

Guaranteed and robust a posteriori error estimates for the reaction–diffusion and heat equations

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The Inria logo is written in a red, cursive script.

Outline

- 1 Introduction
- 2 The reaction–diffusion equation
 - Equivalence between error and dual norm of the residual
 - Guaranteed upper bound
 - Local efficiency and robustness
 - Numerical experiments
- 3 The heat equation
 - Equivalence between error and dual norm of the residual
 - High-order discretization & Radau reconstruction
 - Guaranteed upper bound
 - Local space-time efficiency and robustness
 - Numerical experiments
- 4 Conclusions and future directions

An optimal a posteriori estimate for steady-state problems

Guaranteed upper bound

- $\|u - u_h\|_{?,\Omega}^2 \leq \sum_{K \in \mathcal{T}} \eta_K(u_h)^2$
- no undetermined constant: **error control**

Global efficiency

- $\sum_{K \in \mathcal{T}} \eta_K(u_h)^2 \leq C_{\text{eff}} \|u - u_h\|_{?,\Omega}^2$
- mathematical **equivalence** between the unknown **error** and known **estimate**

Robustness

- C_{eff} independent of the domain Ω , solutions u, u_h , **data**, meshes size and form

Small evaluation cost

- estimators $\eta_K(u_h)$ can be **evaluated cheaply** (locally) from u_h

Asymptotic exactness

- $\sum_{K \in \mathcal{T}} \eta_K(u_h)^2 / \|u - u_h\|_{?,\Omega}^2 \searrow 1$
- overestimation factor goes to one with increasing effort

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Local efficiency

- $\eta_K(u_h) \leq C_{\text{eff}} \|u - u_h\|_{?, \text{neighbors of } K}$
- **local** error lower bound (optimal space **mesh refinement**)

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Previous results (reaction–diffusion equation)

- Verfürth (1998) / Ainsworth and Babuška (1999): **robustness** wrt. singular perturbation
- Grosman (2006): robustness & **anisotropic meshes**, polynomial degree $p = 1$
- Cheddadi, Fučík, Prieto, Vohralík (2009): **guaranteed upper bound** & robustness, $p = 1$
- Ainsworth and Vejchodský (2011, 2014): **guaranteed upper bound** & robustness but requires submesh (complicated), (2019) without submesh (simple but with restrictions), $p = 1$
- Kopteva (2017): guaranteed upper bound, robustness, & **anisotropic meshes**, $p = 1$

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The reaction–diffusion equation

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Find $u : \Omega \subset \mathbb{R}^d \rightarrow \mathbb{R}$, $d \geq 1$, such that

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

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

- $f \in L^2(\Omega)$, $\varepsilon > 0$, $\kappa \geq 0$ fixed real parameters

Singular perturbation

- $\varepsilon \ll \kappa$

Weak solution

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

$$\varepsilon^2 (\nabla u, \nabla v) + \kappa^2 (u, v) = (f, v) \quad \forall v \in H_0^1(\Omega)$$

Finite element approximation

Find $u_h \in V_h := \mathcal{P}_p(\mathcal{T}) \cap H_0^1(\Omega)$, $p \geq 1$, such that

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Equivalence between error and residual

Energy norm

$$\|\varphi\|^2 := \varepsilon^2 \|\nabla \varphi\|^2 + \kappa^2 \|\varphi\|^2 \quad \varphi \in H_0^1(\Omega)$$

$$\|\varphi\| = \sup_{v \in H_0^1(\Omega); \|v\|=1} \{\varepsilon^2 (\nabla \varphi, \nabla v) + \kappa^2 (\varphi, v)\} \quad \varphi \in H_0^1(\Omega)$$

Residual of $u_h \in H_0^1(\Omega)$

- $\mathcal{R}(u_h) \in H^{-1}(\Omega)$, the **misfit** of u_h in the **weak formulation**:

$$\langle \mathcal{R}(u_h), v \rangle := (f, v) - \varepsilon^2 (\nabla u_h, \nabla v) - \kappa^2 (u_h, v) \quad v \in H_0^1(\Omega)$$

- dual norm of the residual

$$\|\mathcal{R}(u_h)\|_{H^{-1}(\Omega)} := \sup_{v \in H_0^1(\Omega); \|v\|=1} \langle \mathcal{R}(u_h), v \rangle$$

Energy error

$$\|(u - u_h)\| = \sup_{v \in H_0^1(\Omega); \|v\|=1} \{(f, v) - \varepsilon^2 (\nabla u_h, \nabla v) - \kappa^2 (u_h, v)\} = \|\mathcal{R}(u_h)\|_{H^{-1}(\Omega)}$$

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Energy error is the dual norm of the residual

$$\|u - u_h\|_{\varepsilon, \kappa} = \sup_{v \in H_0^1(\Omega); \|v\|=1} \{\varepsilon^2 (\nabla(u - u_h), \nabla v) + \kappa^2 (u - u_h, v)\} = \|\mathcal{R}(u_h)\|_{H^{-1}(\Omega)}$$

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Upper bound: motivation

Bound on the residual

- let $\sigma_h \in \mathbf{H}(\text{div}, \Omega)$ and $\phi_h \in L^2(\Omega)$ be such that $\nabla \cdot \sigma_h + \kappa^2 \phi_h = f$

- σ_h : **equilibrated flux reconstruction**, $\approx -\varepsilon^2 \nabla U$

- ϕ_h : **potential reconstruction**, $\approx U$

- Green theorem $(\nabla \cdot \sigma_h, v) + (\sigma_h, \nabla v) = 0$ for $v \in H_0^1(\Omega)$:

$$\begin{aligned} \langle \mathcal{R}(u_h), v \rangle &= (f, v) - \varepsilon^2 (\nabla u_h, \nabla v) - \kappa^2 (u_h, v) \\ &= -(\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h, \varepsilon \nabla v) - (\kappa(u_h - \phi_h), \kappa v) \\ &\leq [\|\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h\|^2 + \|\kappa(u_h - \phi_h)\|^2]^{\frac{1}{2}} \|v\| \end{aligned}$$

- then

$$\|(u - u_h)\| = \|\mathcal{R}(u_h)\|_{H^{-1}(\Omega)} \leq [\|\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h\|^2 + \|\kappa(u_h - \phi_h)\|^2]^{\frac{1}{2}}$$

- how to obtain suitable practical (inexpensive) σ_h and ϕ_h ?
- counter-example** where $\|\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h\|$ can largely overestimate the error

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Bound on the residual

- let $\sigma_h \in \mathbf{H}(\text{div}, \Omega)$ and $\phi_h \in L^2(\Omega)$ be such that $\nabla \cdot \sigma_h + \kappa^2 \phi_h = f$
- σ_h : **equilibrated flux reconstruction**, $\approx -\varepsilon^2 \nabla u$
- ϕ_h : **potential reconstruction**, $\approx u$
- Green theorem $(\nabla \cdot \sigma_h, v) + (\sigma_h, \nabla v) = 0$ for $v \in H_0^1(\Omega)$:

$$\begin{aligned} \langle \mathcal{R}(u_h), v \rangle &= (f, v) - \varepsilon^2 (\nabla u_h, \nabla v) - \kappa^2 (u_h, v) \\ &= -(\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h, \varepsilon \nabla v) - (\kappa(u_h - \phi_h), \kappa v) \\ &\leq [\|\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h\|^2 + \|\kappa(u_h - \phi_h)\|^2]^{\frac{1}{2}} \|v\| \end{aligned}$$

- then

$$\|(u - u_h)\| = \|\mathcal{R}(u_h)\|_{H^{-1}(\Omega)} \leq [\|\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h\|^2 + \|\kappa(u_h - \phi_h)\|^2]^{\frac{1}{2}}$$

- how to obtain suitable **practical** (inexpensive) σ_h and ϕ_h ?
- **counter-example** where $\|\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h\|$ can largely overestimate the error

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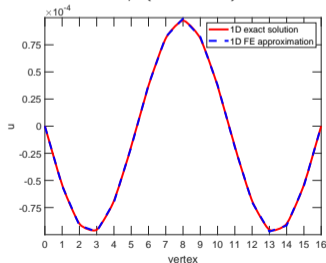
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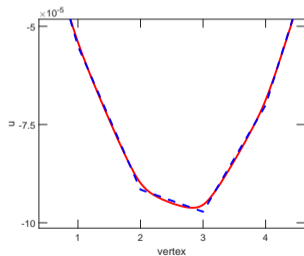
Counter-example ($-\varepsilon^2 \Delta u + \kappa^2 u = f$ in Ω , $u = 0$ on $\partial\Omega$)

Data

- $\Omega := (-1/2, 1/2)$, $d = 1$
- odd integer m
- f : piecewise affine Lagrange int. of $\cos(m\pi x)$
- uniform mesh \mathcal{T} with $2N = (m+1)^2$ intervals
- $h = 1/(m+1)^2$



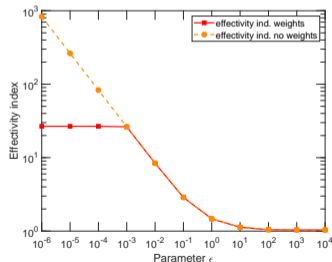
$$\varepsilon = 1, \kappa = 10^2, m = 3$$



detailed view

Finite element approximation

- $V_h := \mathcal{P}_1(\mathcal{T}) \cap H_0^1(\Omega)$
- $\mu_h := \frac{6}{2 + \cos(m\pi h)} \frac{1 - \cos(m\pi h)}{h^2}$
- $u_h = (\varepsilon^2 \mu_h + \kappa^2)^{-1} f$



$$\kappa = 10^2, m = 3, \text{ eff. ind.}$$

Equilibrated flux and potential reconstructions

Definition (Flux σ_h and potential ϕ_h)

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

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

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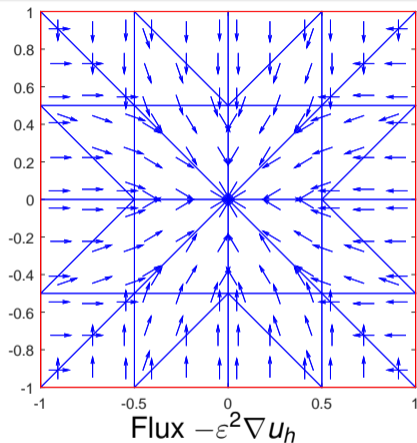
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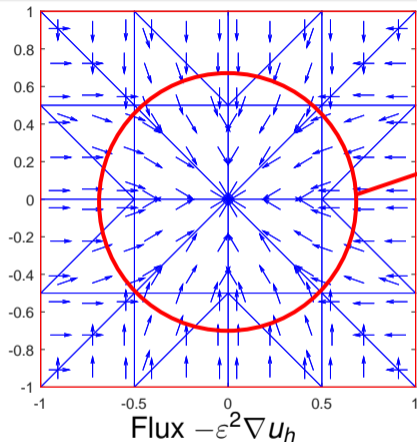
Equilibrated flux reconstruction



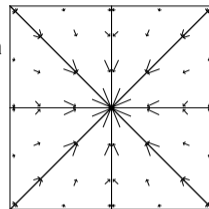
$$-\varepsilon^2 \nabla u_h \in \mathcal{RTN}_p(\mathcal{T}), f \in L^2(\Omega)$$

$$(f, \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} - \varepsilon^2 (\nabla u_h, \nabla \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} - \kappa^2 (u_h, \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} = 0 \quad \forall \mathbf{a} \in \mathcal{V}^{\text{int}}$$

Equilibrated flux reconstruction



vertex patch \mathcal{T}^a

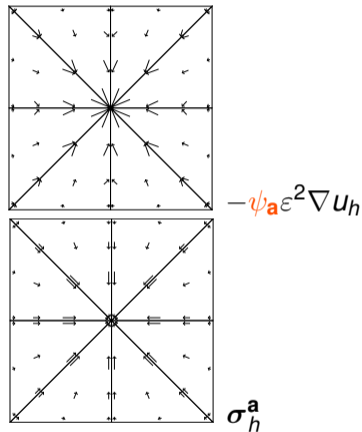
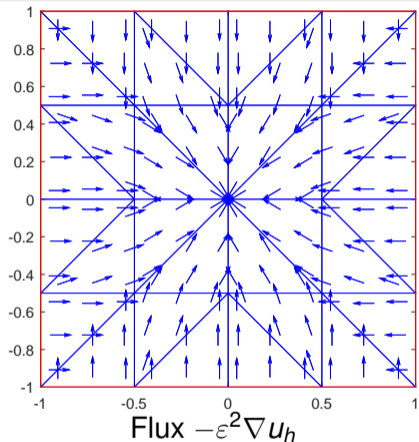


$$-\psi_a \varepsilon^2 \nabla u_h$$

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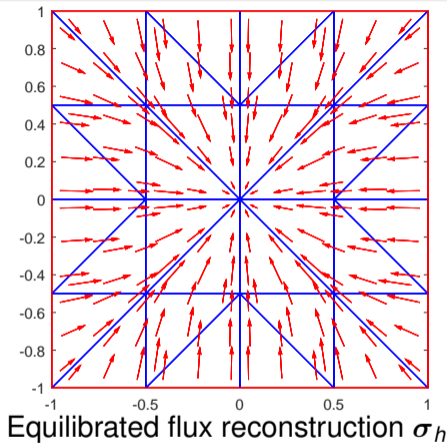
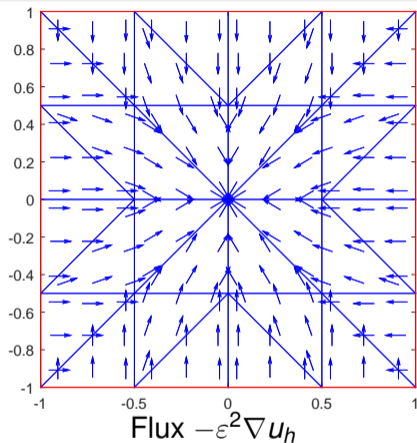
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$$\underbrace{-\epsilon^2 \nabla u_h \in \mathcal{RTN}_p(T), f \in L^2(\Omega)}_{(f, \psi_a)_{\omega_a} - \epsilon^2 (\nabla u_h, \nabla \psi_a)_{\omega_a} - \kappa^2 (u_h, \psi_a)_{\omega_a} = 0 \quad \forall a \in \mathcal{V}^{\text{int}}} \rightarrow \sigma_h \in \mathcal{RTN}_p(T) \cap \mathbf{H}(\text{div}, \Omega), \nabla \cdot \sigma_h + \kappa^2 \phi_h = \Pi_h f$$

Guaranteed a posteriori error estimate

Theorem (Guaranteed a posteriori error estimate)

Let u be the weak solution and let $u_h \in V_h$ be its finite element approximation. Let $\sigma_h \in \mathcal{RTN}_p(\mathcal{T}) \cap \mathbf{H}(\operatorname{div}, \Omega)$ and $\phi_h \in \mathcal{P}_p(\mathcal{T})$ be the flux and potential reconstructions. Then

$$\|u - u_h\|^2 \leq \sum_{K \in \mathcal{T}} [w_K \|\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h\|_K + \|\kappa(u_h - \phi_h)\|_K + \tilde{w}_K \|f - \Pi_h f\|_K]^2$$

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- guaranteed upper bound on the unknown error
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Let f be a piecewise polynomial for simplicity. Then, for all $K \in \mathcal{T}$,

$$w_K \|\varepsilon \nabla u_h + \varepsilon^{-1} \sigma_h\|_K + \|\kappa (u_h - \phi_h)\|_K \leq C_{\text{eff}} \|u - u_h\|_{\omega_K},$$

where the constant C_{eff} only depends on the space dimension d , the shape-regularity constant $\vartheta_{\mathcal{T}}$ of the mesh \mathcal{T} , and on the polynomial degree p of u_h .

Comments

- the computable elementwise estimators are **local lower bounds** for the unknown error
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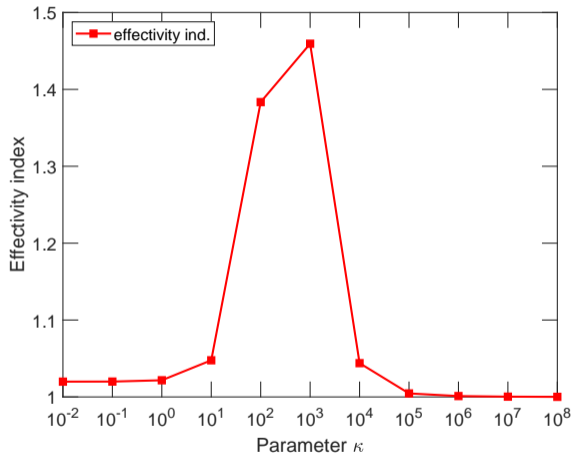
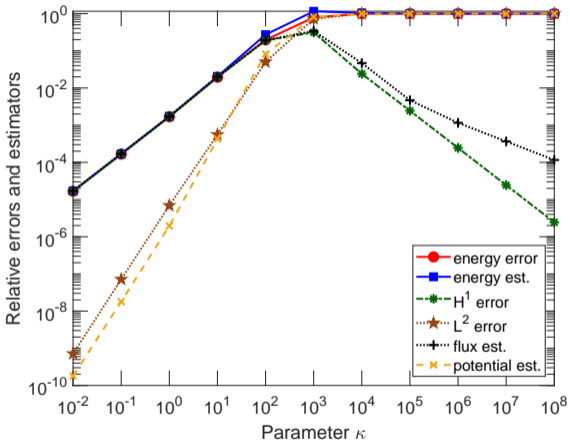
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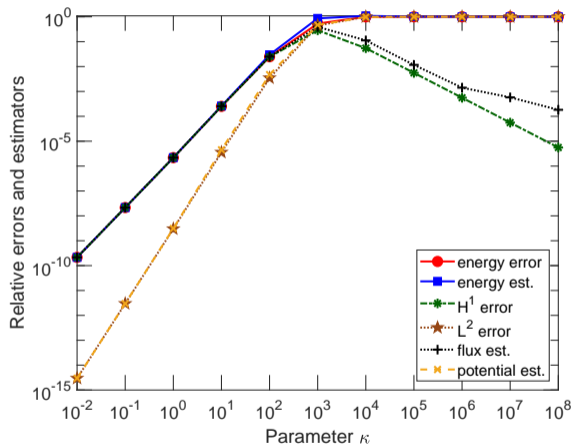


Relative energy errors and estimates

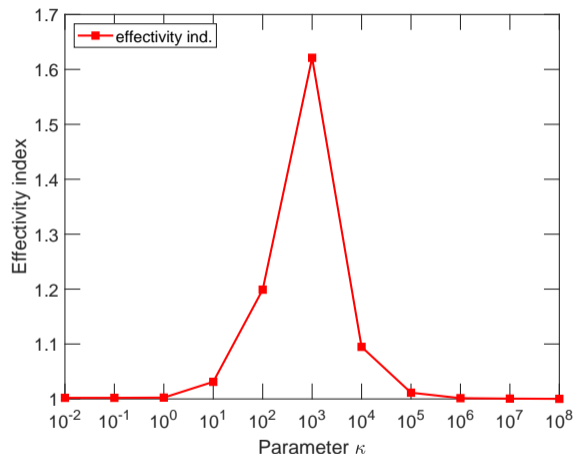
Effectivity indices $\eta(u_h)/\|u - u_h\|$



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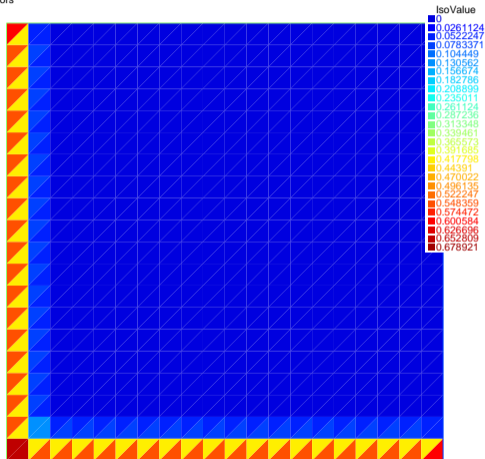
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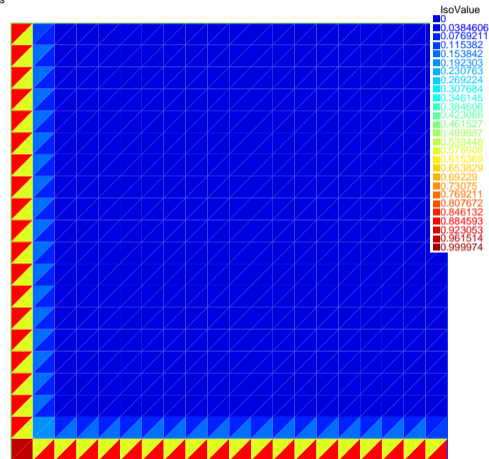
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energy errors



Exact en. error on each mesh element

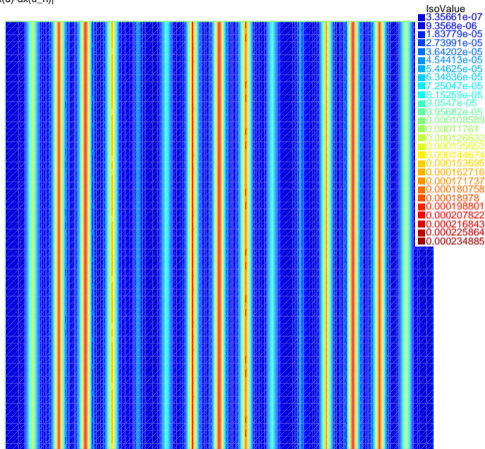
estimators



Estimated en. error on each mesh element

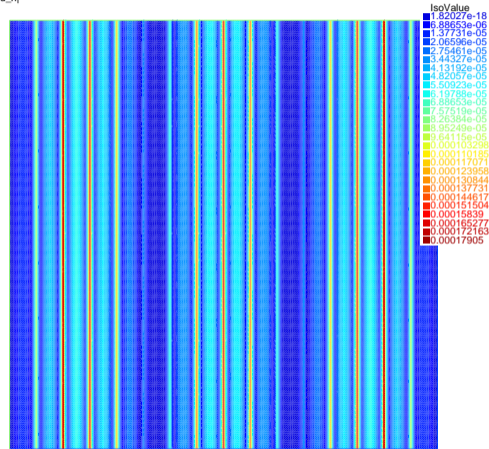
Counter-example with $\varepsilon = 1$, $\kappa = 10^2$, $m = 3$, $p = 1$

$\text{epsilon}^*|\text{dx}(u)-\text{dx}(u_h)|$



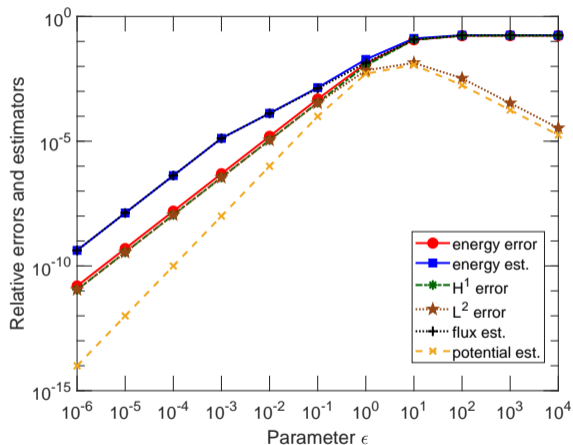
Pointwise H^1 -seminorm errors

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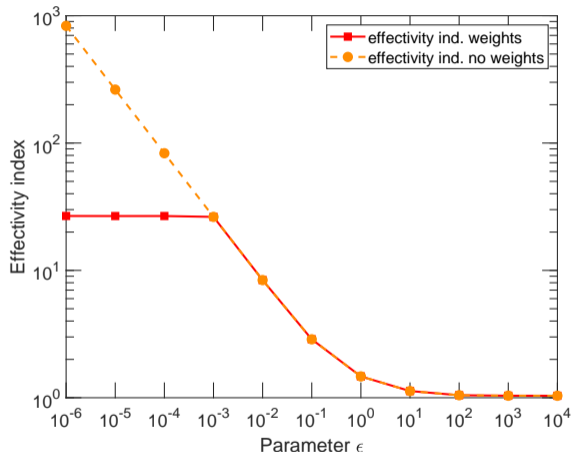


Pointwise $\kappa \times L^2$ -norm errors

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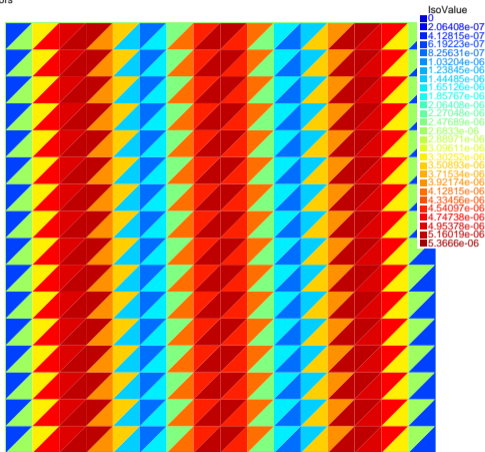
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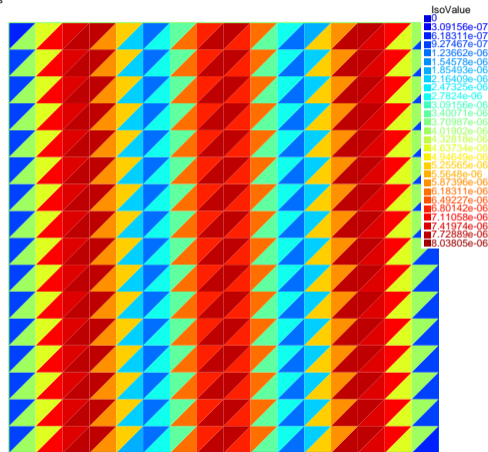
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The heat equation ($f \in L^2(0, T; L^2(\Omega))$, $u_0 \in L^2(\Omega)$)

The heat equation

$$\begin{aligned}\partial_t u - \Delta u &= f && \text{in } \Omega \times (0, T), \\ u &= 0 && \text{on } \partial\Omega \times (0, T), \\ u(0) &= u_0 && \text{in } \Omega\end{aligned}$$

Spaces

$$X := L^2(0, T; H_0^1(\Omega)),$$

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Weak solution

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

$$\int_0^T \langle \partial_t u, v \rangle + (\nabla u, \nabla v) dt = \int_0^T (f, v) dt \quad \forall v \in X$$

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Guaranteed upper bound

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

Local efficiency

- $\eta_K^n(u_{h\tau}) \leq C_{\text{eff}} \|u - u_{h\tau}\|_{?,\text{neighbors of } K \times (t^{n-1}, t^n)}$
- optimal space-time mesh refinement
- **local** in **time** and in **space** error lower bound

Robustness

- C_{eff} independent of data, domain Ω , **final time** T , meshes, solutions u , $u_{h\tau}$, **polynomial degrees** of $u_{h\tau}$ in space p and in time q

Small evaluation cost

- estimators $\eta_K^n(u_{h\tau})$ can be **evaluated cheaply** (locally) **from** $u_{h\tau}$

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- Verfürth (2003) (cf. also Bergam, Bernardi, and Mghazli (2005)), work with the Y norm:
 - ✓ upper bound $\|u - u_{h\tau}\|_Y^2 \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}^n} \eta_K^n(u_{h\tau})^2$
 - ✓ efficiency $\sum_{K \in \mathcal{T}^n} \eta_K^n(u_{h\tau})^2 \leq C \|u - u_{h\tau}\|_{Y(I_h)}^2$
 - ✓ **robustness** with respect to the **final time** T , no link $h \leftrightarrow \tau$
 - ✗ efficiency **local in time** but **global in space**
- Makridakis and Nochetto (2006): **Radau reconstruction**
- Ern and Vohralík (2010): **unified framework** for different spatial discretizations (FEs, NCFEs, DGs, MFEs, FVs)

Previous results

- Picasso / Verfürth (1998), work with the energy norm X :
 - ✓ upper bound $\|u - u_{h\tau}\|_X^2 \leq C \sum_{n=1}^N \sum_{K \in \mathcal{T}^n} \eta_K^n(u_{h\tau})^2$
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Equivalence between error and residual

The heat equation

$$\begin{aligned}\partial_t u - \Delta u &= f && \text{in } \Omega \times (0, T), \\ u &= 0 && \text{on } \partial\Omega \times (0, T), \\ u(0) &= u_0 && \text{in } \Omega\end{aligned}$$

Spaces

$$X := L^2(0, T; H_0^1(\Omega)),$$

$$\|v\|_X^2 := \int_0^T \|\nabla v\|^2 dt,$$

$$Y := L^2(0, T; H_0^1(\Omega)) \cap H^1(0, T; H^{-1}(\Omega)),$$

$$\|v\|_Y^2 := \int_0^T \|\partial_t v\|_{H^{-1}(\Omega)}^2 + \|\nabla v\|^2 dt + \|v(T)\|^2$$

Weak solution

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

$$\int_0^T \langle \partial_t u, v \rangle + (\nabla u, \nabla v) dt = \int_0^T (f, v) dt \quad \forall v \in X$$

Equivalence between error and residual

Theorem (Parabolic inf–sup identity)

For every $\varphi \in Y$, we have

$$\|\varphi\|_Y^2 = \left[\sup_{v \in X, \|v\|_X=1} \int_0^T \langle \partial_t \varphi, v \rangle + (\nabla \varphi, \nabla v) dt \right]^2 + \|\varphi(0)\|^2.$$

Residual of $u_{hT} \in Y$

- $\mathcal{R}(u_{hT}) \in X'$, the misfit of u_{hT} in the weak formulation:

$$\langle \mathcal{R}(u_{hT}), v \rangle := \int_0^T (f, v) - \langle \partial_t u_{hT}, v \rangle - (\nabla u_{hT}, \nabla v) dt \quad v \in X$$

- dual norm of the residual

$$\|\mathcal{R}(u_{hT})\|_{X'} := \sup_{v \in X, \|v\|_X=1} \langle \mathcal{R}(u_{hT}), v \rangle$$

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

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

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

Proof.

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

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



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Approximate solution and Radau reconstruction



Approximate solution

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

Radau reconstruction

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

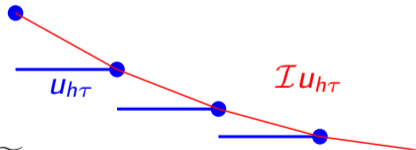
$$\int_{I_n} (\partial_t \mathcal{I}u_{h\tau}, v_{h\tau}) + (\nabla \mathcal{I}u_{h\tau}, \nabla v_{h\tau}) \, dt = \int_{I_n} (f, v_{h\tau}) \, dt \quad \forall v_{h\tau} \in \mathcal{Q}_{q_n}(I_n; V_h^n)$$

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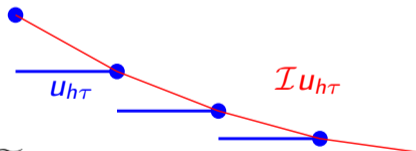
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Results in the Y norm

Theorem (Guaranteed upper bound in the Y norm)

Suppose no data oscillation (f and u_0 piecewise polynomial). Then, for any $\sigma_{h\tau} \in L^2(0, T; \mathbf{H}(\text{div}, \Omega))$ with $\nabla \cdot \sigma_{h\tau} = f - \partial_t \mathcal{I}u_{h\tau}$, there holds

$$\|u - \mathcal{I}u_{h\tau}\|_Y^2 \leq \int_0^T \|\sigma_{h\tau} + \nabla \mathcal{I}u_{h\tau}\|^2 dt.$$

Proof of the upper bound

Proof.

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

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

- Green theorem

$$\int_0^T (\sigma_{h\tau}, \nabla \mathcal{I}u_{h\tau}) + (\nabla \cdot \sigma_{h\tau}, \mathcal{I}u_{h\tau}) dt = 0$$

- residual definition, Cauchy–Schwarz inequality:

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

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Equilibrated flux reconstruction

Definition (Equilibrated flux reconstruction)

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

$$\sigma_{h\tau}^{\mathbf{a},n} := \arg \min_{\mathbf{v}_h \in \mathbf{V}_{h\tau}^{\mathbf{a},n}} \int_{I_n} \|\mathbf{v}_h + \psi_{\mathbf{a}} \nabla u_{h\tau}\|_{\omega_{\mathbf{a}}}^2 dt.$$

$$\nabla \cdot \mathbf{v}_h = \psi_{\mathbf{a}} (f - \partial_t \mathcal{I} u_{h\tau}) - \nabla \psi_{\mathbf{a}} \cdot \nabla u_{h\tau}$$

Then set

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

Comments

- ✓ satisfies $\sigma_{h\tau} \in L^2(0, T; \mathbf{H}(\text{div}, \Omega))$ with $\nabla \cdot \sigma_{h\tau} = f - \partial_t \mathcal{I} u_{h\tau}$
- ✗ a priori a local space-time problem, $\mathbf{V}_{h\tau}^{\mathbf{a},n} := \mathcal{Q}_{q_n}(I_n; \mathbf{V}_h^{\mathbf{a},n})$
- ✓ uncouples to q_n elliptic problems posed in $\mathbf{V}_h^{\mathbf{a},n}$

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Comments

- ✓ satisfies $\sigma_{h\tau} \in L^2(0, T; \mathbf{H}(\text{div}, \Omega))$ with $\nabla \cdot \sigma_{h\tau} = f - \partial_t \mathcal{I}u_{h\tau}$
- ✗ a priori a local space-time problem, $\mathbf{V}_{h\tau}^{\mathbf{a},n} := \mathcal{Q}_{q_n}(I_n; \mathbf{V}_h^{\mathbf{a},n})$
- ✓ uncouples to q_n elliptic problems posed in $\mathbf{V}_h^{\mathbf{a},n}$

Equilibrated flux reconstruction

Definition (Equilibrated flux reconstruction)

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

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

Then set

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

Comments

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Global efficiency \sim missing Galerkin orthogonality

Efficiency

There holds

$$\int_{I_n} \|\sigma_{h\tau} + \nabla \mathcal{I}u_{h\tau}\|_{\Omega}^2 dt \leq C_{\text{eff}}^2 \|u - \mathcal{I}u_{h\tau}\|_{Y(I_n)} \quad \forall 1 \leq n \leq N.$$

\times local-in-time but **global-in-space** only (as in Verfürth & Bergam–Bernardi–Mghazli)

Reason

\times $\mathcal{I}u_{h\tau}$ misses the Galerkin orthogonality:

$$\int_{I_n} (f, v_{h\tau}) - (\partial_t \mathcal{I}u_{h\tau}, v_{h\tau}) - (\nabla \mathcal{I}u_{h\tau}, \nabla v_{h\tau}) dt$$

if the misfit is known: $u_{h\tau} - \mathcal{I}u_{h\tau}$

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Guaranteed upper bound

A decisive trick

Define the final norm as

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

Theorem (Guaranteed upper bound)

Suppose no data oscillation (f and u_0 piecewise polynomial). Then there holds

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

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Local space-time efficiency and robustness

Local error contributions

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

Theorem (Local space-time efficiency and robustness)

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

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

Comments

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

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recall

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

Local space-time efficiency and robustness

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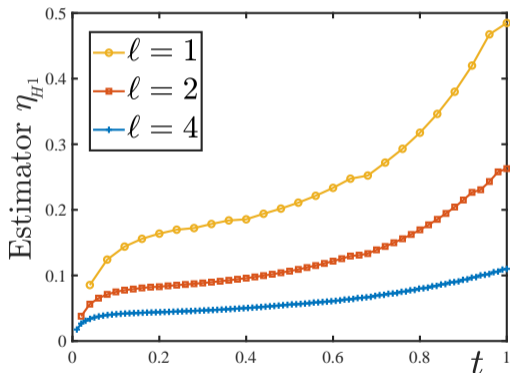
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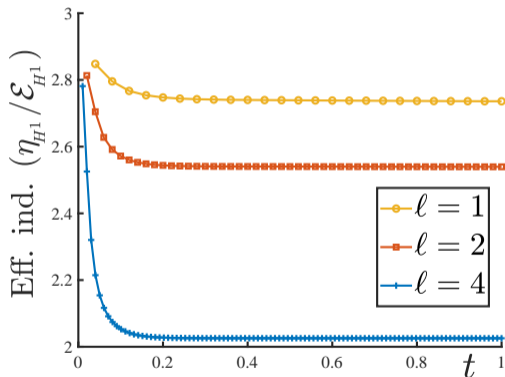
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Richards equation $\partial_t \mathcal{S}(u) - \nabla \cdot [\kappa(\mathcal{S}(u)) (\nabla u + \mathbf{g})] = f$ (results by K. Mitra, three levels of uniform space-time mesh refinement)

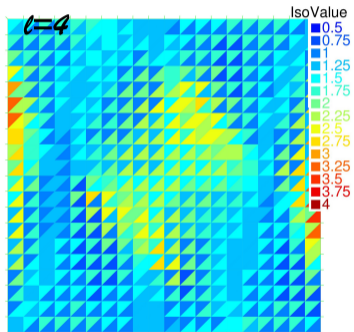
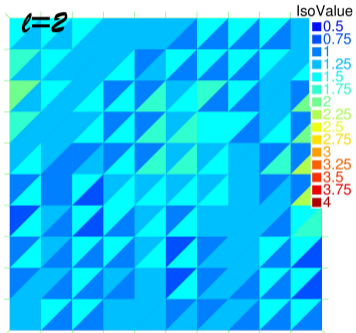
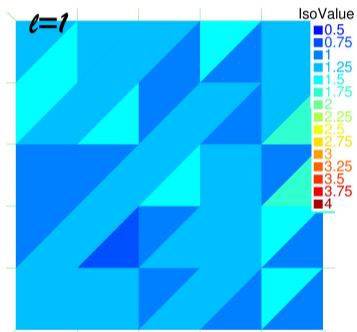


Estimators $\eta(u_{h\tau})$ as a function of T



Effectivity indices $\eta(u_{h\tau}) / \|u - u_{h\tau}\|_{\mathcal{E}_Y}$

Richards equation, local space-time effectivity indices



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- ✓ **guaranteed** upper bound
- ✓ **local efficiency** and **robustness** with respect to reaction and diffusion parameters
- ✓ **simple** form (no submesh), local estimators minimization, any polynomial degree

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- nonlinear and coupled problems

Conclusions and future directions

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- ERN A., SMEARS, I., VOHRALÍK M., Guaranteed, locally space-time efficient, and polynomial-degree robust a posteriori error estimates for high-order discretizations of parabolic problems, *SIAM J. Numer. Anal.* **55** (2017), 2811–2834.
- ERN A., SMEARS, I., VOHRALÍK M., Discrete p -robust $\mathbf{H}(\text{div})$ -liftings and a posteriori estimates for elliptic problems with H^{-1} source terms, *Calcolo* **54** (2017), 1009–1025.

Thank you for your attention!

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Thank you for your attention!

Fundamental results on a reference tetrahedron

Bounded right inverse of the divergence operator

- polynomial volume data
- Costabel & McIntosh (2010):

Let $K \in \mathcal{T}$ and $r \in \mathcal{P}_p(K)$. Then there exists $\xi_h \in \mathcal{RTN}_p(K)$ s.t. $\nabla \cdot \xi_h = r$ and

$$\|\xi_h\|_K \leq C \|r\|_{H^{-1}(K)} = \sup_{v \in H_0^1(K), \|\nabla v\|_K=1} (r, v)_K.$$

Polynomial extensions in $H(\text{div})$

- polynomial boundary data
- Demkowicz, Gopalakrishnan, Schöberl (2012):

Let $K \in \mathcal{T}$ and $r \in \mathcal{P}_p(\mathcal{F}_K)$ satisfying $(r, 1)_{\partial K} = 0$. Then there exists $\xi_h \in \mathcal{RTN}_p(K)$ s.t. $\xi_h \cdot \mathbf{n}_K = r$ on ∂K , $\nabla \cdot \xi_h = 0$ in K , and

$$\|\xi_h\|_K \leq C \|r\|_{H^{-1/2}(\partial K)} = \sup_{v \in H^1(K), \|\nabla v\|_K=1} (r, v)_{\partial K}.$$

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General result on a physical tetrahedron

Lemma ($\mathbf{H}(\text{div})$ polynomial extension on a tetrahedron)

Let $K \in \mathcal{T}$, $\mathcal{F}_K^N \subset \mathcal{F}_K$. Let $r \in \mathcal{P}_p(\mathcal{F}_K^N) \times \mathcal{P}_p(K)$, satisfying $\sum_{F \in \mathcal{F}_K} (r_F, \mathbf{1})_F = (r_K, \mathbf{1})_K$ if $\mathcal{F}_K^N = \mathcal{F}_K$. Then for $C = C(\kappa_K) > 0$,

$$\min_{\substack{\mathbf{v}_h \in \mathbf{RTN}_p(K) \\ \mathbf{v}_h \cdot \mathbf{n}_K = r_F \quad \forall F \in \mathcal{F}_K^N \\ \nabla \cdot \mathbf{v}_h = r_K}} \|\mathbf{v}_h\|_K \leq C \min_{\substack{\mathbf{v} \in \mathbf{H}(\text{div}, K) \\ \mathbf{v} \cdot \mathbf{n}_K = r_F \quad \forall F \in \mathcal{F}_K^N \\ \nabla \cdot \mathbf{v} = r_K}} \|\mathbf{v}\|_K .$$

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Context

$$\begin{aligned} -\Delta \zeta_K &= r_K && \text{in } K, \\ -\nabla \zeta_K \cdot \mathbf{n}_K &= r_F && \text{on all } F \in \mathcal{F}_K^N, \\ \zeta_K &= 0 && \text{on all } F \in \mathcal{F}_K \setminus \mathcal{F}_K^N. \end{aligned}$$

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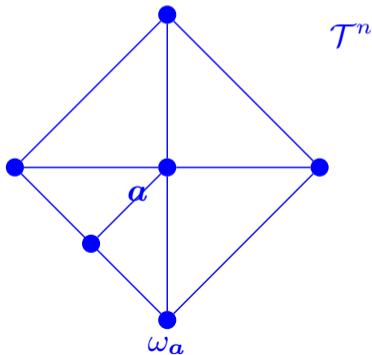
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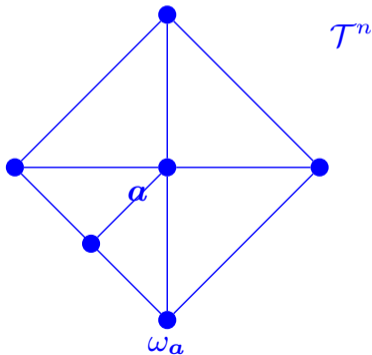
Stable broken $\mathbf{H}(\text{div})$ polynomial extension on a patch

- Braess, Pillwein, & Schöberl (2009), 2D
- Ern & V. (2016), 3D
- Ern, Smears, & V. (2017), 2-3D, patches with subrefinement



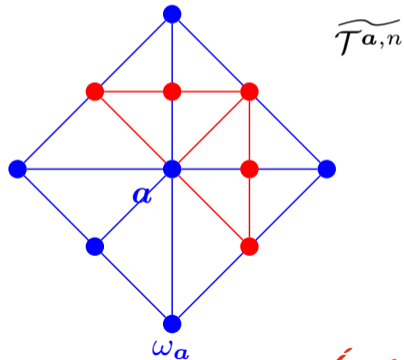
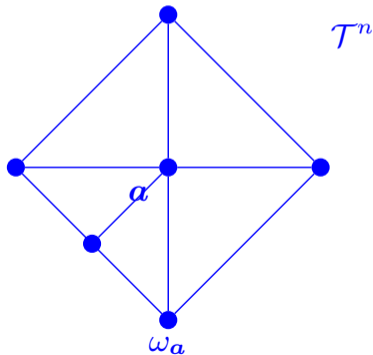
Stable broken $\mathbf{H}(\text{div})$ polynomial extension on a patch

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High-order space-time discretization

CG in space & DG in time

- p -degree **continuous** piecewise polynomials in **space**

$$V_h^n := \{v_h \in H_0^1(\Omega), v_h|_K \in \mathcal{P}_{p_K}(K) \quad \forall K \in \mathcal{T}^n\}$$

- q -degree **discontinuous** piecewise polynomials in **time**

$$\mathcal{Q}_{q_n}(I_n; V) := \{V\text{-valued polys of degree at most } q_n \text{ over } I_n\}$$

High-order discretization

Find $u_{h\tau}|_{I_n} \in \mathcal{Q}_{q_n}(I_n; V_h^n)$ with $u_{h\tau}(0) = \Pi_h u_0$ such that

$$\begin{aligned} & \int_{I_n} (\partial_t u_{h\tau}, v_{h\tau}) + (\nabla u_{h\tau}, \nabla v_{h\tau}) dt - ((u_{h\tau})_{n-1}, v_{h\tau}(t_{n-1}^+)) \\ &= \int_{I_n} (f, v_{h\tau}) dt \quad \forall v_{h\tau} \in \mathcal{Q}_{q_n}(I_n; V_h^n) \quad \forall 1 \leq n \leq N. \end{aligned}$$

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Augmented norm

- augment the norm: $\|v\|_{\mathcal{E}_Y}^2 := \|\mathcal{I}v\|_Y^2 + \|v - \mathcal{I}v\|_X^2$, $v \in Y + V_{h\tau}$

- $\mathcal{I}u = u \Rightarrow$

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

- we are adding to Y norm the time jumps in X norm (Schötzau–Wihler):

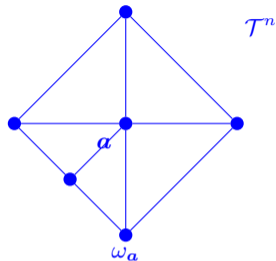
$$\begin{aligned}\|u_{h\tau} - \mathcal{I}u_{h\tau}\|_{X(I_n)}^2 &= \int_{I_n} \|\nabla(u_{h\tau} - \mathcal{I}u_{h\tau})\|^2 dt \\ &= \frac{\tau_n(q_n+1)}{(2q_n+1)(2q_n+3)} \|\nabla(u_{h\tau})_{n-1}\|^2\end{aligned}$$

Theorem (Global equivalence)

Suppose *no source term oscillation* or *no coarsening*. Then there holds

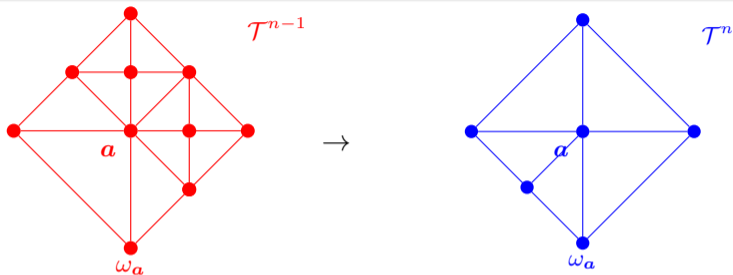
$$\|u - \mathcal{I}u_{h\tau}\|_Y \leq \|u - u_{h\tau}\|_{\mathcal{E}_Y} \leq 3\|u - \mathcal{I}u_{h\tau}\|_Y$$

- the two norms $\|\cdot\|_Y$ and $\|\cdot\|_{\mathcal{E}_Y}$ still may **differ locally**
- in general, an additional source term oscillation **or** coarsening term appears



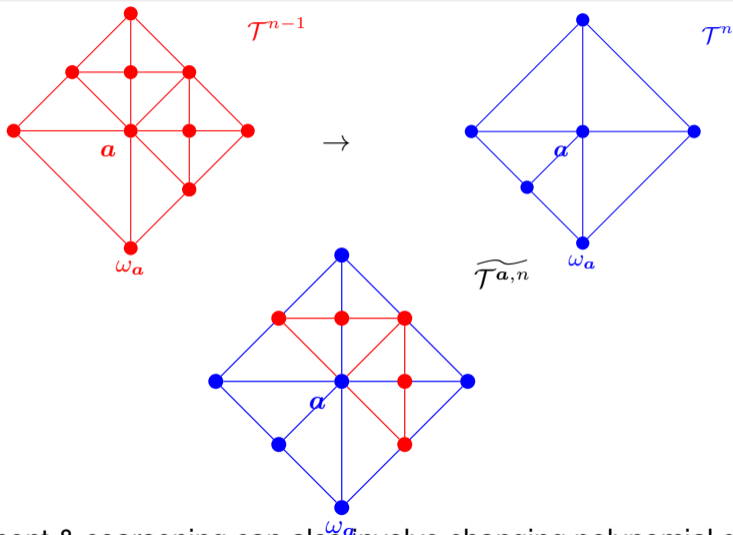
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Handling mesh adaptivity



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