Complementarity – the way towards guaranteed error estimates

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Outline

- A posteriori error estimates
- Primal problem:

$$-\Delta u = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega$$

- Complementary problem:

$$-\operatorname{div} \mathbf{y} = f \quad \text{in } \Omega \quad \text{and more}$$

- Error estimate:

$$|\!|\!| u - u_h |\!|\!| \leq \eta(u_h, \mathbf{y}_h) \quad \forall u_h \in V \quad \forall \mathbf{y}_h \in \mathbf{Q}(f)$$

$$\eta(u_h, \mathbf{y}_h) = \|\mathbf{y}_h - \boldsymbol{\nabla} u_h\|_0$$

- Numerical examples
- Conclusions

A posteriori error estimates

- GOAL: Solve the problem with prescribed accuracy.

A posteriori error estimates

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- Adaptive algorithm
  1. Initialize: Construct the initial mesh $\mathcal{T}_h$.
  2. Solve: Find u_h on $\mathcal{T}_h$.
  3. Estimate error: Compute η_K for all $K \in \mathcal{T}_h$. $\eta^2 = \sum_{K \in \mathcal{T}_h} \eta_K^2$.
  4. Stopping criterion: If $\quad \eta \leq \mathrm{TOL} \quad \Rightarrow \quad$ STOP.
  5. Mark: If $\quad \eta_K \geq \Theta \max_{K \in \mathcal{T}_h} \eta_K \quad \Rightarrow \quad$ mark K. $\qquad 0 < \Theta < 1$
  6. Refine: Refine marked elements and build the new mesh $\mathcal{T}_h$.
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  Guaranteed lower bound: $\|u - u_h\| \geq \eta \geq \mathrm{TOL}$

Reference solution (Runge ≈ 1900)

- u_h on $\mathcal{T}_h$
- u_h^{ref} on $\mathcal{T}_h^{\mathrm{ref}}$
- $\|u - u_h\| \approx \|u_h^{\mathrm{ref}} - u_h\|$

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- u_h on $\mathcal{T}_h$
- u_h^{ref} on $\mathcal{T}_h^{\mathrm{ref}}$
- $|||u - u_h||| \geq |||u_h^{\mathrm{ref}} - u_h|||$
- $|||u_h^{\mathrm{ref}} - u_h|||$ small $\quad\Rightarrow\quad$ $|||u - u_h|||$ small.

Primal Problem

Strong form.:

$$-\Delta u = f \quad \text{in } \Omega \subset \mathbb{R}^d$$
$$u = 0 \quad \text{on } \partial\Omega$$

Weak form.: $u \in V: \quad \mathcal{B}(u,v) = \mathcal{F}(v) \quad \forall v \in V$

Lemma: $f \in L^2(\Omega) \quad \Rightarrow \quad \boldsymbol{\nabla} u \in \mathbf{H}(\mathrm{div},\Omega)$

Notation:

- $V = H_0^1(\Omega)$
- $\mathcal{B}(u,v) = (\boldsymbol{\nabla} u, \boldsymbol{\nabla} v) \qquad (\mathbf{p},\mathbf{q}) = \int_\Omega \mathbf{p}\cdot\mathbf{q}\,\mathrm{d}x$
- $\mathcal{F}(v) = (f,v) \qquad (f,v) = \int_\Omega fv\,\mathrm{d}x$
- $\|v\|^2 = \mathcal{B}(v,v)$

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Weak form.: $u \in V: \quad \mathcal{B}(u,v) = \mathcal{F}(v) \quad \forall v \in V$

Lemma: $f \in L^2(\Omega) \quad \Rightarrow \quad \boldsymbol{\nabla} u \in \mathbf{H}(\mathrm{div}, \Omega)$

Proof:

$$\mathbf{H}(\mathrm{div}, \Omega) = \{\mathbf{y} \in [L^2(\Omega)]^d : \mathrm{div}\, \mathbf{y} \in L^2(\Omega)\}$$

$$\mathrm{div}\, \mathbf{y} \in L^2(\Omega) \quad \Leftrightarrow \quad \exists z \in L^2(\Omega) \ : \ (v, z) = -(\boldsymbol{\nabla} v, \mathbf{y}) \quad \forall v \in C_0^\infty(\Omega)$$
$$\mathrm{div}\, \mathbf{y} = z$$

Derivation of the estimate

Divergence theorem: $v \in H^1(\Omega) \quad \mathbf{y} \in \mathbf{H}(\mathrm{div}, \Omega)$

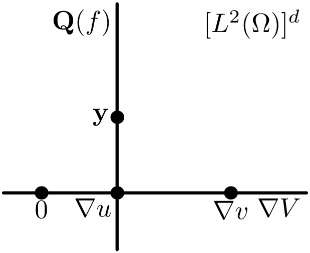
$$\int_\Omega v \,\mathrm{div}\, \mathbf{y} \,\mathrm{d}x + \int_\Omega \mathbf{y} \cdot \nabla v \,\mathrm{d}x - \int_{\partial\Omega} v\mathbf{y} \cdot \mathbf{n} \,\mathrm{d}x = 0$$

$$\mathbf{Q}(f) = \{\mathbf{y} \in \mathbf{H}(\mathrm{div}, \Omega) : (\mathbf{y}, \nabla v) = (f, v) \quad \forall v \in V\}$$

Orthogonality:

$$\int_\Omega (\nabla u - \mathbf{y}) \cdot \nabla v \,\mathrm{d}x = 0$$

$$\forall v \in V, \ \forall \mathbf{y} \in \mathbf{Q}(f)$$



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$$v \in V, \quad \mathbf{y} \in \mathbf{Q}(f) = \{\mathbf{y} \in \mathbf{H}(\mathrm{div}, \Omega) : (\mathbf{y}, \nabla v) = (f, v) \quad \forall v \in V\}$$

$$\begin{aligned}
\mathcal{B}(u - u_h, v) &= (f, v) - (\nabla u_h, \nabla v) + (v, \mathrm{div}\, \mathbf{y}) + (\mathbf{y}, \nabla v) \\
&= (f + \mathrm{div}\, \mathbf{y}, v) + (\mathbf{y} - \nabla u_h, \nabla v) \\
&= (\mathbf{y} - \nabla u_h, \nabla v) \\
&\le \|\mathbf{y} - \nabla u_h\|_0 \, \|\nabla v\|_0
\end{aligned}$$

$$|\!|\!| u - u_h |\!|\!| \le \|\mathbf{y} - \nabla u_h\|_0 \qquad \forall u_h \in V$$

The estimator

Definition: $\eta(u_h, \mathbf{y}_h) = \|\mathbf{y}_h - \boldsymbol{\nabla} u_h\|_0$

Theorem: $|\!|\!| u - u_h |\!|\!| \leq \eta(u_h, \mathbf{y}_h) \qquad \forall u_h \in V \quad \forall \mathbf{y}_h \in \mathbf{Q}(f)$

Complementary problem:

(A) Find $\mathbf{y} \in \mathbf{Q}(f) : \eta(u_h, \mathbf{y}) \leq \eta(u_h, \mathbf{w}) \quad \forall \mathbf{w} \in \mathbf{Q}(f)$

(B) Find $\mathbf{y} \in \mathbf{Q}(f) : \frac{1}{2}\|\mathbf{y}\|_0^2 \leq \frac{1}{2}\|\mathbf{w}\|_0^2 \quad \forall \mathbf{w} \in \mathbf{Q}(f)$

(C) Find $\mathbf{y} \in \mathbf{Q}(f) : (\mathbf{y}, \mathbf{w}^0) = 0 \quad \forall \mathbf{w}^0 \in \mathbf{Q}(0)$

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Lemma 1: (A) $\Leftrightarrow$ (B) $\Leftrightarrow$ (C)

Proof: (A) $\Leftrightarrow$ (B)

$$\|\mathbf{y} - \nabla u_h\|_0^2 \leq \|\mathbf{w} - \nabla u_h\|_0^2$$

$$\|\mathbf{y}\|_0^2 - 2(\mathbf{y}, \nabla u_h) + \|\nabla u_h\|_0^2 \leq \|\mathbf{w}\|_0^2 - 2(\mathbf{w}, \nabla u_h) + \|\nabla u_h\|_0^2$$

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$$\begin{aligned} \|\mathbf{y} - \nabla u_h\|_0^2 &\leq \|\mathbf{w} - \nabla u_h\|_0^2 \\ \|\mathbf{y}\|_0^2 - 2(\mathbf{y}, \nabla u_h) &\leq \|\mathbf{w}\|_0^2 - 2(\mathbf{w}, \nabla u_h) \end{aligned}$$

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$$\|\mathbf{y}\|_0^2 - 2(f, u_h) \leq \|\mathbf{w}\|_0^2 - 2(f, u_h)$$

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Proof: (B) $\Rightarrow$ (C)

$J(t) = \left\|\mathbf{y} + t\mathbf{w}^0\right\|_0^2, \qquad J(t)$ has minimum at $t = 0$

$$0 = J'(0) = \lim_{t \to 0} \frac{\left\|\mathbf{y} + t\mathbf{w}^0\right\|_0^2 - \|\mathbf{y}\|_0^2}{t}$$

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Theorem: $|\!|\!| u - u_h |\!|\!| \le \eta(u_h, \mathbf{y}_h) \qquad \forall u_h \in V \quad \forall \mathbf{y}_h \in \mathbf{Q}(f)$

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Lemma 1: (A) $\Leftrightarrow$ (B) $\Leftrightarrow$ (C)
Proof: (C) $\Rightarrow$ (B)

$$\mathbf{w} \in \mathbf{Q}(f), \quad \exists \mathbf{w}^0 \in \mathbf{Q}(0) : \mathbf{w} = \mathbf{y} + \mathbf{w}^0, \qquad (\mathbf{y}, \mathbf{w}) = \|\mathbf{y}\|_0^2$$

$$0 \leq \|\mathbf{w} - \mathbf{y}\|_0^2 = \|\mathbf{w}\|_0^2 - 2(\mathbf{y}, \mathbf{w}) + \|\mathbf{y}\|_0^2 = \|\mathbf{w}\|_0^2 - \|\mathbf{y}\|_0^2$$

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Theorem: $|||u - u_h||| \leq \eta(u_h, \mathbf{y}_h) \qquad \forall u_h \in V \quad \forall \mathbf{y}_h \in \mathbf{Q}(f)$

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(C) Find $\mathbf{y} \in \mathbf{Q}(f) : (\mathbf{y}, \mathbf{w}^0) = 0 \quad \forall \mathbf{w}^0 \in \mathbf{Q}(0)$

Lemma 2: $\mathbf{y} = \boldsymbol{\nabla} u \in \mathbf{Q}(f)$ is the unique solution of (A)–(C)

Proof:

If $\mathbf{y}_1 \in \mathbf{Q}(f)$ and $\mathbf{y}_2 \in \mathbf{Q}(f)$ satisfy (C):

$\Rightarrow \mathbf{y}_2 - \mathbf{y}_1 \in \mathbf{Q}(0)$ and $(\mathbf{y}_2 - \mathbf{y}_1, \mathbf{w}^0) = 0$

$\Rightarrow \|\mathbf{y}_2 - \mathbf{y}_1\|_0^2 = 0 \quad \Rightarrow \quad \mathbf{y}_2 = \mathbf{y}_1$

The estimator

Definition: $\eta(u_h, \mathbf{y}_h) = \|\mathbf{y}_h - \boldsymbol{\nabla} u_h\|_0$

Theorem: $|\!|\!| u - u_h |\!|\!| \leq \eta(u_h, \mathbf{y}_h) \qquad \forall u_h \in V \quad \forall \mathbf{y}_h \in \mathbf{Q}(f)$

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(C) Find $\mathbf{y} \in \mathbf{Q}(f) : (\mathbf{y}, \mathbf{w}^0) = 0 \quad \forall \mathbf{w}^0 \in \mathbf{Q}(0)$

Lemma 3: $\eta^2(u, \mathbf{y}_h) + \eta^2(u_h, \mathbf{y}) = \eta^2(u_h, \mathbf{y}_h) \qquad \forall u_h \in V,\ \mathbf{y}_h \in \mathbf{Q}(f)$

$$\|\mathbf{y}_h - \mathbf{y}\|_0^2 + \|\boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\|_0^2 = \|\mathbf{y}_h - \boldsymbol{\nabla} u_h\|_0^2$$

Proof:

$$\|\mathbf{y}_h - \boldsymbol{\nabla} u + \boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\|_0^2 = \|\mathbf{y}_h - \boldsymbol{\nabla} u\|_0^2 + \|\boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\|_0^2$$

$$(\mathbf{y}_h - \boldsymbol{\nabla} u, \boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h) = 0$$

Equivalent formulations

$$\mathcal{B}(u,v) = (\nabla u, \nabla v), \qquad \mathcal{F}(v) = (f,v), \qquad \mathcal{B}^*(\mathbf{y},\mathbf{w}) = (\mathbf{y},\mathbf{w})$$

Weak formulation:

(Prim) $u \in V : \mathcal{B}(u,v) = \mathcal{F}(v) \quad \forall v \in V$

(Comp) $\mathbf{y} \in \mathbf{Q}(f) : \mathcal{B}^*(\mathbf{y},\mathbf{w}^0) = 0 \quad \forall \mathbf{w}^0 \in \mathbf{Q}(0)$

Variational formulation:

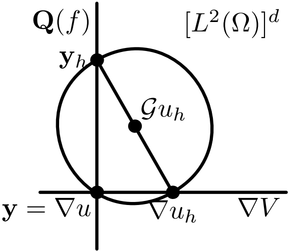
(Prim) $u \in V : J(u) = \min_{v \in V} J(v), \quad J(v) = \frac{1}{2}\mathcal{B}(v,v) - \mathcal{F}(v)$

(Comp) $\mathbf{y} \in \mathbf{Q}(f) : J^*(\mathbf{y}) = \min_{\mathbf{w} \in \mathbf{Q}(f)} J^*(\mathbf{w}), \quad J^*(\mathbf{w}) = \frac{1}{2}\mathcal{B}^*(\mathbf{w},\mathbf{w})$

Complementarity of energies:

$$J(u) + J^*(\mathbf{y}) = -\frac{1}{2}\mathcal{B}(u,u) + \frac{1}{2}\mathcal{B}^*(\nabla u, \nabla u) = 0$$

Method of hypercircle



Theorem: If

- $u \in V$ is primal solution
- $u_h \in V$, $\mathbf{y}_h \in \mathbf{Q}(f)$ arbitrary
- $\mathcal{G}u_h = (\mathbf{y}_h + \boldsymbol{\nabla} u_h)/2$

Then

$$\|\boldsymbol{\nabla} u - \mathcal{G}u_h\|_0 = \frac{1}{2}\eta(u_h, \mathbf{y}_h).$$

Proof:

$$\begin{aligned}4\,\|\boldsymbol{\nabla} u - \mathcal{G}u_h\|_0^2 &= \|\boldsymbol{\nabla} u - \mathbf{y}_h + \boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\|_0^2 \\ &= \|\boldsymbol{\nabla} u - \mathbf{y}_h\|_0^2 + \|\boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\|_0^2 = \|\boldsymbol{\nabla} u_h - \mathbf{y}_h\|_0^2\end{aligned}$$

Handelling $\mathbf{Q}(f)$, $d = 2$, Ω simply connected

$$\overline{\mathbf{q}}(x_1, x_2) = -\left(\int_0^{x_1} f(s, x_2)\,\mathrm{d}s, 0\right)^T \quad \Rightarrow \quad -\operatorname{div}\overline{\mathbf{q}} = f$$

$$\mathbf{Q}(0) = \mathbf{curl}\, H^1(\Omega), \qquad \mathbf{curl} = (\partial_2, -\partial_1)^\top$$

$$\mathbf{Q}(f) = \overline{\mathbf{q}} + \mathbf{Q}(0) = \overline{\mathbf{q}} + \mathbf{curl}\, H^1(\Omega)$$

(Comp) $\quad \mathbf{y} = \overline{\mathbf{q}} + \mathbf{curl}\, z \in \mathbf{Q}(f) : (\mathbf{y}, \mathbf{w}^0) = 0 \quad \forall \mathbf{w}^0 \in \mathbf{Q}(0)$

(Comp) $\quad z \in H^1(\Omega) : \underbrace{(\mathbf{curl}\, z, \mathbf{curl}\, v)}_{(\boldsymbol{\nabla} z, \boldsymbol{\nabla} v)} = -(\overline{\mathbf{q}}, \mathbf{curl}\, v) \quad \forall v \in H^1(\Omega)$

Error majorants (Friedrichs' inequality)

Friedrichs' inequality: $\|v\|_0 \le C_\Omega \|\nabla v\|_0 \quad \forall v \in V$

Remark: $C_\Omega \le \frac{1}{\pi}\left(\frac{1}{|a_1|} + \cdots + \frac{1}{|a_d|}\right)^{-1/2}, \quad \Omega \subset a_1 \times \cdots \times a_d$

Derivation:

$$\begin{aligned}
\mathcal{B}(u - u_h, v) &= (f + \operatorname{div} \mathbf{y}, v) + (\mathbf{y} - \nabla u_h, \nabla v) \\
&\le \left(C_\Omega \|f + \operatorname{div} \mathbf{y}\|_0 + \|\mathbf{y} - \nabla u_h\|_0\right) |||v||| \\
|||u - u_h||| &\le \widehat{\eta}(u_h, \mathbf{y}) \qquad\qquad \forall \mathbf{y} \in \mathbf{H}(\operatorname{div}, \Omega)
\end{aligned}$$

Majorant:

$$\widehat{\eta}(u_h, \mathbf{y}) = C_\Omega \|f + \operatorname{div} \mathbf{y}\|_0 + \|\mathbf{y} - \nabla u_h\|_0$$

$$\widehat{\eta}^2(u_h, \mathbf{y}) \le \left(1 + \frac{1}{\beta}\right) C_\Omega^2 \|f + \operatorname{div} \mathbf{y}\|_0^2 + (1 + \beta)\|\mathbf{y} - \nabla u_h\|_0^2 \qquad \forall \beta > 0$$

Numerical examples

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

Estimators:

$$\eta(u_h, \mathbf{y}) = \|\mathbf{y} - \nabla u_h\|_0 \qquad \mathbf{y} \in \mathbf{Q}(f, u_h)$$

$$\widehat{\eta}(u_h, \widehat{\mathbf{y}}) = C_\Omega \left\|f - \kappa^2 u_h + \operatorname{div} \widehat{\mathbf{y}}\right\|_0 + \|\widehat{\mathbf{y}} - \nabla u_h\|_0 \qquad \widehat{\mathbf{y}} \in \mathbf{H}(\operatorname{div}, \Omega)$$

$$\widetilde{\eta}^2(u_h, \widetilde{\mathbf{y}}) = \left\|\kappa^{-1}(f - \kappa^2 u_h + \operatorname{div} \widetilde{\mathbf{y}})\right\|_0^2 + \|\widetilde{\mathbf{y}} - \nabla u_h\|_0^2 \quad \widetilde{\mathbf{y}} \in \mathbf{H}(\operatorname{div}, \Omega)$$

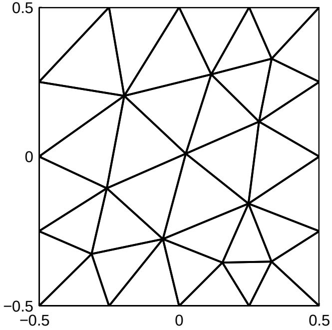
(MA,TV 2010)

- Based on equilibrated residuals
- Combination of η and $\widetilde{\eta}$
- Explicit formulas for $\mathbf{y}$

Example 1

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

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

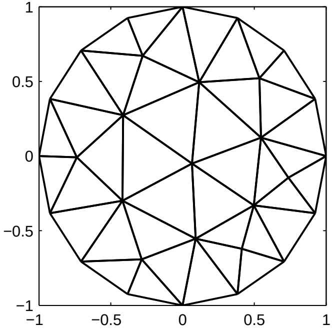


Example 2

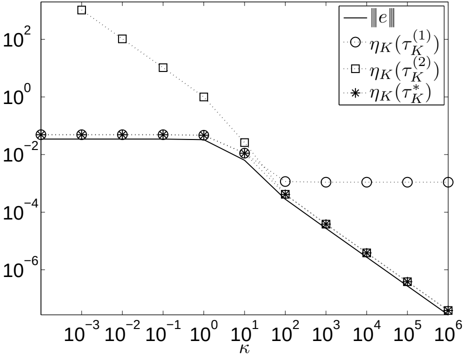
$$-\Delta u + \kappa^2 u = f \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \partial\Omega$$

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

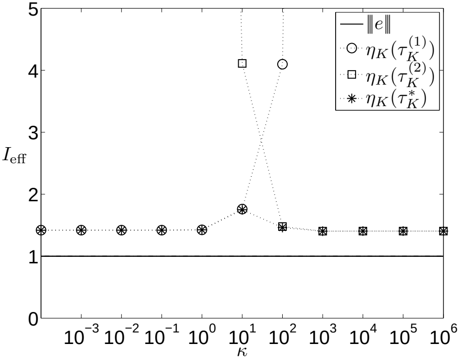
  $u = \dfrac{1 - x_1^2 - x_2^2}{4} \quad \text{for } \kappa = 0$
- $C_\Omega = 1/\pi$



Example 1



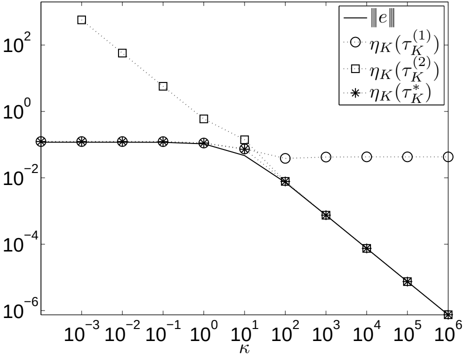
Error estimators



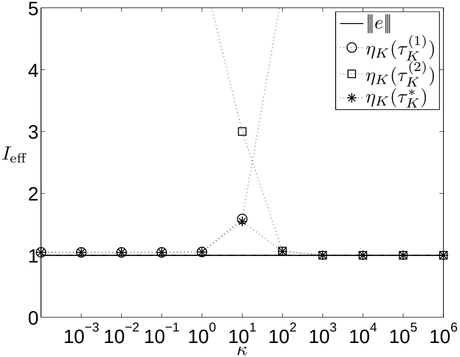
Effectivity index

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

Example 2



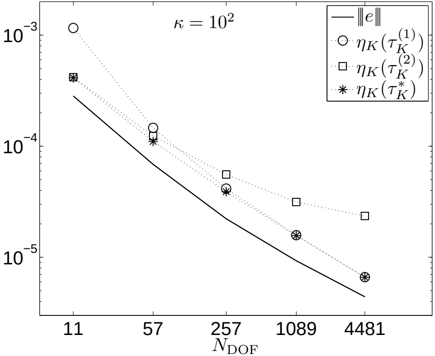
Error estimators



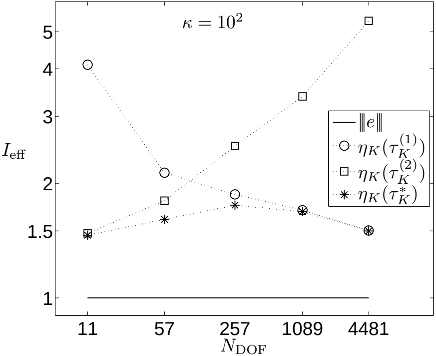
Effectivity index

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

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

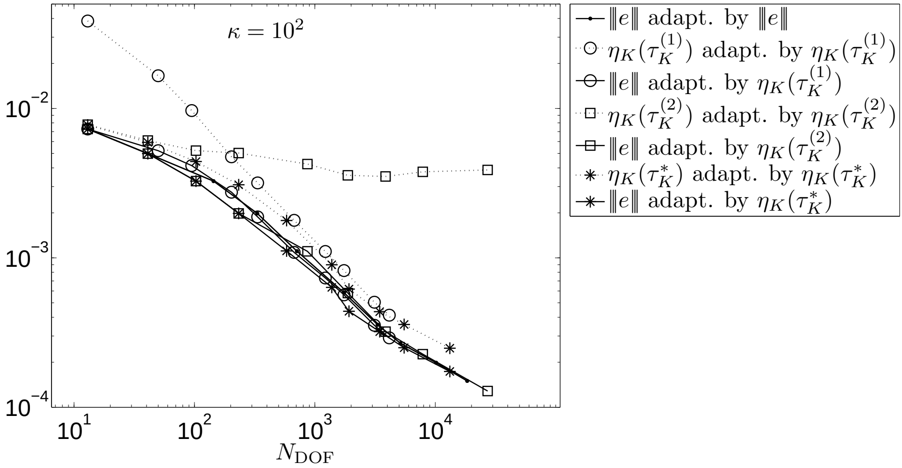


Error estimators



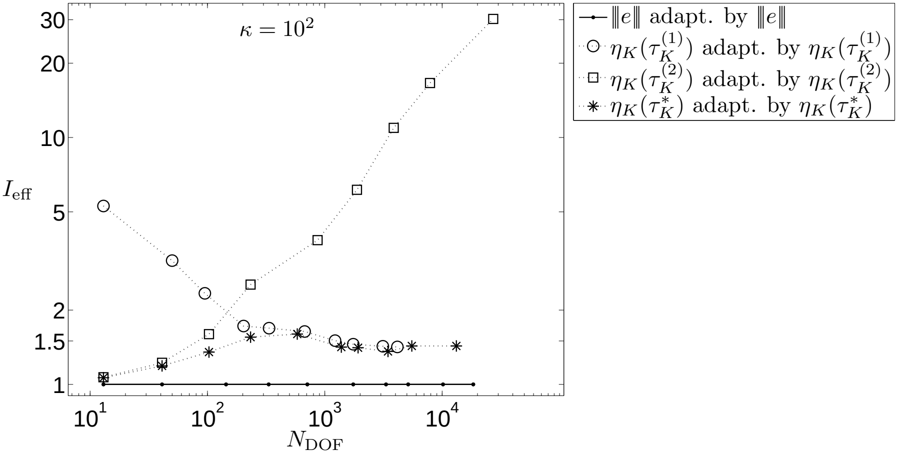
Effectivity index

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



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

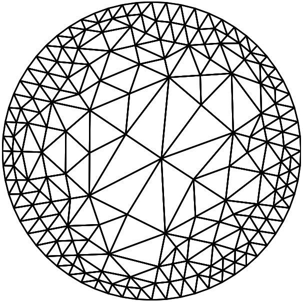
Example 2, adaptive refinement, $\kappa = 100$



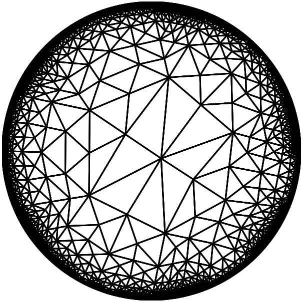
Effectivity indices.

Example 2, adaptivity driven by true error

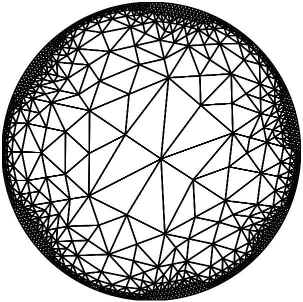
$\kappa = 100$



Step 3



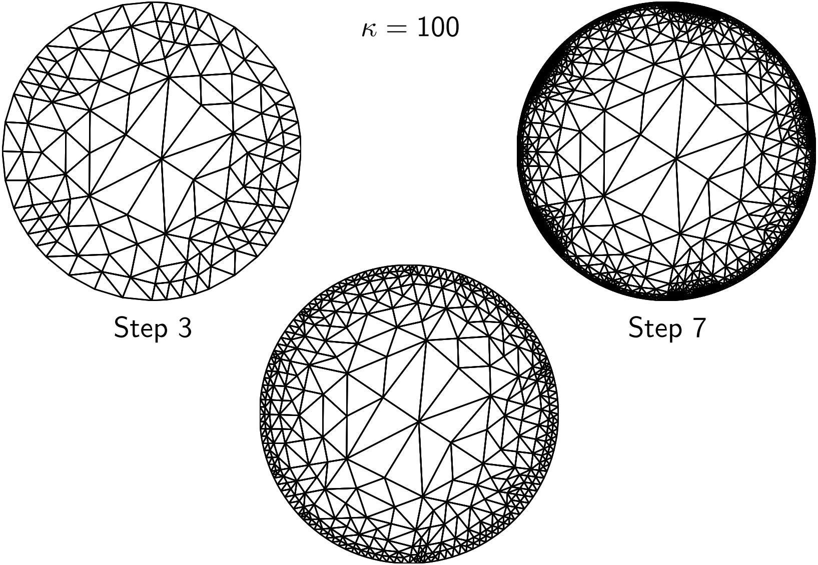
Step 7



Step 5

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

$\kappa = 100$



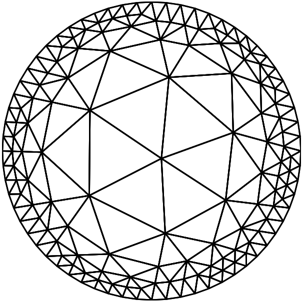
Step 3

Step 5

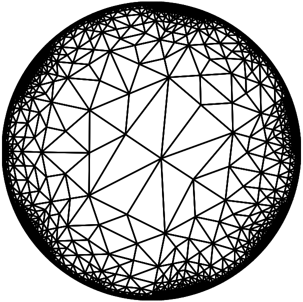
Step 7

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

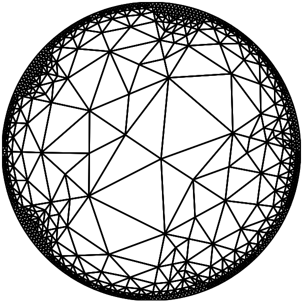
$\kappa = 100$



Step 3



Step 7



Step 5

Generalizations

- General elliptic problem (nonsymmetric)
- Elasticity
- Stokes problem (incompressible viscous fluids)
- Variational inequalities
- Nonlinear problems (special)
- Differential equations of higher order
- Equations with curl
- Linear evolutionary problems
- Optimal control

History

1947 W. Prager and J.L. Synge

1957 J.L. Synge

1971 J.P. Aubin and H.G. Burchard

1976- I. Hlaváček (M. Křížek, J. Vacek, J. Weisz, . . .)

2000- S. Repin (S. Korotov, J. Valdman, S. Sauter, M. Frolov, . . .)

M. Vohralík (R. Fučík, I. Cheddadi, M.I. Prieto, . . .)

Conclusions

$$\|u - u_h\| \leq \eta(u_h, \mathbf{y}_h)$$

- Guaranteed upper bounds
- Optimal $\mathbf{y}$ solves a complementary problem
- Postprocessing of ∇u_h
  $\Rightarrow$ fast algorithms for $\mathbf{y}_h$ (many open problems)
- $u_h \in V$ arbitrary
  $\Rightarrow$ including algebraic errors, quadrature errors, human errors

Thank you for your attention

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