Two types of guaranteed (and robust) a posteriori estimates for finite volume methods

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Outline

1. Introduction
   - Classical a posteriori estimates
2. Flux-based/cell-centered estimates
   - A posteriori error estimates and their efficiency
   - Numerical experiments
3. Potential-based/vertex-centered estimates
   - A posteriori error estimates and their efficiency
   - Numerical experiments
4. Extensions
   - Cell-centered convection–diffusion–reaction estimates
   - Vertex-centered reaction–diffusion estimates
   - Estimates including the algebraic error
5. Conclusions and future work

Outline

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 upper bound)

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

Local efficiency (local lower bound)

- $\eta_K(p_h)^2 \le C_{\mathrm{eff},K}^2 \sum_{L \text{ close to } K} \|p - p_h\|_L^2$

Asymptotic exactness

- $\sum_{K \in \mathcal{T}_h} \eta_K(p_h)^2 / \|p - p_h\|_\Omega^2 \to 1$

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

Discontinuous finite elements

- Karakashian and Pascal (2003), Becker, Hansbo, and Larson (2003), residual-based estimates
- Ainsworth (2007), Kim (2007), Lazarov, Repin, and Tomar (2008), Cochez-Dhondt and Nicaise (2008), equilibrated fluxes estimates

Finite volumes

- Ohlberger (2001), non-energy norm estimates
- Nicaise (2004), reconstruction-based estimates

Problems with discontinuous coefficients

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

Convection–diffusion problems

- Verfürth (1998, 2005), conforming finite elements
- Sangalli (2008), conforming finite elements

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Residual estimates for $-\triangle p = f$

Corollary (Classical residual error estimate in FEs)

There holds (cf. Verfürth 96)

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

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.

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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)

There holds (cf. Zienkiewicz–Zhu 87)

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

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

Drawbacks

- No error upper bound (neither guaranteed, nor reliable).
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Equilibrated residuals estimate for $-\nabla \cdot (\mathbf{S}\nabla p) = f$

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

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

Then there holds (cf. Ainsworth and Oden 00)

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

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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A model problem

Problem

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\begin{aligned}
-\nabla\cdot(\mathbf{S}\nabla p) &= f \quad \text{in } \Omega,\\
p &= g \quad \text{on } \Gamma_{\mathrm{D}},\\
-\mathbf{S}\nabla p\cdot\mathbf{n} &= u \quad \text{on } \Gamma_{\mathrm{N}}
\end{aligned}
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Assumptions

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a polygonal domain
- $\mathbf{S}|_K$ is a constant SPD matrix, $c_{\mathbf{S},K}$ its smallest, and $C_{\mathbf{S},K}$ its largest eigenvalue on each $K \in \mathcal{T}_h$

Difficulties

- $\mathbf{S}$ is a piecewise constant matrix, inhomogeneous and anisotropic

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Bilinear form, weak solution, and energy norm

Definition (Bilinear form $\mathcal{B}$)

We define a bilinear form $\mathcal{B}$ for $p, \varphi \in H^1(\mathcal{T}_h)$ by

$$\mathcal{B}(p, \varphi) := \sum_{K \in \mathcal{T}_h} (\mathbf{S} \nabla p, \nabla \varphi)_K .$$

Definition (Weak solution)

Weak solution: $p \in H^1(\Omega)$ with $p|_{\Gamma_{\mathrm{D}}} = g$ such that

$$\mathcal{B}(p, \varphi) = (f, \varphi) - \langle u, \varphi \rangle_{\Gamma_{\mathrm{N}}} \qquad \forall \varphi \in H^1_{\mathrm{D}}(\Omega).$$

Definition (Energy (semi-)norm)

We define the energy (semi-)norm for $\varphi \in H^1(\mathcal{T}_h)$ by

$$|||\varphi|||^2 := \sum_{K \in \mathcal{T}_h} |||\varphi|||_K^2, \ |||\varphi|||_K^2 := \left\| \mathbf{S}^{\frac{1}{2}} \nabla \varphi \right\|_K^2 .$$

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General cell-centered finite volume scheme

Definition (FV scheme for $-\nabla \cdot (\mathbf{S}\nabla p) = f$)

Find p_K, $K \in \mathcal{T}_h$, such that

$$\sum_{\sigma \in \mathcal{E}_K} S_{K,\sigma} = f_K |K| \qquad \forall K \in \mathcal{T}_h\,.$$

- $S_{K,\sigma}$: diffusive flux — no specific form, just conservativity needed
- $f_K := (f, 1)/|K|$

Example

- $S_{K,\sigma} = -s_{K,L} \frac{|\sigma_{K,L}|}{d_{K,L}} (p_L - p_K)$

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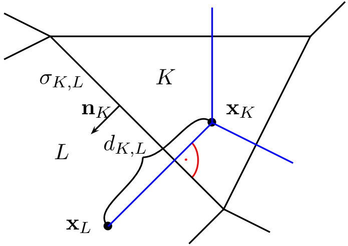
$$\sum_{\sigma \in \mathcal{E}_K} S_{K,\sigma} = f_K|K| \qquad \forall K \in \mathcal{T}_h\,.$$

- $S_{K,\sigma}$: diffusive flux
- $f_K := (f, 1)/|K|$

no specific form,
just conservativity needed

Example

- $S_{K,\sigma} = -s_{K,L}\frac{|\sigma_{K,L}|}{d_{K,L}}(p_L - p_K)$



A locally postprocessed scalar variable $\tilde{p}_h$

Definition (Postprocessed scalar variable $\tilde{p}_h$)

We define $\tilde{p}_h$ such that, separately on each $K \in \mathcal{T}_h$,

$$\begin{aligned} -\nabla\cdot(\mathbf{S}\nabla\tilde{p}_h) &= \frac{1}{|K|}\sum_{\sigma\in\mathcal{E}_K} S_{K,\sigma}, \\ (1-\mu_K)(\tilde{p}_h,1)_K/|K| + \mu_K\tilde{p}_h(\mathbf{x}_K) &= p_K, \\ -\mathbf{S}\nabla\tilde{p}_h|_K\cdot\mathbf{n} &= S_{K,\sigma}/|\sigma| \quad \forall\sigma\in\mathcal{E}_K\,. \end{aligned}$$

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- $\tilde{p}_h$ exists and is unique
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- $\tilde{p}_h \notin H^1(\Omega)$, only $\in H^1(\mathcal{T}_h)$ in general
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Outline

Optimal abstract estimate for $-\nabla \cdot (\mathbf{S}\nabla p) = f$

Theorem (Optimal abstract estimate, hom. Dir. BC)

Let p be the weak solution and let $\tilde{p}_h \in H^1(\mathcal{T}_h)$ be arbitrary but such that $-\mathbf{S}\nabla \tilde{p}_h \in \mathbf{H}(\mathrm{div}, \Omega)$. Then

$$\begin{aligned} |||p - \tilde{p}_h||| &\leq \inf_{s \in H_0^1(\Omega)} |||\tilde{p}_h - s||| + \sup_{\varphi \in H_0^1(\Omega),\, |||\varphi|||=1} (f + \nabla \cdot (\mathbf{S}\nabla \tilde{p}_h), \varphi) \\ &\leq |||p - \tilde{p}_h||| + \sup_{\varphi \in H_0^1(\Omega),\, |||\varphi|||=1} (f + \nabla \cdot (\mathbf{S}\nabla \tilde{p}_h), \varphi). \end{aligned}$$

Properties

- Guaranteed upper bound (no undetermined constant).
- Robust and exact up to a higher-order term.
- Not computable (infimum over an infinite-dimensional space).

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A first computable estimate for $-\nabla \cdot (\mathbf{S}\nabla p) = f$

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$$|||p - \tilde{p}_h||| \leq \frac{C_{\mathrm{F},\Omega}^{1/2} h_\Omega}{c_{\mathbf{S},\Omega}^{1/2}} \|f + \nabla \cdot (\mathbf{S}\nabla \tilde{p}_h)\| + |||\tilde{p}_h - s_h|||.$$

Properties

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- Advantage: very general (not even a local conservativity used).
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Optimal a posteriori error estimate for $-\nabla \cdot (\mathbf{S}\nabla p) = f$

Theorem (A posteriori error estimate)

Let p be the weak solution and let $\tilde{p}_h \in H^1(\mathcal{T}_h)$ be arbitrary but such that $-\mathbf{S}\nabla\tilde{p}_h \in \mathbf{H}(\mathrm{div},\Omega)$, $-\mathbf{S}\nabla\tilde{p}_h \cdot \mathbf{n} = u_\sigma$ for all $\sigma \in \mathcal{E}_h^{\mathrm{N}}$, and $-(\nabla \cdot (\mathbf{S}\nabla\tilde{p}_h), 1)_K = (f, 1)_K$ for all $K \in \mathcal{T}_h$. Then

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- **nonconformity estimator**
  - $\eta_{\mathrm{NC},K} := |||\tilde{p}_h - \mathcal{I}_{\mathrm{Os}}^{\Gamma_{\mathrm{D}}}(\tilde{p}_h)|||_K$
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Local efficiency for $-\nabla \cdot (\mathbf{S}\nabla p) = f$

Theorem (Local efficiency)

There holds

$$\eta_{\mathrm{R},K} + \eta_{\mathrm{NC},K} \leq C\sqrt{\frac{C_{\mathbf{S},K}}{c_{\mathbf{S},\mathcal{T}_K}}}\left(|||p - \tilde{p}_h|||_{\mathcal{T}_K} + |||p - \tilde{p}_h|||_{\#,\mathcal{E}_K^{\mathrm{int}}}\right) + |||\mathcal{I}_{\mathrm{Os}}(\tilde{p}_h) - \mathcal{I}_{\mathrm{Os}}^{\Gamma_{\mathrm{D}}}(\tilde{p}_h)|||_K,$$

where the constant C depends only on the space dimension d, on the shape regularity parameter $\kappa_{\mathcal{T}}$, and on the polynomial degree k of f and where

$$|||p - \tilde{p}_h|||^2_{\#,\mathcal{E}_K^{\mathrm{int}}} := c_{\mathbf{S},\mathcal{T}_K} \sum_{\sigma \in \mathcal{E}_K^{\mathrm{int}}} h_\sigma^{-1} \|\langle [\![p - \tilde{p}_h]\!], 1\rangle_\sigma |\sigma|^{-1}\|^2_\sigma.$$

- nonconformity and residual estimators are **locally efficient** (lower bound for error on K and its neighbors) and **semi-robust** ($C_{\mathrm{eff},K}$ depends on local inhomogeneities and anisotropies)

Local efficiency for $-\nabla \cdot (\mathbf{S}\nabla p) = f$

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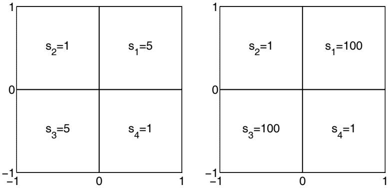
Outline

Discontinuous diffusion tensor and finite volumes

- consider the pure diffusion equation

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

- discontinuous and inhomogeneous **S**, two cases:

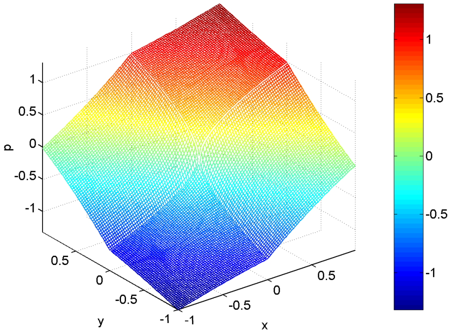


- analytical solution: singularity at the origin

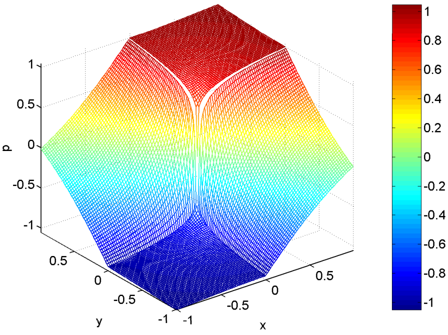
$$p(r,\theta)|_{\Omega_i} = r^{\alpha}(a_i \sin(\alpha\theta) + b_i \cos(\alpha\theta))$$

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

Analytical solutions

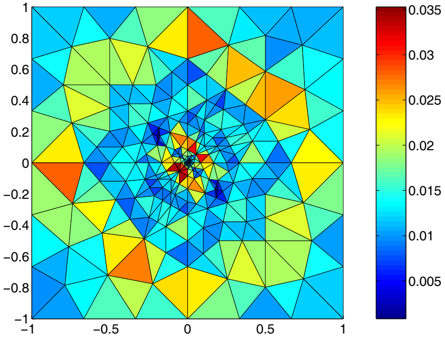


Case 1

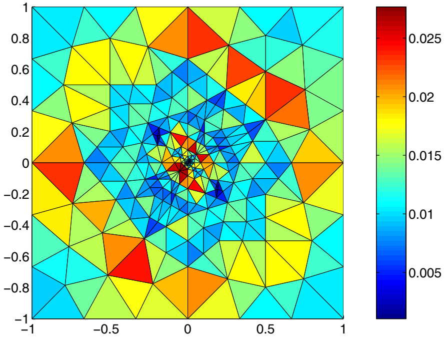


Case 2

Error distribution on an adaptively refined mesh, case 1

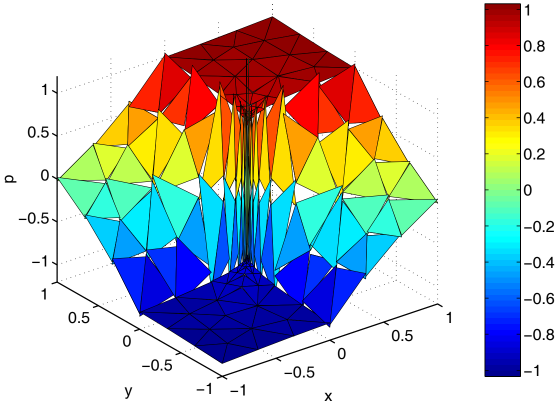


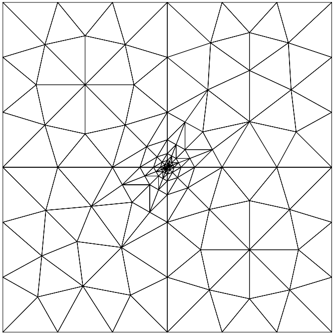
Estimated error distribution



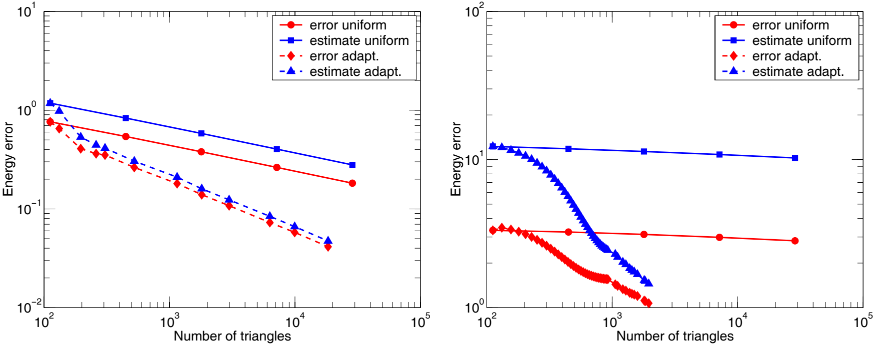
Exact error distribution

Approximate solution and the corresponding adaptively refined mesh, case 2



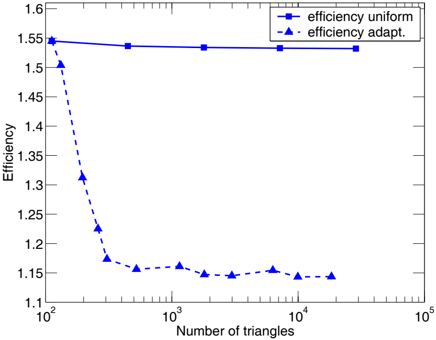


Estimated and actual errors in uniformly/adaptively refined meshes



Case 1 Case 2

Effectivity indices in uniformly/adaptively refined meshes



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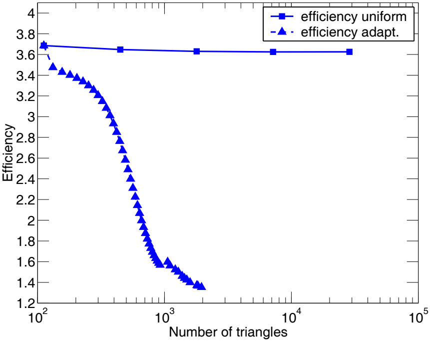

Case 2

Outline

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

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Bilinear form, energy norm, and a weak solution

Definition (Bilinear form $\mathcal{B}$)

We define a bilinear form $\mathcal{B}$ for $p, \varphi \in H_0^1(\Omega)$ by

$$\mathcal{B}(p, \varphi) := (a\nabla p, \nabla \varphi) .$$

Definition (Energy norm)

The associated energy norm for $\varphi \in H_0^1(\Omega)$ is given by

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

Definition (Weak solution)

Weak solution: $p \in H_0^1(\Omega)$ such that

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

Theorem (Optimal abstract estimate, potential-based)

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

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

Properties

- Guaranteed upper bound (no undetermined constant).
- Exact and robust.
- Not computable (infimum over an infinite-dimensional space).

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Properties

- Guaranteed upper bound ($C_{\mathrm{F},\Omega} \le 1$, Friedrichs constant).
- $\mathbf{t}_h \in \mathbf{H}(\mathrm{div}, \Omega)$ unconstrained, $\nabla \cdot \mathbf{t}_h \ne f$ $\times$ Prager & Synge.
- $\|a^{\frac{1}{2}} \nabla p_h + a^{-\frac{1}{2}} \mathbf{t}_h\|$ penalizes $-a \nabla p_h \notin \mathbf{H}(\mathrm{div}, \Omega)$.
- $\|f - \nabla \cdot \mathbf{t}_h\|$ is a residual term, evaluated for $\mathbf{t}_h$.
- Advantage: scheme-independent (works for all schemes) (promoted by Repin).
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Optimal a posteriori error estimate for $-\nabla \cdot (a\nabla p) = f$

Theorem (Optimal a posteriori error estimate)

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

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

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  - $\eta_{\mathrm{DF},D} := \|a^{\frac{1}{2}} \nabla p_h + a^{-\frac{1}{2}} \mathbf{t}_h\|_D$
  - penalizes the fact that $-a\nabla p_h \notin \mathbf{H}(\mathrm{div}, \Omega)$
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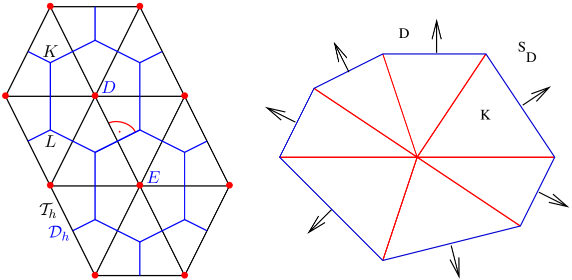
Cell-centered finite volumes for $-\nabla \cdot (a\nabla p) = f$

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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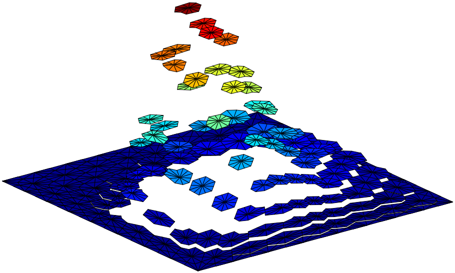
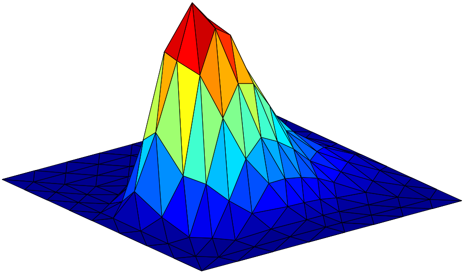
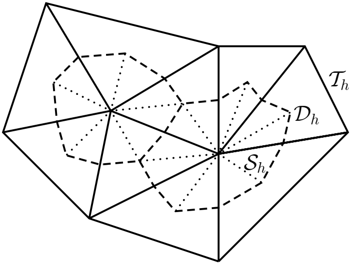


p_D piecewise constant on $\mathcal{D}_h$



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

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

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

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

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

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

Robustness when $a \neq 1$.

- 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, with better constants

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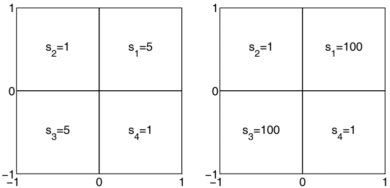
Outline

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:

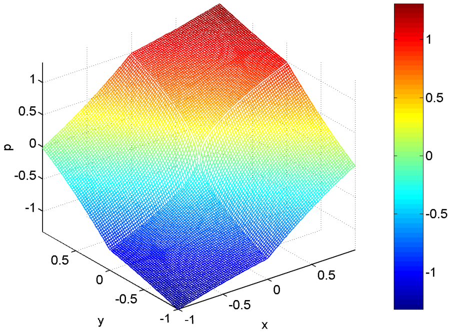


- analytical solution: singularity at the origin

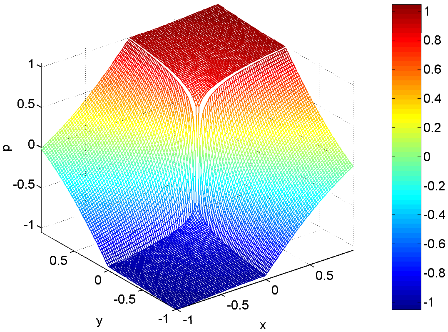
$$p(r, \theta)|_{\Omega_i} = r^{\alpha}(a_i \sin(\alpha\theta) + b_i \cos(\alpha\theta))$$

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

Analytical solutions

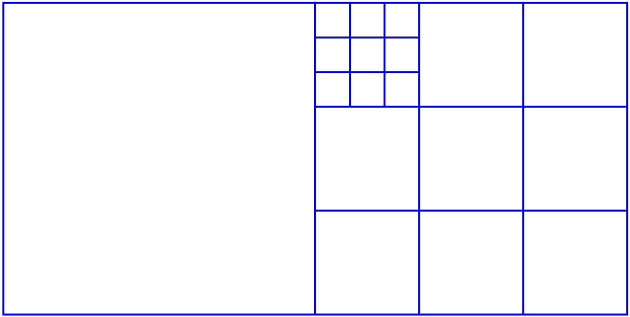


Case 1



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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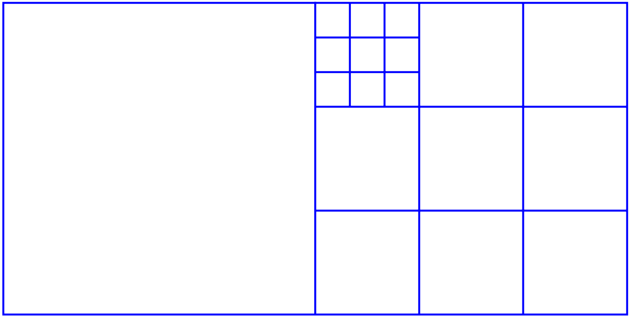

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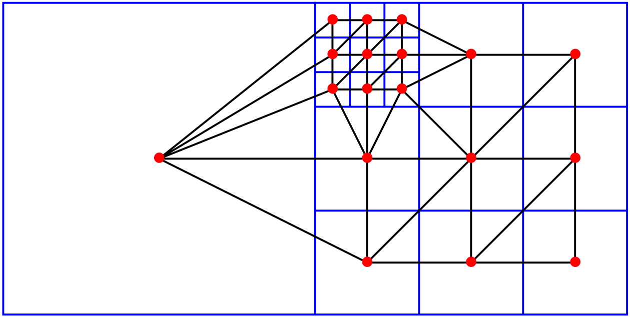

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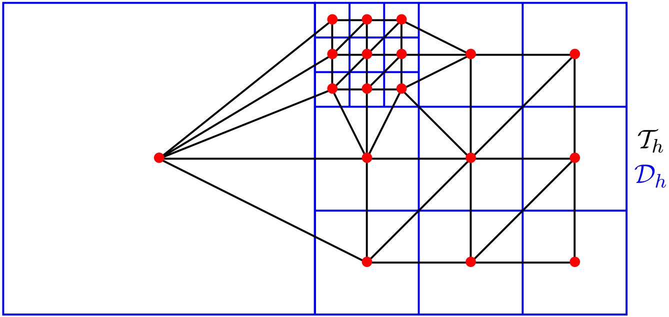

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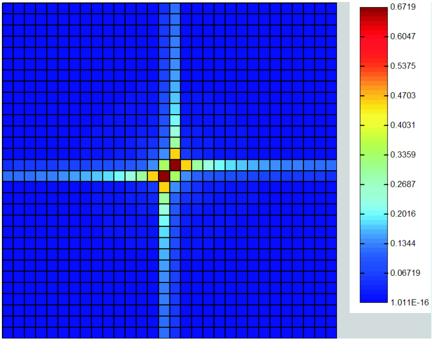
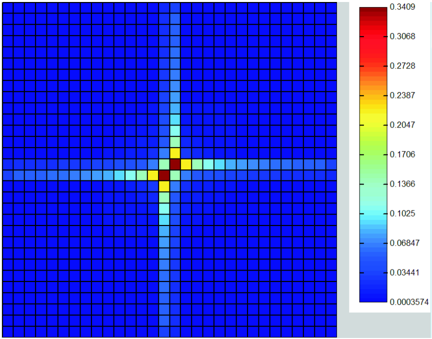
Error distribution on a uniformly refined mesh, case 1

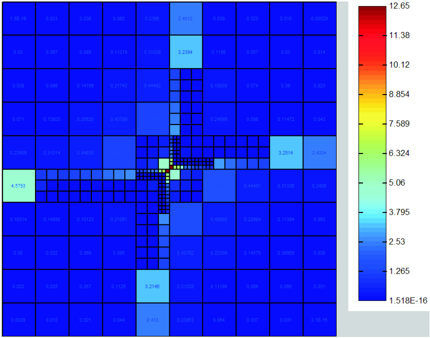


Estimated error distribution



Exact error distribution

Error distribution on an adaptively refined mesh, case 2



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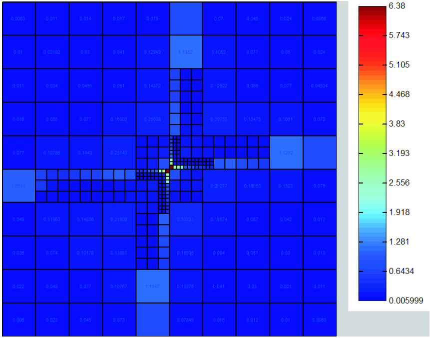
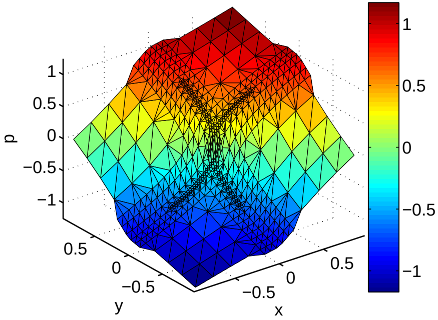


Exact error distribution

Approximate solutions on adaptively refined meshes



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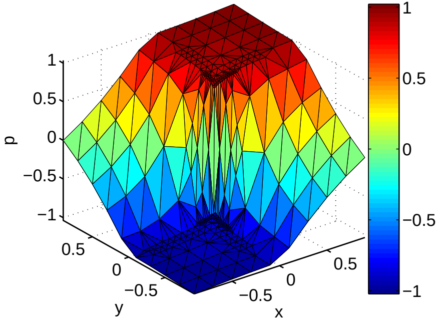
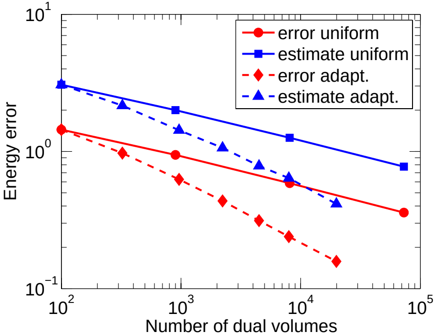


Case 2

Estimated and actual errors in uniformly/adaptively refined meshes



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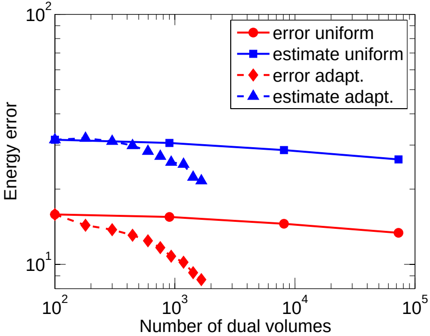
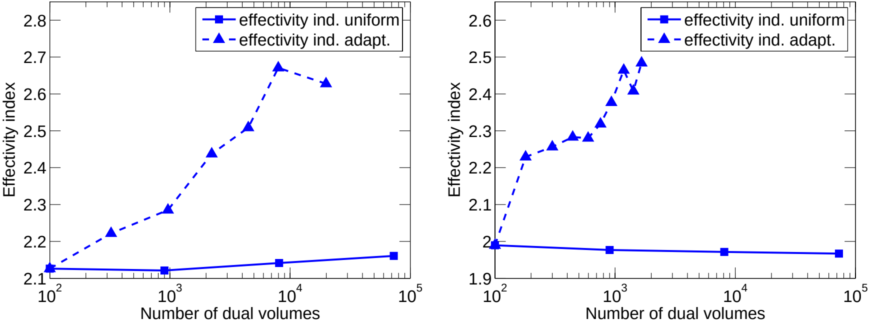


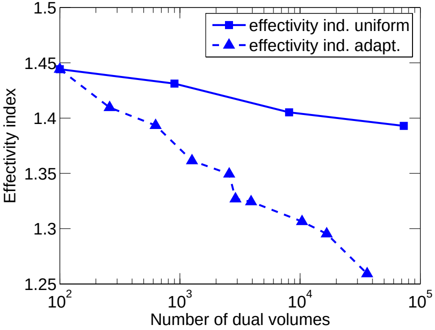
Case 2

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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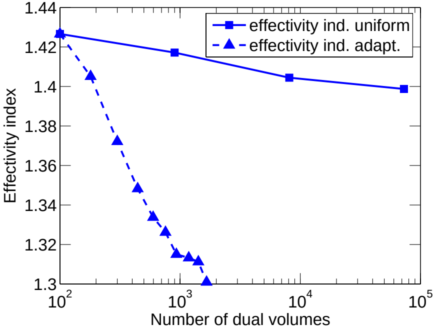

Case 2

Outline

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A convection–diffusion–reaction problem with general boundary conditions

Problem

$$
\begin{aligned}
-\nabla \cdot (\mathbf{S}\nabla p) + \nabla \cdot (p\mathbf{w}) + rp &= f \quad \text{in } \Omega, \\
p &= g \quad \text{on } \Gamma_{\mathrm{D}}, \\
-\mathbf{S}\nabla p \cdot \mathbf{n} &= u \quad \text{on } \Gamma_{\mathrm{N}}
\end{aligned}
$$

Assumptions

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a polygonal domain
- $\mathbf{S}|_K$ is a constant SPD matrix, $c_{\mathbf{S},K}$ its smallest, and $C_{\mathbf{S},K}$ its largest eigenvalue on each $K \in \mathcal{T}_h$
- $\left(\frac{1}{2}\nabla \cdot \mathbf{w} + r\right)|_K \geq c_{\mathbf{w},r,K} \geq 0$ on each $K \in \mathcal{T}_h$ (from pure diffusion to convection–diffusion–reaction cases)

Difficulties

- $\mathbf{S}$ is a piecewise constant matrix, inhomogeneous and anisotropic
- $\mathbf{w}$ is dominating

A convection–diffusion–reaction problem with general boundary conditions

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- **S** is a piecewise constant matrix, inhomogeneous and anisotropic
- **w** is dominating

Bilinear form, weak solution, and energy norm

Definition (Bilinear form $\mathcal{B}$)

We define a bilinear form $\mathcal{B}$ for $p, \varphi \in H^1(\mathcal{T}_h)$ by

$$\mathcal{B}(p, \varphi) := \sum_{K \in \mathcal{T}_h} \left\{ (\mathbf{S} \nabla p, \nabla \varphi)_K + (\nabla \cdot (\mathbf{w} p), \varphi)_K + (rp, \varphi)_K \right\}.$$

Definition (Weak solution)

Weak solution: $p \in H^1(\Omega)$ with $p|_{\Gamma_{\mathrm{D}}} = g$ such that

$$\mathcal{B}(p, \varphi) = (f, \varphi) - \langle u, \varphi \rangle_{\Gamma_{\mathrm{N}}} \qquad \forall \varphi \in H^1_{\mathrm{D}}(\Omega).$$

Definition (Energy (semi-)norm)

We define the energy (semi-)norm for $\varphi \in H^1(\mathcal{T}_h)$ by

$$|||\varphi|||^2 := \sum_{K \in \mathcal{T}_h} |||\varphi|||_K^2, \; |||\varphi|||_K^2 := \left\| \mathbf{S}^{\frac{1}{2}} \nabla \varphi \right\|_K^2 + \left\| \left(\tfrac{1}{2} \nabla \cdot \mathbf{w} + r \right)^{\frac{1}{2}} \varphi \right\|_K^2.$$

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General finite volume scheme

Definition (FV scheme for $-\nabla \cdot (\mathbf{S}\nabla p) + \nabla \cdot (p\mathbf{w}) + rp = f$)

Find p_K, $K \in \mathcal{T}_h$, such that

$$\sum_{\sigma \in \mathcal{E}_K} S_{K,\sigma} + \sum_{\sigma \in \mathcal{E}_K} W_{K,\sigma} + r_K p_K |K| = f_K |K| \qquad \forall K \in \mathcal{T}_h .$$

- $\left.\begin{array}{ll} S_{K,\sigma}: & \text{diffusive flux} \\ W_{K,\sigma}: & \text{convective flux} \end{array}\right\}$ no specific form, just conservativity needed
- $r_K := (r, 1)/|K|$
- $f_K := (f, 1)/|K|$

Example

- $S_{K,\sigma} = -s_{K,L} \frac{|\sigma_{K,L}|}{d_{K,L}} (p_L - p_K)$
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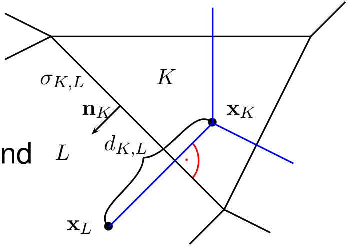

A locally postprocessed scalar variable $\tilde{p}_h$

Definition (Postprocessed scalar variable $\tilde{p}_h$)

We define $\tilde{p}_h$ such that, separately on each $K \in \mathcal{T}_h$,

$$\begin{aligned} -\nabla \cdot (\mathbf{S}\nabla \tilde{p}_h) &= \frac{1}{|K|} \sum_{\sigma \in \mathcal{E}_K} S_{K,\sigma}, \\ (1-\mu_K)(\tilde{p}_h, 1)_K/|K| + \mu_K \tilde{p}_h(\mathbf{x}_K) &= p_K, \\ -\mathbf{S}\nabla \tilde{p}_h|_K \cdot \mathbf{n} &= S_{K,\sigma}/|\sigma| \quad \forall \sigma \in \mathcal{E}_K\,. \end{aligned}$$

Properties of $\tilde{p}_h$

- $\tilde{p}_h$ exists and is unique
- flux of $\tilde{p}_h$ is given by $S_{K,\sigma}$, point or mean value by p_K
- $\tilde{p}_h \notin H^1(\Omega)$, only $\in H^1(\mathcal{T}_h)$ in general
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- $-\mathbf{S} \nabla \tilde{p}_h \in \mathbf{H}(\mathrm{div}, \Omega)$
- given on $\mathcal{T}_h$, no need for a dual mesh
- for simplices or rectangular parallelepipeds when $\mathbf{S}$ is diagonal: $\tilde{p}_h$ is a piecewise second-order polynomial

A locally postprocessed scalar variable $\tilde{p}_h$

Definition (Postprocessed scalar variable $\tilde{p}_h$)

We define $\tilde{p}_h$ such that, separately on each $K \in \mathcal{T}_h$,

$$\begin{aligned} -\nabla \cdot (\mathbf{S}\nabla \tilde{p}_h) &= \frac{1}{|K|} \sum_{\sigma \in \mathcal{E}_K} S_{K,\sigma}, \\ (1-\mu_K)(\tilde{p}_h, 1)_K/|K| + \mu_K \tilde{p}_h(\mathbf{x}_K) &= p_K, \\ -\mathbf{S}\nabla \tilde{p}_h|_K \cdot \mathbf{n} &= S_{K,\sigma}/|\sigma| \quad \forall \sigma \in \mathcal{E}_K . \end{aligned}$$

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A post. estimate for $-\nabla\cdot(\mathbf{S}\nabla p)+\nabla\cdot(p\mathbf{w})+rp=f$

Theorem (A posteriori error estimate)

There holds

$$|||p-\tilde{p}_h|||\leq\left\{\sum_{K\in\mathcal{T}_h}\eta_{\mathrm{NC},K}^2\right\}^{\frac{1}{2}}+\left\{\sum_{K\in\mathcal{T}_h}(\eta_{\mathrm{R},K}+\eta_{\mathrm{C},K}+\eta_{\mathrm{U},K}+\eta_{\mathrm{RQ},K}+\eta_{\Gamma_{\mathrm{N}},K})^2\right\}^{\frac{1}{2}}.$$

- **nonconformity estimator**
  - $\eta_{\mathrm{NC},K}:=|||\tilde{p}_h-\mathcal{I}_{\mathrm{Os}}^{\Gamma_{\mathrm{D}}}(\tilde{p}_h)|||_K$
  - $\mathcal{I}_{\mathrm{Os}}^{\Gamma_{\mathrm{D}}}(\tilde{p}_h)$: Oswald int. operator (Burman and Ern '07)
- **residual estimator**
  - $\eta_{\mathrm{R},K}:=m_K\|f+\nabla\cdot(\mathbf{S}_K\nabla\tilde{p}_h)-\nabla\cdot(\tilde{p}_h\mathbf{w})-r\tilde{p}_h\|_K$
  - $m_K^2:=\min\left\{C_{\mathrm{P}}\frac{h_K^2}{c_{\mathbf{S},K}},\frac{1}{c_{\mathbf{w},r,K}}\right\}$
- **convection estimator**
  - $\eta_{\mathrm{C},K}:=\min\left\{\frac{\|\nabla\cdot(v\mathbf{w})-\frac{1}{2}v\nabla\cdot\mathbf{w}\|_K+\|\nabla\cdot(v\mathbf{w})\|_K}{\sqrt{c_{\mathbf{w},r,K}}},\left(\frac{C_{\mathrm{P}}h_K^2\|\nabla v\cdot\mathbf{w}\|_K^2}{c_{\mathbf{S},K}}+\frac{9\|v\nabla\cdot\mathbf{w}\|_K^2}{4c_{\mathbf{w},r,K}}\right)^{\frac{1}{2}}\right\}$
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A post. estimate for $-\nabla\cdot(\mathbf{S}\nabla p)+\nabla\cdot(p\mathbf{w})+rp=f$

- **upwinding estimator**
  - $\eta_{\mathrm{U},K} := \sum_{\sigma\in\mathcal{E}_K\setminus\mathcal{E}_h^{\mathrm{N}}} m_\sigma \|(W_{K,\sigma} - \langle \mathcal{I}_{\mathrm{Os}}^{\Gamma}(\tilde{p}_h)\mathbf{w}\cdot\mathbf{n},1\rangle_\sigma)|\sigma|^{-1}\|_\sigma$
  - $W_{K,\sigma} = p_\sigma\langle\mathbf{w}\cdot\mathbf{n},1\rangle_\sigma$: weighted-upwind
  - m_σ: function of $c_{\mathbf{S},K}$, $c_{\mathbf{w},r,K} = \left(\frac{1}{2}\nabla\cdot\mathbf{w}+r\right)|_K$, d, h_K, $|\sigma|$, $|K|$
  - all dependencies evaluated explicitly
- **reaction quadrature estimator**
  - $\eta_{\mathrm{RQ},K} := \frac{1}{\sqrt{c_{\mathbf{w},r,K}}}\|r_K p_K - (r\tilde{p}_h,1)_K|K|^{-1}\|_K$
  - disappears when r pw constant and $\tilde{p}_h$ fixed by mean
- **Neumann boundary estimator**
  - $\eta_{\Gamma_{\mathrm{N}},K} := 0 + \frac{\sqrt{h_K}}{\sqrt{c_{\mathbf{S},K}}}\sum_{\sigma\in\mathcal{E}_K\cap\mathcal{E}_h^{\mathrm{N}}}\sqrt{C_{\mathrm{t},K,\sigma}}\|u_\sigma - u\|_\sigma$

A post. estimate for $-\nabla\cdot(\mathbf{S}\nabla p)+\nabla\cdot(p\mathbf{w})+rp=f$

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Convection-dominated problem

- consider the convection–diffusion–reaction equation

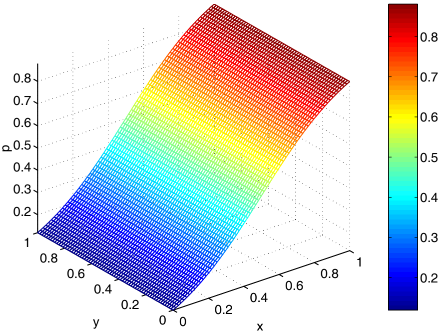
$$-\varepsilon\triangle p + \nabla\cdot(p(0,1)) + p = f \quad \text{in} \quad \Omega = (0,1)\times(0,1)$$

- analytical solution: layer of width a

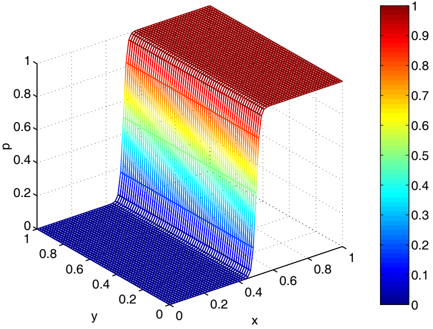
$$p(x,y) = 0.5\left(1 - \tanh\left(\frac{0.5 - x}{a}\right)\right)$$

- consider
  - $\varepsilon = 1$, $a = 0.5$
  - $\varepsilon = 10^{-2}$, $a = 0.05$
  - $\varepsilon = 10^{-4}$, $a = 0.02$
- unstructured grid of 46 elements given, uniformly/adaptively refined

Analytical solutions

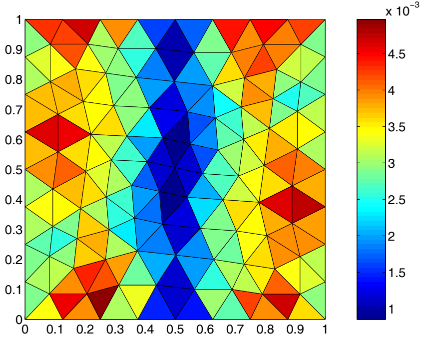


Case $\varepsilon = 1$, $a = 0.5$

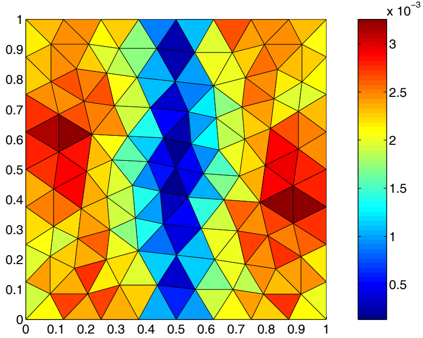


Case $\varepsilon = 10^{-4}$, $a = 0.02$

Error distribution on a uniformly refined mesh, $\varepsilon = 1$, $a = 0.5$

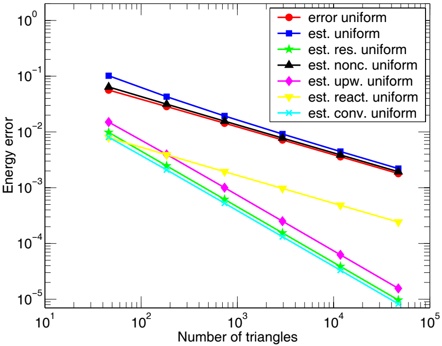


Estimated error distribution

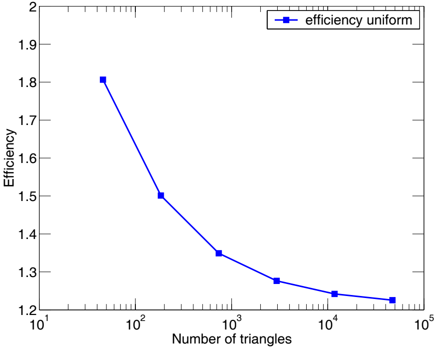


Exact error distribution

Estimated and actual errors and the effectivity index, $\varepsilon = 1$, $a = 0.5$

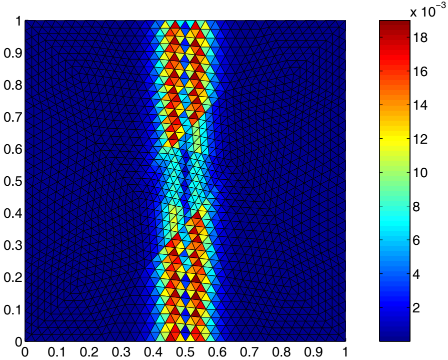


The different estimators

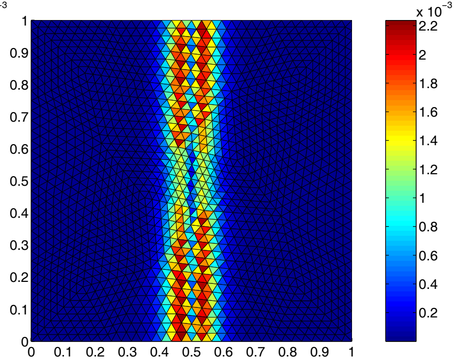


Effectivity index

Error distribution on a uniformly refined mesh, $\varepsilon = 10^{-2}$, $a = 0.05$

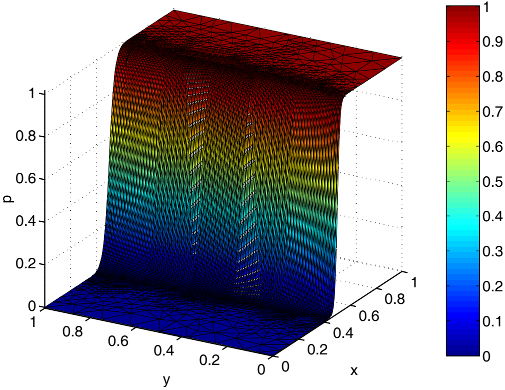


Estimated error distribution

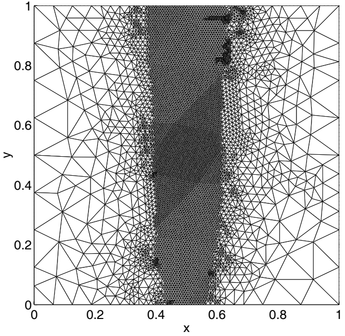


Exact error distribution

Approximate solution and the corresponding adaptively refined mesh, $\varepsilon = 10^{-4}$, $a = 0.02$

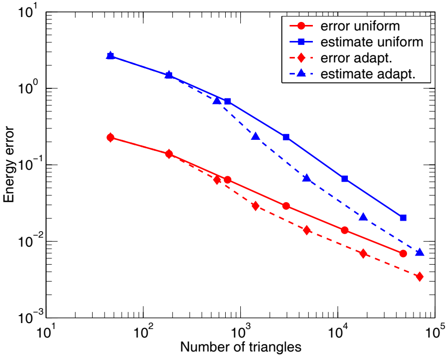


Approximate solution

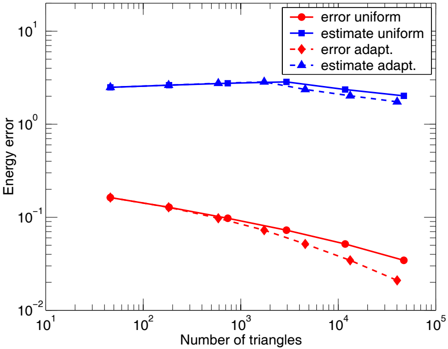


Adaptively refined mesh

Estimated and actual errors in uniformly/adaptively refined meshes

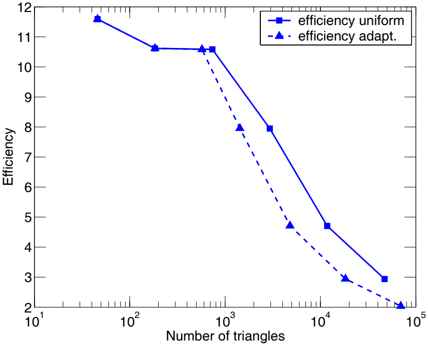


Case $\varepsilon = 10^{-2}$, $a = 0.05$



Case $\varepsilon = 10^{-4}$, $a = 0.02$

Effectivity indices in uniformly/adaptively refined meshes



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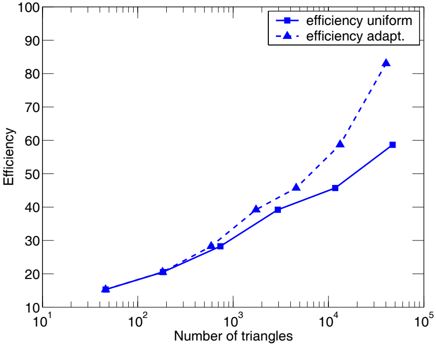

Case $\varepsilon = 10^{-4}$, $a = 0.02$

Outline

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 $D \in \mathcal{D}_h$, $0 \leq c_{r,D} \leq r \leq C_{r,D}$, a.e. in D

Bilinear form, energy norm, and weak solution

Definition (Bilinear form $\mathcal{B}$)

We define a bilinear form $\mathcal{B}$ for $p, \varphi \in H_0^1(\Omega)$ by

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

Definition (Energy norm)

The associated energy norm for $\varphi \in H_0^1(\Omega)$ is given by

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

Definition (Weak solution)

Weak solution: $p \in H_0^1(\Omega)$ such that

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

Bilinear form, energy norm, and weak solution

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Residual and diffusive flux estimators

Define:

- **residual estimator**

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

- **diffusive flux estimator**

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

where

$$\eta^{(1)}_{\mathrm{DF},D} := \|\nabla p_h + \mathbf{t}_h\|_D$$

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

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

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 $C_{r,D}/c_{r,D}$.

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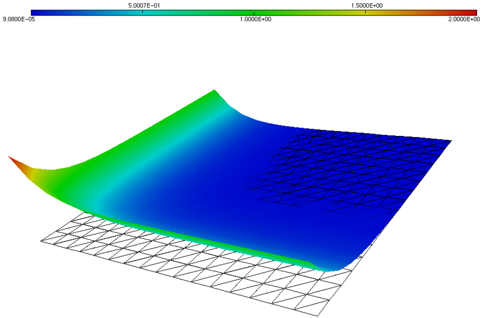
Problem and exact solution

Problem

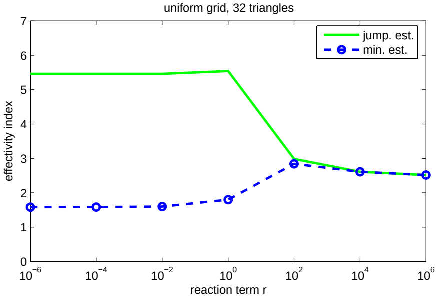
$$-\triangle p + rp = 0, \qquad \text{in } \Omega$$
$$p = p_0, \qquad \text{on } \partial\Omega$$

Solution

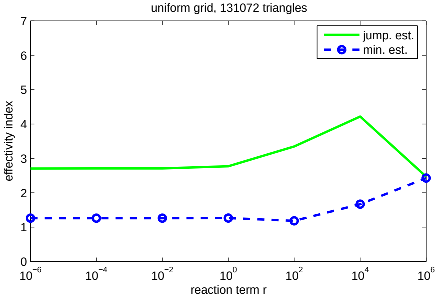
$$p_0(x,y) = e^{-\sqrt{r}x} + e^{-\sqrt{r}y}$$



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

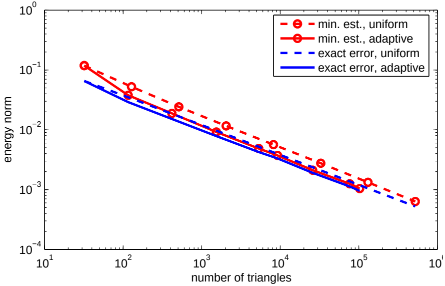


Mesh with 32 triangles

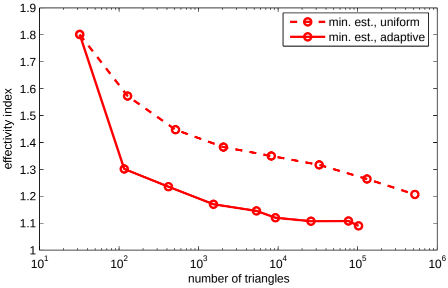


Mesh with 131072 triangles

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



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



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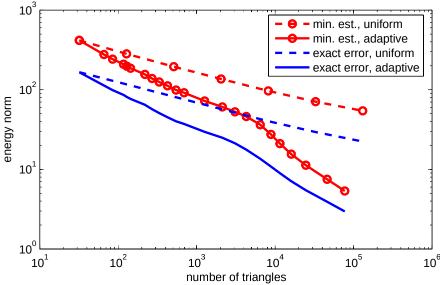
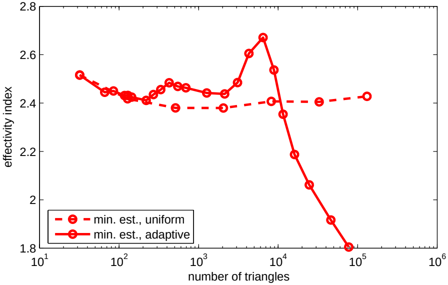
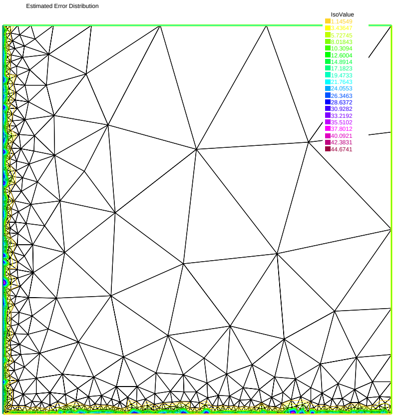


Est. and act. errors, $r = 10^6$

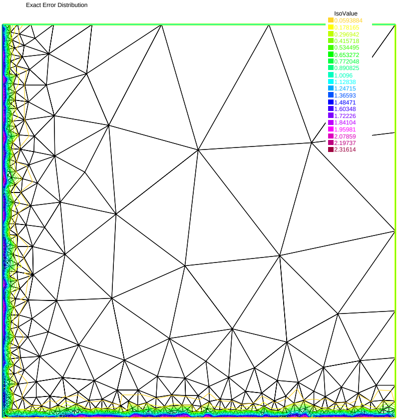


Effectivity indices, $r = 10^6$

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



Estimated error distribution



Exact error distribution

Outline

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, $R := B - \mathbb{A}X^*$

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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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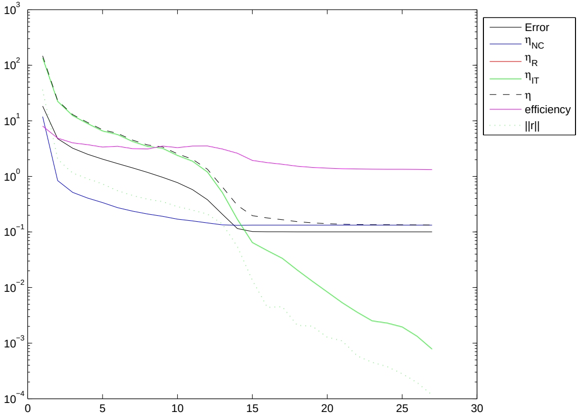
Finite volume estimates including inexact linear systems solution



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

Outline

Comments on the estimates and their efficiency

General comments

- $p \in H^1(\Omega)$, no additional regularity
- no convexity of Ω needed
- no saturation assumption
- no Helmholtz decomposition
- no shape-regularity and polynomial data needed for the upper bounds (only for the efficiency proofs)
- polynomial degree-independent upper bound
- no "monotonicity" hypothesis on inhomogeneities distribution
- the only important tools: Cauchy–Schwarz and optimal Poincaré–Friedrichs and trace inequalities
- holds from diffusion to convection–diffusion–reaction cases

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 $\mathbf{t}_h$
- for optimality, $\mathbf{t}_h$ has to be locally conservative
- 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
- additional nonsymmetric term for convection
- use problem-dependent energy norms

Conclusions and future work

Conclusions

- a posteriori error estimates: not only a tool to refine mesh
- **error control**
  - guaranteed upper bound
  - almost asymptotically exact
  - fully robust with respect to inhomogeneities
  - directly and easily computable estimators
- one can
  - increase considerably calculation precision and decrease calculation cost
  - give optimal algorithms which will automatically guarantee that the final error error is below a user-defined precision

Future work

- anisotropies
- extensions to other types of problems
- nonlinear (degenerate) cases
- systems of equations

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Thank you for your attention!