ell) \leq C_{\text{eff}} \|\nabla(u - u_\ell)\|_{\omega_K} \qquad \forall K \in \mathcal{T}_\ell$$

- C_{eff} a generic constant only dependent on d and shape regularity of $\mathcal{T}_\ell$ and thus independent of Ω, u, u_ℓ, ℓ, p
- computable bound on C_{eff} available, $C_{\text{eff}} \approx 5$ in 2D

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A posteriori error estimates: discretization error control

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

$$-\Delta u = f \quad \text{in} \quad \Omega,$$
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Guaranteed error upper bound (reliability) ($u_\ell \in \mathcal{P}_p(\mathcal{T}_\ell) \cap H_0^1(\Omega)$, $p \geq 1$, FEs)

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

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

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Error characterization

Theorem (Error characterization)

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

$$\|\nabla(u-u_\ell)\|^2 = \underbrace{\min_{\substack{\boldsymbol{v}\in\boldsymbol{H}(\mathrm{div},\Omega)\\ \nabla\cdot\boldsymbol{v}=f}} \|\nabla u_\ell + \boldsymbol{v}\|^2}_{\substack{\text{constrained distance to } \boldsymbol{H}(\mathrm{div},\Omega)\\ =\max_{\substack{v\in H_0^1(\Omega)\\ \|\nabla v\|=1}}\{(f,v)-(\nabla u_\ell,\nabla v)\}^2\\ \text{dual norm of the PDE residual}}} + \underbrace{\min_{v\in H_0^1(\Omega)} \|\nabla(u_\ell - v)\|^2}_{\text{distance to } H_0^1(\Omega)=\text{nonconformity residual}}.$$

Comments

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dual norm of the **PDE residual**

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constrained distance to $\boldsymbol{H}(\mathrm{div},\Omega)$

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distance to $H_0^1(\Omega)$ = **nonconformity residual**

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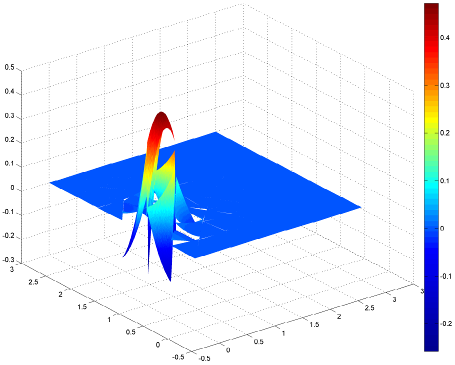
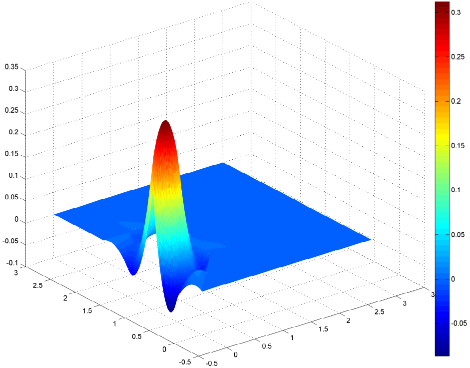
Outline

Potential reconstruction



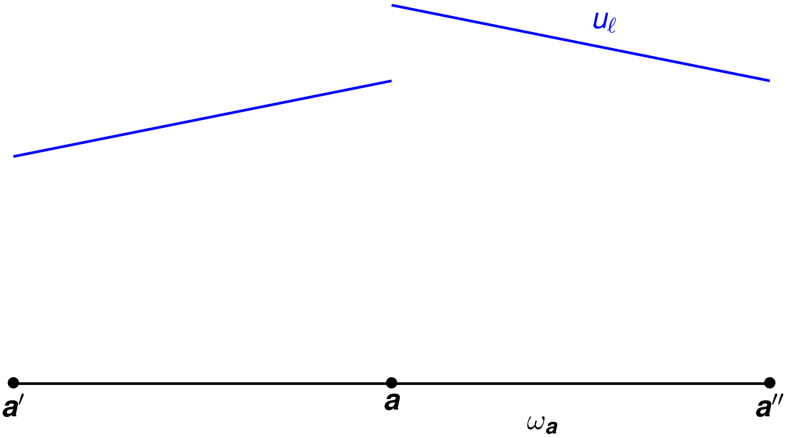
Potential u_ℓ



Potential reconstruction s_ℓ

$$u_\ell \in \mathcal{P}_p(\mathcal{T}_\ell) \to s_\ell \in \mathcal{P}_{p+1}(\mathcal{T}_\ell) \cap H_0^1(\Omega)$$

Potential reconstruction in 1D, $p = 1$



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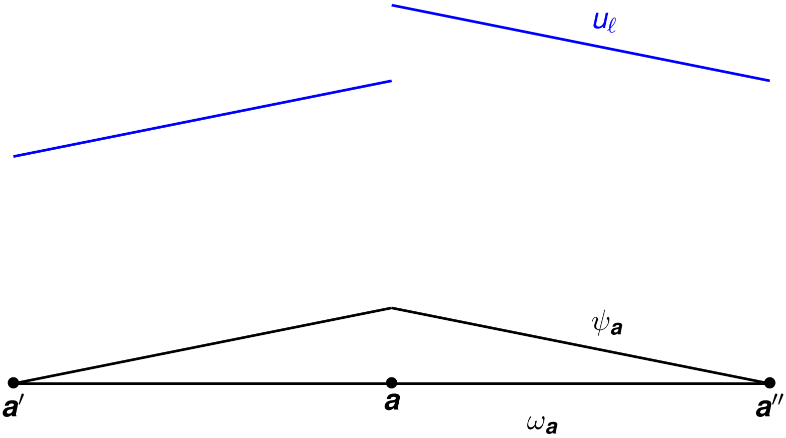

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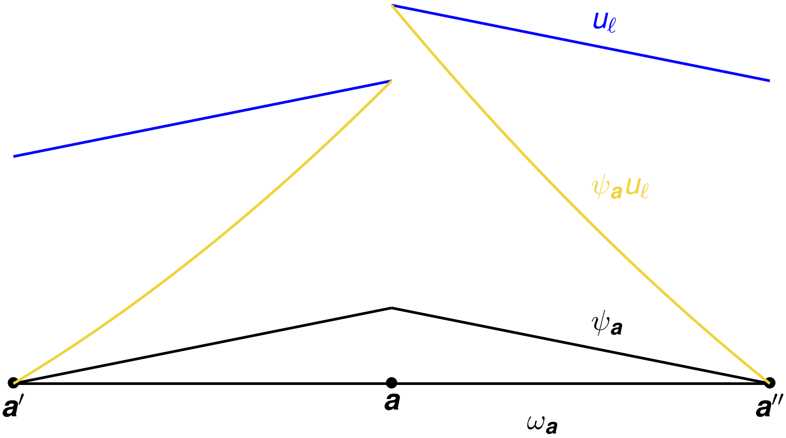

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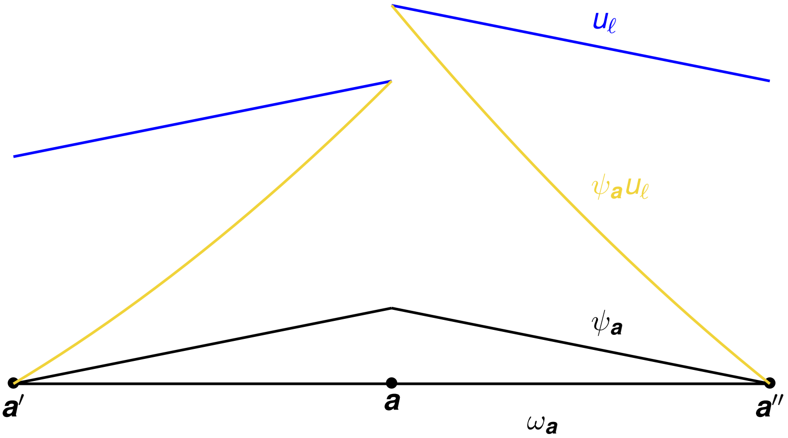

Potential reconstruction: datum $u_\ell \in \mathcal{P}_p(\mathcal{T}_\ell)$, $p \geq 1$

Definition (Nonconformity residual lifting s_ℓ Ern & V. (2015), ≈ Carstensen and Merdon (2013))

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

$$s_\ell^{\mathbf{a}} := \arg \min_{v_\ell \in V_\ell^{\mathbf{a}} := \mathcal{P}_{p+1}(\mathcal{T}^{\mathbf{a}}) \cap H_0^1(\omega_{\mathbf{a}})} \|\nabla(\psi_{\mathbf{a}} u_\ell - v_\ell)\|_{\omega_{\mathbf{a}}}$$

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Equivalent form: conforming FEs

Find $s_\ell^{\mathbf{a}} \in V_\ell^{\mathbf{a}}$ such that

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Key points

- localization to patches $\mathcal{T}^{\mathbf{a}}$
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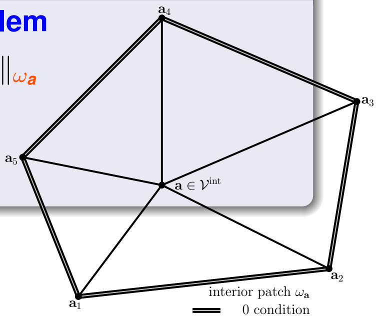

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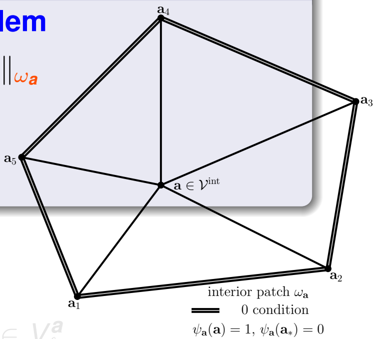

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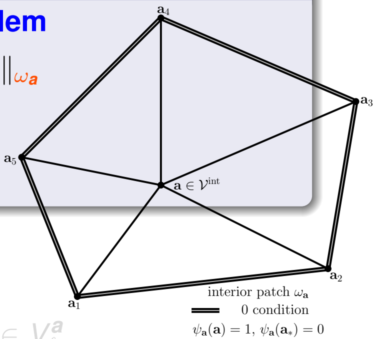

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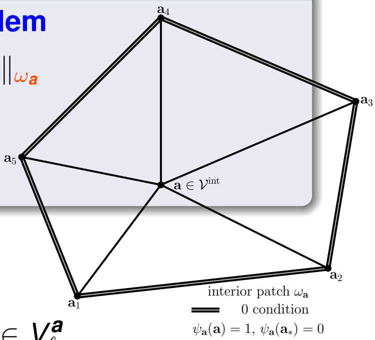

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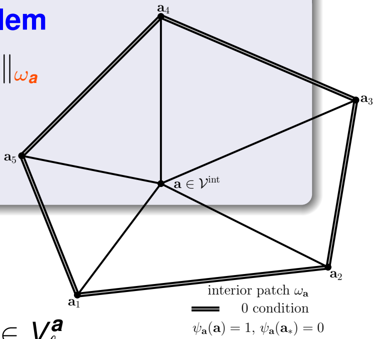

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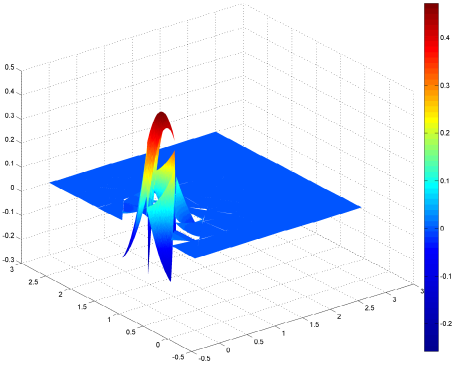
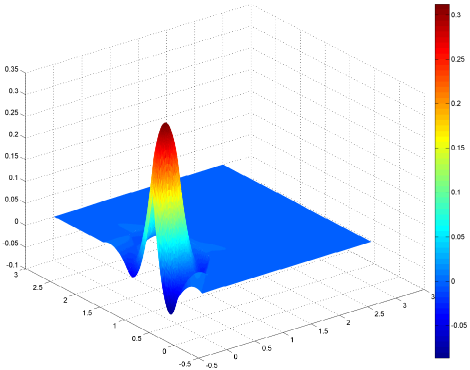


Potential u_ℓ

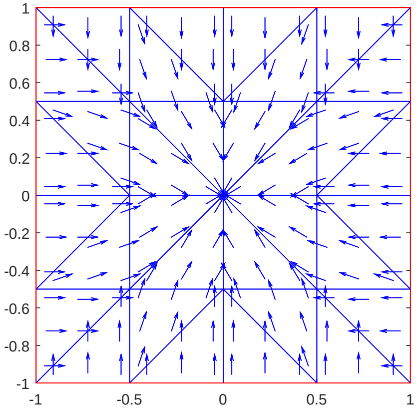


Potential reconstruction s_ℓ

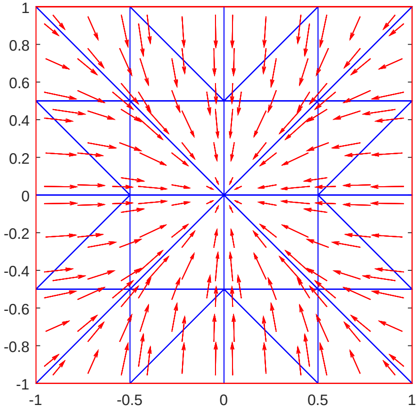
$$u_\ell \in \mathcal{P}_p(\mathcal{T}_\ell) \to s_\ell \in \mathcal{P}_{p+1}(\mathcal{T}_\ell) \cap H_0^1(\Omega)$$

Outline

Equilibrated flux reconstruction



Flux $-\nabla u_\ell$



Equilibrated flux reconstruction $\boldsymbol{\sigma}_\ell$

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

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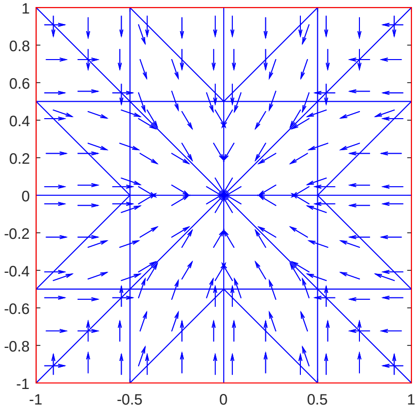

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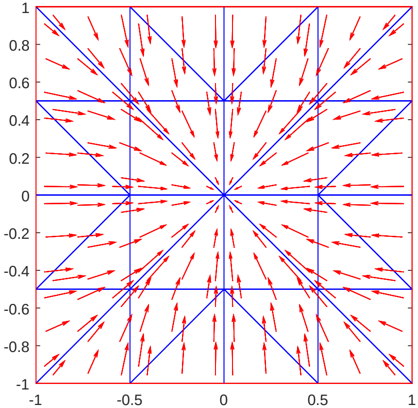

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Assumption (Orthogonality wrt hat functions)

There holds

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

$$\boldsymbol{\sigma}_\ell^{\boldsymbol{a}} := \arg \min_{\substack{\boldsymbol{v}_\ell \in \mathcal{RT}_p(\mathcal{T}_{\boldsymbol{a}}) \cap \boldsymbol{H}_0(\mathrm{div}, \omega_{\boldsymbol{a}}) \\ \nabla \cdot \boldsymbol{v}_\ell = \Pi_p(f\psi_{\boldsymbol{a}} - \nabla u_\ell \cdot \nabla \psi_{\boldsymbol{a}})}} \|\psi_{\boldsymbol{a}} \nabla u_\ell + \boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}}$$

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Key points

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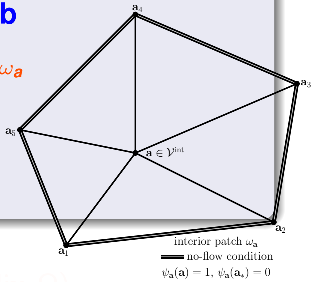

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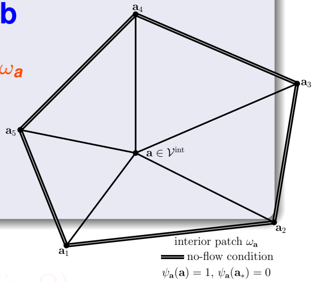

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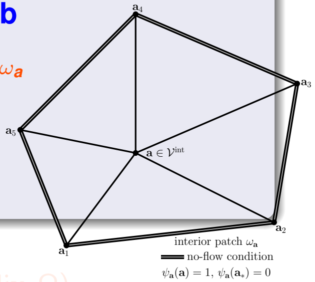

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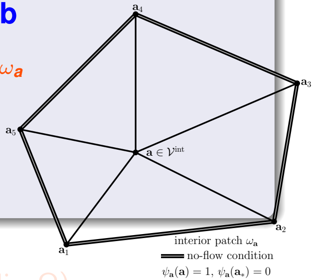

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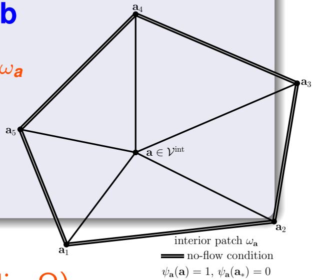

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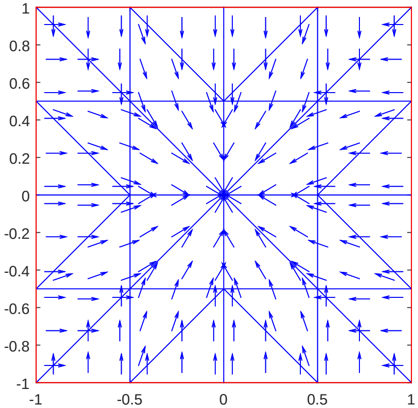

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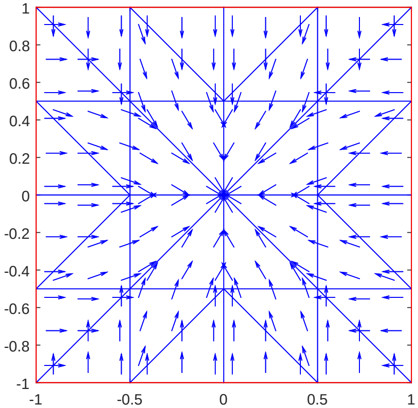

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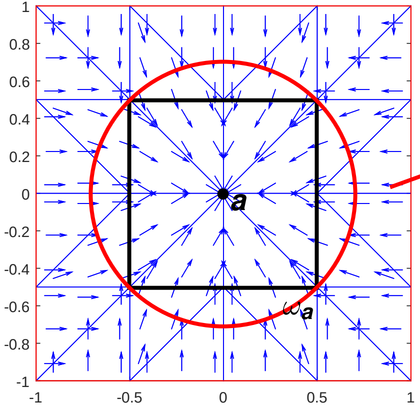

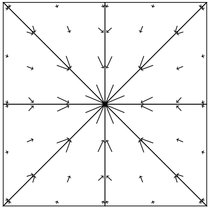

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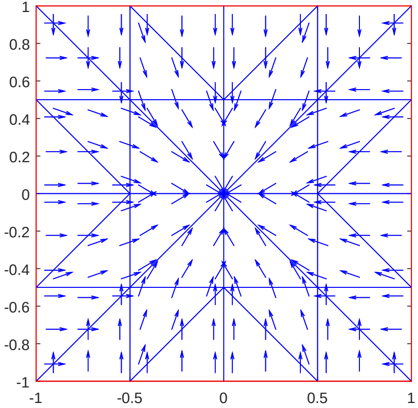

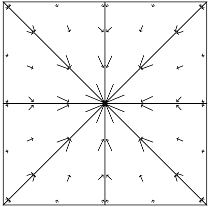

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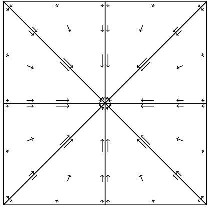

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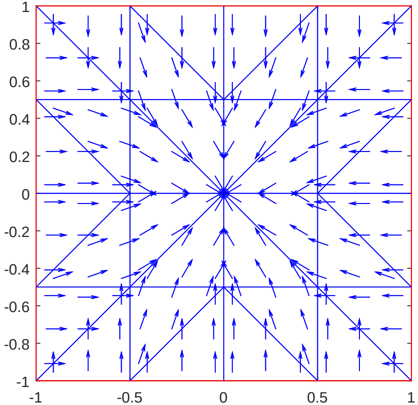

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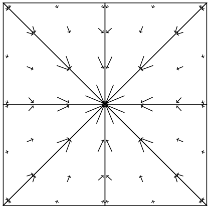

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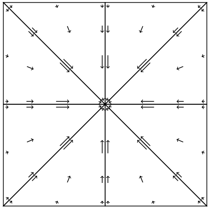

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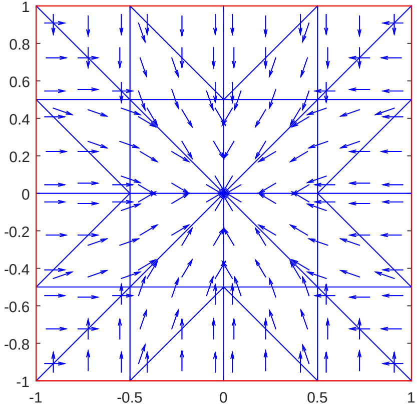

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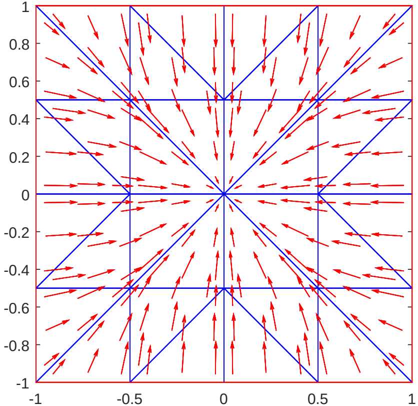

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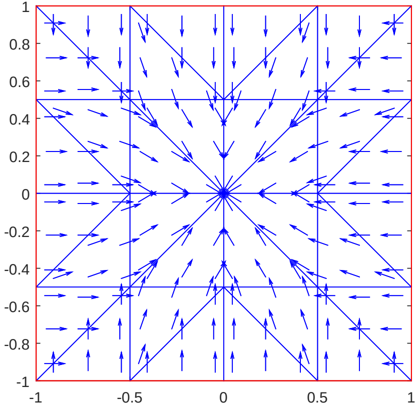

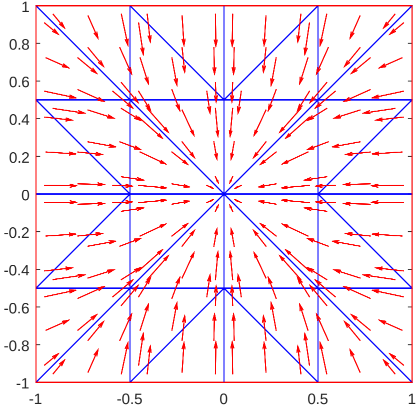

Flux $-\nabla u_\ell \notin \mathbf{H}(\mathrm{div}, \Omega)$, $\nabla \cdot (-\nabla u_\ell) \neq f$ Equilibrated flux rec. $\boldsymbol{\sigma}_\ell \in \mathbf{H}(\mathrm{div}, \Omega)$, $\nabla \cdot \boldsymbol{\sigma}_\ell = f$

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

Outline

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

ℓ	p	$\eta(u_\ell)$	rel. error estimate $\frac{\eta(u_\ell)}{\|\nabla u_\ell\|}$	$\|\nabla(u-u_\ell)\|$	rel. error $\frac{\|\nabla(u-u_\ell)\|}{\|\nabla u_\ell\|}$	$I^{\rm eff} = \frac{\eta(u_\ell)}{\|\nabla(u-u_\ell)\|}$
0	1	1.25	28%	1.07	24%	1.17
1		[illegible]				
2		[illegible]				
3		[illegible]				
1	2	[illegible]				
2	3	[illegible]				
3	4	[illegible]				

A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

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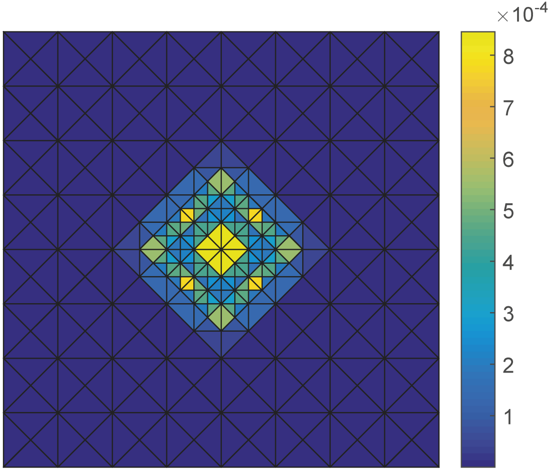
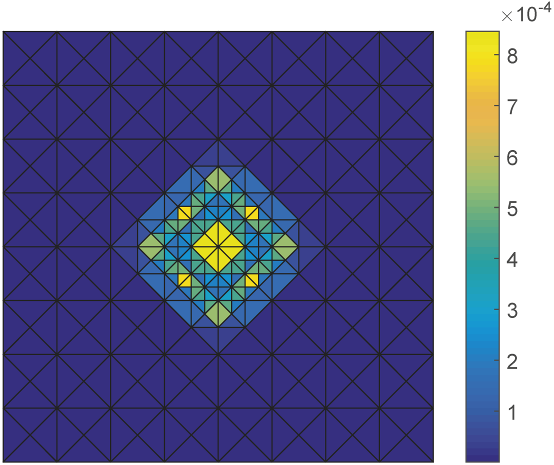
Outline

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



Estimated error distribution $\eta_K(u_\ell)$



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

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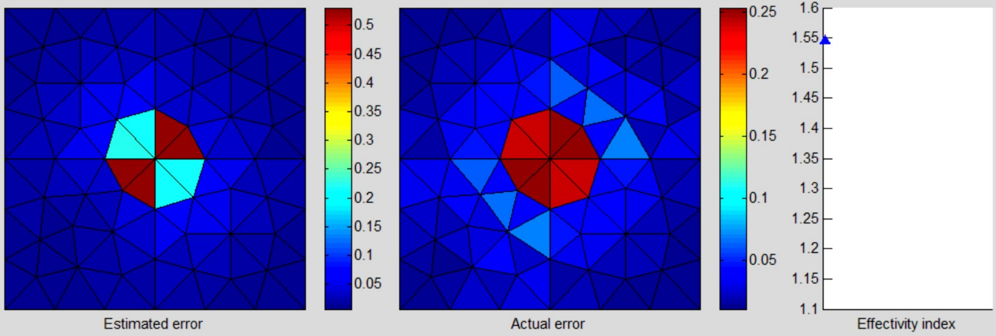
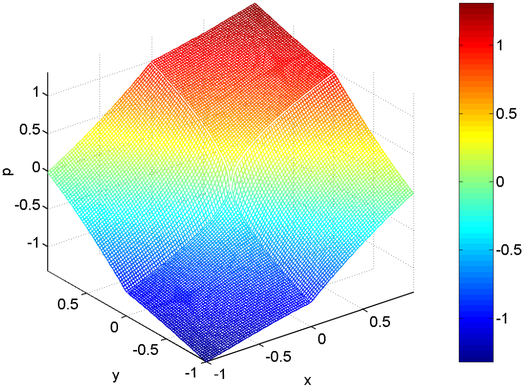
Can we **decrease the error efficiently**? (adaptive mesh refinement)

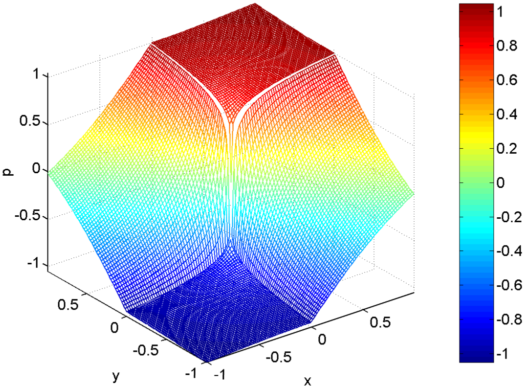


M. Vohralík, SIAM Journal on Numerical Analysis (2007)

Singular solutions

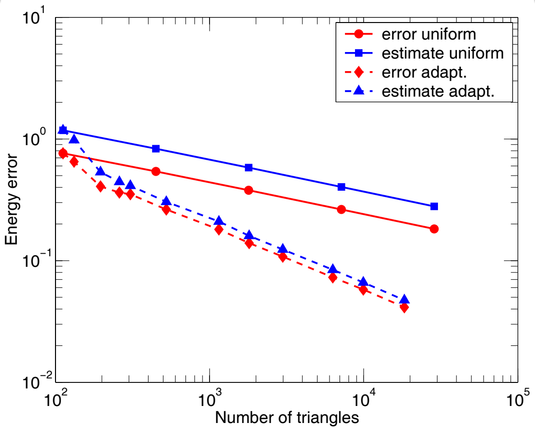


$H^{1.54}$ singularity



$H^{1.13}$ singularity

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



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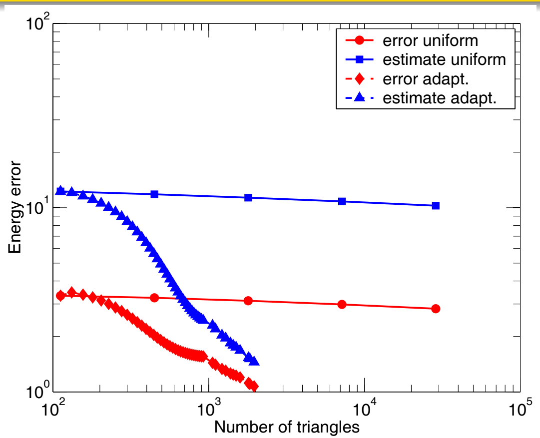

$H^{1.13}$ singularity

M. Vohralík, SIAM Journal on Numerical Analysis (2008)

Adaptive mesh refinement

Adaptive mesh refinement

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Adaptive mesh refinement

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

Adaptive mesh refinement

Adaptive mesh refinement

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

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

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Convergence on a sequence of adaptively refined meshes

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

Adaptive mesh refinement

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Optimal error decay rate wrt degrees of freedom

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

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1. Introduction: adaptive iterative approximation
   - A posteriori error estimates and adaptivity
   - Achievements and example results
   - Real life comparison
2. Linear diffusion: discretization error, mesh and polynomial degree adaptivity
   - A posteriori error estimates
   - Potential reconstruction
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   - A posteriori error control
   - Balancing error components: mesh adaptivity
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3. Nonlinear diffusion: overall error and solvers adaptivity
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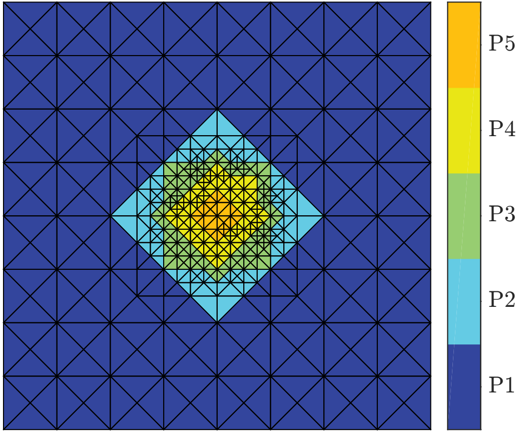
4. Conclusions

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



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

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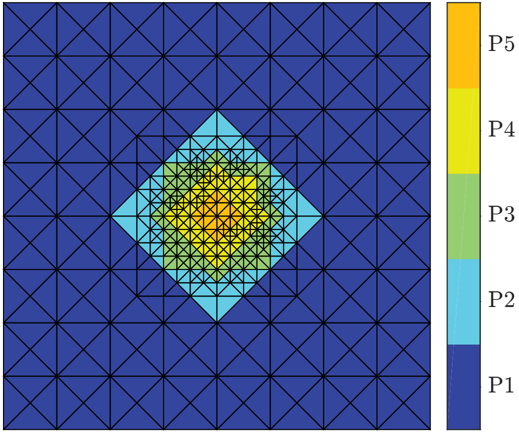

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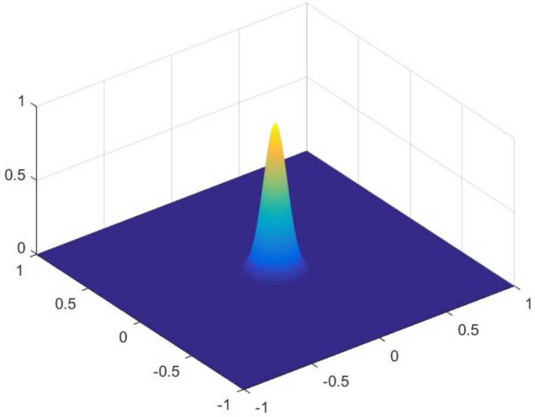

Exact solution

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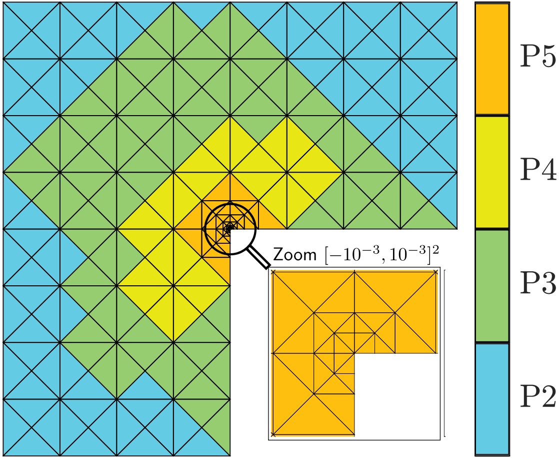
Best-possible error decrease: *hp* adaptivity, (singular solution)



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

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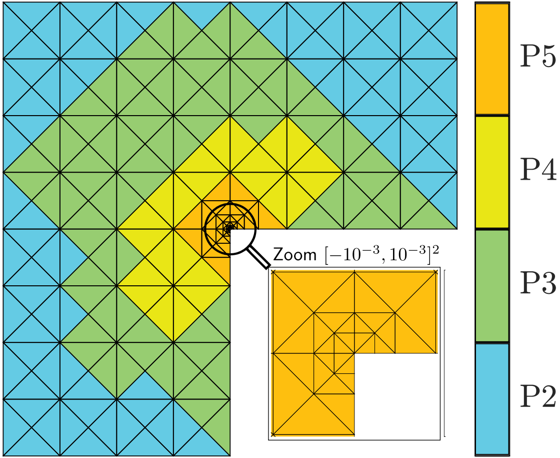

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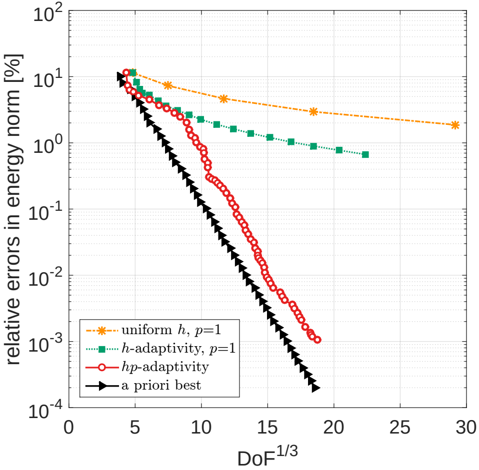

Relative error as a function of DoF

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

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A model nonlinear problem

Find $u \in H_0^1(\Omega)$ such that

$$\underbrace{(a(|\nabla u|)\nabla u, \nabla v)}_{\langle \mathcal{A}(u), v\rangle:\ \text{nonlinear operator}} = (f, v) \qquad \forall v \in H_0^1(\Omega).$$

A model nonlinear problem

Find $u \in H_0^1(\Omega)$ such that

$$\underbrace{(a(|\nabla u|)\nabla u, \nabla v)}_{\langle \mathcal{A}(u), v\rangle:\ \text{nonlinear operator}} = (f, v) \qquad \forall v \in H_0^1(\Omega).$$

Assumption (Gradient-dependent diffusivity)

Function $a : [0, \infty) \to (0, \infty)$, for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$,

$$|a(|\mathbf{x}|)\mathbf{x} - a(|\mathbf{y}|)\mathbf{y}| \leq a_{\mathrm{c}} |\mathbf{x} - \mathbf{y}| \qquad \textit{(Lipschitz continuity)},$$

$$(a(|\mathbf{x}|)\mathbf{x} - a(|\mathbf{y}|)\mathbf{y}) \cdot (\mathbf{x} - \mathbf{y}) \geq a_{\mathrm{m}} |\mathbf{x} - \mathbf{y}|^2 \qquad \textit{(strong monotonicity)}.$$

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- $a_{\mathrm{m}} \le a(r) \le a_{\mathrm{c}}$, $a_{\mathrm{m}} \le (a(r)r)' \le a_{\mathrm{c}}$

Example of the nonlinear function a

Example (Mean curvature nonlinearity)

$$a(r) := a_{\mathrm{m}} + \frac{a_{\mathrm{c}} - a_{\mathrm{m}}}{\sqrt{1 + r^2}}.$$

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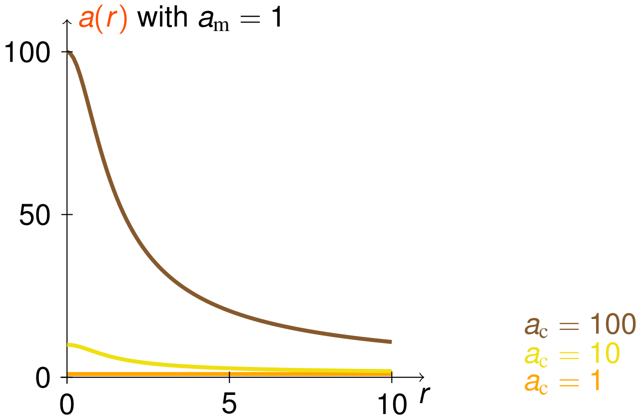

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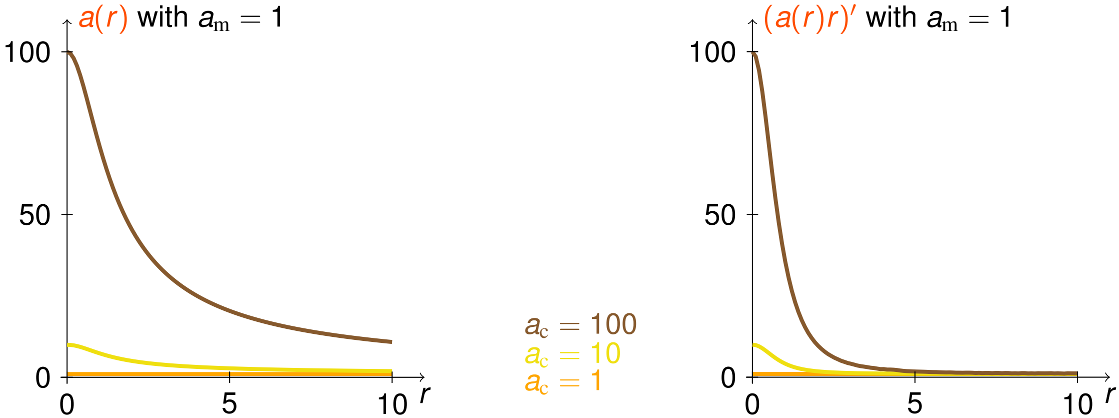

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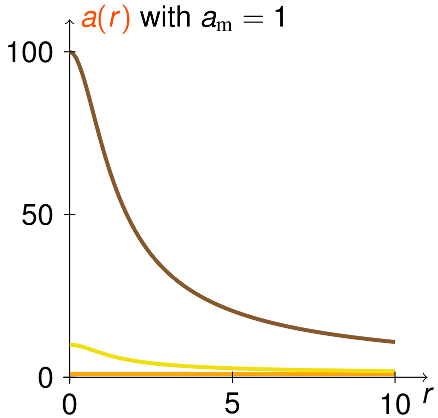
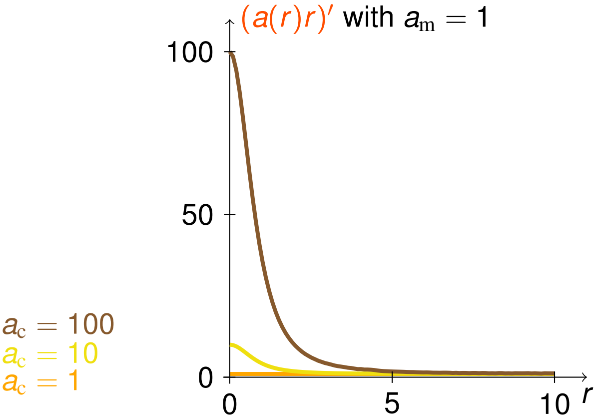
Strength of the nonlinearity

$$\frac{a_{\mathrm{c}}}{a_{\mathrm{m}}} = \frac{\text{Lipschitz continuity}}{\text{strong monotonicity}}$$





Finite element discretization

Definition (Finite element discretization)

Find $u_\ell \in V_\ell$ such that

$$\underbrace{\big(a(|\nabla u_\ell|)\nabla u_\ell, \nabla v_\ell\big)}_{\langle \mathcal{A}(u_\ell), v_\ell\rangle:\ \text{nonlinear operator}} = (f, v_\ell) \qquad \forall v_\ell \in V_\ell.$$

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- $p \geq 1$ polynomial degree
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- system of **nonlinear algebraic equations**

Iterative linearization

Definition (Linearized finite element approximation)

Find $u_\ell^k \in V_\ell$ such that

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Iterative algebraic solver

Definition (Iterative algebraic solver)

Find $u_\ell^{k,i} \in V_\ell$ such that

$$(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell) = (f, v_\ell) - \underbrace{(r_\ell^{k,i}, v_\ell)}_{\langle \mathcal{R}^{\mathrm{alg}}(u_\ell^{k,i}), v_\ell\rangle:\ \text{algebraic residual}} \qquad \forall v_\ell \in V_\ell.$$

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- algebraic residual: discrete, known

Outline

Error measure, error components

Definition (Intrinsic measure of error)

$$|||u - u_\ell^{k,i}||| := \max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\|=1}} \Big\{ \underbrace{(f, v) - (a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i}, \nabla v)} \Big\}$$

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Error components

$$\underbrace{(f, v) - \langle \mathcal{A}(u_\ell^{k,i}), v\rangle}_{\langle \mathcal{R}(u_\ell^{k,i}),v\rangle:\ \text{total residual}} = \underbrace{(f, v) - \langle \mathcal{A}^{k-1}(u_\ell^{k,i}), v\rangle - \langle \mathcal{R}^{\mathrm{alg}}(u_\ell^{k,i}), v\rangle}_{\langle \mathcal{R}^{\mathrm{disc}}(u_\ell^{k,i}),v\rangle:\ \text{discretization residual}}$$

$$+ \underbrace{\langle \mathcal{A}^{k-1}(u_\ell^{k,i}), v\rangle - \langle \mathcal{A}(u_\ell^{k,i}), v\rangle}_{\langle \mathcal{R}^{\mathrm{lin}}(u_\ell^{k,i}),v\rangle:\ \text{linearization residual}}$$

$$+ \underbrace{\langle \mathcal{R}^{\mathrm{alg}}(u_\ell^{k,i}), v\rangle}_{\text{algebraic residual}}$$

Reminder from the linear case

Theorem (Error characterization)

Let $u \in H_0^1(\Omega)$ be the weak solution and let $u_\ell \in H_0^1(\Omega)$ be arbitrary. Then

$$\|\nabla(u-u_\ell)\|^2 = \underbrace{\min_{\substack{\mathbf{v}\in \mathbf{H}(\mathrm{div},\Omega)\\ \nabla\cdot\mathbf{v}=f}} \|\nabla u_\ell + \mathbf{v}\|^2}_{\text{constrained distance to } \mathbf{H}(\mathrm{div},\Omega)} = \underbrace{\max_{\substack{v\in H_0^1(\Omega)\\ \|\nabla v\|=1}} \{(f,v)-(\nabla u_\ell,\nabla v)\}^2}_{\text{dual norm of the PDE residual}}.$$

Comments

- It is enough to choose suitable (discrete, piecewise polynomial) $\sigma_\ell \in \mathbf{H}(\mathrm{div},\Omega)$ with $\nabla\cdot\sigma_\ell = f$ to get the guaranteed upper bound $\|\nabla(u-u_\ell)\| \le \|\nabla u_\ell + \sigma_\ell\|$.

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dual norm of the **PDE residual**

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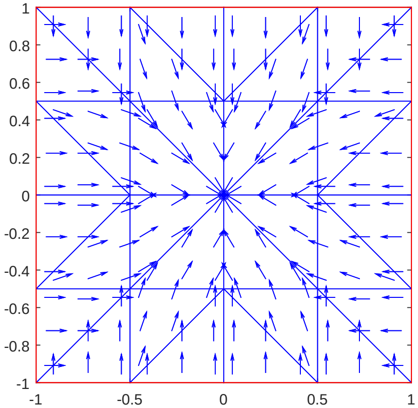
Equilibrated flux reconstruction: $-\nabla u_\ell \in \mathcal{RT}_{p-1}(\mathcal{T}_\ell)$, $p \geq 1$, $f \in L^2(\Omega)$



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

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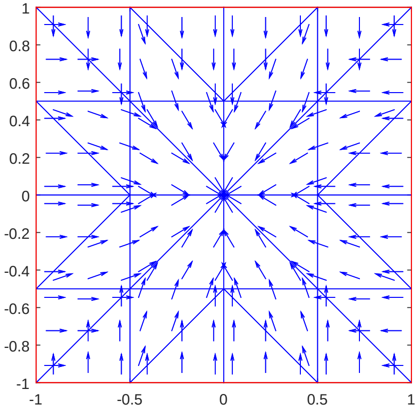

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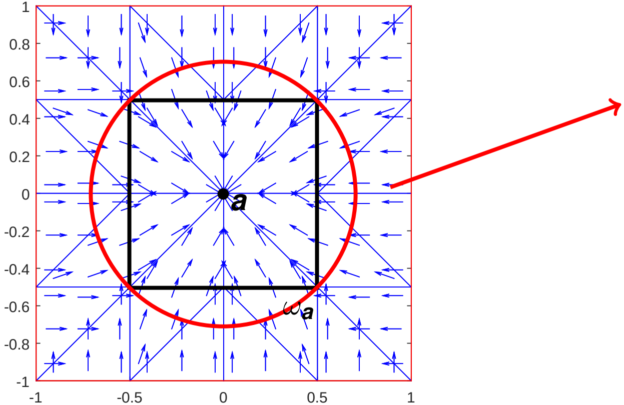

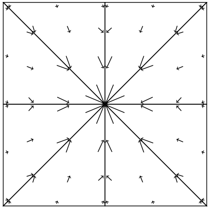

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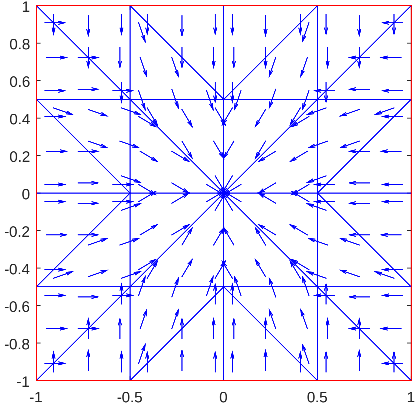
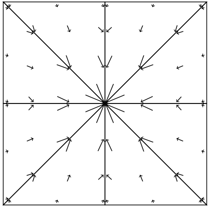
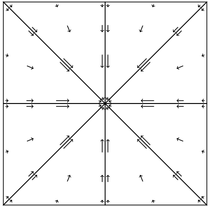




$-\psi_{\boldsymbol{a}} \nabla u_\ell$

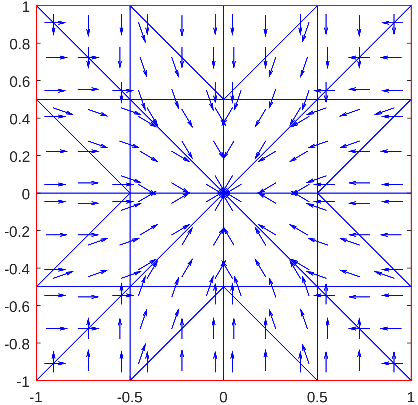


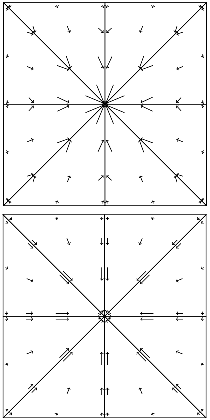
$\boldsymbol{\sigma}_\ell^{\boldsymbol{a}}$

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

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

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





$-\psi_{\boldsymbol{a}} \nabla u_\ell$

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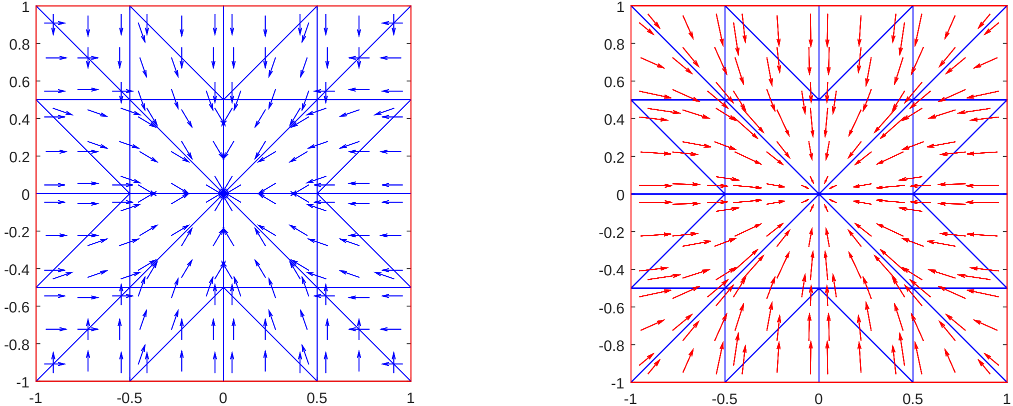

Flux $-\nabla u_\ell \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot(-\nabla u_\ell) \neq f$ Equilibrated flux rec. $\boldsymbol{\sigma}_\ell$

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

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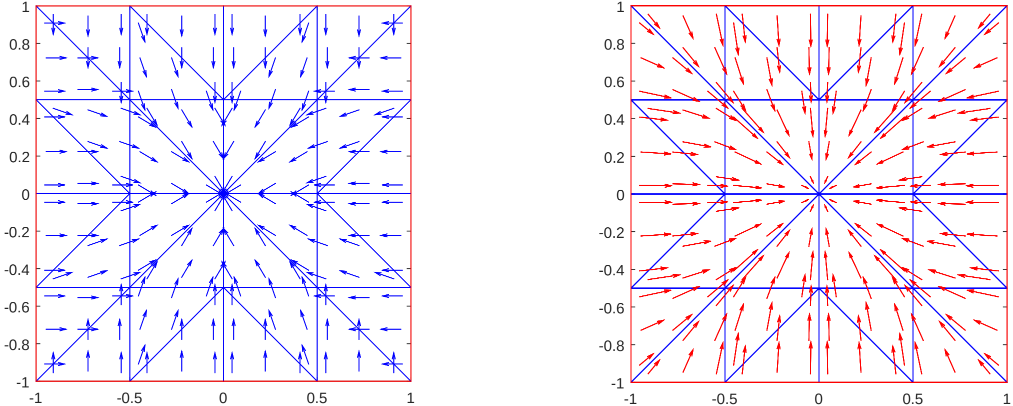

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Flux reconstructions (residual liftings)

Definition (Discretization residual lifting $\boldsymbol{\sigma}^{k,i}_{\mathrm{disc},\ell}$)

For each $\boldsymbol{a} \in \mathcal{V}_\ell$, solve the local constrained minimization pb

$$\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{disc},\ell} := \arg \min_{\substack{\boldsymbol{v}_\ell \in \boldsymbol{\mathcal{RT}}_p(\mathcal{T}^{\boldsymbol{a}}) \cap \boldsymbol{H}_0(\mathrm{div},\omega_{\boldsymbol{a}}) \\ \nabla\cdot\boldsymbol{v}_\ell = \Pi_p((f - r^{k,i}_\ell)\psi_{\boldsymbol{a}} - (\boldsymbol{A}^{k-1}_\ell \nabla u^{k,i}_\ell - \boldsymbol{b}^{k-1}_\ell)\cdot\nabla\psi_{\boldsymbol{a}})}} \|\psi_{\boldsymbol{a}}(\boldsymbol{A}^{k-1}_\ell \nabla u^{k,i}_\ell - \boldsymbol{b}^{k-1}_\ell) + \boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}}$$

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Algebraic error flux reconstruction, two-level setting

Definition (Coarse grid solve)

Find $\rho_{\mathrm{alg},0}^{k,i} \in \mathcal{P}_1(\mathcal{T}_0) \cap H_0^1(\Omega)$ s.t.

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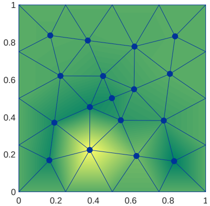
- $\mathcal{P}_1$ FE solve on coarse mesh $\mathcal{T}_0$



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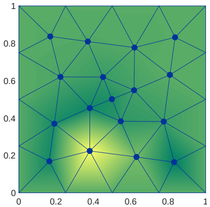

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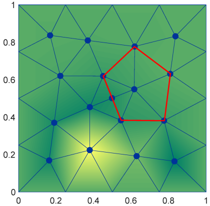

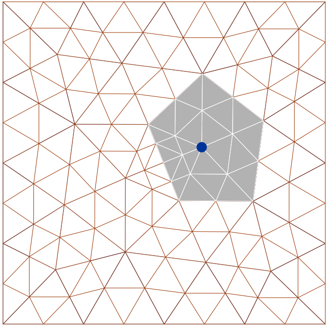

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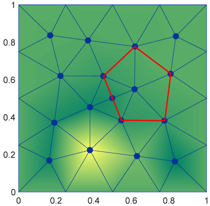
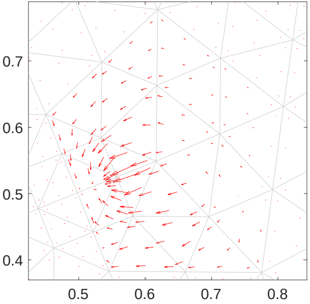


local alg. error flux reconstruction, $\sigma_{h,\mathrm{alg}}^{\mathrm{a},i}$



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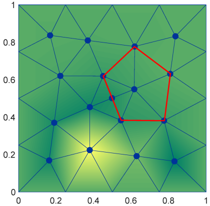
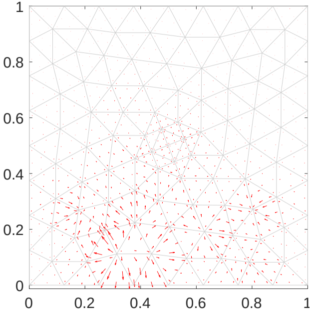
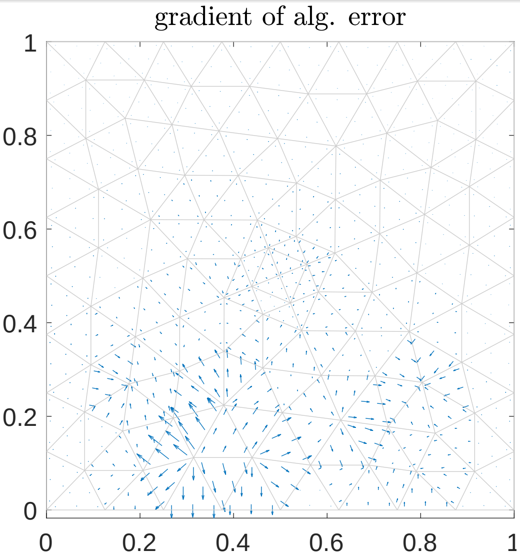
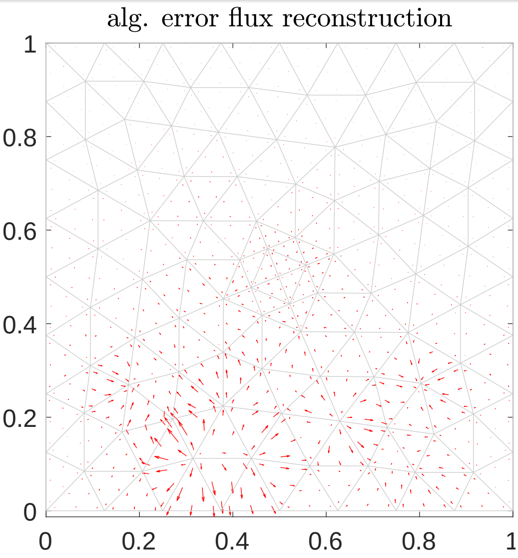


alg. error flux reconstruction



Algebraic error flux reconstruction, two-level setting





A posteriori error estimate distinguishing the error components

Theorem (A posteriori error estimate)

Let $u_\ell^{k,i} \in V_\ell$ *be given.*

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$$|||u - u_\ell^{k,i}||| \le \underbrace{\|a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i} + \boldsymbol{\sigma}_\ell^{k,i}\|}_{\eta\left(u_\ell^{k,i}\right)}$$

$$\le \underbrace{\|a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i} + \boldsymbol{\sigma}_{\mathrm{disc},\ell}^{k,i}\|}_{\eta_{\mathrm{disc}}\left(u_\ell^{k,i}\right)} + \underbrace{\|\boldsymbol{\sigma}_{\mathrm{lin},\ell}^{k,i}\|}_{\eta_{\mathrm{lin}}\left(u_\ell^{k,i}\right)} + \underbrace{\|\boldsymbol{\sigma}_{\mathrm{alg},\ell}^{k,i}\|}_{\eta_{\mathrm{alg}}\left(u_\ell^{k,i}\right)}.$$

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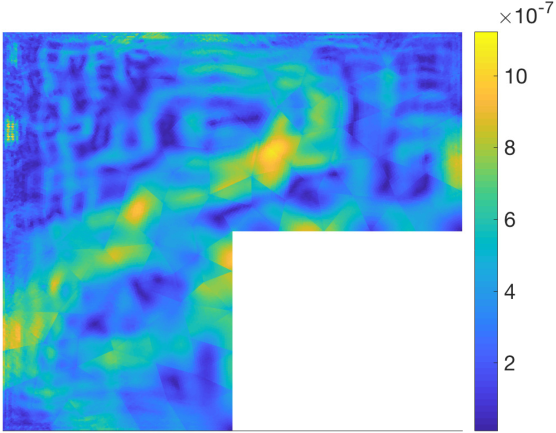
&\le \underbrace{\|a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i} + \boldsymbol{\sigma}_{\text{disc},\ell}^{k,i}\|}_{\eta_{\text{disc}}\left(u_\ell^{k,i}\right)} + \underbrace{\|\boldsymbol{\sigma}_{\text{lin},\ell}^{k,i}\|}_{\eta_{\text{lin}}\left(u_\ell^{k,i}\right)} + \underbrace{\|\boldsymbol{\sigma}_{\text{alg},\ell}^{k,i}\|}_{\eta_{\text{alg}}\left(u_\ell^{k,i}\right)}.
\end{aligned}$$

Moreover, the estimates are **locally efficient** *and* **robust** *with respect to the* **strength of nonlinearities**

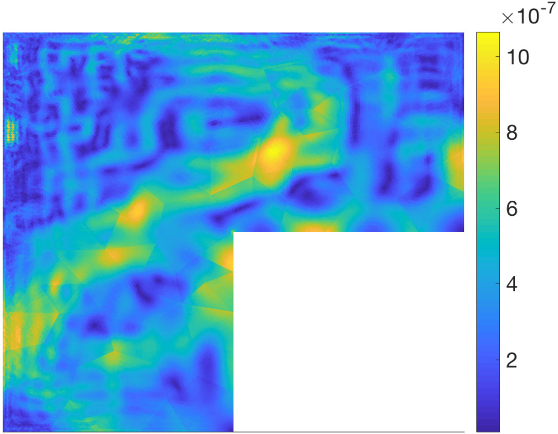
$$\eta_K\left(u_\ell^{k,i}\right) \le C_{\text{eff}} |||u - u_\ell^{k,i}|||_{\omega_K} \qquad \forall K \in \mathcal{T}_\ell, \qquad C_{\text{eff}} \text{ independent of } \frac{a_{\text{c}}}{a_{\text{m}}}.$$

Outline

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



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



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

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

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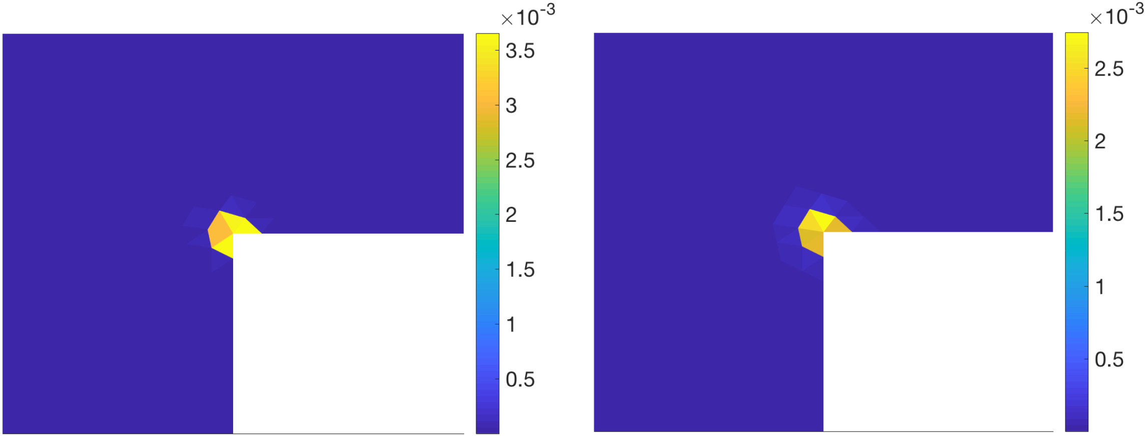

Estimated total errors $\eta_K(u_\ell^i)$ Exact total errors $\|\nabla(u - u_\ell^i)\|_K$

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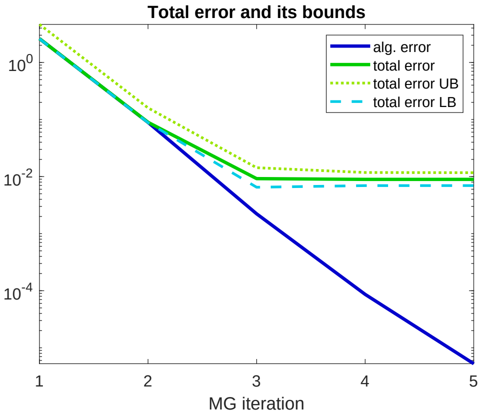
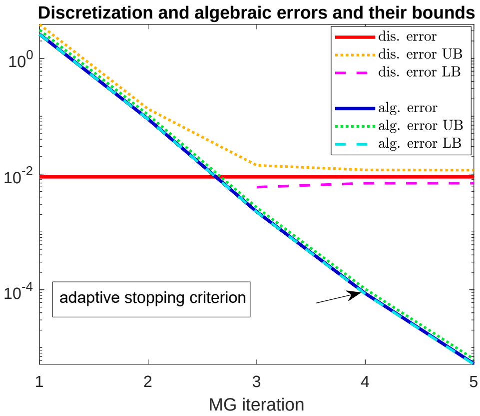


Total error



Error components and adaptive st. crit.

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

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

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

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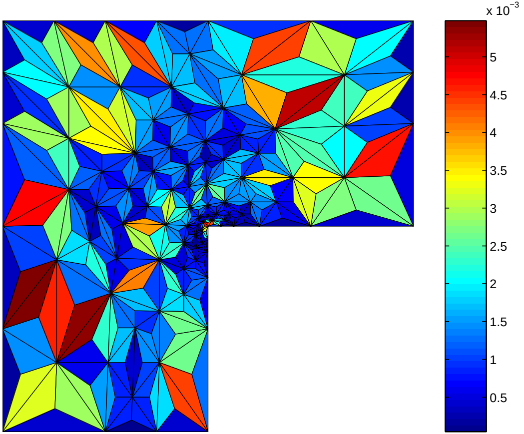
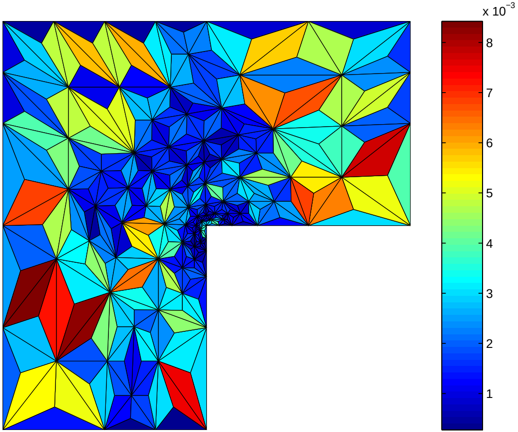


Estimated errors $\eta_K(u_\ell^{k,i})$



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

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

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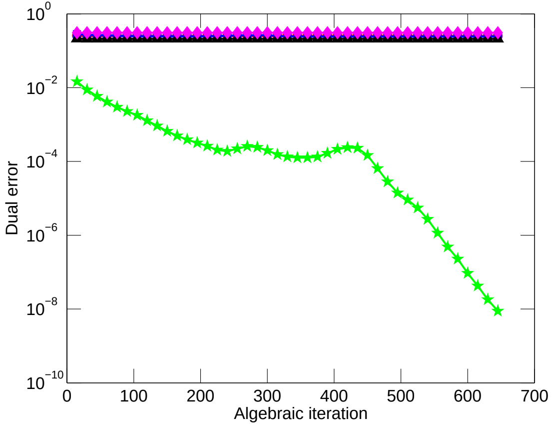
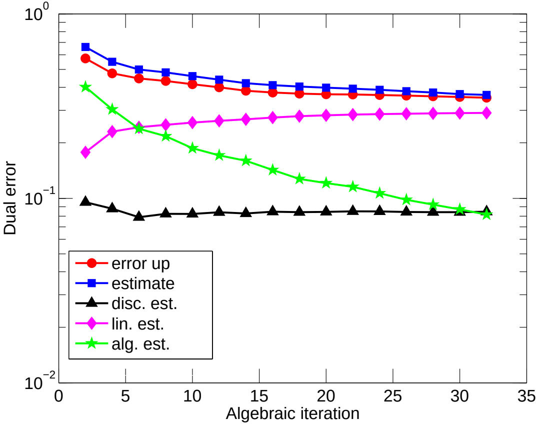


Newton



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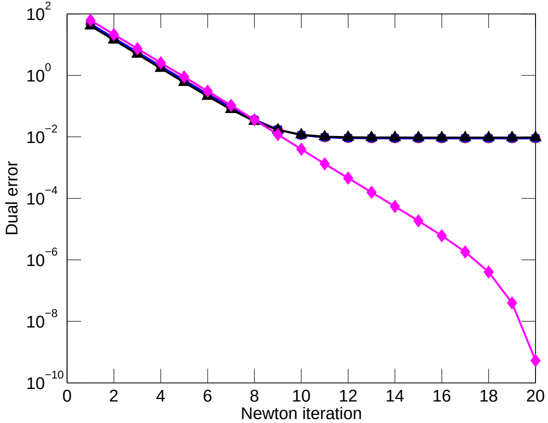

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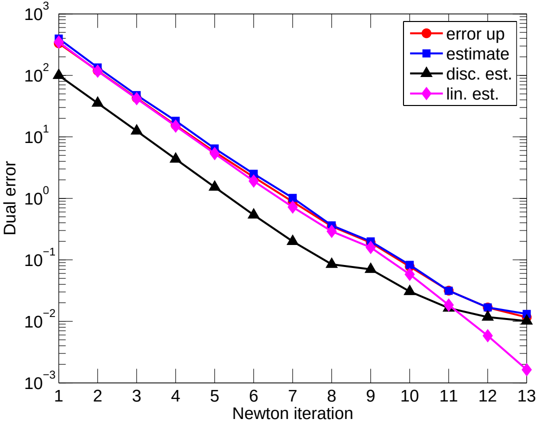

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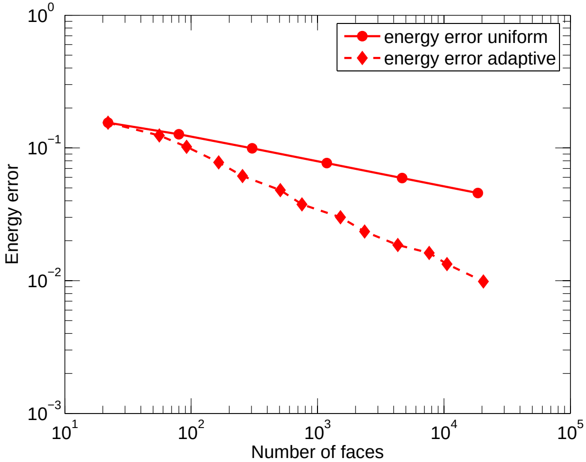
Optimal decay rate wrt degrees of freedom & computational cost



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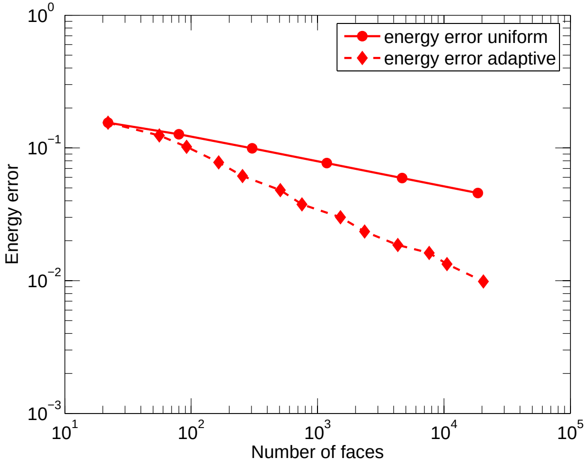

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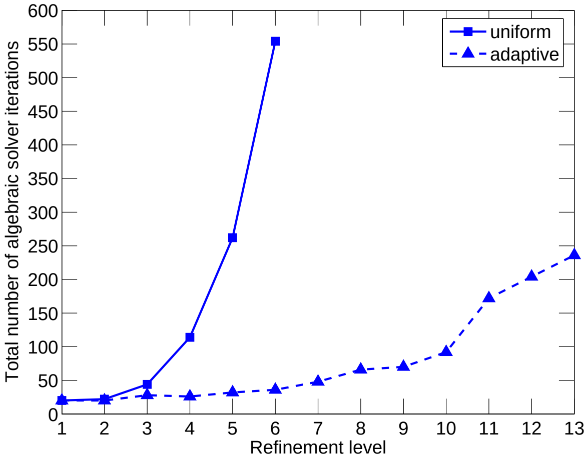

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Thank you for your attention!

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