Estimations a posteriori garanties et robustes pour des problèmes à coefficients discontinus et à la réaction dominante

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Outline

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1. Introduction
2. Pure diffusion problems
   - Classical a posteriori estimates
   - Optimal abstract framework and a first estimate
   - Optimal a posteriori error estimate
   - Remarks on finite elements and finite volumes
   - Efficiency of the a posteriori error estimate
   - Numerical experiments
3. Reaction–diffusion problems
   - Problem and estimates
   - Numerical experiments
4. Estimates including the algebraic error
   - Problem and estimates
   - Numerical experiments
5. Conclusions and future work

What is an a posteriori error estimate

A posteriori error estimate

- Let p be a weak solution of a PDE.
- Let p_h be its approximate numerical solution.
- A priori error estimate: $\|p - p_h\|_\Omega \leq f(p)h^q$. Dependent on p, not computable. Useful in theory.
- A posteriori error estimate: $\|p - p_h\|_\Omega \lesssim f(p_h)$. Only uses p_h, computable. Great in practice.

Usual form

- $f(p_h)^2 = \sum_{K \in \mathcal{T}_h} \eta_K(p_h)^2$, where $\eta_K(p_h)$ is an element indicator.
- Can be used to determine mesh elements with large error.
- We can then refine these elements: mesh adaptivity.

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What an a posteriori error estimate should fulfill

Guaranteed upper bound (global error upper bound)

- $\|p - p_h\|_{\Omega}^2 \leq \sum_{K\in\mathcal{T}_h} \eta_K(p_h)^2$
- no undetermined constant: error control
- remark (reliability): $\|p - p_h\|_{\Omega}^2 \leq C \sum_{K\in\mathcal{T}_h} \eta_K(p_h)^2$

Local efficiency (local error lower bound)

- $\eta_K(p_h)^2 \leq C_{\mathrm{eff},K}^2 \sum_{L \text{ close to } K} \|p - p_h\|_L^2$
- necessary for optimal mesh refinement

Asymptotic exactness

- $\sum_{K\in\mathcal{T}_h} \eta_K(p_h)^2 / \|p - p_h\|_{\Omega}^2 \to 1$
- overestimation factor goes to one with mesh size

Robustness

- $C_{\mathrm{eff},K}$ does not depend on data, mesh, or solution

Negligible evaluation cost

- estimators can be evaluated locally

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Previous results

Continuous finite elements

- Babuška and Rheinboldt (1978), introduction
- Ladevèze and Leguillon (1983), equilibrated fluxes estimates (equality of Prager and Synge (1947))
- Zienkiewicz and Zhu (1987), averaging-based estimates
- Verfürth (1996, book), residual-based estimates
- Repin (1997), functional a posteriori error estimates
- Destuynder and Métivet (1999), equilibrated fluxes estimates
- Ainsworth and Oden (2000, book), equilibrated residual estimates
- Luce and Wohlmuth (2004), equilibrated fluxes estimates
- Braess and Schöberl (2008), equilibrated fluxes estimates

Previous results

Finite volumes

- Ohlberger (2001), non-energy norm estimates

Problems with discontinuous coefficients

- Bernardi and Verfürth (2000), conforming finite elements
- Ainsworth (2005), nonconforming finite elements

Reaction–diffusion problems

- Verfürth (1998), conforming finite elements & residual estimates
- Grosman (2006), conforming finite elements & equilibrated residual estimates

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A model problem with discontinuous coefficients

Model problem with discontinuous coefficients

$$\begin{aligned} -\nabla\cdot(a\nabla p) &= f \quad \text{in } \Omega,\\ p &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

Assumptions

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a polygonal domain
- a is a piecewise constant scalar, inhomogeneous

Bilinear form $\mathcal{B}$

$$\mathcal{B}(p,\varphi) := (a\nabla p, \nabla\varphi), \qquad p, \varphi \in H_0^1(\Omega)\,.$$

Weak solution

Find $p \in H_0^1(\Omega)$ such that $\mathcal{B}(p,\varphi) = (f,\varphi) \qquad \forall \varphi \in H_0^1(\Omega)$.

Energy norm

$$|||\varphi|||^2 := \mathcal{B}(\varphi,\varphi) = \|a^{\frac{1}{2}}\nabla\varphi\|^2, \qquad \varphi \in H_0^1(\Omega).$$

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Residual estimates for $-\triangle p = f$

Corollary (Classical residual error estimate in FEs)

Let $a = 1$. Then there holds (cf. Verfürth 96)

$$\begin{aligned} |||p - p_h||| \quad \leq \quad & C_1 \left\{ \sum_{K \in \mathcal{T}_h} h_K^2 \|f + \triangle p_h\|_K^2 \right\}^{1/2} \\ & + C_2 \left\{ \sum_{\sigma \in \mathcal{E}_h} h_\sigma \|[\nabla p_h \cdot \mathbf{n}]\|_\sigma^2 \right\}^{1/2} . \end{aligned}$$

Drawbacks

- What are C_1 and C_2?
- If C_1 and C_2 evaluated: overestimation by a factor of 30 (uniform refinement) and 60 (adaptive refinement).
- $\triangle p_h = 0$: $h_K \|f\|_K$ as estimator gives no good sense.
- Not robust for inhomogeneities when a is discontinuous.

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FEs residual constants C_1 and C_2

Constants C_1 and C_2, Carstensen and Funken 00

$$
\begin{aligned}
C_V &:= \begin{cases} C_{\mathrm{P},\mathcal{T}_V}^{\frac{1}{2}} h_{\mathcal{T}_V} & V \in \mathcal{V}_h^{\mathrm{int}}, \\ C_{\mathrm{F},\mathcal{T}_V,\partial\Omega}^{\frac{1}{2}} h_{\mathcal{T}_V} & V \in \mathcal{V}_h^{\mathrm{ext}}, \end{cases} \\
C_1 &:= \max_{K\in\mathcal{T}_h} \left\{ \sum_{V\in\mathcal{V}_K} C_V^2 / \min_{K\in\mathcal{T}_V} h_K^2 \right\}^{\frac{1}{2}}, \\
C_2^2 &:= 3 C_1 \max_{K\in\mathcal{T}_h} \max_{\sigma\in\mathcal{E}_K} \{ h_K / h_\sigma h_K^2 / |K| \} \\
&\quad + \frac{1}{2} 3^{\frac{3}{2}} C_1^2 \max_{K\in\mathcal{T}_h} \max_{\sigma\in\mathcal{E}_K} \{ h_K / h_\sigma h_K^2 / |K| (3 + h_K^2 / |K|) \}.
\end{aligned}
$$

Zienkiewicz–Zhu averaging estimate for $-\triangle p = f$

Corollary (Zienkiewicz–Zhu averaging error estimate in FEs)

Let $a = 1$. Then there holds (cf. Zienkiewicz–Zhu 87)

$$|||p - p_h||| \lesssim \|\nabla p_h + \mathbf{t}_h\|,$$

where $\mathbf{t}_h$ is an averaged smooth flux.

Drawbacks

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Equilibrated residuals estimate for $-\nabla \cdot (a\nabla p) = f$

Corollary (Equilibrated residuals error estimate in FEs)

Let $\phi_K \in H^1(K)$, $\phi_K = 0$ on $\partial\Omega$, $K \in \mathcal{T}_h$, be the solutions of the local problems

$$\mathcal{B}_K(\phi_K, v_K) = (f, v_K)_K - \mathcal{B}_K(p_h, v_K) + \langle g_K, v_K\rangle_{\partial K} \qquad \forall v_K \in H^1(K),\ v_K = 0 \text{ on } \partial\Omega.$$

Then there holds (cf. Ainsworth and Oden 00)

$$|||p - p_h||| \le \left\{ \sum_{K\in\mathcal{T}_h} |||\phi_K|||_K^2 \right\}^{1/2}.$$

Drawbacks

- Infinite-dimensional local problems would need to be solved to get a guaranteed upper bound.
- Their approximation may be quite expensive.

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Optimal abstract framework for $-\nabla\cdot(a\nabla p) = f$

Theorem (Optimal abstract framework, conf. & pure dif. case)

Let $p, p_h \in H^1_0(\Omega)$ *be arbitrary. Then*

$$|||p - p_h||| \le \sup_{\varphi\in H^1_0(\Omega),\, |||\varphi|||=1} \mathcal{B}(p - p_h, \varphi) \le |||p - p_h|||.$$

Proof.

We have

$$\begin{aligned} |||p - p_h||| &= \mathcal{B}\left(p - p_h, \frac{p - p_h}{|||p - p_h|||}\right) \\ &\le \sup_{\varphi\in H^1_0(\Omega),\, |||\varphi|||=1} \mathcal{B}(p - p_h, \varphi) \\ &\le |||p - p_h||| \sup_{\varphi\in H^1_0(\Omega),\, |||\varphi|||=1} |||\varphi||| \\ &= |||p - p_h|||. \end{aligned}$$

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Optimal abstract estimate for $-\nabla \cdot (a\nabla p) = f$

Theorem (Optimal abstract estimate, conf. & pure dif. case)

Let p be the weak solution and let $p_h \in H_0^1(\Omega)$ be arbitrary. Then

$$|||p - p_h||| \leq \inf_{\mathbf{t}\in\mathbf{H}(\mathrm{div},\Omega)} \sup_{\varphi\in H_0^1(\Omega),\, |||\varphi|||=1} \{(f - \nabla\cdot\mathbf{t}, \varphi) - (a\nabla p_h + \mathbf{t}, \nabla\varphi)\}$$

$$\leq |||p - p_h|||.$$

Proof.

Upper bound: put $\varphi := p - p_h / |||p - p_h|||$ and take $\mathbf{t} \in \mathbf{H}(\mathrm{div},\Omega)$ arbitrary. Then

$$\begin{aligned}\mathcal{B}(p - p_h, \varphi) &= (f, \varphi) - (a\nabla p_h, \nabla\varphi) && //\mathcal{B} \text{ lin., weak sol. def.}\\ &= (f, \varphi) - (a\nabla p_h + \mathbf{t}, \nabla\varphi) + (\mathbf{t}, \nabla\varphi) && // \pm (\mathbf{t}, \nabla\varphi)\\ &= (f - \nabla\cdot\mathbf{t}, \varphi) - (a\nabla p_h + \mathbf{t}, \nabla\varphi)\,. && //\text{Green th.}\end{aligned}$$

Lower bound: put $\mathbf{t} = -a\nabla p$ and use the Schwarz inequality.

Optimal abstract estimate for $-\nabla \cdot (a\nabla p) = f$

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- Guaranteed upper bound (no undetermined constant).
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A first computable estimate for $-\nabla \cdot (a\nabla p) = f$

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Let p be the weak solution and let $p_h \in H_0^1(\Omega)$ be arbitrary. Take any $\mathbf{t}_h \in \mathbf{H}(\mathrm{div}, \Omega)$. Then

$$|||p - p_h||| \leq \frac{C_{\mathrm{F},\Omega}^{1/2} h_\Omega}{c_{a,\Omega}^{1/2}} \|f - \nabla \cdot \mathbf{t}_h\| + \|a^{\frac{1}{2}} \nabla p_h + a^{-\frac{1}{2}} \mathbf{t}_h\|.$$

Proof.

- $|||p - p_h||| \leq \sup_{\varphi \in H_0^1(\Omega),\, |||\varphi|||=1} \{(f - \nabla \cdot \mathbf{t}_h, \varphi) - (a\nabla p_h + \mathbf{t}_h, \nabla\varphi)\};$
- Friedrichs inequality: $\|\varphi\| \leq C_{\mathrm{F},\Omega}^{1/2} h_\Omega \|\nabla\varphi\| \leq \frac{C_{\mathrm{F},\Omega}^{1/2} h_\Omega}{c_{a,\Omega}^{1/2}} |||\varphi|||;$
- use this and the Schwarz inequality:

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Outline

Optimal a posteriori error estimate for $-\nabla \cdot (a\nabla p) = f$

Theorem (Optimal a posteriori error estimate)

Let

- *p be the weak solution,*
- *$p_h \in H_0^1(\Omega)$ be arbitrary,*
- *$\mathcal{D}_h = \mathcal{D}_h^{\mathrm{int}} \cup \mathcal{D}_h^{\mathrm{ext}}$ be a partition of Ω,*
- *$\mathbf{t}_h \in \mathbf{H}(\mathrm{div}, \Omega)$ be arbitrary but such that $(\nabla \cdot \mathbf{t}_h, 1)_D = (f, 1)_D$ for all $D \in \mathcal{D}_h^{\mathrm{int}}$.*

Then

$$|||p - p_h||| \leq \left\{ \sum_{D \in \mathcal{D}_h} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^2 \right\}^{1/2}.$$

Optimal a posteriori error estimate for $-\nabla\cdot(a\nabla p) = f$

Estimators

- *diffusive flux estimator*
  - $\eta_{\mathrm{DF},D} := \|a^{\frac{1}{2}}\nabla p_h + a^{-\frac{1}{2}}\mathbf{t}_h\|_D$
  - penalizes the fact that $-a\nabla p_h \notin \mathbf{H}(\mathrm{div},\Omega)$
- *residual estimator*
  - $\eta_{\mathrm{R},D} := m_{D,a}\|f - \nabla\cdot\mathbf{t}_h\|_D$
  - residue evaluated for $\mathbf{t}_h$
  - $m_{D,a}^2 := C_{\mathrm{P},D}{h_D}^2/c_{a,D}$ for $D\in\mathcal{D}_h^{\mathrm{int}}$, $C_{\mathrm{P},D} = 1/\pi^2$ if D convex
  - $m_{D,a}^2 := C_{\mathrm{F},D}{h_D}^2/c_{a,D}$ for $D\in\mathcal{D}_h^{\mathrm{ext}}$, $C_{\mathrm{F},D} = 1$ in general
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Proof of the optimal estimate for $-\nabla \cdot (a\nabla p) = f$

Proof, part 1.

- Recall that

$$|||p - p_h||| \leq \sup_{\varphi \in H_0^1(\Omega),\, |||\varphi|||=1} \{(f - \nabla\cdot\mathbf{t}_h, \varphi) - (a\nabla p_h + \mathbf{t}_h, \nabla\varphi)\};$$

- Poincaré inequality

$$\|\varphi - \varphi_D\|_D^2 \leq C_{\mathrm{P},D} h_D^2 \|\nabla\varphi\|_D^2,$$

where φ_D is the mean value of φ over D;

- Friedrichs inequality

$$\|\varphi\|_D^2 \leq C_{\mathrm{F},D,\partial\Omega} h_D^2 \|\nabla\varphi\|_D^2,$$

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$$|||p - p_h||| \le \sup_{\varphi \in H_0^1(\Omega),\, |||\varphi|||=1} \{(f - \nabla{\cdot}\mathbf{t}_h, \varphi) - (a\nabla p_h + \mathbf{t}_h, \nabla\varphi)\};$$

- Poincaré inequality

$$\|\varphi - \varphi_D\|_D^2 \le C_{\mathrm{P},D} h_D^2 \|\nabla\varphi\|_D^2,$$

  where φ_D is the mean value of φ over D;
- Friedrichs inequality

$$\|\varphi\|_D^2 \le C_{\mathrm{F},D,\partial\Omega} h_D^2 \|\nabla\varphi\|_D^2,$$

  where $\varphi = 0$ on $\partial\Omega \cap \partial D \neq \emptyset$;
- energy norm:

$$\|\nabla\varphi\|_D^2 \le \frac{1}{c_{a,D}} |||\varphi|||_D^2;$$

Proof of the optimal estimate for $-\nabla \cdot (a\nabla p) = f$

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Proof of the optimal estimate for $-\nabla \cdot (a\nabla p) = f$

Proof, part 2.

- $D \in \mathcal{D}_h^{\mathrm{int}}$: conservativity of $\mathbf{t}_h$, i.e. $(\nabla\cdot\mathbf{t}_h, 1)_D = (f, 1)_D$, Schwarz inequality, and Poincaré inequality:

$$\begin{aligned}(f - \nabla\cdot\mathbf{t}_h, \varphi)_D =&(f - \nabla\cdot\mathbf{t}_h, \varphi - \varphi_D)_D \le \|f - \nabla\cdot\mathbf{t}_h\|_D \|\varphi - \varphi_D\|_D\\ \le&\|f - \nabla\cdot\mathbf{t}_h\|_D C_{\mathrm{P},D}^{\frac{1}{2}} h_D \|\nabla\varphi\|_D\\ \le& m_{D,a}\|f - \nabla\cdot\mathbf{t}_h\|_D |||\varphi|||_D;\end{aligned}$$

- $D \in \mathcal{D}_h^{\mathrm{ext}}$: Schwarz and Friedrichs inequalities:

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- the Schwarz inequality for the second term:

$$-(a\nabla p_h + \mathbf{t}_h, \nabla\varphi)_D \le \|a^{\frac{1}{2}}\nabla p_h + a^{-\frac{1}{2}}\mathbf{t}_h\|_D |||\varphi|||_D.$$

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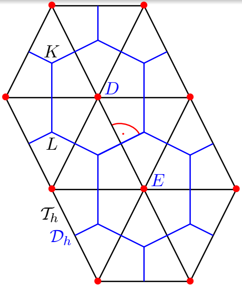
Outline

Finite element and cell-centered finite volume methods



$$
\begin{aligned}
-\nabla\cdot(a\nabla p) &= f \quad \text{in } \Omega\\
p &= 0 \quad \text{on } \partial\Omega
\end{aligned}
$$

Finite elements

$$(a\nabla p_h, \nabla\varphi_h) = (f, \varphi_h) \quad \forall \varphi_h \in V_h$$

- $-a\nabla p_h \notin \mathbf{H}(\mathrm{div}, \Omega) \Rightarrow$ not locally conservative
- $p_h \in H_0^1(\Omega) \Rightarrow$ conforming
- Galerkin orthogonality
- arithmetic averaging of a

Cell-centered finite volumes

$$-\sum_{E\in\mathcal{N}(D)} \{a\}_\omega \frac{|\sigma_{D,E}|}{d_{D,E}}(p_E - p_D) = (f, 1)_D \quad \forall D \in \mathcal{D}_h^{\mathrm{int}}$$

- locally conservative
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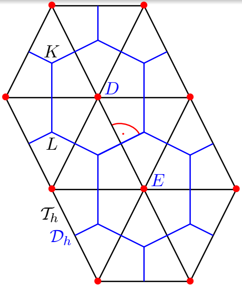
Finite element and cell-centered finite volume methods



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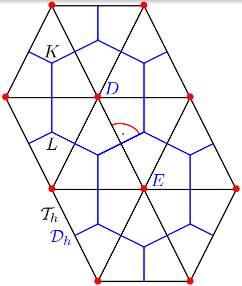

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Equivalence between FEs and FVs

Theorem (Equivalence between FEs and FVs, Eymard, Gallouët, and Herbin 00)

Let $d = 2$, let $a = 1$, let $\mathcal{T}_h$ be Delaunay and let $\mathcal{D}_h$ be its Voronoï dual (given by the orthogonal bisectors of the edges from $\mathcal{T}_h$). Let next f be piecewise constant on $\mathcal{T}_h$. Then FEs and FVs produce the same discrete systems.

Consequences:

- interpretation of the results
- local conservativity of FEs on $\mathcal{D}_h$
- general f: equivalence up to numerical quadrature

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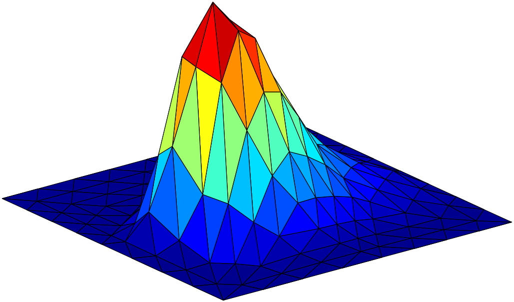
Finite elements for $-\nabla \cdot (a\nabla p) = f$

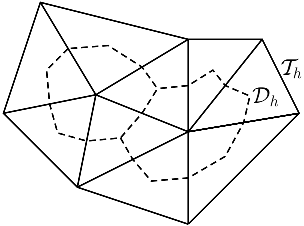
Finite element method

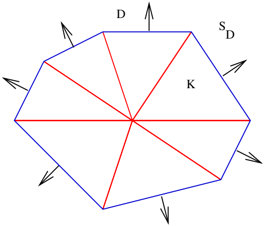
- Find $p_h \in V_h$ such that
$$(a\nabla p_h, \nabla \varphi_h) = (f, \varphi_h) \qquad \forall \varphi_h \in V_h.$$
- $p_h \in H_0^1(\Omega)$:



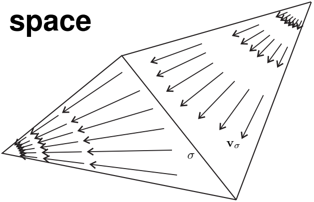
Choice of $\mathbf{t}_h \in \mathbf{H}(\mathrm{div}, \Omega)$

Recall the equivalence with finite volumes





Raviart–Thomas–Nédélec space



Choice of $\mathbf{t}_h$ based on the equivalence with FVs

- using the FV fluxes on $\mathcal{D}_h$, construct $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{S}_h)$; $\langle \mathbf{t}_h \cdot \mathbf{n}, 1 \rangle_{\partial D} = (\nabla \cdot \mathbf{t}_h, 1)_D = (f, 1)_D \quad \forall D \in \mathcal{D}_h^{\mathrm{int}}$.

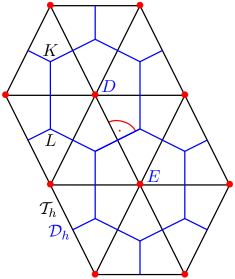
Cell-centered finite volumes for $-\nabla\cdot(a\nabla p) = f$

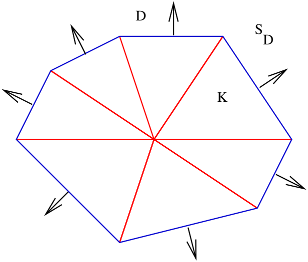
Cell-centered finite volume method

- Find $\{p_D\}_{D\in\mathcal{D}_h^{\rm int}}$ such that

$$-\{a\}_\omega \sum_{E\in\mathcal{N}(D)} \frac{|\sigma_{D,E}|}{d_{D,E}}(p_E - p_D) = (f,1)_D \quad \forall D\in\mathcal{D}_h^{\rm int}.$$

- $\{a\}_\omega$: harmonic averaging of the diffusion tensor.
- We immediately have $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{S}_h)$ which verifies $\langle \mathbf{t}_h\cdot\mathbf{n}, 1\rangle_{\partial D} = (\nabla\cdot\mathbf{t}_h, 1)_D = (f,1)_D \quad \forall D\in\mathcal{D}_h^{\rm int}$.





Interpretation of $\{p_D\}_{D\in\mathcal{D}_h^{\mathrm{int}}}$ as $p_h \in V_h$

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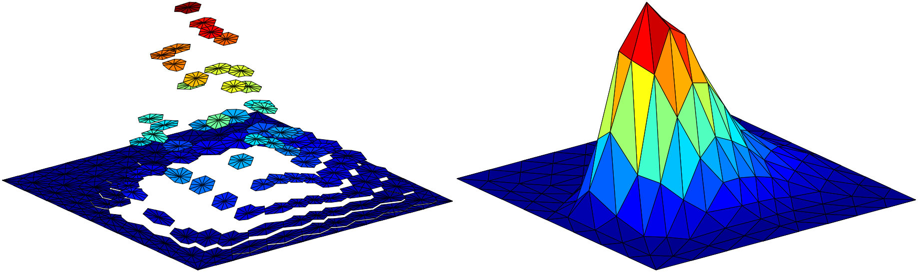


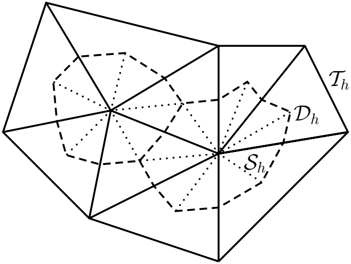
p_D piecewise constant on $\mathcal{D}_h$

p_h piecewise linear on $\mathcal{T}_h$

Outline

1. Introduction
2. Pure diffusion problems
   - Classical a posteriori estimates
   - Optimal abstract framework and a first estimate
   - Optimal a posteriori error estimate
   - Remarks on finite elements and finite volumes
   - Efficiency of the a posteriori error estimate
   - Numerical experiments
3. Reaction–diffusion problems
   - Problem and estimates
   - Numerical experiments
4. Estimates including the algebraic error
   - Problem and estimates
   - Numerical experiments
5. Conclusions and future work

Local efficiency of the estimates for $-\nabla \cdot (a\nabla p) = f$



Theorem (Local efficiency)

Let $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{S}_h)$, $\mathbf{t}_h \cdot \mathbf{n}_\sigma := -\{a\nabla p_h \cdot \mathbf{n}_\sigma\}_\omega$ for all sides σ of $\mathcal{S}_h$. Then

$$\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D} \le C|||p - p_h|||_{\mathcal{T}_{V_D}},$$

where C depends only on the space dimension d, on the shape regularity parameter $\kappa_\mathcal{T}$, and on the polynomial degree m of f. Moreover, when $a = 1$, one actually has

$$\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D} \le C|||p - p_h|||_D.$$

Local efficiency of the estimates for $-\nabla \cdot (a\nabla p) = f$

Proof (diffusive flux estimator, case $a = 1$).

- for each $\mathbf{v}_h \in \mathbf{RTN}(K)$, $\|\mathbf{v}_h\|_K^2 \le C h_K \sum_{\sigma \in \mathcal{E}_K} \|\mathbf{v}_h \cdot \mathbf{n}\|_\sigma^2$ (equivalence of norms on finite-dimensional spaces)
- put $\mathbf{v}_h = \nabla p_h + \mathbf{t}_h$; then $\|\nabla p_h + \mathbf{t}_h\|_K^2 = \|\mathbf{v}_h\|_K^2$ $\le C h_K \sum_{\sigma \in \mathcal{E}_K \cap \mathcal{E}_h^{\mathrm{int}}} \|[\![\nabla p_h \cdot \mathbf{n}_\sigma]\!]\|_\sigma^2 \Rightarrow \eta_{\mathrm{DF},D}$ is a lower bound for the classical mass balance estimator
- side bubble functions technique of Verfürth: $h_K^{\frac{1}{2}} \|[\![\nabla p_h \cdot \mathbf{n}_\sigma]\!]\|_\sigma \le C \sum_{M \in \{K,L\}} |||p - p_h|||_M$ for $\sigma \in \mathcal{E}_K \cap \mathcal{E}_h^{\mathrm{int}}$

Proof (residual estimator, case $a = 1$).

- element bubble functions technique of Verfürth: $\|f - \nabla \cdot \mathbf{t}_h\|_K \le C h_K^{-1} \|\nabla p + \mathbf{t}_h\|_K$
- $\|\nabla p + \mathbf{t}_h\|_D \le |||p - p_h|||_D + \|\nabla p_h + \mathbf{t}_h\|_D$
- complete the proof by the previous result

Local efficiency of the estimates for $-\nabla \cdot (a \nabla p) = f$

Proof (diffusive flux estimator, case $a = 1$).

- for each $\mathbf{v}_h \in \mathbf{RTN}(K)$, $\|\mathbf{v}_h\|_K^2 \leq C h_K \sum_{\sigma \in \mathcal{E}_K} \|\mathbf{v}_h \cdot \mathbf{n}\|_\sigma^2$ (equivalence of norms on finite-dimensional spaces)
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Proof (diffusive flux estimator, case $a = 1$).

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Local efficiency of the estimates for $-\nabla \cdot (a\nabla p) = f$

Proof (diffusive flux estimator, case $a = 1$).

- for each $\mathbf{v}_h \in \mathbf{RTN}(K)$, $\|\mathbf{v}_h\|_K^2 \leq Ch_K \sum_{\sigma \in \mathcal{E}_K} \|\mathbf{v}_h \cdot \mathbf{n}\|_\sigma^2$ (equivalence of norms on finite-dimensional spaces)
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Proof (residual estimator, case $a = 1$).

- element bubble functions technique of Verfürth: $\|f - \nabla \cdot \mathbf{t}_h\|_K \leq C h_K^{-1} \|\nabla p + \mathbf{t}_h\|_K$
- $\|\nabla p + \mathbf{t}_h\|_D \leq |||p - p_h|||_D + \|\nabla p_h + \mathbf{t}_h\|_D$
- complete the proof by the previous result

Local efficiency of the estimates for $-\nabla \cdot (a\nabla p) = f$

Proof (case $a \neq 1$).

- the discontinuities have to be aligned with the dual mesh
- harmonic averaging has to be used in the scheme
- harmonic averaging has to be used in the construction of $\mathbf{t}_h$: $\mathbf{t}_h \cdot \mathbf{n}_\sigma = -\{\nabla p_h \cdot \mathbf{n}_\sigma\}_\omega$

Properties

- **guaranteed upper bound**
- local efficiency
- **full robustness**
- negligible evaluation cost
- locally, our estimator is a lower bound for the classical residual one

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The estimate in 1D

Model problem

$$\begin{aligned} -p'' &= \pi^2 sin(\pi x) \quad \text{in }]0,1[, \\ p &= 0 \quad \text{in } 0,1 \end{aligned}$$

Exact solution

$$p(x) = sin(\pi x)$$

Discretization

N given, $h = 1/(N+1)$, $x_k = kh$, $k = 0, \ldots, N+1$ ($x_0 = 0$ and $x_{N+1} = 1$), $x_{k+\frac{1}{2}} = (k+\frac{1}{2})h$, $k = 0, \ldots, N$, $x_{-\frac{1}{2}} = 0$, $x_{N+1+\frac{1}{2}} = 1$

Choice of t_h

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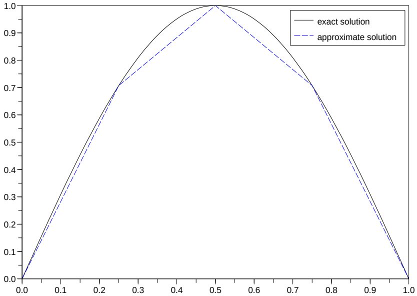
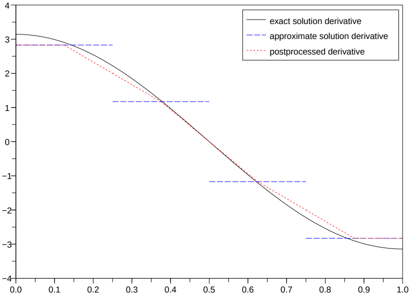
Plots of p, p_h, and $-t_h$

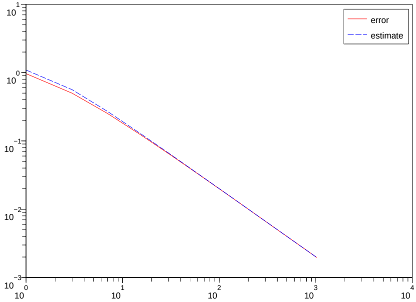


Plot of p and p_h

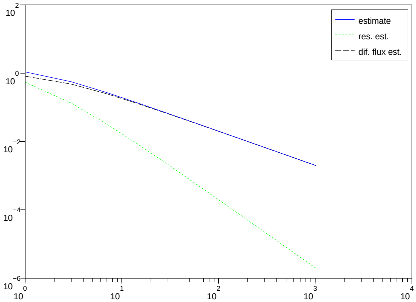


Plot of p', p'_h, and $-t_h$

The optimal estimate in 1D

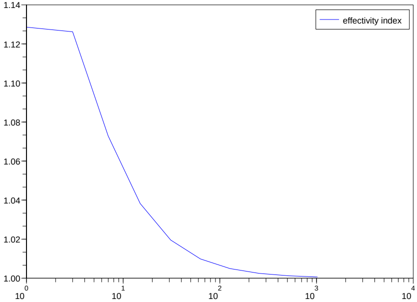


Estimated and actual errors



Estimated error and residual and diffusive flux estimators

The optimal estimate in 1D



Effectivity index

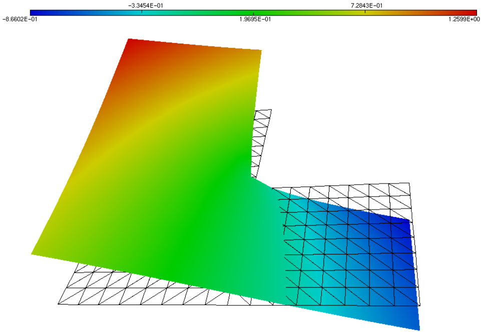
L-shape domain example and finite elements

Problem

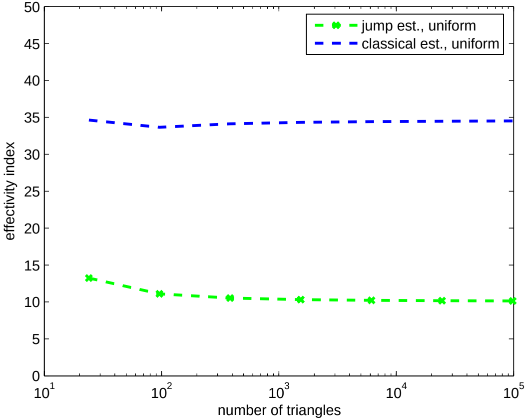
$$\begin{aligned} -\triangle p &= 0, && \text{in } \Omega \\ p &= p_0, && \text{on } \partial\Omega \end{aligned}$$

Exact solution
(polar coordinates)

$$p_0(r, \varphi) = r^{-\frac{2}{3}} \sin\left(\frac{2}{3}\varphi\right)$$



Effectivity index – comparison, uniform refinement

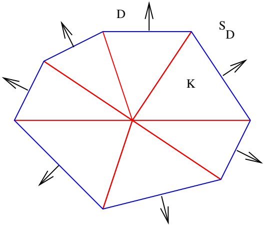


Effectivity indices for the jump and classical estimators

Improvement by local minimization

Observation

- Fluxes of $\mathbf{t}_h$ need to be prescribed on the boundary of dual volumes only to get $(\nabla \cdot \mathbf{t}_h, 1)_D = (f, 1)_D$.
- We can choose them on other edges.



Local minimization (for each vertex)

- solve local linear problem (size = number of vertex sides)
- compute the estimators
- the whole estimate still has a linear cost

No linear system solution

- choose $\mathbf{t}_h$ such that $(\nabla \cdot \mathbf{t}_h, 1)_K = (f, 1)_K$ for all $K \in \mathcal{S}_h$

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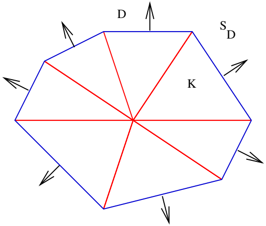

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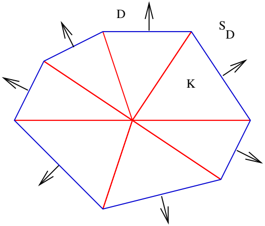

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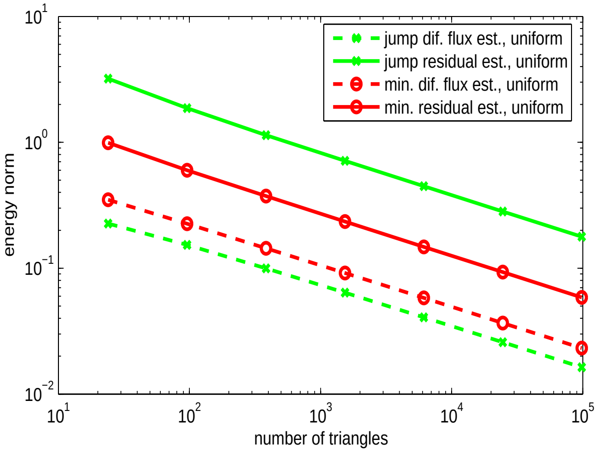
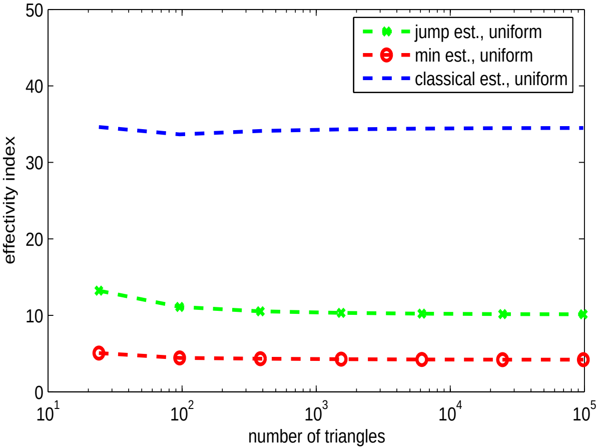
Residual and diffusive flux estimators, uniform refinement



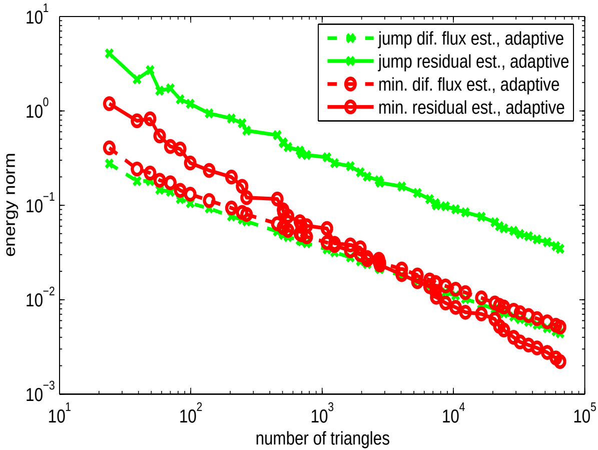
Residual and diffusive flux estimators comparison

Effectivity index – comparison, uniform refinement



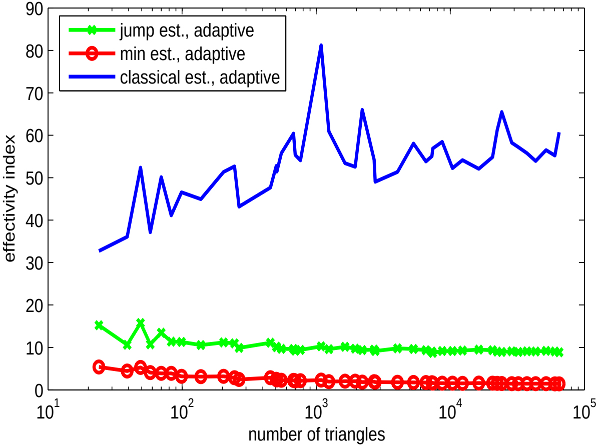
Effectivity indices for the jump, minimization, and classical estimators

Residual and diffusive flux estimators, uniform refinement



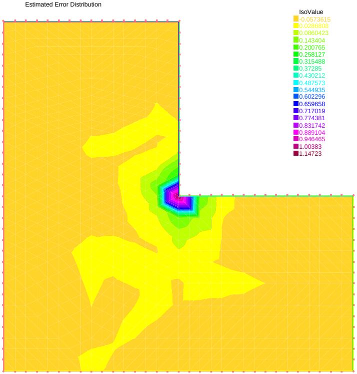
Residual and diffusive flux estimators comparison

Effectivity index – comparison, adaptive refinement

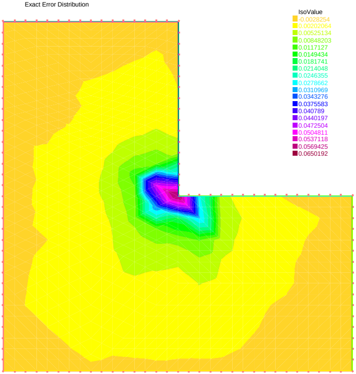


Effectivity indices for the jump, minimization, and classical estimators

Error distribution on a uniformly refined mesh

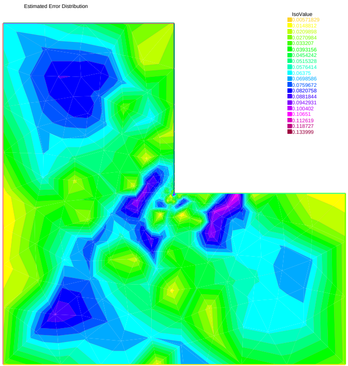


Estimated error distribution



Exact error distribution

Error distribution on an adaptively refined mesh



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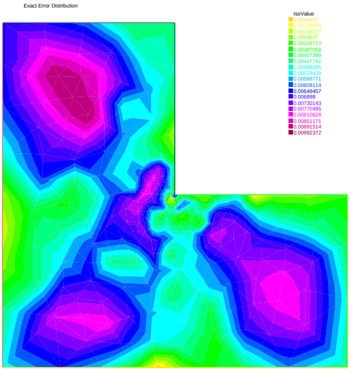
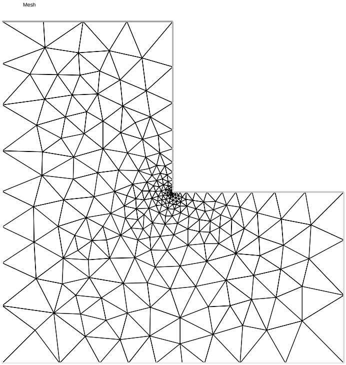


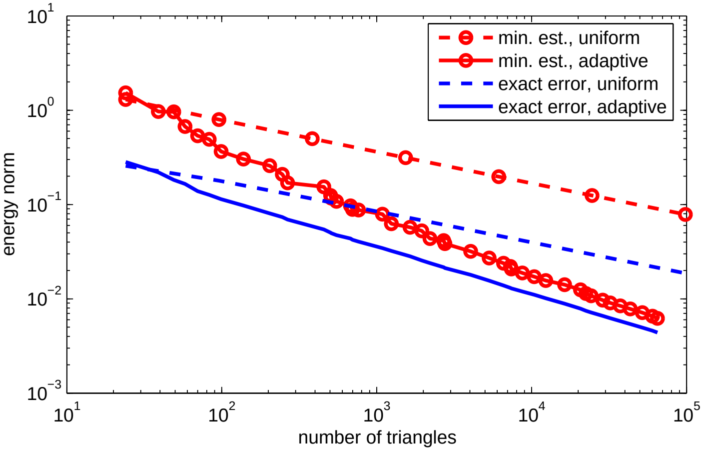
Exact error distribution

Adaptively refined mesh



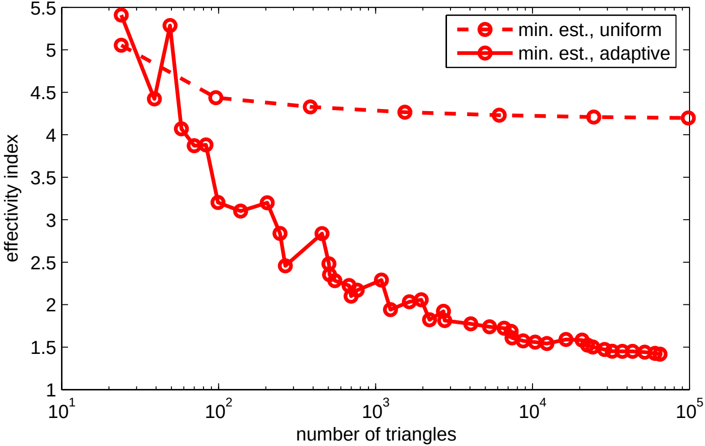
Corresponding adaptively refined mesh

Energy error



Estimated and actual energy error,
uniformly/adaptively refined meshes

Effectivity index



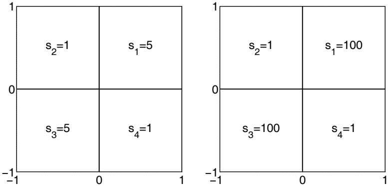
Effectivity index, uniformly/adaptively refined meshes

Discontinuous diffusion tensor and vertex-centered finite volumes

- consider the pure diffusion equation

$$-\nabla \cdot (a \nabla p) = 0 \quad \text{in} \quad \Omega = (-1,1) \times (-1,1)$$

- discontinuous and inhomogeneous a, two cases:

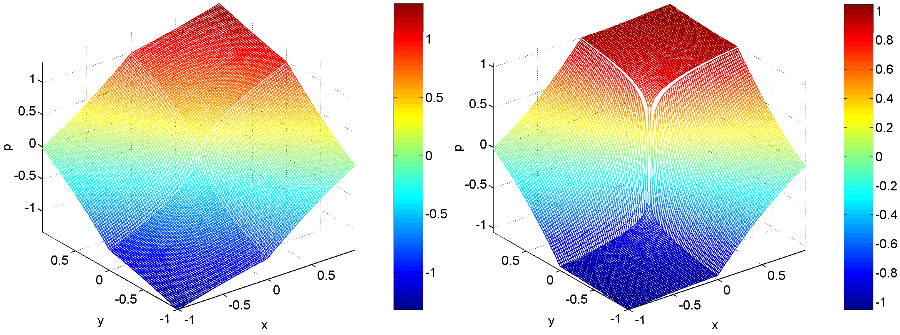


- analytical solution: singularity at the origin

$$p(r,\theta)|_{\Omega_i} = r^{\alpha}(a_i \sin(\alpha\theta) + b_i \cos(\alpha\theta))$$

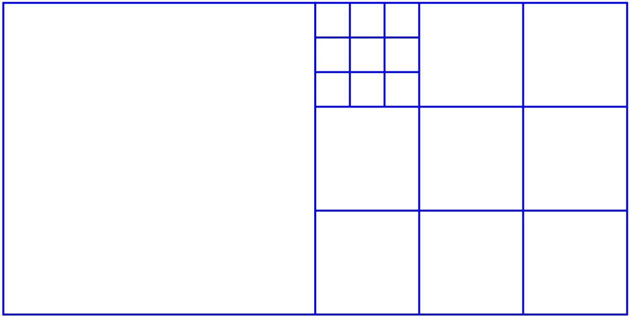
  - (r,θ) polar coordinates in Ω
  - a_i, b_i constants depending on Ω_i
  - α regularity of the solution

Analytical solutions



Case 1 Case 2

A vertex-centered FV scheme on nonmatching grids



A vertex-centered FV scheme on nonmatching grids

- Suppose that a (nonmatching) grid $\mathcal{D}_h$ is given.
- Construct a conforming simplicial mesh $\mathcal{T}_h$ given by the "centers" of $\mathcal{D}_h$.
- Find $p_h \in V_h$ such that

$$-\langle \{a\}_\omega \nabla p_h \cdot \mathbf{n}, 1 \rangle_{\partial D} = (f, 1)_D \qquad \forall D \in \mathcal{D}_h^{\mathrm{int}}.$$

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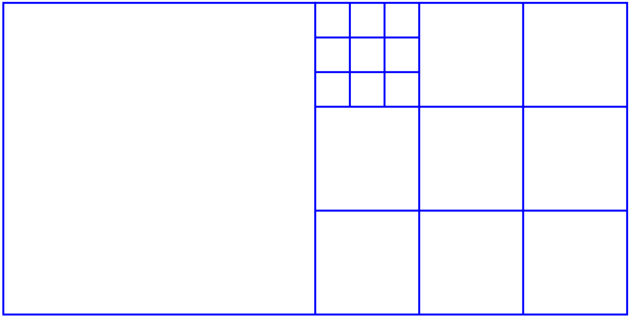

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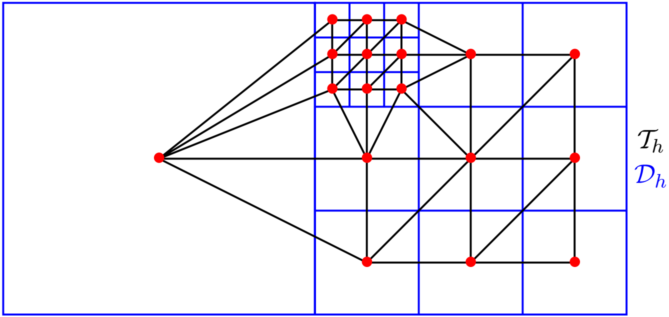

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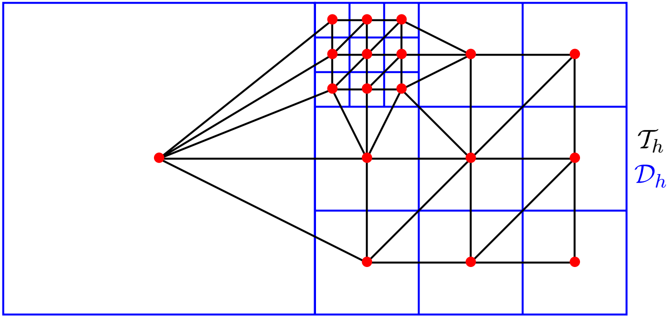

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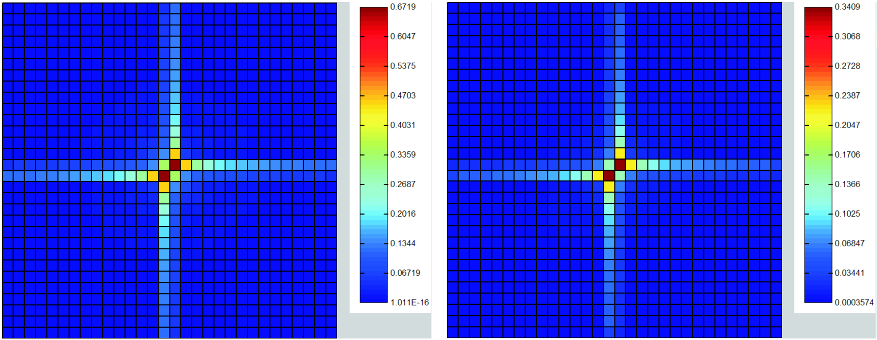
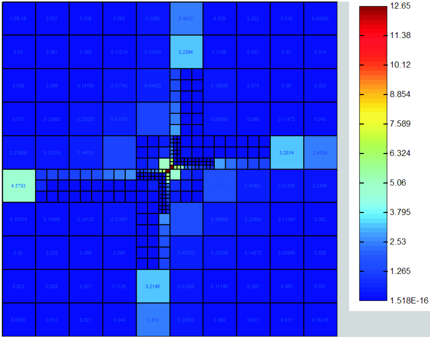
Error distribution on a uniformly refined mesh, case 1



Estimated error distribution Exact error distribution

Error distribution on an adaptively refined mesh, case 2



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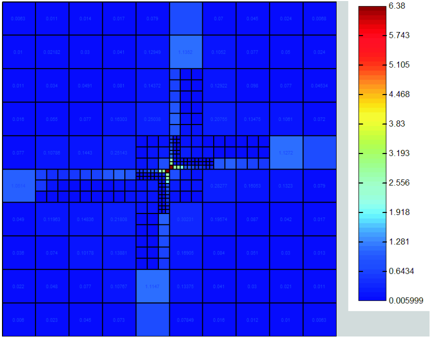
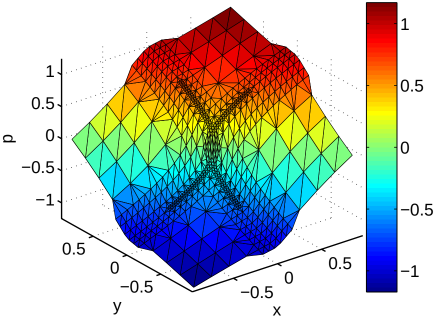
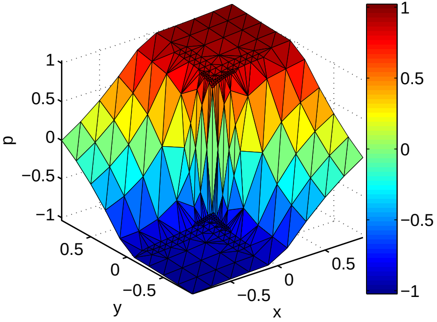


Exact error distribution

Approximate solutions on adaptively refined meshes

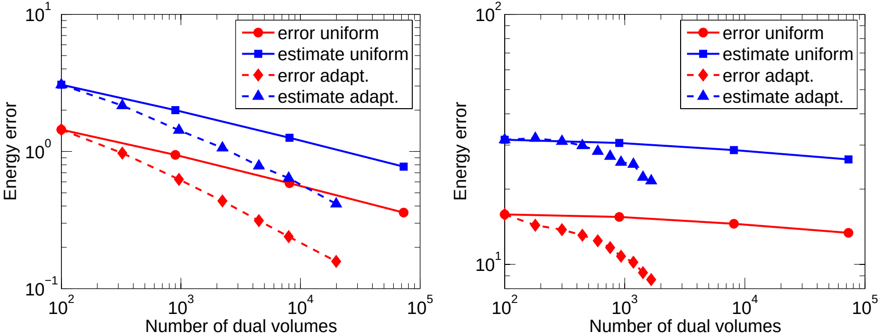


Case 1



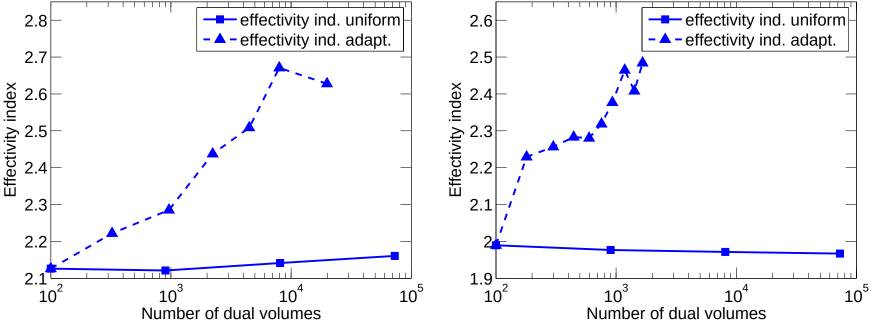
Case 2

Estimated and actual errors in uniformly/adaptively refined meshes



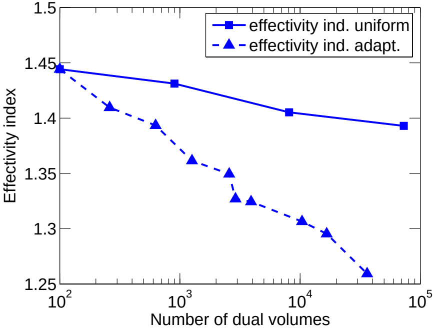
Case 1 Case 2

Original effectivity indices in uniformly/adaptively refined meshes



Case 1 Case 2

Effectivity indices in uniformly/adaptively refined meshes using a simple (no linear system solution) local minimization



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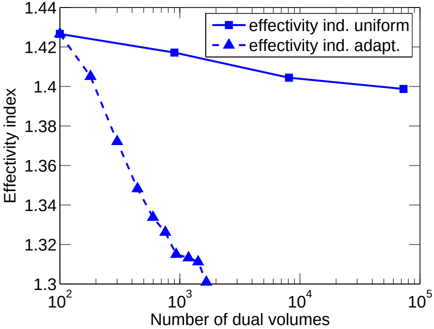

Case 2

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4. Estimates including the algebraic error
    - Problem and estimates
    - Numerical experiments
5. Conclusions and future work

A reaction–diffusion problem

Problem

$$\begin{aligned} -\triangle p + rp &= f \quad \text{in } \Omega\,,\\ p &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

Assumptions

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a polygonal domain
- $r \in L^\infty(\Omega)$ such that for each $D \in \mathcal{D}_h$, $0 \le c_{r,D} \le r \le C_{r,D}$, a.e. in D

Bilinear form $\mathcal{B}$

$$\mathcal{B}(p,\varphi) := (\nabla p, \nabla\varphi)_\Omega + (r^{1/2}p, r^{1/2}\varphi)_\Omega, \qquad p, \varphi \in H_0^1(\Omega).$$

Weak solution

Find $p \in H_0^1(\Omega)$ such that $\mathcal{B}(p,\varphi) = (f,\varphi)_\Omega \qquad \forall \varphi \in H_0^1(\Omega)$.

Energy norm

$$|||\varphi|||_\Omega^2 := \mathcal{B}(\varphi,\varphi), \qquad \varphi \in H_0^1(\Omega).$$

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Residual and diffusive flux estimators

Estimators

- *residual estimator*

$$\eta_{\mathrm{R},D} := m_D \|f - \nabla \cdot \mathbf{t}_h - r p_h\|_D$$

- *diffusive flux estimator*

$$\eta_{\mathrm{DF},D} := \min\left\{\eta^{(1)}_{DF,D}, \eta^{(2)}_{DF,D}\right\}$$

$$\begin{aligned} \eta^{(1)}_{\mathrm{DF},D} &:= \|\nabla p_h + \mathbf{t}_h\|_D \\ \eta^{(2)}_{\mathrm{DF},D} &:= \left\{\sum_{K \in \mathcal{S}_D} \left(m_K \|\triangle p_h + \nabla \cdot \mathbf{t}_h - (\triangle p_h + \nabla \cdot \mathbf{t}_h)_K\|_K \right.\right. \\ &\qquad \left.\left. + \widetilde{m}_K^{\frac{1}{2}} \sum_{\sigma \in \mathcal{E}_K \cap \mathcal{G}_h^{\mathrm{int}}} C_{\mathrm{t},K,\sigma}^{\frac{1}{2}} \|(\nabla p_h + \mathbf{t}_h) \cdot \mathbf{n}\|_\sigma \right)^2 \right\}^{\frac{1}{2}} \end{aligned}$$

Robust a posteriori error estimates for $-\triangle p + rp = f$

Theorem (A posteriori error estimate)

There holds

$$|||p - p_h|||_\Omega \leq \left\{ \sum_{D \in \mathcal{D}_h} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^2 \right\}^{\frac{1}{2}} .$$

Theorem (Local efficiency)

There holds

$$\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D} \leq C|||p - p_h|||_D ,$$

where C depends only on d, $\kappa_\mathcal{T}$, m, and $C_{r,D}/c_{r,D}$.

Properties

- **guaranteed upper bound**
- local efficiency
- **robustness**
- negligible evaluation cost

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- **guaranteed upper bound**
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Constants and inequalities

Poincaré inequality

- $\|\varphi - \varphi_D\|_D^2 \leq C_{\mathrm{P},D} h_D^2 \|\nabla\varphi\|_D^2 \qquad \forall \varphi \in H^1(D)$
- $D \in \mathcal{D}_h^{\mathrm{int}}$
- φ_D: mean of φ over D
- $C_{\mathrm{P},D} = 1/\pi^2$ if D is convex

Friedrichs inequality

- $\|\varphi\|_D^2 \leq C_{\mathrm{F},D,\partial\Omega} h_D^2 \|\nabla\varphi\|_D^2 \qquad \forall \varphi \in H^1(D) \cap H_0^1(\Omega)$
- $D \in \mathcal{D}_h^{\mathrm{ext}}$
- $C_{\mathrm{F},D,\partial\Omega} = 1$ in general

Trace inequality

- $\|\varphi\|_\sigma^2 \leq C_{\mathrm{t},K,\sigma}(h_K^{-1}\|\varphi\|_K^2 + \|\varphi\|_K \|\nabla\varphi\|_K) \qquad \forall \varphi \in H^1(K)$
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Constants and inequalities

Lemma (Auxiliary estimates on simplices)

Let $K \in \mathcal{S}_h$, $\sigma \in \mathcal{E}_K$, $\varphi \in H^1(K)$, *and* $\varphi_K := (\varphi, 1)_K / |K|$. *Then*

$$\|\varphi - \varphi_K\|_K \leq m_K |||\varphi|||_K$$

with

$$m_K := \min\left\{ C_{\mathrm{P},K}^{1/2} h_K, c_{r,K}^{-1/2} \right\}.$$

Moreover,

$$\|\varphi - \varphi_K\|_\sigma \leq C_{\mathrm{t},K,\sigma}^{1/2} \widetilde{m}_K^{1/2} |||\varphi|||_K$$

with

$$\widetilde{m}_K := \min\left\{ \left(C_{\mathrm{P},K} + C_{\mathrm{P},K}^{1/2} \right) h_K, c_{r,K}^{-1} h_K^{-1} + \frac{1}{2} c_{r,K}^{-1/2} \right\}.$$

Constants and inequalities

Lemma (Auxiliary estimates on dual volumes)

Let $D \in \mathcal{D}_h$, $\varphi \in H^1(D)$, and $\varphi_D := (\varphi, 1)_D/|D|$. Then,

$$\begin{aligned} \|\varphi - \varphi_D\|_D &\le m_D |||\varphi|||_D, \quad D \in \mathcal{D}_h^{\mathrm{int}}, \\ \|\varphi\|_D &\le m_D |||\varphi|||_D, \quad D \in \mathcal{D}_h^{\mathrm{ext}}, \end{aligned}$$

where

$$\begin{aligned} m_D &:= \min\left\{ C_{\mathrm{P},D}^{1/2} h_D, c_{r,D}^{-1/2} \right\}, \quad D \in \mathcal{D}_h^{\mathrm{int}}, \\ m_D &:= \min\left\{ C_{\mathrm{F},D,\partial\Omega}^{1/2} h_D, c_{r,D}^{-1/2} \right\}, \quad D \in \mathcal{D}_h^{\mathrm{ext}}. \end{aligned}$$

Outline

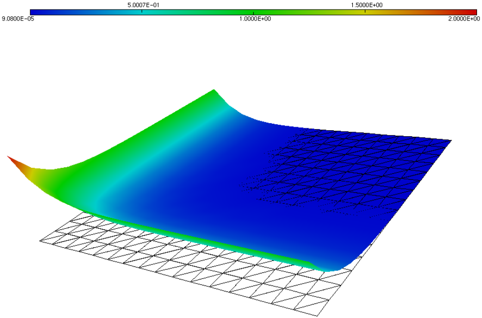
Problem and exact solution

Problem

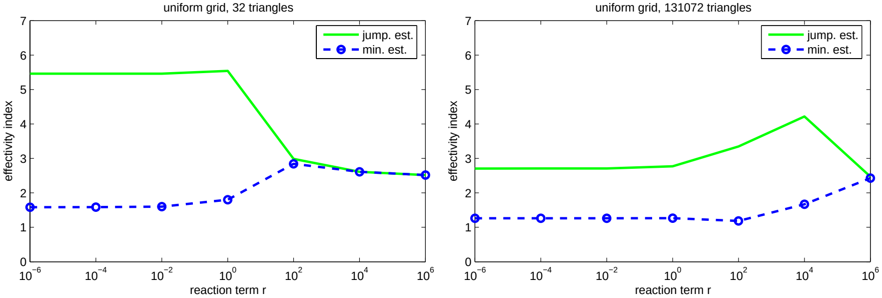
$$-\triangle p + rp = 0, \qquad \text{in } \Omega$$
$$p = p_0, \qquad \text{on } \partial\Omega$$

Solution

$$p_0(x, y) = e^{-\sqrt{r}x} + e^{-\sqrt{r}y}$$



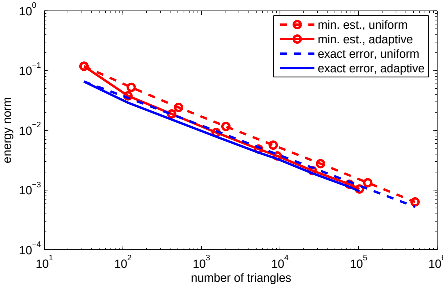
Effectivity indices for the original estimate and for the minimization estimate in dependence on *r*



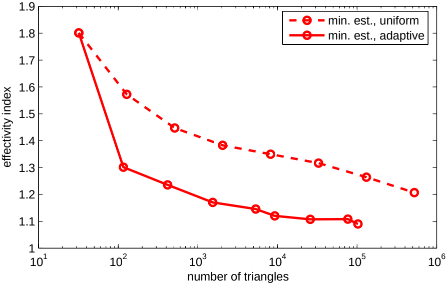
Mesh with 32 triangles

Mesh with 131072 triangles

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



Est. and act. errors, $r = 1$



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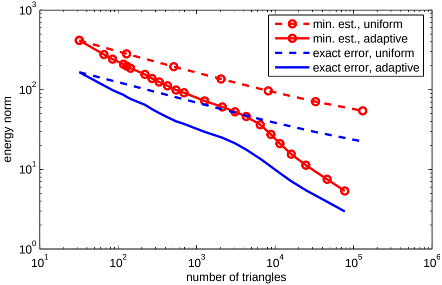
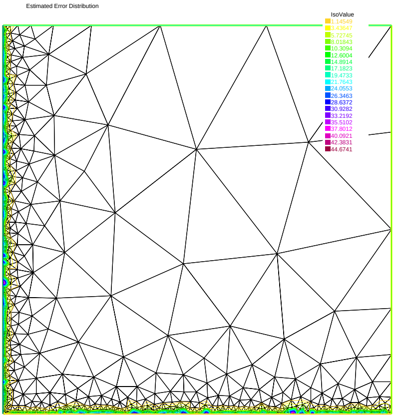
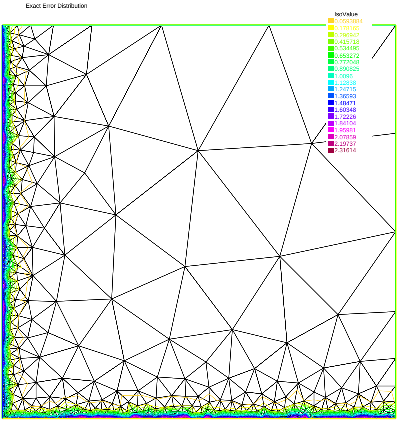


Est. and act. errors, $r = 10^6$ Effectivity indices, $r = 10^6$

Error distribution on an adaptively refined mesh, $r = 10^6$



Estimated error distribution



Exact error distribution

Outline

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1. Introduction
2. Pure diffusion problems
   - Classical a posteriori estimates
   - Optimal abstract framework and a first estimate
   - Optimal a posteriori error estimate
   - Remarks on finite elements and finite volumes
   - Efficiency of the a posteriori error estimate
   - Numerical experiments
3. Reaction–diffusion problems
   - Problem and estimates
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4. Estimates including the algebraic error
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5. Conclusions and future work

A model pure diffusion problem

A model pure diffusion problem

$$\begin{aligned} -\nabla\cdot(\mathbf{S}\nabla p) &= f \quad \text{in } \Omega,\\ p &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

Algebraic problem

- at some point, we shall solve $\mathbb{A}X = B$
- we only solve it inexactly, $\mathbb{A}X^* \approx B$
- we know the algebraic residual, $R := B - \mathbb{A}X^*$

Goals

- take into account the algebraic error
- efficiently stop the iterative solver
- **certified error bound and huge computational savings**

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Estimate including inexact linear systems error

Theorem (A posteriori error estimate including inexact linear systems solution error, cell-centered FVs or MFEs)

There holds

$$|||p - \tilde{p}_h^*||| \leq \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{NC},K}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{R},K}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{AE},K}^2 \right\}^{\frac{1}{2}}.$$

- **nonconformity estimator**
  - $\eta_{\mathrm{NC},K} := |||\tilde{p}_h^* - \mathcal{I}_{\mathrm{Os}}(\tilde{p}_h^*)|||_K$
- **residual estimator**
  - $\eta_{\mathrm{R},K} := m_K \|f + \nabla \cdot (\mathbf{S}_K \nabla \tilde{p}_h^*)\|_K$
  - $m_K^2 := C_{\mathrm{P}} \frac{h_K^2}{c_{\mathbf{S},K}}$
- **algebraic error estimator**
  - $\eta_{\mathrm{AE},K} := \|\mathbf{S}^{-\frac{1}{2}} \mathbf{t}_h\|_K$
  - $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{T}_h)$ is such that $\nabla \cdot \mathbf{t}_h|_K = \frac{R_K}{|K|}$
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$$|||p - \tilde{p}_h^*||| \le \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{NC},K}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{R},K}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{AE},K}^2 \right\}^{\frac{1}{2}}.$$

- **nonconformity estimator**
  - $\eta_{\mathrm{NC},K} := |||\tilde{p}_h^* - \mathcal{I}_{\mathrm{Os}}(\tilde{p}_h^*)|||_K$
- **residual estimator**
  - $\eta_{\mathrm{R},K} := m_K \|f + \nabla \cdot (\mathbf{S}_K \nabla \tilde{p}_h^*)\|_K$
  - $m_K^2 := C_{\mathrm{P}} \frac{h_K^2}{c_{\mathbf{S},K}}$
- **algebraic error estimator**
  - $\eta_{\mathrm{AE},K} := \|\mathbf{S}^{-\frac{1}{2}} \mathbf{t}_h\|_K$
  - $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{T}_h)$ is such that $\nabla \cdot \mathbf{t}_h|_K = \frac{R_K}{|K|}$
  - R is the residual vector

Estimate including inexact linear systems error

Theorem (A posteriori error estimate including inexact linear systems solution error, cell-centered FVs or MFEs)

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$$|||p - \tilde{p}_h^*||| \leq \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{NC},K}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{R},K}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{K \in \mathcal{T}_h} \eta_{\mathrm{AE},K}^2 \right\}^{\frac{1}{2}}.$$

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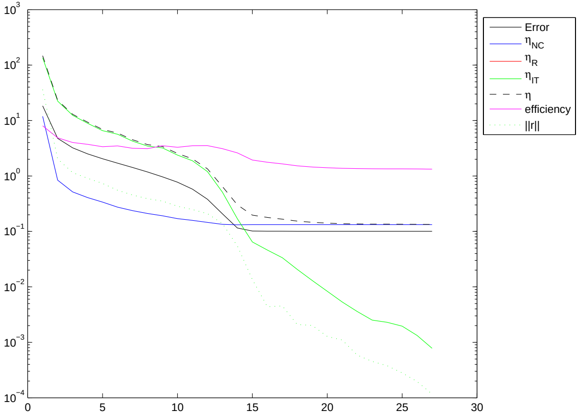
Outline

Finite volume estimates including inexact linear systems solution



Different estimators, error, and effectivity index as a function of the number of CG iterations

Outline

1. Introduction
2. Pure diffusion problems
   - Classical a posteriori estimates
   - Optimal abstract framework and a first estimate
   - Optimal a posteriori error estimate
   - Remarks on finite elements and finite volumes
   - Efficiency of the a posteriori error estimate
   - Numerical experiments
3. Reaction–diffusion problems
   - Problem and estimates
   - Numerical experiments
4. Estimates including the algebraic error
   - Problem and estimates
   - Numerical experiments
5. Conclusions and future work

Comments on the estimates and their efficiency

General comments

- $p \in H^1(\Omega)$, no additional regularity
- no saturation assumption
- no Helmholtz decomposition
- polynomial degree-independent upper bound
- the only important tools: Cauchy–Schwarz and optimal Poincaré–Friedrichs and trace inequalities
- holds from diffusion to convection–diffusion–reaction cases
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Essentials of the estimates

Essentials of the estimates

- nonconformity estimate: compare the approximate solution p_h to a $H^1(\Omega)$-conforming potential s_h
- diffusive flux estimate: compare the flux of the approximate solution $-\mathbf{S}\nabla p_h$ to a $\mathbf{H}(\mathrm{div}, \Omega)$-conforming flux $\mathbf{t}_h$
- evaluate the residue for $\mathbf{t}_h$
- in conforming methods ($p_h \in H^1(\Omega)$), there is no nonconformity estimate
- in flux-conforming methods ($-\mathbf{S}\nabla p_h \in \mathbf{H}(\mathrm{div}, \Omega)$), there is no diffusive flux estimate

Conclusions and future work

Conclusions

- guaranteed, locally efficient, and robust a posteriori error estimates
- directly and locally computable
- almost asymptotically exact
- optimal framework (exact and robust)
- works for all major numerical schemes
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Future work

- asymptotic exactness
- nonlinear (degenerate) cases
- extensions to other types of problems (Stokes, Maxwell)
- multi-scale, multi-numerics, multi-physics, mortars

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Merci de votre attention !