Fast, fully computable, and robust guaranteed error bounds for diffusion-reaction problems

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Model problem

- Classical formulation: $\kappa = \text{const.} > 0$

$$
\begin{aligned}
-\Delta u + \kappa^2 u &= f \quad \text{in } \Omega \subset \mathbb{R}^2 \\
u &= 0 \quad \text{on } \partial\Omega
\end{aligned}
$$

- Weak formulation:
$V = H_0^1(\Omega), \quad \mathcal{B}(u,v) = \int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}\mathbf{x} + \kappa^2 \int_\Omega uv \,\mathrm{d}\mathbf{x}$

$$
u \in V: \quad \mathcal{B}(u,v) = \int_\Omega fv \,\mathrm{d}\mathbf{x} \quad \forall v \in V
$$

- Linear triangular FEM:
$V_h = \{v_h \in V : v_h|_K \in P^1(K), K \in \mathcal{T}_h\}$

$$
u_h \in V_h: \quad \mathcal{B}(u_h,v_h) = \int_\Omega fv_h \,\mathrm{d}\mathbf{x} \quad \forall v_h \in V_h
$$

Upper bound

Theorem 1.

$$|||u - u_h|||^2 \le \sum_{K \in \mathcal{T}_h} \left[\eta_K(\mathbf{y}_K) + \mathrm{osc}_K(f) \right]^2 \quad \forall \mathbf{y}_K \in \mathbf{\Sigma}_K$$

where

- $\eta_K^2(\mathbf{y}_K) = \|\mathbf{y}_K - \nabla u_h\|_{0,K}^2 + \kappa^{-2} \left\| \Pi_K f - \kappa^2 u_h + \operatorname{div} \mathbf{y}_K \right\|_{0,K}^2$
- $\mathrm{osc}_K(f) = \min\left\{ h_K/\pi, \kappa^{-1} \right\} \|f - \Pi_K f\|_{0,K}$
- $\mathbf{\Sigma}_K = \{ \mathbf{y}_K \in \mathbf{H}(\mathrm{div}, K) : \mathbf{n}_K \cdot \mathbf{y}_K = g_K \text{ on } \partial K \}$
- $\Pi_K f \in P^1(K) : \quad \int_K (f - \Pi_K f) \varphi \, \mathrm{d}\mathbf{x} = 0 \quad \forall \varphi \in P^1(K)$
- $g_K \approx \mathbf{n}_K \cdot \nabla u$ ... piecewise linear boundary flux functions

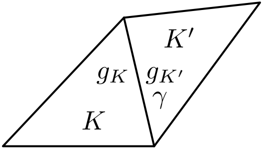
- Notation: $|||v|||^2 = \mathcal{B}(v, v), \qquad \|v\|_{0,K}^2 = \int_K v^2 \, \mathrm{d}\mathbf{x}$

Boundary fluxes g_K

Fast algorithm for g_K [Ainsworth, Oden, 2000]:

Linearity:

- $g_K \in P^1(\gamma), \quad \gamma \in \partial\mathcal{T}_h$



Consistency:

- $g_K + g_{K'} = 0$ on $\gamma = \partial K \cap \partial K'$

Equilibration:

- $\mathcal{B}_K(u_h, \theta_n) - \int_K f\theta_n \,\mathrm{d}\mathbf{x} - \int_{\partial K} g_K \theta_n \,\mathrm{d}\mathbf{x} = 0 \quad \forall \theta_n \in V_h$

Notation: $\mathcal{B}_K(u, v) = \int_K \nabla u \cdot \nabla v \,\mathrm{d}\mathbf{x} + \kappa^2 \int_K uv \,\mathrm{d}\mathbf{x}$

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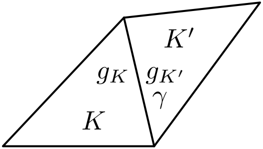

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NOT ROBUST FOR $\kappa \to \infty$ [Babuška, Ainsworth, 1999]

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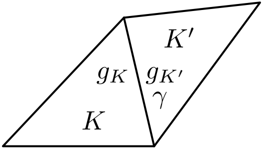
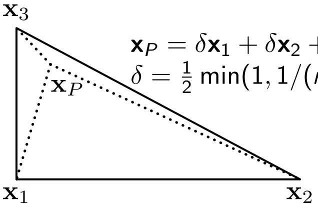


Consistency:

- $g_K + g_{K'} = 0$ on $\gamma = \partial K \cap \partial K'$

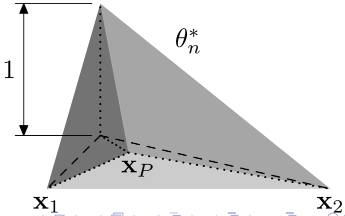
Robust equilibration:

- $\mathcal{B}_K(u_h, \theta_n^*) - \int_K f\theta_n^* \,\mathrm{d}\mathbf{x} - \int_{\partial K} g_K \theta_n^* \,\mathrm{d}\mathbf{x} \approx 0 \qquad \forall \theta_n^*$



$\mathbf{x}_P = \delta\mathbf{x}_1 + \delta\mathbf{x}_2 + (1-2\delta)\mathbf{x}_3$

$\delta = \frac{1}{2}\min(1, 1/(\kappa\rho_K))$



Flux construction #1

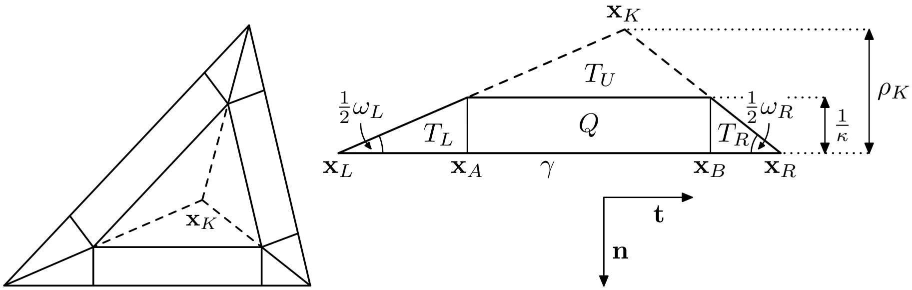
$$\mathbf{y}_K^{(1)} = \boldsymbol{\nabla} u_h|_K + \mathbf{y}_K^L + \mathbf{y}_K^Q$$

- $\mathbf{y}_K^L = \dfrac{1}{2|K|}\left(\varrho_1^{(K)}\lambda_1 + \varrho_2^{(K)}\lambda_2 + \varrho_3^{(K)}\lambda_3\right)$
- $\varrho_i^{(K)} = |\gamma_k|\left(g_K - \dfrac{\partial u_h}{\partial \mathbf{n}_K}\right)\Big|_{\gamma_k}(\mathbf{x}_i)\mathbf{t}_j - |\gamma_j|\left(g_K - \dfrac{\partial u_h}{\partial \mathbf{n}_K}\right)\Big|_{\gamma_j}(\mathbf{x}_i)\mathbf{t}_k$
  $i = 1,2,3, \quad j = (i \bmod 3) + 1, \qquad k = (j \bmod 3) + 1$
- $\mathbf{y}_K^Q = \dfrac{1}{3}\left(\beta_1 \mathbf{t}_1 \mathbf{t}_1^T + \beta_2 \mathbf{t}_2 \mathbf{t}_2^T + \beta_3 \mathbf{t}_3 \mathbf{t}_3^T\right) \boldsymbol{\nabla}(\Pi_K f - \kappa^2 u_h)(\bar{\mathbf{x}}_K)$
- $\beta_1 = \lambda_2\lambda_3, \quad \beta_2 = \lambda_3\lambda_1, \quad \beta_3 = \lambda_1\lambda_2$
  $\bar{\mathbf{x}}_K$ ... centroid of K
  $\lambda_1, \lambda_2, \lambda_3$ ... barycentric coordinates in K
  $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$ ... edge vectors of K

Flux construction #2

$$\mathbf{y}_K^{(2)} = \nabla u_h|_K + \mathbf{y}_K^O$$

- $\mathbf{n}_K \cdot \mathbf{y}_K^O = R_K^O = g_K - \mathbf{n}_K \cdot \nabla u_h|_K \quad \Rightarrow \quad \mathbf{n}_K \cdot \mathbf{y}_K^{(2)} = g_K$



Flux construction #2

$$\mathbf{y}_K^{(2)} = \nabla u_h|_K + \mathbf{y}_K^O$$

- $\mathbf{n}_K \cdot \mathbf{y}_K^O = R_K^O = g_K - \mathbf{n}_K \cdot \nabla u_h|_K \quad \Rightarrow \quad \mathbf{n}_K \cdot \mathbf{y}_K^{(2)} = g_K$
- $\mathbf{y}_K^O(\mathbf{x}) = R_K^O|_\gamma(\mathbf{x}_L)\lambda_L(\mathbf{x}) \left(\mathbf{n} - \mathbf{t} \cot \frac{1}{2}\omega_L\right) + R_K^O|_\gamma(\mathbf{x}_A)\lambda_A(\mathbf{x})\mathbf{n}, \quad \mathbf{x} \in T_L$
- $\mathbf{y}_K^O(\mathbf{x}) = R_K^O|_\gamma(\mathbf{x}_A + x\mathbf{t})(1 - \kappa y)\mathbf{n}, \quad \mathbf{x} \in Q$
- $\mathbf{y}_K^O(\mathbf{x}) = R_K^O|_\gamma(\mathbf{x}_R)\lambda_R(\mathbf{x}) \left(\mathbf{n} + \mathbf{t} \cot \frac{1}{2}\omega_R\right) + R_K^O|_\gamma(\mathbf{x}_B)\lambda_B(\mathbf{x})\mathbf{n}, \quad \mathbf{x} \in T_R$
- $\mathbf{y}_K^O(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} \in T_U$

Final estimator

$$\overline{\eta}_K = \min \left\{ \eta_K\left(\mathbf{y}_K^{(1)}\right),\ \eta_K\left(\mathbf{y}_K^{(2)}\right) \right\}$$

Theorem 1. (Upper bound)

$$|||u - u_h|||^2 \le \sum_{K \in \mathcal{T}_h} \left[\overline{\eta}_K + \mathrm{osc}_K(f) \right]^2$$

Theorem 2. (Local efficiency)

$$\overline{\eta}_K \le C \left[|||u - u_h|||_{\widetilde{K}} + \mathrm{osc}_{\widetilde{K}}(f) \right]$$

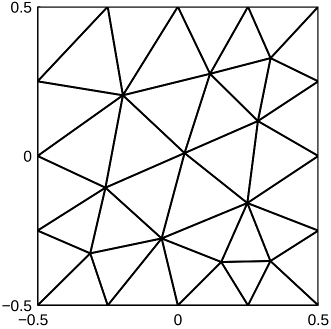
where

- $\mathrm{osc}^2_{\widetilde{K}}(f) = \min\{h_K^2, \kappa^{-2}\} \sum_{K \subset \widetilde{K}} \|f - \Pi_K f\|^2_{0,K}$
- $\widetilde{K} = \cup\{L \in \mathcal{T}_h : L \cap K \neq \emptyset\}$ ... patch of elements around K

Example 1

$$
\begin{aligned}
-\Delta u + \kappa^2 u &= f \quad \text{in } \Omega \\
u &= 0 \quad \text{on } \partial\Omega
\end{aligned}
$$

- $\Omega = (-1/2, 1/2)^2$
- $f = \cos(\pi x_1)\cos(\pi x_2)$
- $u = \dfrac{\cos(\pi x_1)\cos(\pi x_2)}{2\pi^2 + \kappa^2}$

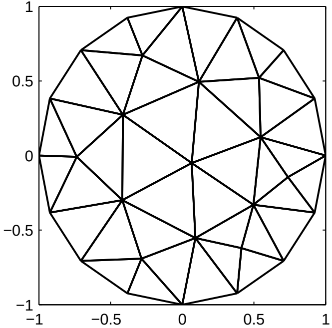


Example 2

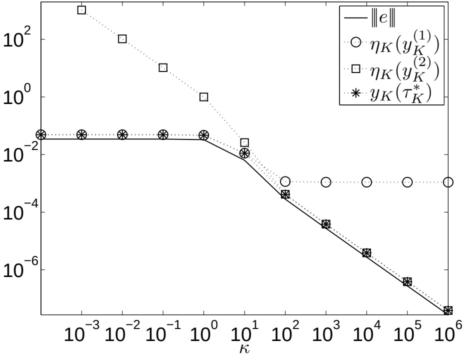
$$-\Delta u + \kappa^2 u = f \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \partial\Omega$$

- $\Omega = \{(x_1, x_2) : r < 1\}$
- $f = 1 \qquad r = \sqrt{x_1^2 + x_2^2}$
- $u = \dfrac{1}{\kappa^2}\left(1 - \dfrac{I_0(\kappa r)}{I_0(\kappa)}\right) \quad \text{for } \kappa > 0$

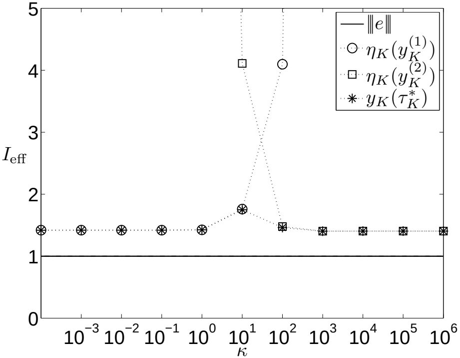
  $u = \dfrac{1 - r^2}{4} \quad \text{for } \kappa = 0$



Example 1



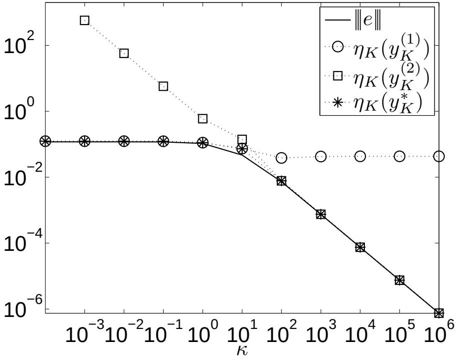
Error estimators



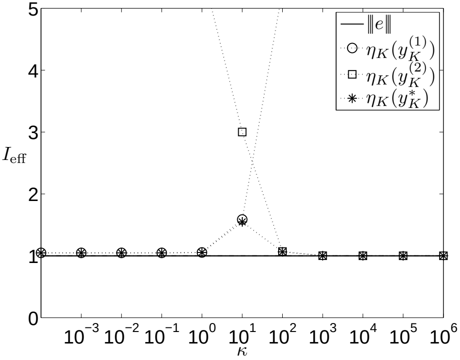
Effectivity index

$$I_{\text{eff}} = \frac{\eta}{\|u - u_h\|}$$

Example 2



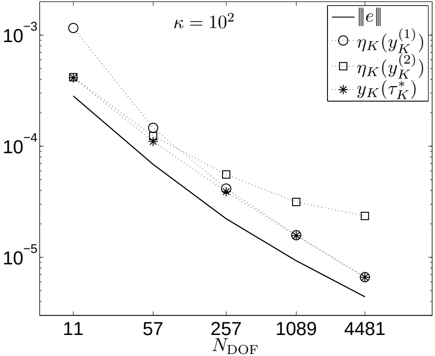
Error estimators



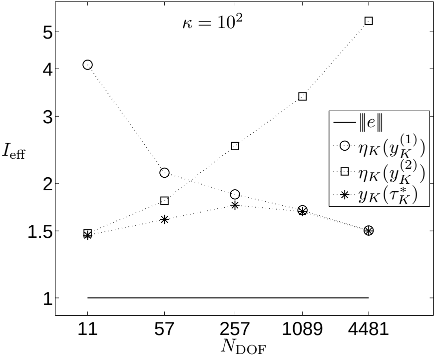
Effectivity index

$$I_{\text{eff}} = \frac{\eta}{\|u - u_h\|}$$

Example 1, uniform refinement, $\kappa = 100$

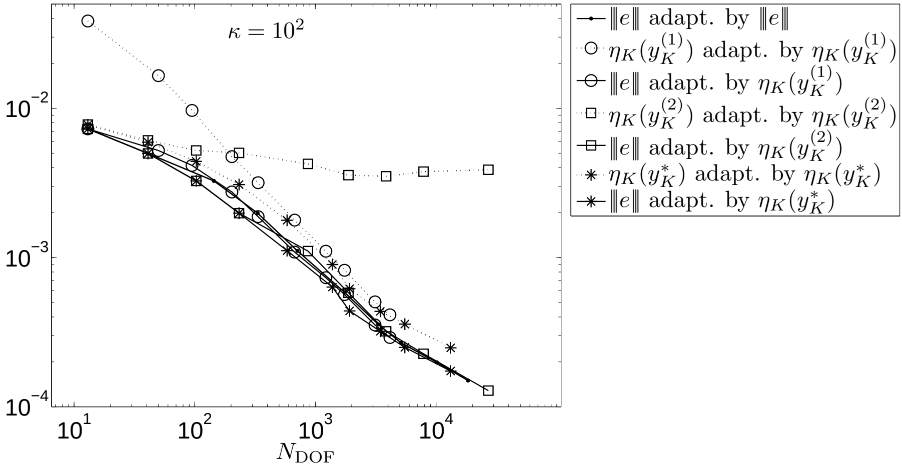


Error estimators



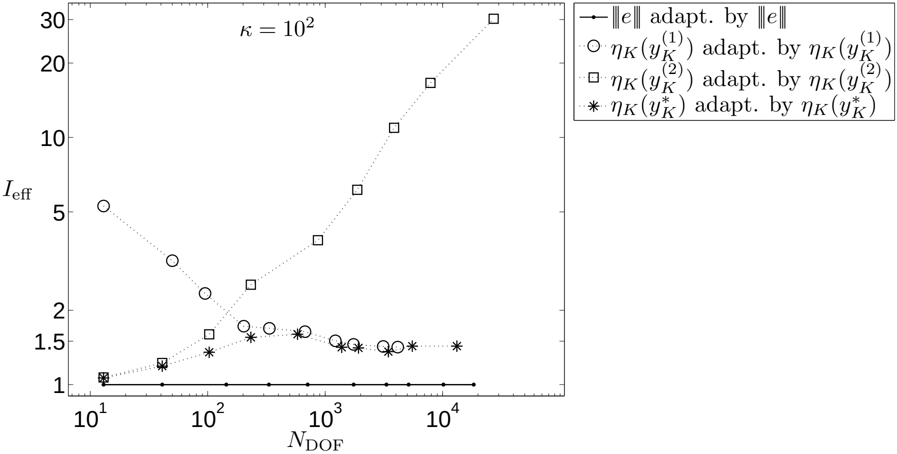
Effectivity index

Example 2, adaptive refinement, $\kappa = 100$



Convergence. Estimators (dotted lines) and true errors (solid lines).

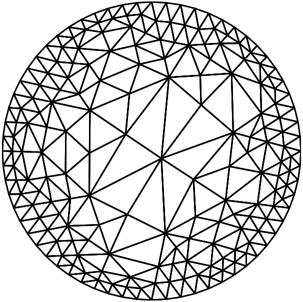
Example 2, adaptive refinement, $\kappa = 100$



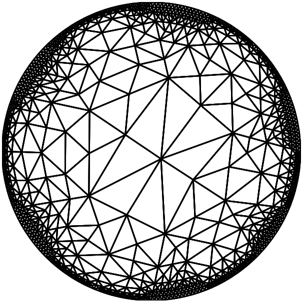
Effectivity indices.

Example 2, adaptivity driven by true error

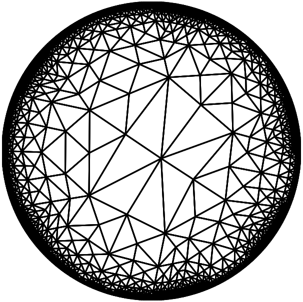
$\kappa = 100$



Step 3



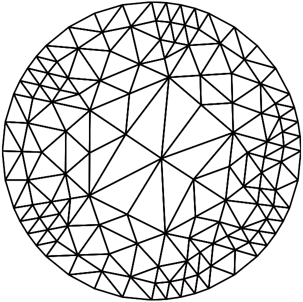
Step 5



Step 7

Example 2, adaptivity driven by $\eta_K(\tau_K^{(1)})$

$\kappa = 100$



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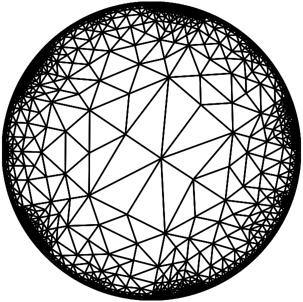

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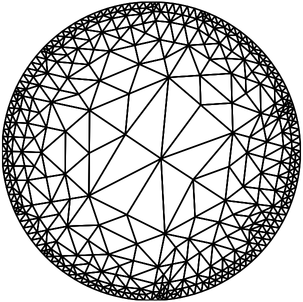
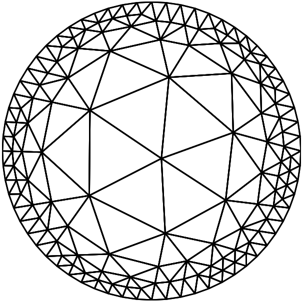


Step 5

Example 2, adaptivity driven by $\eta_K(\tau_K^*)$

$\kappa = 100$



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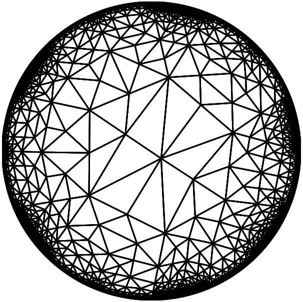

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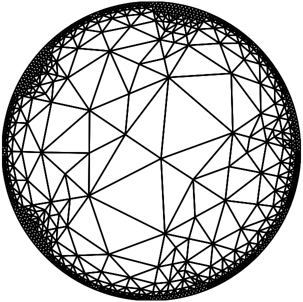

Step 5

Conclusions

- Guaranteed upper bound
- Local efficiency
- Robustness
- No constants
- Fast algorithm

Outlook

- 3D
- Higher-order

For details see:

M. Ainsworth, T.V.: *Fully computable robust a posteriori error bounds for singularly perturbed reaction–diffusion problems*, accepted by Numer. Math. 2011.

Preprint available at:

http://www.math.cas.cz/preprints/pre-208.pdf

Thank you for your attention

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