

# Computing guaranteed upper bounds of the approximation error

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June 28, 2010, ESCO 2010, Plzeň



- ▶ A posteriori error estimates
- ▶ Primal problem:  $-\mathcal{L}\mathbf{u} = f$  in  $\Omega$  + b.c.
- ▶ Complementary problem:  $-\mathcal{L}^*\mathbf{y} = f$  in  $\Omega$  + b.c.
- ▶ Error estimate:  $\|\mathbf{u} - \mathbf{u}_h\| \leq \eta(\mathbf{u}_h, \mathbf{y}_h) \quad \forall \mathbf{u}_h \in \mathbf{V} \quad \forall \mathbf{y}_h \in \mathbf{W}$
- ▶ Numerical examples
- ▶ Conclusions

# A posteriori error estimates



- ▶ GOAL: Solve the problem **with prescribed accuracy**.



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- ▶ Adaptive algorithm
  1. **Initialize:** Construct the initial mesh  $\mathcal{T}_h$ .
  2. **Solve:** Find  $\mathbf{u}_h$  on  $\mathcal{T}_h$ .
  3. **Estimate error:** Compute  $\eta_K$  for all  $K \in \mathcal{T}_h$ .  $\eta^2 = \sum_{K \in \mathcal{T}_h} \eta_K^2$ .
  4. **Stopping criterion:** If  $\eta \leq \text{TOL} \Rightarrow \text{STOP}$ .
  5. **Mark:** If  $\eta_K \geq \Theta \max_{K \in \mathcal{T}_h} \eta_K \Rightarrow \text{mark } K$ .  $0 < \Theta < 1$
  6. **Refine:** Refine marked elements and build the new mesh  $\mathcal{T}_h$ .
  7. GO TO 2.

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- ▶ Guaranteed upper bound:  $\|\mathbf{u} - \mathbf{u}_h\| \leq \eta \leq \text{TOL}$
- ▶ Verification

# Primal Problem



$$\Omega \subset \mathbb{R}^d$$

$$-\operatorname{div}(\mathcal{A}^{11} \nabla u^1) \cdots -\operatorname{div}(\mathcal{A}^{1N} \nabla u^N) + c^{11} u^1 \cdots + c^{1N} u^N = f^1$$

$$-\operatorname{div}(\mathcal{A}^{21} \nabla u^1) \cdots -\operatorname{div}(\mathcal{A}^{2N} \nabla u^N) + c^{21} u^1 \cdots + c^{2N} u^N = f^2$$

⋮

$$-\operatorname{div}(\mathcal{A}^{N1} \nabla u^1) \cdots -\operatorname{div}(\mathcal{A}^{NN} \nabla u^N) + c^{N1} u^1 \cdots + c^{NN} u^N = f^N$$

$$u^1 = u^2 = \cdots = u^N = 0 \quad \text{on } \partial\Omega$$

# Primal Problem



$$\begin{aligned} -\operatorname{div}(\overline{\mathcal{A}} \overline{\nabla u}) + C \mathbf{u} &= \mathbf{f} \quad \text{in } \Omega \\ \mathbf{u} &= \mathbf{0} \quad \text{on } \partial\Omega \end{aligned}$$

$$\mathbf{u} = \begin{pmatrix} u^1 \\ \vdots \\ u^N \end{pmatrix} \quad \overline{\nabla u} = \begin{pmatrix} \nabla u^1 \\ \vdots \\ \nabla u^N \end{pmatrix} \quad \overline{\mathbf{y}} = \begin{pmatrix} \mathbf{y}^1 \\ \vdots \\ \mathbf{y}^N \end{pmatrix} \quad \operatorname{div} \overline{\mathbf{y}} = \begin{pmatrix} \operatorname{div} \mathbf{y}^1 \\ \vdots \\ \operatorname{div} \mathbf{y}^N \end{pmatrix}$$

$$\overline{\mathcal{A}} = \begin{pmatrix} \mathcal{A}^{11} & \dots & \mathcal{A}^{1N} \\ \vdots & & \vdots \\ \mathcal{A}^{N1} & \dots & \mathcal{A}^{NN} \end{pmatrix} \quad C = \begin{pmatrix} c^{11} & \dots & c^{1N} \\ \vdots & & \vdots \\ c^{N1} & \dots & c^{NN} \end{pmatrix} \quad \mathbf{f} = \begin{pmatrix} f^1 \\ \vdots \\ f^N \end{pmatrix}$$

**Assumptions:**  $\overline{\mathcal{A}} = \overline{\mathcal{A}}^{\frac{1}{2}} \overline{\mathcal{A}}^{\frac{1}{2}}$  is uniformly s.p.d.  $C = K^T K$  is s.p.d.

Strong form.: 
$$-\operatorname{div}(\overline{\mathcal{A}} \overline{\nabla u}) + C\mathbf{u} = \mathbf{f} \quad \text{in } \Omega$$
$$\mathbf{u} = \mathbf{0} \quad \text{on } \partial\Omega$$

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

Notation:

- ▶  $\mathbf{V} = [H_0^1(\Omega)]^N$
- ▶  $B(\mathbf{u}, \mathbf{v}) = (\overline{\mathcal{A}} \overline{\nabla u}, \overline{\nabla v}) + (C\mathbf{u}, \mathbf{v}) \quad (\overline{\mathbf{p}}, \overline{\mathbf{q}}) = \int_{\Omega} \overline{\mathbf{p}} \cdot \overline{\mathbf{q}} \, dx$
- ▶  $\mathcal{F}(\mathbf{v}) = (\mathbf{f}, \mathbf{v})$
- ▶  $\|\mathbf{v}\|^2 = B(\mathbf{v}, \mathbf{v})$





# Derivation of the estimate

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

$$\int_{\Omega} v \operatorname{div} \mathbf{y} \, dx + \int_{\Omega} \mathbf{y} \cdot \nabla v \, dx - \int_{\partial\Omega} v \mathbf{y} \cdot \mathbf{n} \, dx = 0$$



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$$\begin{aligned} \mathcal{B}(\mathbf{u}, \mathbf{v}) &= \\ &= (\mathbf{f}, \mathbf{v}) \end{aligned}$$



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$$\begin{aligned} \mathcal{B}(\mathbf{u} - \mathbf{u}_h, \mathbf{v}) &= \\ &= (\mathbf{f}, \mathbf{v}) - (\overline{\mathcal{A} \nabla u_h}, \overline{\nabla v}) - (C \mathbf{u}_h, \mathbf{v}) \end{aligned}$$



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$$= (\mathbf{f}, \mathbf{v}) - (\overline{\mathcal{A} \nabla u_h}, \overline{\nabla v}) - (C \mathbf{u}_h, \mathbf{v}) + (\operatorname{div} \bar{\mathbf{y}}, \mathbf{v}) + (\bar{\mathbf{y}}, \overline{\nabla v})$$



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$$= ([\mathbf{f} - C \mathbf{u}_h + \operatorname{div} \bar{\mathbf{y}}], \mathbf{v}) + ([\bar{\mathbf{y}} - \overline{\mathcal{A} \nabla u_h}], \overline{\nabla v})$$



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$$= \left( K^{-T} [\mathbf{f} - C \mathbf{u}_h + \operatorname{div} \bar{\mathbf{y}}], K \mathbf{v} \right) + \left( \overline{\mathcal{A}^{-\frac{1}{2}} [\bar{\mathbf{y}} - \overline{\mathcal{A} \nabla u_h}]}, \overline{\mathcal{A}^{\frac{1}{2}} \nabla v} \right)$$



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$$\leq \underbrace{\left( \left\| \mathbf{f} - C \mathbf{u}_h + \operatorname{div} \bar{\mathbf{y}} \right\|_{C^{-1}}^2 + \left\| \bar{\mathbf{y}} - \overline{\mathcal{A} \nabla u_h} \right\|_{\overline{\mathcal{A}^{-1}}}^2 \right)^{\frac{1}{2}}}_{\eta(\mathbf{u}_h, \bar{\mathbf{y}})} \left\| \mathbf{v} \right\|$$





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$$\left\| \mathbf{u} - \mathbf{u}_h \right\| \leq \eta(\mathbf{u}_h, \bar{\mathbf{y}}) \quad \forall \mathbf{u}_h \in \mathbf{V} \quad \forall \bar{\mathbf{y}} \in \mathbf{W} = [\mathbf{H}(\text{div}, \Omega)]^N$$



# The estimator

**Definition:**  $\eta^2(\mathbf{u}_h, \bar{\mathbf{y}}_h) = \|\mathbf{f} - \mathbf{C}\mathbf{u}_h + \mathbf{div} \bar{\mathbf{y}}\|_{\mathbf{C}^{-1}}^2 + \|\bar{\mathbf{y}} - \overline{\mathcal{A} \nabla u_h}\|_{\overline{\mathcal{A}}}^2$

**Theorem:**  $\|\mathbf{u} - \mathbf{u}_h\| \leq \eta(\mathbf{u}_h, \bar{\mathbf{y}}_h) \quad \forall \mathbf{u}_h \in \mathbf{V} \quad \forall \bar{\mathbf{y}}_h \in \mathbf{W}$

Complementary problem:

(A) Find  $\bar{\mathbf{y}} \in \mathbf{W} : \eta(\mathbf{u}_h, \bar{\mathbf{y}}) = \min_{\bar{\mathbf{w}} \in \mathbf{W}} \eta(\mathbf{u}_h, \bar{\mathbf{w}})$

(B) Find  $\bar{\mathbf{y}} \in \mathbf{W} : \mathcal{B}^*(\bar{\mathbf{y}}, \bar{\mathbf{w}}) = \mathcal{F}^*(\bar{\mathbf{w}}) \quad \forall \bar{\mathbf{w}} \in \mathbf{W}$

▶  $\mathbf{W} = [\mathbf{H}(\text{div}, \Omega)]^N$

▶  $\mathcal{B}^*(\bar{\mathbf{y}}, \bar{\mathbf{w}}) = (\mathbf{C}^{-1} \mathbf{div} \bar{\mathbf{y}}, \mathbf{div} \bar{\mathbf{w}}) + (\overline{\mathcal{A}^{-1}} \bar{\mathbf{y}}, \bar{\mathbf{w}})$

▶  $\mathcal{F}^*(\bar{\mathbf{w}}) = -(\mathbf{C}^{-1} \mathbf{f}, \mathbf{div} \bar{\mathbf{w}})$

▶  $\|\bar{\mathbf{w}}\|_*^2 = \mathcal{B}^*(\bar{\mathbf{w}}, \bar{\mathbf{w}})$



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**Theorem:**  $\|\mathbf{u} - \mathbf{u}_h\| \leq \eta(\mathbf{u}_h, \bar{\mathbf{y}}_h) \quad \forall \mathbf{u}_h \in \mathbf{V} \quad \forall \bar{\mathbf{y}}_h \in \mathbf{W}$

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

**Lemma 2:**  $\bar{\mathbf{y}} = \overline{\mathcal{A} \nabla \mathbf{u}} \in \mathbf{W}$  is the unique solution of (A)–(B)

**Lemma 3:**  $\eta^2(\mathbf{u}_h, \bar{\mathbf{y}}) + \eta^2(\mathbf{u}, \bar{\mathbf{y}}_h) = \eta^2(\mathbf{u}_h, \bar{\mathbf{y}}_h) \quad \forall \mathbf{u}_h \in \mathbf{V}, \bar{\mathbf{y}}_h \in \mathbf{W}$   
 $\|\mathbf{u} - \mathbf{u}_h\|^2 + \|\bar{\mathbf{y}}_h - \bar{\mathbf{y}}\|_*^2 = \eta^2(\mathbf{u}_h, \bar{\mathbf{y}}_h)$

Theorem: If

- ▶  $\mathbf{u} \in \mathbf{V}$  is primal solution
- ▶  $\mathbf{u}_h \in \mathbf{V}$ ,  $\bar{\mathbf{y}}_h \in \mathbf{W}$  arbitrary
- ▶  $\tilde{\mathbf{u}}_h = [C^{-1}(\mathbf{f} + \mathbf{div} \bar{\mathbf{y}}_h) + \mathbf{u}_h]/2$
- ▶  $\mathcal{G}\tilde{\mathbf{u}}_h = (\bar{\mathbf{y}}_h + \overline{\mathcal{A} \nabla u_h})/2$

Then

$$\left\| \overline{\nabla u} - \overline{\mathcal{A}^{-1} \mathcal{G}\tilde{\mathbf{u}}_h} \right\|_{\overline{\mathcal{A}}}^2 + \|\mathbf{u} - \tilde{\mathbf{u}}_h\|_C^2 = \frac{1}{4} \eta^2(\mathbf{u}_h, \bar{\mathbf{y}}_h).$$



## Other variants (good for $C$ singular)

$$(1) \quad \eta^2(\mathbf{u}_h, \bar{\mathbf{y}}_h) = \|\mathbf{f} - C\mathbf{u}_h + \mathbf{div} \bar{\mathbf{y}}_h\|_{C^{-1}}^2 + \|\bar{\mathbf{y}}_h - \overline{\mathcal{A} \nabla u_h}\|_{\mathcal{A}^{-1}}^2$$

$$(2) \quad \tilde{\eta}(\mathbf{u}_h, \tilde{\mathbf{y}}_h) = \|\tilde{\mathbf{y}}_h - \overline{\mathcal{A} \nabla u_h}\|_{\mathcal{A}^{-1}} \quad \tilde{\mathbf{y}}_h \in \mathbf{Q}(\mathbf{f}, \mathbf{u}_h)$$
$$\mathbf{Q}(\mathbf{f}, \mathbf{u}_h) = \{\tilde{\mathbf{y}} \in \mathbf{W} : \mathbf{f} - C\mathbf{u}_h + \mathbf{div} \tilde{\mathbf{y}} = 0\}$$

$$(3) \quad \hat{\eta}(\mathbf{u}_h, \hat{\mathbf{y}}_h) = \frac{\gamma_F}{\lambda} \|\mathbf{f} - C\mathbf{u}_h + \mathbf{div} \hat{\mathbf{y}}_h\|_0 + \|\hat{\mathbf{y}}_h - \overline{\mathcal{A} \nabla u_h}\|_{\mathcal{A}^{-1}}$$

$$\text{Friedrichs ineq.: } \|v\|_0 \leq \gamma_F \|\nabla v\|_0 \quad \forall v \in H_0^1(\Omega)$$

$$\text{Ellipticity: } (\overline{\mathcal{A} \mathbf{w}}, \mathbf{w}) \geq \lambda^2 \|\mathbf{w}\|_0^2 \quad \forall \mathbf{w} \in \mathbf{W}$$

$$\text{Lemma: } \|\mathbf{u} - \mathbf{u}_h\| \leq \min \{\eta(\mathbf{u}_h, \bar{\mathbf{y}}_h), \tilde{\eta}(\mathbf{u}_h, \tilde{\mathbf{y}}_h), \hat{\eta}(\mathbf{u}_h, \hat{\mathbf{y}}_h)\}$$
$$\forall \mathbf{u}_h \in \mathbf{V} \quad \forall \bar{\mathbf{y}}_h \in \mathbf{W} \quad \forall \tilde{\mathbf{y}}_h \in \mathbf{Q}(\mathbf{f}, \mathbf{u}_h) \quad \forall \hat{\mathbf{y}}_h \in \mathbf{W}$$

# Numerical example



## Primal problem

$$- (\overline{\mathcal{A}}\mathbf{u}')' + C\mathbf{u} = \mathbf{f}$$
$$\mathbf{u}(0) = \mathbf{u}(1) = \mathbf{0}$$

$$\overline{\mathcal{A}} = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 2 & 0 \\ -2 & 0 & 6 \end{pmatrix} \quad C = \kappa^2 \begin{pmatrix} 4 & 1 & -1 \\ 1 & 2 & 1 \\ -1 & 1 & 4 \end{pmatrix} \quad \mathbf{f} = \begin{pmatrix} 4 \\ 4 \\ 4 \end{pmatrix}$$

$$\mathbf{u} = \begin{pmatrix} u^1 \\ u^2 \\ u^3 \end{pmatrix} = \frac{1}{\kappa^2} \left( 1 - \frac{\sinh \kappa(1-x) + \sinh \kappa x}{\sinh \kappa} \right) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

# Numerical example



## Primal problem

$$-(\bar{\mathcal{A}}\mathbf{u}')' + \mathbf{C}\mathbf{u} = \mathbf{f}$$
$$\mathbf{u}(0) = \mathbf{u}(1) = \mathbf{0}$$

## Complementary problem

$$-(\mathbf{C}^{-1}\mathbf{y}')' + \bar{\mathcal{A}}^{-1}\mathbf{y} = (\mathbf{C}^{-1}\mathbf{f})' \quad \text{in } (0, 1)$$
$$\mathbf{y}'(0) = -\mathbf{f}(0) \quad \mathbf{y}'(1) = -\mathbf{f}(1)$$

$$\bar{\mathcal{A}} = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 2 & 0 \\ -2 & 0 & 6 \end{pmatrix} \quad \mathbf{C} = \kappa^2 \begin{pmatrix} 4 & 1 & -1 \\ 1 & 2 & 1 \\ -1 & 1 & 4 \end{pmatrix} \quad \mathbf{f} = \begin{pmatrix} 4 \\ 4 \\ 4 \end{pmatrix}$$

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$$\mathbf{y} = \bar{\mathcal{A}}\mathbf{u}'$$

# Numerical example



Primal problem

$$\begin{aligned} -(\overline{\mathcal{A}}\mathbf{u}')' + \mathbf{C}\mathbf{u} &= \mathbf{f} \\ \mathbf{u}(0) = \mathbf{u}(1) &= \mathbf{0} \end{aligned}$$

Complementary problem

$$\begin{aligned} -(C^{-1}\mathbf{y}')' + \overline{\mathcal{A}}^{-1}\mathbf{y} &= (C^{-1}\mathbf{f})' \quad \text{in } (0, 1) \\ \mathbf{y}'(0) = -\mathbf{f}(0) \quad \mathbf{y}'(1) &= -\mathbf{f}(1) \end{aligned}$$

FEM mesh

$$0 = x_0 < x_1 < \dots < x_M = 1 \quad K_i = [x_{i-1}, x_i], \quad i = 1, 2, \dots, M$$

Primal FEM

$$\mathbf{V}_h = \{v_h \in H_0^1(0, 1) : v_h|_{K_i} \in P^1(K_i) \quad \forall K_i\}^3$$

$$\mathbf{u}_h \in \mathbf{V}_h : (\overline{\mathcal{A}}\mathbf{u}'_h, \mathbf{v}'_h) + (\mathbf{C}\mathbf{u}_h, \mathbf{v}_h) = (\mathbf{f}, \mathbf{v}_h) \quad \forall \mathbf{v}_h \in \mathbf{V}_h$$

Complementary FEM

$$\mathbf{W}_h = \{w_h \in H^1(0, 1) : w_h|_{K_i} \in P^1(K_i) \quad \forall K_i\}^3$$

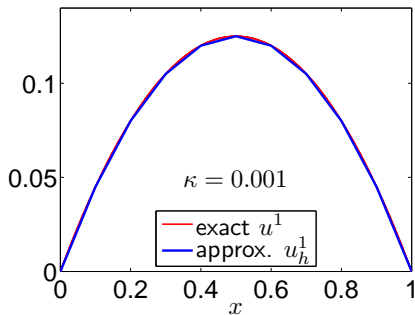
$$\mathbf{y}_h \in \mathbf{W}_h : (C^{-1}\mathbf{y}'_h, \mathbf{w}'_h) + (\overline{\mathcal{A}}^{-1}\mathbf{y}_h, \mathbf{w}_h) = -(C^{-1}\mathbf{f}, \mathbf{w}'_h) \quad \forall \mathbf{w}_h \in \mathbf{W}_h$$



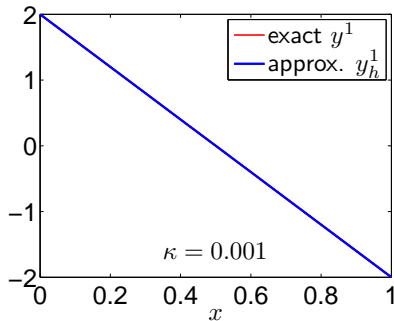
# Primal and complementary solutions



Primal solution



Complementary sol.



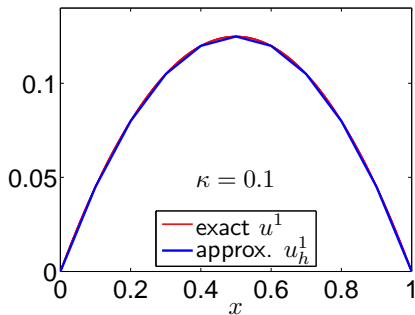
$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}_h\|} \leq \frac{\eta}{\|\mathbf{u}_h\|} = 9.486\%$$

$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}\|} = 9.440\% \quad \frac{\eta}{\|\mathbf{u}\|} = 9.440\% \quad l_{eff} = 1.000$$

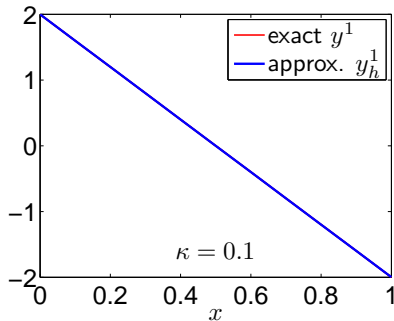
# Primal and complementary solutions



Primal solution



Complementary sol.



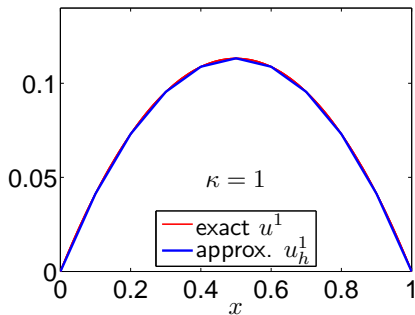
$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}_h\|} \leq \frac{\eta}{\|\mathbf{u}_h\|} = 9.486\%$$

$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}\|} = 9.436\% \quad \frac{\eta}{\|\mathbf{u}\|} = 9.439\% \quad l_{eff} = 1.0003$$

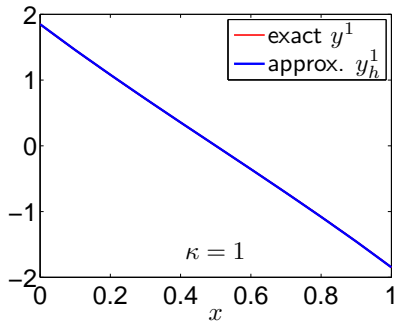
# Primal and complementary solutions



Primal solution



Complementary sol.



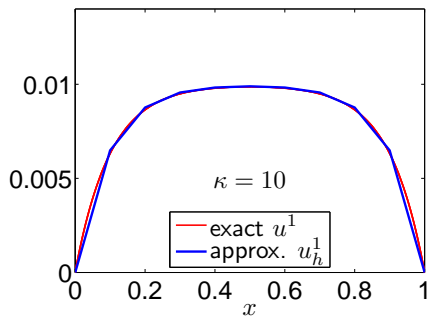
$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}_h\|} \leq \frac{\eta}{\|\mathbf{u}_h\|} = 9.530\%$$

$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}\|} = 9.158\% \quad \frac{\eta}{\|\mathbf{u}\|} = 9.487\% \quad l_{eff} = 1.036$$

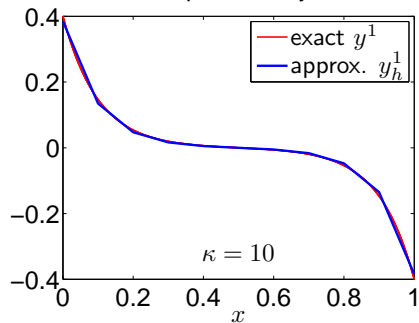
# Primal and complementary solutions



Primal solution



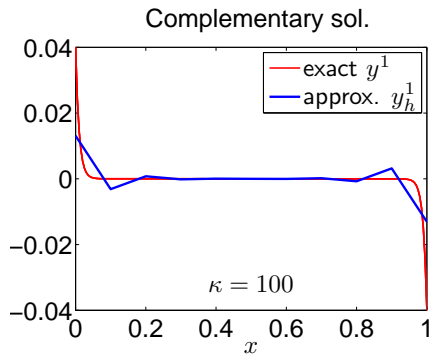
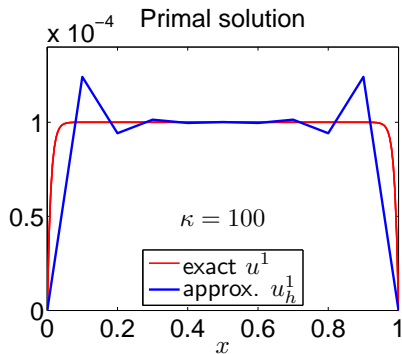
Complementary sol.



$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}_h\|} \leq \frac{\eta}{\|\mathbf{u}_h\|} = 13.45\%$$

$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}\|} = 9.617\% \quad \frac{\eta}{\|\mathbf{u}\|} = 13.39\% \quad l_{eff} = 1.392$$

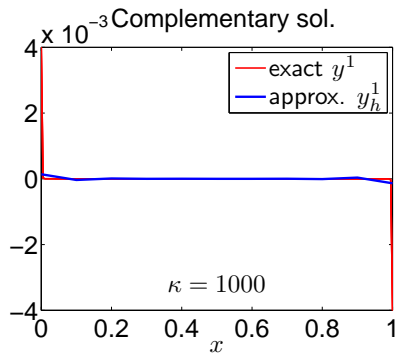
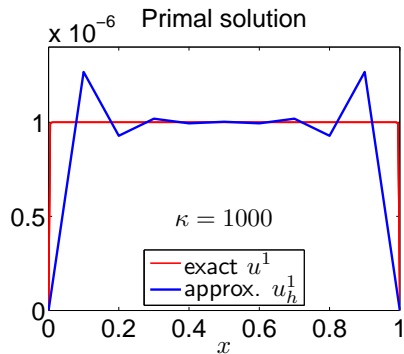
# Primal and complementary solutions



$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}_h\|} \leq \frac{\eta}{\|\mathbf{u}_h\|} = 22.26\%$$

$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}\|} = 15.48\% \quad \frac{\eta}{\|\mathbf{u}\|} = 21.99\% \quad l_{eff} = 1.420$$

# Primal and complementary solutions



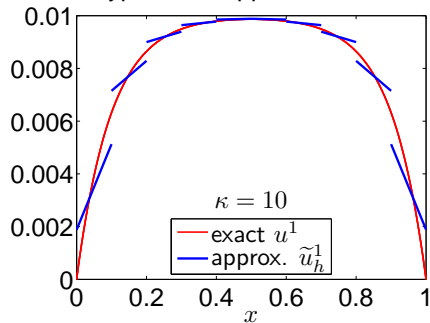
$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}_h\|} \leq \frac{\eta}{\|\mathbf{u}_h\|} = 22.23\%$$

$$\frac{\|\mathbf{u} - \mathbf{u}_h\|}{\|\mathbf{u}\|} = 19.86\% \quad \frac{\eta}{\|\mathbf{u}\|} = 21.90\% \quad l_{eff} = 1.103$$

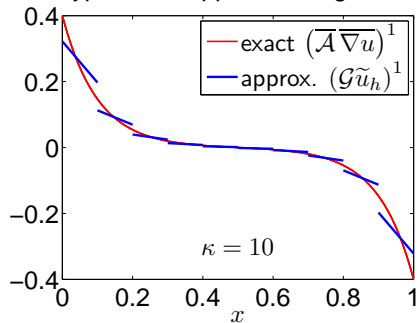
# Method of hypercircle



Hypercircle approx. of values



Hypercircle approx. of cogradient

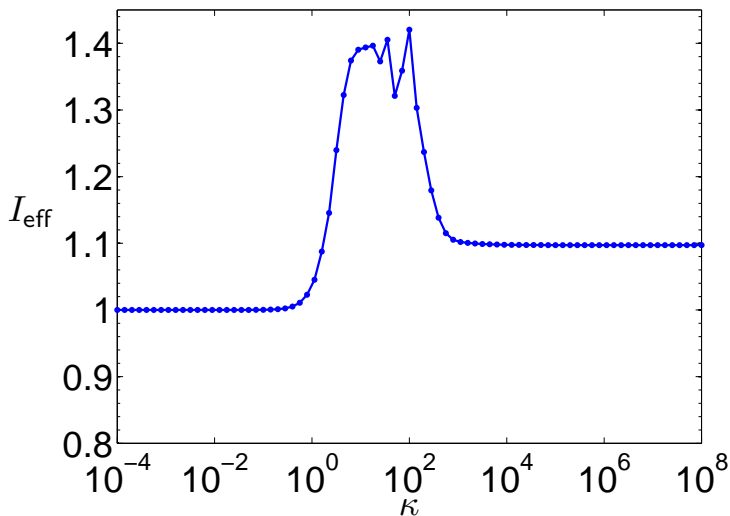


$$\frac{\|[\mathbf{u} - \tilde{\mathbf{u}}_h, \overline{\nabla} u - \mathcal{G}\tilde{\mathbf{u}}_h]\|_{hc}}{\|\mathbf{u}_h\|} = \frac{1}{2} \frac{\eta}{\|\mathbf{u}_h\|} = 6.72\%$$

# Effectivity index



Effectivity vs.  $\kappa$







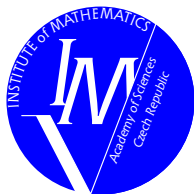
$$\|\mathbf{u} - \mathbf{u}_h\| \leq \eta(\mathbf{u}_h, \bar{\mathbf{y}}_h)$$

- ▶ Computable guaranteed upper bounds
- ▶ Optimal  $\bar{\mathbf{y}}$  solves a complementary problem
- ▶ Postprocessing of  $\overline{\mathcal{A} \nabla u_h}$   
⇒ fast algorithms for  $\bar{\mathbf{y}}_h$  (many open problems)
- ▶  $\mathbf{u}_h \in \mathbf{V}$  arbitrary  
⇒ including algebraic errors, human errors
- ▶ Exist generalizations to other classes of problems

Thank you for your attention

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June 28, 2010, ESCO 2010, Plzeň