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

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Outline

An optimal a posteriori estimate for singular problems

Guaranteed upper bound

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

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)

Robustness

- C_{eff} independent of domain Ω, meshes, solution u, **data**

Asymptotic exactness

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

Small evaluation cost

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

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Previous results (reaction–diffusion equation)

- Verfürth (1998) / Ainsworth and Babuška (1999): robustness wrt. singular perturbation
- 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); $p = 1$
- Grosman (2006) / Kopteva (2017): anisotropic meshes

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The reaction–diffusion equation

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

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

Finite element approximation

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

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Equivalence between error and residual

Energy norm

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

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:

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

- dual norm of the residual

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

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

Energy error is the dual norm of the residual

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

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

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

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Upper bound: motivation

Bound on the residual

- let $\boldsymbol{\sigma}_h \in \boldsymbol{H}(\mathrm{div}, \Omega)$ and $\phi_h \in L^2(\Omega)$ be such that

$$\nabla \cdot \boldsymbol{\sigma}_h + \kappa^2 \phi_h = f$$

- $\boldsymbol{\sigma}_h$: equilibrated flux reconstruction, $\approx -\varepsilon^2 \nabla u$
- ϕ_h: potential reconstruction, $\approx u$
- Green theorem $(\nabla \cdot \boldsymbol{\sigma}_h, v) + (\boldsymbol{\sigma}_h, \nabla v) = 0$ for $v \in H_0^1(\Omega)$:

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

- how to obtain suitable practical $\boldsymbol{\sigma}_h$ and ϕ_h?
- counter-example where $\|\varepsilon \nabla u_h + \varepsilon^{-1} \boldsymbol{\sigma}_h\|$ can largely overestimate the error: need to do better

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Flux and potential reconstructions

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

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

$$(\boldsymbol{\sigma}_h^{\mathbf{a}}, \phi_h^{\mathbf{a}}) := \arg \min_{(\boldsymbol{v}_h, q_h) \in \boldsymbol{V}_h^{\mathbf{a}} \times Q_h^{\mathbf{a}} \subset \boldsymbol{H}_0(\mathrm{div}, \omega_{\mathbf{a}}) \times L^2(\omega_{\mathbf{a}})}$$

$$\mathcal{J}_{u_h}^{\mathbf{a}}(\boldsymbol{v}_h, q_h) := w_{\mathbf{a}}^2 \|\varepsilon \psi_{\mathbf{a}} \nabla u_h + \varepsilon^{-1} \boldsymbol{v}_h\|_{\omega_{\mathbf{a}}}^2 + \|\kappa [\Pi_h(\psi_{\mathbf{a}} u_h) - q_h]\|_{\omega_{\mathbf{a}}}^2$$

Comments

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

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

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

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- **local discrete** constrained minimization problems
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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 $\sigma_h \in \mathbf{RTN}_p(\mathcal{T}) \cap \boldsymbol{H}(\mathrm{div}, \Omega)$ and $\phi_h \in \mathcal{P}_p(\mathcal{T})$ be the flux and potential reconstructions. Then

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Outline

Local efficiency and robustness

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Let u be the weak solution, $u_h \in V_h$ its finite element approximation, and $\boldsymbol{\sigma}_h \in \mathbf{RTN}_p(\mathcal{T}) \cap \boldsymbol{H}(\mathrm{div}, \Omega)$ and $\phi_h \in \mathcal{P}_p(\mathcal{T})$ the flux and potential reconstructions. Let f be a piecewise polynomial for simplicity. Then, for all $K \in \mathcal{T}$,

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where the constant C depends only 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.

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- the computable elementwise estimators are **local** lower bounds for the unknown error
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\partial_t u - \Delta u &= f \quad \text{in } \Omega \times (0,T),\\
u &= 0 \quad \text{on } \partial\Omega \times (0,T),\\
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$$f \in L^2(0,T;L^2(\Omega)), \quad u_0 \in L^2(\Omega)$$

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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

$$\int_0^T \langle \partial_t u, v \rangle + (\nabla u, \nabla v) \, \mathrm{d}t = \int_0^T (f, v) \, \mathrm{d}t \qquad \forall v \in X$$

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An optimal a posteriori estimate for evolutive problems

Guaranteed upper bound

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

Local efficiency

- $\eta_K^n(u_{h\tau}) \leq C_{\mathrm{eff}} \|u - u_{h\tau}\|_{?,\text{neighbors of } K\times(t^{n-1},t^n)}$
- 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, solution u, **polynomial degrees** of $u_{h\tau}$ in space and in time

Asymptotic exactness

- $\sum_{n=1}^{N} \sum_{K\in\mathcal{T}^n} \eta_K^n(u_{h\tau})^2 / \|u - u_{h\tau}\|^2_{?,\Omega\times(0,T)} \searrow 1$
- overestimation factor goes to one with increasing effort

Small evaluation cost

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

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- $\sum_{n=1}^{N} \sum_{K\in\mathcal{T}^n} \eta_K^n(u_{h\tau})^2 / \|u - u_{h\tau}\|^2_{?,\Omega\times(0,T)} \searrow 1$
- overestimation factor goes to one with increasing effort

Small evaluation cost

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

An optimal a posteriori estimate for evolutive problems

Guaranteed upper bound

- $\|u - u_{h\tau}\|^2_{?,\Omega\times(0,T)} \leq \sum_{n=1}^{N} \sum_{K\in\mathcal{T}^n} \eta_K^n(u_{h\tau})^2$
- 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

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- 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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Outline

Equivalence between error and residual

The heat equation

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

Spaces

$$\begin{aligned} X &:= L^2(0,T;H_0^1(\Omega)), \\ \|v\|_X^2 &:= \int_0^T \|\nabla v\|^2 \,\mathrm{d}t, \\ Y &:= L^2(0,T;H_0^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega)), \\ \|v\|_Y^2 &:= \int_0^T \|\partial_t v\|_{H^{-1}(\Omega)}^2 + \|\nabla v\|^2 \,\mathrm{d}t + \|v(T)\|^2 \end{aligned}$$

Weak solution

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

$$\int_0^T \langle \partial_t u, v \rangle + (\nabla u, \nabla v) \,\mathrm{d}t = \int_0^T (f, v) \,\mathrm{d}t \qquad \forall\, v \in X$$

Equivalence between error and residual

Theorem (Parabolic inf–sup identity)

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

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

Residual of $u_{h\tau} \in Y$

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

$$\langle \mathcal{R}(u_{h\tau}), v \rangle := \int_0^T (f, v) - \langle \partial_t u_{h\tau}, v \rangle - (\nabla u_{h\tau}, \nabla v)\, \mathrm{d}t \qquad v \in X$$

- dual norm of the residual

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

Y norm error is the dual X norm of the residual + IC error

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

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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 $(0, T)$,

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

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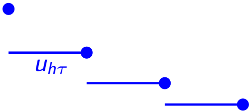
Outline

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)

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

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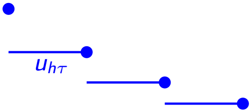

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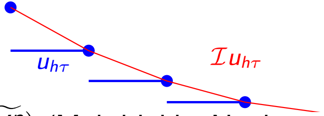

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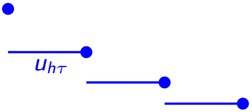
$$\int_{I_n} (\partial_t \mathcal{I}u_{h\tau}, v_{h\tau}) + (\nabla u_{h\tau}, \nabla v_{h\tau})\,\mathrm{d}t = \int_{I_n} (f, v_{h\tau})\,\mathrm{d}t \quad \forall\, v_{h\tau} \in \mathcal{Q}_{q_n}(I_n; V_h^n)$$

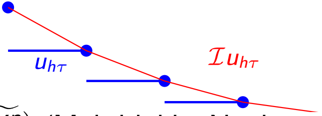
- ✓ final norm: $\|u - u_{h\tau}\|_{\mathcal{E}_Y}^2 := \|u - \mathcal{I}u_{h\tau}\|_Y^2 + \underbrace{\|u_{h\tau} - \mathcal{I}u_{h\tau}\|_X^2}_{\text{known, computable}}$

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 $\|u - u_{h\tau}\|_Y$



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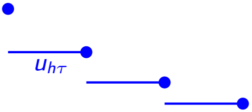
Approximate solution and Radau reconstruction



Approximate solution

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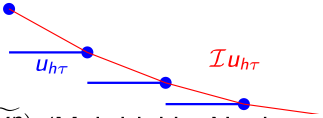

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$$\int_{I_n} (\partial_t \mathcal{I} u_{h\tau}, v_{h\tau}) + (\nabla u_{h\tau}, \nabla v_{h\tau})\, \mathrm{d}t = \int_{I_n} (f, v_{h\tau})\, \mathrm{d}t \quad \forall v_{h\tau} \in \mathcal{Q}_{q_n}(I_n; V_h^n)$$

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Outline

Results in the Y norm

Theorem (Reliability in the Y norm)

Suppose no data oscillation for simplicity. Then, for any $\boldsymbol{\sigma}_{h\tau} \in L^2(0, T; \boldsymbol{H}(\mathrm{div}, \Omega))$ with $\nabla\cdot\boldsymbol{\sigma}_{h\tau} = f - \partial_t \mathcal{I} u_{h\tau}$, there holds

$$\|u - \mathcal{I}u_{h\tau}\|_Y^2 \leq \int_0^T \|\boldsymbol{\sigma}_{h\tau} + \nabla \mathcal{I} u_{h\tau}\|^2 \,\mathrm{d}t.$$

Proof of the upper bound

Proof.

- equivalence error-residual (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

$$\int_0^T (\boldsymbol{\sigma}_{h\tau}, \nabla \mathcal{I}u_{h\tau}) + (\nabla \cdot \boldsymbol{\sigma}_{h\tau}, \mathcal{I}u_{h\tau}) \,\mathrm{d}t = 0$$

- residual definition, Cauchy–Schwarz inequality:

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

Proof of the upper bound

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$$\leq \left\{ \int_0^T \|\boldsymbol{\sigma}_{h\tau} + \nabla \mathcal{I}u_{h\tau}\|^2\,\mathrm{d}t \right\}^{\frac{1}{2}} \|v\|_X$$

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- Green theorem

$$\int_0^T (\boldsymbol{\sigma}_{h\tau}, \nabla \mathcal{I}u_{h\tau}) + (\nabla\cdot\boldsymbol{\sigma}_{h\tau}, \mathcal{I}u_{h\tau})\,\mathrm{d}t = 0$$

- residual definition, Cauchy–Schwarz inequality:

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

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

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

Then set

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

Comments

- ✓ satisfies $\boldsymbol{\sigma}_{h\tau} \in L^2(0,T;\boldsymbol{H}(\mathrm{div},\Omega))$ with $\nabla\cdot\boldsymbol{\sigma}_{h\tau} = f - \partial_t \mathcal{I} u_{h\tau}$
- works on the common refinement $\widetilde{\mathcal{T}}^{\mathbf{a},n}$ of the patch $\omega_{\mathbf{a}}$
- ✓ uncouples to q_n elliptic problems posed in $\boldsymbol{V}_h^{\mathbf{a},n}$

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Guaranteed upper bound

Theorem (Guaranteed upper bound)

In the absence of data oscillation (f and u_0 piecewise polynomial), there holds

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

Outline

Local space-time efficiency and robustness

Local error contributions

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

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,

$$\int_{I_n} \|\boldsymbol{\sigma}_{h\tau} + \nabla\mathcal{I}u_{h\tau}\|^2_K + \|\nabla(u_{h\tau} - \mathcal{I}u_{h\tau})\|^2_K \mathrm{d}t \le C^2_{\mathrm{eff}} \sum_{\mathbf{a}\in\mathcal{V}_K} |u - u_{h\tau}|^2_{\mathcal{E}_Y^{\mathbf{a},n}}.$$

Comments

- ✓ **local** in **space** and **time**
- ✓ C_{eff} only depends on shape regularity ⇒ **robustness** w.r.t the final time T and the **polynomial degrees** p and q
- ✓ **no restriction on coarsening** between $\mathcal{T}^{n-1}$ and $\mathcal{T}^n$

Local space-time efficiency and robustness

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recall

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

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Outline

Numerics: smooth case

Model problem

$$-\Delta u = f \quad \text{in } \Omega := (0,1)^2,$$
$$u = 0 \quad \text{on } \partial\Omega$$

Exact solution

$$u(x,y) = \sin(2\pi x)\sin(2\pi y)$$

Discretization

- symmetric interior penalty discontinuous Galerkin method: $u_h \notin H_0^1(\Omega)$
- unstructured triangular grids
- uniform h and p refinement

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How large is the overall error? (model pb, known sol.)

h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\|\nabla u_h\|}$	$\|\nabla(u-u_h)\|$	rel. error $\frac{\|\nabla(u-u_h)\|}{\|\nabla u_h\|}$	$I^{\rm eff} = \frac{\eta(u_h)}{\|\nabla(u-u_h)\|}$
h_0	1	1.3	$2.8 \times 10^{1}\%$	1.1	$2.4 \times 10^{1}\%$	1.17
$\approx h_0/2$		[illegible]				
$\approx h_0/4$		[illegible]				
$\approx h_0/8$		[illegible]				
h_0	2	[illegible]				
$\approx h_0/2$	2	[illegible]				
h_0	3	[illegible]				
$\approx h_0/4$	3	[illegible]				
h_0	4	[illegible]				
$\approx h_0/8$	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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h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\lVert\nabla u_h\rVert}$	$\lVert\nabla(u-u_h)\rVert$	rel. error $\frac{\lVert\nabla(u-u_h)\rVert}{\lVert\nabla u_h\rVert}$	$I^{\mathrm{eff}} = \frac{\eta(u_h)}{\lVert\nabla(u-u_h)\rVert}$
h_0	1	1.3	$2.8 \times 10^1\%$	1.1	$2.4 \times 10^1\%$	1.17
$\approx h_0/2$		6.1×10^{-1}	[illegible]	5.6×10^{-1}		
$\approx h_0/4$		3.1×10^{-1}	[illegible]	2.9×10^{-1}		
$\approx h_0/8$		1.5×10^{-1}	[illegible]	1.4×10^{-1}		
h_0	2	1.6×10^{-1}	[illegible]	1.5×10^{-1}		
$\approx h_0/2$	2	4.2×10^{-2}	[illegible]	4.1×10^{-2}		
h_0	3	1.4×10^{-2}	[illegible]	1.4×10^{-2}		
$\approx h_0/4$	3	2.6×10^{-4}	[illegible]	2.6×10^{-4}		
h_0	4	1.0×10^{-3}	[illegible]	9.9×10^{-4}		
$\approx h_0/8$	4	2.6×10^{-7}	[illegible]	2.6×10^{-7}		

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h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\|\nabla u_h\|}$	$\|\nabla(u-u_h)\|$	rel. error $\frac{\|\nabla(u-u_h)\|}{\|\nabla u_h\|}$	$I^{\mathrm{eff}} = \frac{\eta(u_h)}{\|\nabla(u-u_h)\|}$
h_0	1	1.3	$2.8 \times 10^{1}\%$	1.1	$2.4 \times 10^{1}\%$	1.17
$\approx h_0/2$		6.1×10^{-1}	$1.4 \times 10^{1}\%$	5.6×10^{-1}	$1.3 \times 10^{1}\%$	
$\approx h_0/4$		3.1×10^{-1}	7.0%	2.9×10^{-1}	6.6%	
$\approx h_0/8$		1.5×10^{-1}	3.3%	1.4×10^{-1}	3.1%	
h_0	2	1.6×10^{-1}	3.7%	1.5×10^{-1}	3.5%	
$\approx h_0/2$	2	4.2×10^{-2}	$9.5 \times 10^{-1}\%$	4.1×10^{-2}	$9.2 \times 10^{-1}\%$	
h_0	3	1.4×10^{-2}	$3.2 \times 10^{-1}\%$	1.4×10^{-2}	$3.1 \times 10^{-1}\%$	
$\approx h_0/4$	3	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	
h_0	4	1.0×10^{-3}	$2.3 \times 10^{-2}\%$	9.9×10^{-4}	$2.2 \times 10^{-2}\%$	
$\approx h_0/8$	4	2.6×10^{-7}	$5.9 \times 10^{-6}\%$	2.6×10^{-7}	$5.8 \times 10^{-6}\%$	

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h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\lVert\nabla u_h\rVert}$	$\lVert\nabla(u-u_h)\rVert$	rel. error $\frac{\lVert\nabla(u-u_h)\rVert}{\lVert\nabla u_h\rVert}$	$I^{\mathrm{eff}} = \frac{\eta(u_h)}{\lVert\nabla(u-u_h)\rVert}$
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$\approx h_0/4$		3.1×10^{-1}	7.0%	2.9×10^{-1}	6.6%	
$\approx h_0/8$		1.5×10^{-1}	3.3%	1.4×10^{-1}	3.1%	
h_0	2	1.6×10^{-1}	3.7%	1.5×10^{-1}	3.5%	
$\approx h_0/2$	2	4.2×10^{-2}	$9.5 \times 10^{-1}\%$	4.1×10^{-2}	$9.2 \times 10^{-1}\%$	
h_0	3	1.4×10^{-2}	$3.2 \times 10^{-1}\%$	1.4×10^{-2}	$3.1 \times 10^{-1}\%$	
$\approx h_0/4$	3	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	
h_0	4	1.0×10^{-3}	$2.3 \times 10^{-2}\%$	9.9×10^{-4}	$2.2 \times 10^{-2}\%$	
$\approx h_0/8$	4	2.6×10^{-7}	$5.9 \times 10^{-6}\%$	2.6×10^{-7}	$5.8 \times 10^{-6}\%$	

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h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\lVert\nabla u_h\rVert}$	$\lVert\nabla(u-u_h)\rVert$	rel. error $\frac{\lVert\nabla(u-u_h)\rVert}{\lVert\nabla u_h\rVert}$	$I^{\text{eff}} = \frac{\eta(u_h)}{\lVert\nabla(u-u_h)\rVert}$
h_0	1	1.3	$2.8 \times 10^1\%$	1.1	$2.4 \times 10^1\%$	1.17
$\approx h_0/2$		6.1×10^{-1}	$1.4 \times 10^1\%$	5.6×10^{-1}	$1.3 \times 10^1\%$	1.09
$\approx h_0/4$		3.1×10^{-1}	7.0%	2.9×10^{-1}	6.6%	[illegible]
$\approx h_0/8$		1.5×10^{-1}	3.3%	1.4×10^{-1}	3.1%	[illegible]
h_0	2	1.6×10^{-1}	3.7%	1.5×10^{-1}	3.5%	[illegible]
$\approx h_0/2$	2	4.2×10^{-2}	$9.5 \times 10^{-1}\%$	4.1×10^{-2}	$9.2 \times 10^{-1}\%$	[illegible]
h_0	3	1.4×10^{-2}	$3.2 \times 10^{-1}\%$	1.4×10^{-2}	$3.1 \times 10^{-1}\%$	[illegible]
$\approx h_0/4$	3	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	[illegible]
h_0	4	1.0×10^{-3}	$2.3 \times 10^{-2}\%$	9.9×10^{-4}	$2.2 \times 10^{-2}\%$	[illegible]
$\approx h_0/8$	4	2.6×10^{-7}	$5.9 \times 10^{-6}\%$	2.6×10^{-7}	$5.8 \times 10^{-6}\%$	[illegible]

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h_0	1	1.3	$2.8 \times 10^1\%$	1.1	$2.4 \times 10^1\%$	**1.17**
$\approx h_0/2$		6.1×10^{-1}	$1.4 \times 10^1\%$	5.6×10^{-1}	$1.3 \times 10^1\%$	**1.09**
$\approx h_0/4$		3.1×10^{-1}	7.0%	2.9×10^{-1}	6.6%	**1.06**
$\approx h_0/8$		1.5×10^{-1}	3.3%	1.4×10^{-1}	3.1%	**1.04**
h_0	2	1.6×10^{-1}	3.7%	1.5×10^{-1}	3.5%	**1.08**
$\approx h_0/2$	2	4.2×10^{-2}	$9.5 \times 10^{-1}\%$	4.1×10^{-2}	$9.2 \times 10^{-1}\%$	**1.04**
h_0	3	1.4×10^{-2}	$3.2 \times 10^{-1}\%$	1.4×10^{-2}	$3.1 \times 10^{-1}\%$	**1.03**
$\approx h_0/4$	3	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	2.6×10^{-4}	$5.9 \times 10^{-3}\%$	**1.01**
h_0	4	1.0×10^{-3}	$2.3 \times 10^{-2}\%$	9.9×10^{-4}	$2.2 \times 10^{-2}\%$	**1.02**
$\approx h_0/8$	4	2.6×10^{-7}	$5.9 \times 10^{-6}\%$	2.6×10^{-7}	$5.8 \times 10^{-6}\%$	**1.01**

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Numerics: smooth case with localized features

Model problem

$$
\begin{aligned}
-\Delta u &= f \quad \text{in } \Omega := (-1,1)^2,\\
u &= 0 \quad \text{on } \partial\Omega
\end{aligned}
$$

Exact solution

$$u(x,y) = (x^2-1)(y^2-1)\exp\left(-100(x^2+y^2)\right)$$

Discretization

- conforming finite elements: $u_h \in H^1(\Omega)$
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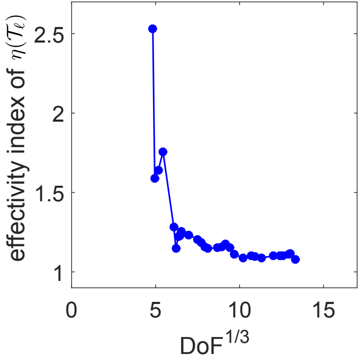
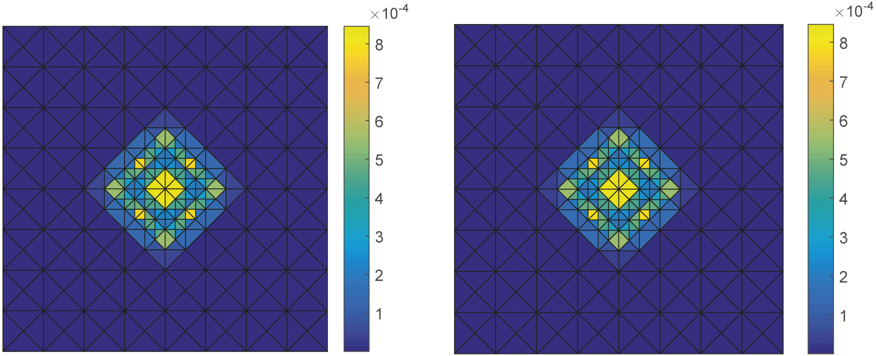
How precise are the estimates?



Effectivity indices on *hp* meshes

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

Where (in space) is the error localized?



Estimated error distribution $\eta_K(u_h)$

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

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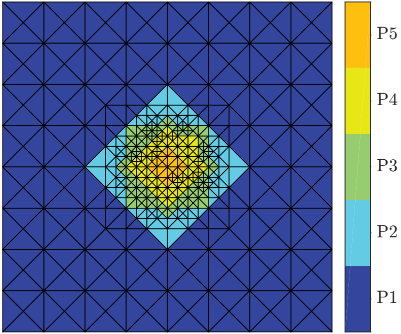
Can we decrease the error efficiently?



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

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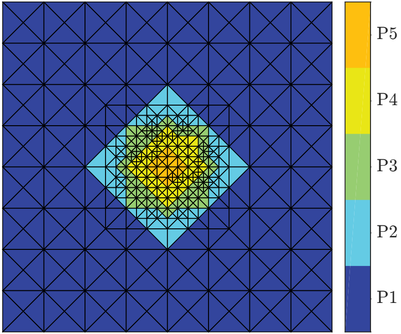

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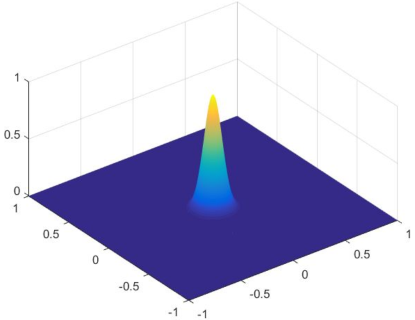

Exact solution

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Numerics: singular case

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$$\begin{aligned} -\Delta u &= 0 \quad \text{in } \Omega := (-1,1)^2 \setminus [0,1]^2, \\ u &= u_{\mathrm{D}} \quad \text{on } \partial\Omega \end{aligned}$$

Exact solution

$$u(r,\phi) = r^{2/3} \sin(2\phi/3)$$

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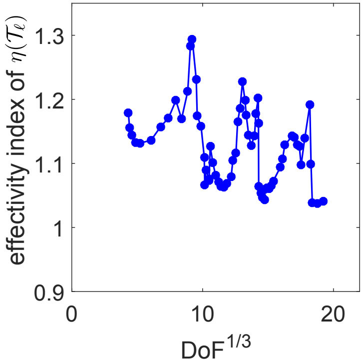

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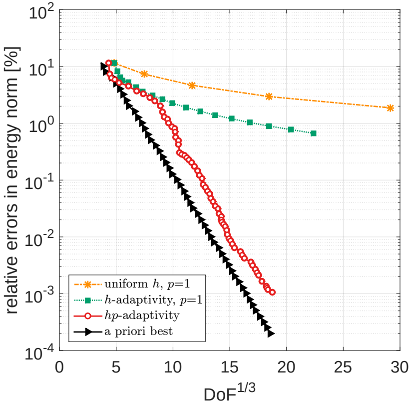

Relative error as a function of no. of unknowns

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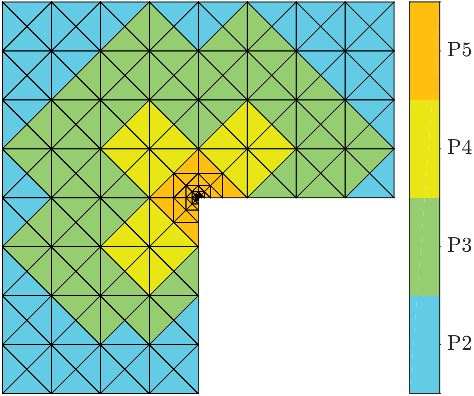

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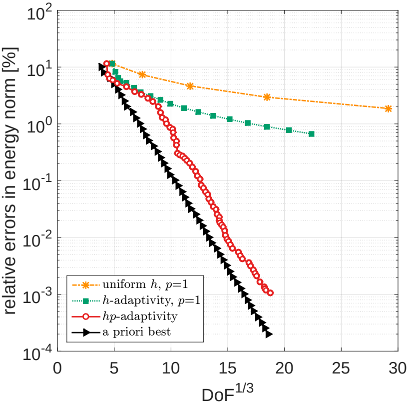


Relative error as a function of no. of unknowns

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

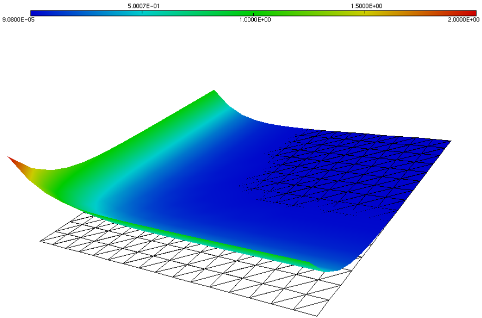
Problem and exact solution

Problem

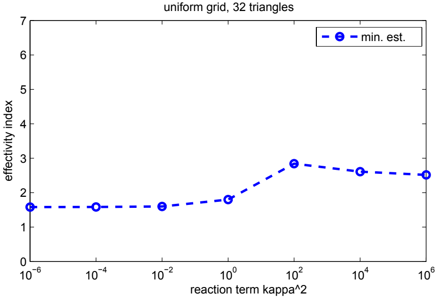
$$-\Delta u + \kappa^2 u = 0 \qquad \text{in } \Omega,$$
$$u = u_{\mathrm{D}} \qquad \text{on } \partial\Omega$$

Solution

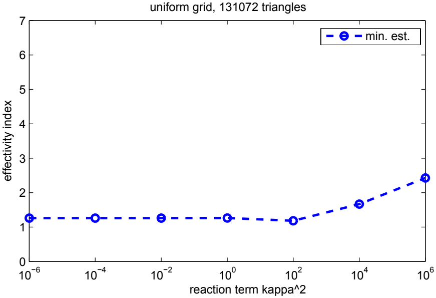
$$u(x, y) = e^{-\kappa x} + e^{-\kappa y}$$



Effectivity indices in dependence on κ: robustness



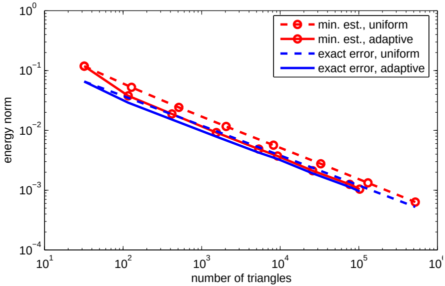
Mesh with 32 triangles



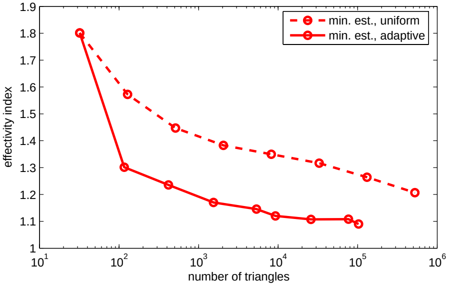
Mesh with 131072 triangles

I. Cheddadi, R. Fučík, M. Prieto, M. Vohralík, M2AN Math. Model. Numer. Anal. (2009)

Estimated and actual errors in uniformly/adaptively refined meshes and effectivity indices



Est. and act. errors, $\kappa = 1$



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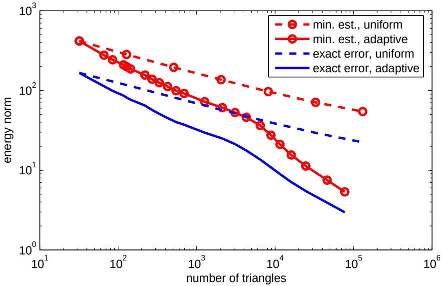
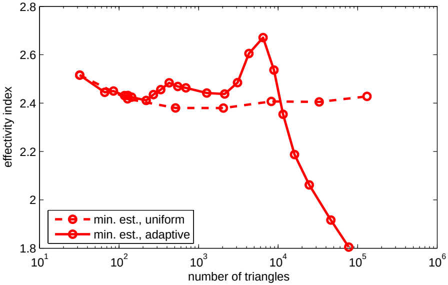


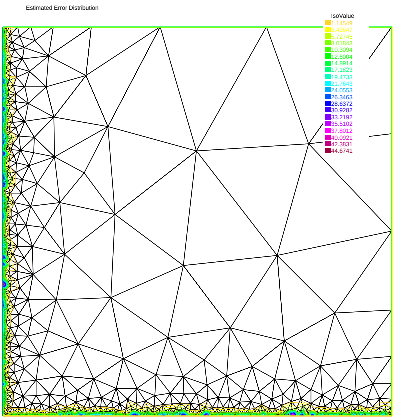
Est. and act. errors, $\kappa = 10^3$



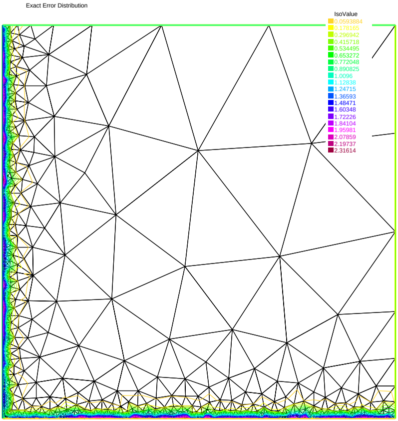
Effectivity indices, $\kappa = 10^3$

I. Cheddadi, R. Fučík, M. Prieto, M. Vohralík, M2AN Math. Model. Numer. Anal. (2009)

Error distribution, adaptively refined mesh, $\kappa = 10^3$



Estimated error distribution



Exact error distribution

I. Cheddadi, R. Fučík, M. Prieto, M. Vohralík, M2AN Math. Model. Numer. Anal. (2009)

Outline

Conclusions and future directions

Conclusions (reaction-diffusion)

- ✓ **guaranteed** upper bound
- ✓ local efficiency and **robustness** with respect to reaction and diffusion parameters
- ✓ simple form, any polynomial degree

Conclusions (heat)

- ✓ **guaranteed** upper bound
- ✓ local **space-time** efficiency
- ✓ **robustness** with respect to both spatial and temporal polynomial degree
- ✓ arbitrarily large **coarsening** allowed

Future directions

- nonlinear and coupled problems

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Bibliography

- SMEARS, I., VOHRALÍK M., Simple and robust equilibrated flux a posteriori estimates for singularly perturbed reaction–diffusion problems, HAL Preprint 01956180, submitted for publication, 2018.
- ERN A., SMEARS, I., VOHRALÍK M., Guaranteed, locally space-time efficient, and polynomial-degree robust a posteriori error estimates for high-order discretizations of parabolic problems, *SIAM J. Numer. Anal.* **55** (2017), 2811–2834.
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Thank you for your attention!

Bibliography

- SMEARS, I., VOHRALÍK M., Simple and robust equilibrated flux a posteriori estimates for singularly perturbed reaction–diffusion problems, HAL Preprint 01956180, submitted for publication, 2018.
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Fundamental results on a reference tetrahedron

Bounded right inverse of the divergence operator

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

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

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General result on a physical tetrahedron

Lemma ($\boldsymbol{H}(\mathrm{div})$ polynomial extension on a tetrahedron)

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

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Context

$$-\Delta \zeta_K = r_K \qquad \text{in } K,$$
$$-\nabla \zeta_K \cdot \mathbf{n}_K = r_F \qquad \text{on all } F \in \mathcal{F}_K^{\mathrm{N}},$$
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- Ern & V. (2016), 3D
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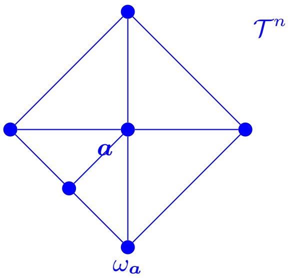

Stable broken $\mathbf{H}(\mathrm{div})$ polynomial extension on a patch

- Braess, Pillwein, & Schöberl (2009), 2D
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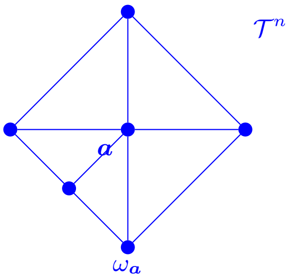

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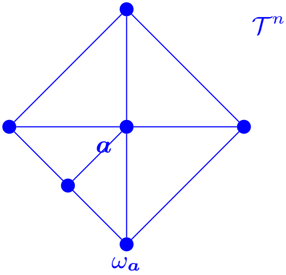

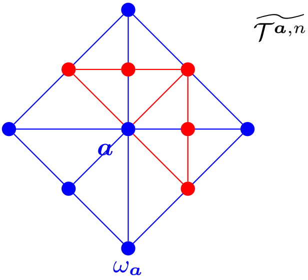

High-order space-time discretization

CG in space & DG in time

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

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

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

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$$= \int_{I_n} (f, v_{h\tau})\, \mathrm{d}t \qquad \forall v_{h\tau} \in \mathcal{Q}_{q_n}(I_n; V_h^n) \qquad \forall 1 \le n \le N.$$

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Global efficiency $\sim$ missing Galerkin orthogonality

Efficiency

For suitable $\boldsymbol{\sigma}_{h\tau}$, there holds

$$\int_{I_n} \|\boldsymbol{\sigma}_{h\tau} + \nabla \mathcal{I} u_{h\tau}\|_{\Omega}^2 \, \mathrm{d}t \leq C_{\mathrm{eff}}^2 \|u - \mathcal{I} u_{h\tau}\|_{Y(I_n)} \qquad \forall 1 \leq n \leq N.$$

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

Reason

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

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

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Remedy

Augmented norm

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

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

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

$$\|u_{h\tau} - \mathcal{I}u_{h\tau}\|^2_{X(I_n)} = \int_{I_n} \|\nabla(u_{h\tau} - \mathcal{I}u_{h\tau})\|^2 \,\mathrm{d}t$$
$$= \frac{\tau_n(q_n+1)}{(2q_n+1)(2q_n+3)} \|\nabla (\!| u_{h\tau} |\!)_{n-1}\|^2$$

Equivalence between the Y and $\mathcal{E}_Y$ norms

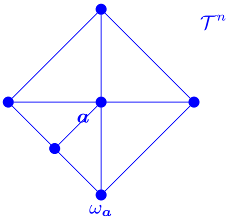
Theorem (Global equivalence)

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

Handling mesh adaptivity



- refinement & coarsening can also involve changing polynomial degrees

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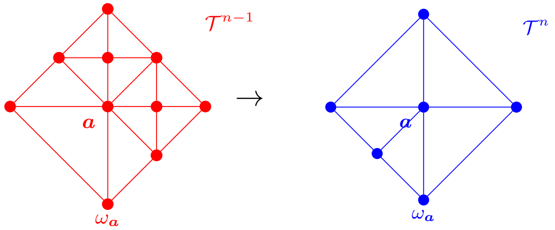

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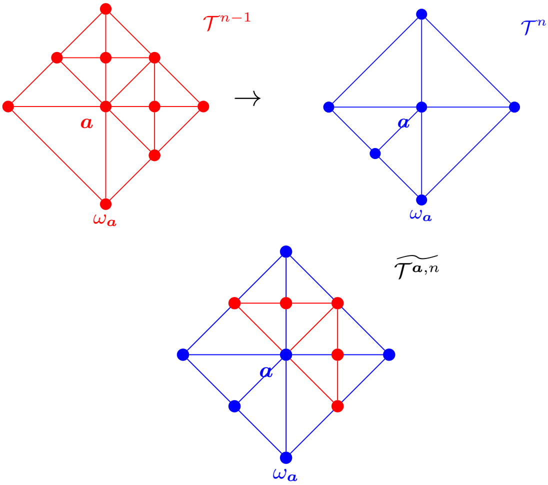

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