A posteriori error estimates

Part I – Overview

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April 17, 2012, Technical University of Ostrava

Outline

- Introduction – reference solution
- Good error indicators
  - Explicit residual estimators
  - Postprocessing
- Lower bounds
  - Hierarchic
  - Implicit residual – Dirichlet
- Upper bounds
  - Implicit residual – Neumann
  - Complementary
- Quantity of interest
- Adaptive algorithm

Introduction

Mathematical modelling:

Reality	—	Mathematical model	—	Numerical model	—	Computer model
	modelling error		discretization error		round-off error algebraic error quadrature error	

- error × uncertainty
- verification × validation

Toy problem

Classical formulation:

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

Weak formulation: $V = H_0^1(\Omega)$

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

Notation:

- $a(u,v) = (\nabla u, \nabla v)$
- $\mathcal{F}(v) = (f, v)$
- $(\varphi, \psi) = \int_\Omega \varphi\psi \, \mathrm{d}x$

Finite elements: $V_h = \{v_h \in V : \text{p.w. linear on } \mathcal{T}_h\} \subset V$

$$u_h \in V_h: \quad a(u_h, v_h) = \mathcal{F}(v_h) \quad \forall v_h \in V_h$$

Error: $e = u - u_h$

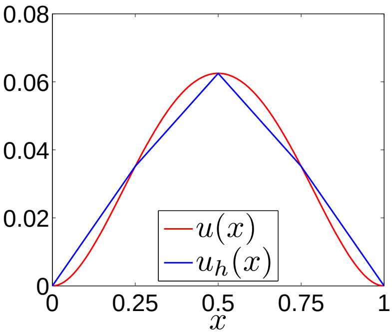
Energy norm: $|||e|||^2 = a(e,e) = (\nabla e, \nabla e) = \|\nabla e\|_0^2$

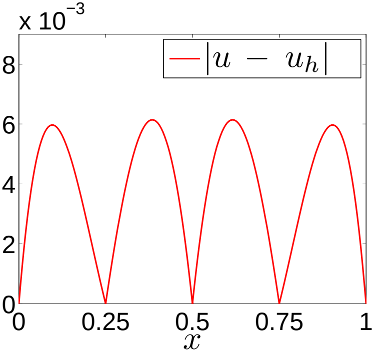
Reference solution (Runge ≈1900)

Idea: replace $u \approx u_h^{\mathrm{ref}}$ and estimate $\|u - u_h\| \approx \|u_h^{\mathrm{ref}} - u_h\|$

$$u_h \in V_h \qquad V_h = \{\text{p.w. linears on a mesh } \mathcal{T}_h\} \subset V$$

$$u_h^{\mathrm{ref}} \in V_h^{\mathrm{ref}} \qquad V_h \subset V_h^{\mathrm{ref}} = \{\text{p.w. linears on a mesh } \mathcal{T}_h^{\mathrm{ref}}\} \subset V$$





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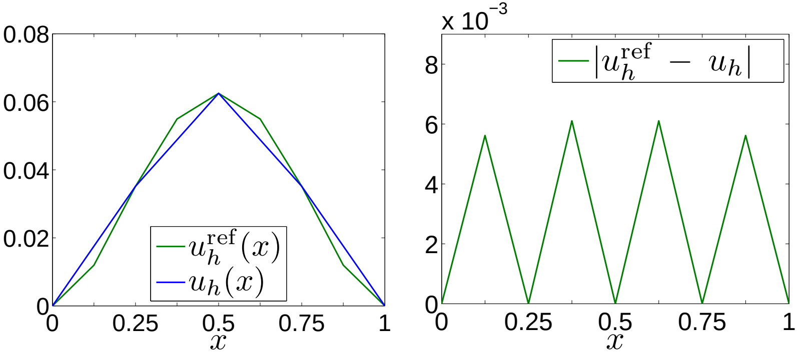

Analysis of the reference solution

Lemma (Galerkin ortho.): Let $V_1 \subset V_2$, $a(\cdot,\cdot)$ be symmetric, and

$$u_1 \in V_1 : \quad a(u_1, v_1) = \mathcal{F}(v_1) \quad \forall v_1 \in V_1$$
$$u_2 \in V_2 : \quad a(u_2, v_2) = \mathcal{F}(v_2) \quad \forall v_2 \in V_2$$

Then

$$a(u_2 - u_1, v_1) = 0 \quad \forall v_1 \in V_1$$
$$|||u_2 - u_1|||^2 = |||u_2|||^2 - |||u_1|||^2$$

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$$|\!|\!| u_2 - u_1 |\!|\!|^2 = |\!|\!| u_2 |\!|\!|^2 - |\!|\!| u_1 |\!|\!|^2$$

Proof:

$$a(u_1, u_2) = a(u_2, u_1) = \mathcal{F}(u_1) = a(u_1, u_1) = |\!|\!| u_1 |\!|\!|^2$$

$$|\!|\!| u_2 - u_1 |\!|\!|^2 = a(u_2 - u_1, u_2) = |\!|\!| u_2 |\!|\!|^2 - |\!|\!| u_1 |\!|\!|^2$$

□

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Then

$$a(u_2 - u_1, v_1) = 0 \quad \forall v_1 \in V_1$$
$$\|u_2 - u_1\|^2 = \|u_2\|^2 - \|u_1\|^2$$

Lemma (lower bound): Let $V_h \subset V_h^{\mathrm{ref}} \subset V$, $a(\cdot,\cdot)$ be symmetric, and

$$u_h \in V_h : \quad a(u_h, v_h) = \mathcal{F}(v_h) \quad \forall v_h \in V_h$$
$$u_h^{\mathrm{ref}} \in V_h^{\mathrm{ref}} : \quad a(u_h^{\mathrm{ref}}, v_h^{\mathrm{ref}}) = \mathcal{F}(v_h^{\mathrm{ref}}) \quad \forall v_h^{\mathrm{ref}} \in V_h^{\mathrm{ref}}$$
$$u \in V : \quad a(u, v) = \mathcal{F}(v) \quad \forall v \in V$$

Then

$$\|u - u_h\|^2 = \|u - u_h^{\mathrm{ref}}\|^2 + \|u_h^{\mathrm{ref}} - u_h\|^2$$

Analysis of the reference solution

Lemma (Galerkin ortho.): $|||u_2 - u_1|||^2 = |||u_2|||^2 - |||u_1|||^2$

Lemma (lower bound): $|||u - u_h|||^2 = |||u - u_h^{\mathrm{ref}}|||^2 + |||u_h^{\mathrm{ref}} - u_h|||^2$

Analysis of the reference solution

Lemma (Galerkin ortho.): $\|u_2 - u_1\|^2 = \|u_2\|^2 - \|u_1\|^2$

Lemma (lower bound): $\|u - u_h\|^2 = \|u - u_h^{\mathrm{ref}}\|^2 + \|u_h^{\mathrm{ref}} - u_h\|^2$

$\Rightarrow \quad \|u_h^{\mathrm{ref}} - u_h\| \leq \|u - u_h\|$

Analysis of the reference solution

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Easy to compute:

$\varphi_1, \varphi_2, \ldots, \varphi_N$ basis of $V_h \quad \Rightarrow \quad u_h = \sum_{i=1}^{N} x_i \varphi_i$

$Ax = F, \quad A_{ij} = a(\varphi_j, \varphi_i), \quad F_i = \mathcal{F}(\varphi_i) \quad \Rightarrow \quad \|u_h\|^2 = x^\top A x$

Analysis of the reference solution

Lemma (Galerkin ortho.): $\|u_2 - u_1\|^2 = \|u_2\|^2 - \|u_1\|^2$

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$\Rightarrow \quad \|u_h^{\mathrm{ref}} - u_h\| \le \|u - u_h\|$

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$Ax = F, \quad A_{ij} = a(\varphi_j, \varphi_i), \quad F_i = \mathcal{F}(\varphi_i) \quad \Rightarrow \quad \|u_h\|^2 = x^\top A x$

Proof: $\|u_h\|^2 = a\left(\sum_{i=1}^{N} x_i \varphi_i, \sum_{j=1}^{N} x_j \varphi_j\right) = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j a(\varphi_i, \varphi_j) = x^\top A x$

A posteriori error estimates

A quantity η is *a posteriori error estimate* if it is

- computable (from u_h, $\mathcal{T}_h$, f, etc.)
- $\|u - u_h\| \approx \eta$

Properties and terminology:

- Efficient and reliable: $C_1\eta \le \|u - u_h\| \le C_2\eta$
- Guaranteed upper (lower) bound: $\|u - u_h\| \le \eta \quad (\eta \le \|u - u_h\|)$
- Robust: C_1, C_2 independent of $\mathcal{T}_h$, coefficients, ...
- Fast: $O(N)$ operations
- Asymptotic exactness: $\lim_{h\to 0} I_{\text{eff}} = 1$
- Index of effectivity: $I_{\text{eff}} = \dfrac{\eta}{\|u - u_h\|}$

Usage

- For efficiency:
  - error indicator
  - adaptive mesh refinement
  - fast, inaccurate
  - efficiency and reliability $\Rightarrow$ convergence of adaptive algorithm
- For reliability:
  - error estimator
  - two-sided error bounds or stopping criterion (in adaptivity)
  - slow, accurate
  - guaranteed upper bound
- Cost:
  - direct
  - indirect – cost for underestimation and overestimation

Types of AEE and what they are good for

- Explicit residual:
  good indicators
- Implicit residual – Dirichlet type:
  guaranteed lower bound, good indicators
- Implicit residual – Neumann:
  upper bound
- Hierarchic:
  guaranteed lower bound, good indicators
- Complementary:
  guaranteed upper bound, good estimators
- Postprocessing:
  good indicators
- Quantity of interest:
  if energy norm not desirable

Good indicators

(A) Explicit residual:

$$\|u - u_h\|^2 \leq C \sum_{K \in \mathcal{T}_h} \left(|K| \, \|r\|_{0,K}^2 + \frac{1}{2} \sum_{\ell \subset \partial K} |\ell| \, \|J_\ell\|_{0,\ell}^2 \right)$$

where $r = f + \Delta u_h \qquad J_\ell = (\nabla u_h^+ - \nabla u_h^-) \cdot \mathbf{n}_\ell$

[Babuška, Rheinboldt, 1979]

(B) Postprocessing:

$$\|u - u_h\| = \|\nabla u - \nabla u_h\|_0 \approx \|\mathcal{G}(u_h) - \nabla u_h\|_0$$

where $\mathcal{G}(u_h)$ is a recovered (postprocessed) gradient ∇u_h

[Zienkiewicz, Zhu, 1992], [Ainsworth, Craig, 1991]

Lower bounds

(C) Hierarchic estimates

$$V_h \subset V_h^{\mathrm{ref}} \subset V \qquad V_h^{\mathrm{ref}} = V_h \oplus \widehat{V}_h$$

$$\widehat{u}_h \in \widehat{V}_h : a(\widehat{u}_h, \widehat{v}_h) = \mathcal{F}(\widehat{v}_h) \quad \forall \widehat{v}_h \in \widehat{V}_h$$

$$e = u - u_h \qquad e_h^{\mathrm{ref}} = u_h^{\mathrm{ref}} - u_h \qquad \widehat{e}_h = \widehat{u}_h - u_h$$

Saturation assumption:
$\exists \beta < 1: \quad \|u - u_h^{\mathrm{ref}}\| \le \beta \|u - u_h\|$

Strengthenned Cauchy-Schwarz inequality:
$\exists \gamma < 1: \quad |a(v_h, \widehat{v}_h)| \le \gamma \|v_h\| \|\widehat{v}_h\| \quad \forall v_h \in V_h, \ \widehat{v}_h \in \widehat{V}_h$

Theorem:

$$\|\widehat{e}_h\| \le \|e_h^{\mathrm{ref}}\| \le \|e\| \le \frac{1}{(1-\beta^2)^{\frac{1}{2}}} \|e_h^{\mathrm{ref}}\| \le \frac{1}{(1-\beta^2)^{\frac{1}{2}}(1-\gamma^2)^{\frac{1}{2}}} \|\widehat{e}_h\|$$

[Bank, Smith, 1993], [Bank, Weiser, 1985]

Lower bounds

(D) Implicit residual – Dirichlet type

Strong: $-\Delta \widehat{u}_K = f$ in K, $\widehat{u}_K = u_h$ on ∂K

Weak: $\widehat{u}_K - u_h \in H_0^1(K)$: $a_K(\widehat{u}_K, \widehat{v}_K) = \mathcal{F}_K(\widehat{v}_K) \quad \forall \widehat{v}_K \in H_0^1(K)$

Notation: $a_K(u,v) = \int_K \nabla u \cdot \nabla v \,\mathrm{d}x$, $\mathcal{F}_K(v) = \int_K f v \,\mathrm{d}x$

[Babuška, Rheinboldt, 1978]

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Lemma: Let $\widehat{u}|_K = \widehat{u}_K$. Then $|\!|\!|\widehat{u} - u_h|\!|\!| \leq |\!|\!|u - u_h|\!|\!|$

Proof: Special case of Hierarchic estimates with

$$\widehat{V}_h = \{v \in V : v|_K \in H_0^1(K)\ \forall K \in \mathcal{T}_h\} \qquad \square$$

[Babuška, Rheinboldt, 1978]

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Strong: $-\Delta \widehat{u}_K = f$ in K, $\quad \widehat{u}_K = u_h$ on ∂K

Weak: $\widehat{u}_K - u_h \in H^1_0(K): \quad a_K(\widehat{u}_K, \widehat{v}_K) = \mathcal{F}_K(\widehat{v}_K) \quad \forall \widehat{v}_K \in H^1_0(K)$

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$$\widehat{V}_h = \{v \in V : v|_K \in H^1_0(K)\ \forall K \in \mathcal{T}_h\} \qquad \square$$

For computations:

Replace $H^1_0(K)$ by a finite dimensional subspace, e.g. $P^3_0(K)$.

$\widehat{V}_h^{p=3} = \{v_h \in \widehat{V}_h : v_h|_K \in P^3_0(K)\ \forall K \in \mathcal{T}_h\} \subset \widehat{V}_h$

$\Rightarrow \quad \widehat{u}^{p=3} \in \widehat{V}_h^{p=3} \quad \Rightarrow \quad |\!|\!|\widehat{u}^{p=3} - u_h|\!|\!| \leq |\!|\!|\widehat{u} - u_h|\!|\!| \leq |\!|\!|u - u_h|\!|\!|$

[Babuška, Rheinboldt, 1978]

Upper bounds

(E) Implicit residual – Neumann:

Strong: $-\Delta\widetilde{u}_K = f$ in K, $\quad \mathbf{n}_K \cdot \nabla\widetilde{u}_K = g_K \approx \mathbf{n}_K \cdot \nabla u$ on ∂K

Weak: $\widetilde{u}_K \in H^1(K): \quad a_K(\widetilde{u}_K, \widetilde{v}_K) = \mathcal{F}_K(\widetilde{v}_K) + \int_{\partial K} g_K \widetilde{v}_K \,\mathrm{d}x \quad \forall \widetilde{v}_K \in H^1(K)$

[Kelly, 1984], [Ladevèze, Leguillon, 1983]

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Lemma: Let $g_K + g_{K'} = 0$ on $\ell = \partial K \cap \partial K'$.
Then $|\!|\!| u - u_h |\!|\!|^2 \leq \sum_{K \in \mathcal{T}_h} |\!|\!| \widetilde{u}_K - u_h |\!|\!|_K^2$.

[Kelly, 1984], [Ladevèze, Leguillon, 1983]

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Lemma: Let $g_K + g_{K'} = 0$ on $\ell = \partial K \cap \partial K'$.
Then $\|u - u_h\|^2 \leq \sum_{K\in\mathcal{T}_h} \|\widetilde{u}_K - u_h\|_K^2$.

Proof: $v \in V$

$$a(u-u_h, v) = \mathcal{F}(v) - a(u_h, v) = \sum_{K\in\mathcal{T}_h}\left(\mathcal{F}_K(v) + \int_{\partial K} g_K v \,\mathrm{d}x - a_K(u_h, v)\right)$$

$$= \sum_{K\in\mathcal{T}_h} a_K(\widetilde{u}_K - u_h, v) \leq \sum_{K\in\mathcal{T}_h} \|\widetilde{u}_K - u_h\|_K \|v\|_K \leq \left(\sum_{K\in\mathcal{T}_h} \|\widetilde{u}_K - u_h\|_K^2\right)^{\frac{1}{2}} \|v\|$$

Set $v = u - u_h$. □

[Kelly, 1984], [Ladevèze, Leguillon, 1983]

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Weak: $\widetilde{u}_K \in H^1(K)$: $\quad a_K(\widetilde{u}_K, \widetilde{v}_K) = \mathcal{F}_K(\widetilde{v}_K) + \int_{\partial K} g_K \widetilde{v}_K \,\mathrm{d}x \quad \forall \widetilde{v}_K \in H^1(K)$

Lemma: Let $g_K + g_{K'} = 0$ on $\ell = \partial K \cap \partial K'$.
Then $\|u - u_h\|^2 \leq \sum_{K\in\mathcal{T}_h} \|\widetilde{u}_K - u_h\|_K^2$.

Technical details:

$\widetilde{u}_K = 0$ on $\partial\Omega \cap \partial K$

Solvability: $\int_K f \,\mathrm{d}x + \int_{\partial K} g_K \,\mathrm{d}x = 0 \quad \Rightarrow \quad$ Equilibration cond. on g_K

For computations:

Replace $H^1(K)$ by a finite dimensional subspace, e.g. $P^2(K)$.

$$\Rightarrow \quad \widetilde{u}_K^{p=2} \in P^2(K) \quad \Rightarrow \quad \|\widetilde{u}^{p=2} - u_h\|_K \leq \|\widetilde{u}_K - u_h\|_K$$

$$\not\Rightarrow \quad \|u - u_h\|^2 \leq \sum_{K\in\mathcal{T}_h} \|\widetilde{u}^{p=2} - u_h\|_K^2$$

[Kelly, 1984], [Ladevèze, Leguillon, 1983]

Upper bounds

(F) Complementary

Divergence thm.: $(\operatorname{div} \mathbf{y}, v) + (\mathbf{y}, \nabla v) = 0 \quad \forall \mathbf{y} \in \mathbf{H}(\operatorname{div}, \Omega), v \in H_0^1(\Omega)$

Friedrichs' inequality: $\|v\|_0 \leq C_{\mathrm{F}} |||v||| \quad \forall v \in H_0^1(\Omega)$

Theorem: Let $u_h \in V$ be arbitrary. Then

$$|||u - u_h||| \leq C_{\mathrm{F}} \|f + \operatorname{div} \mathbf{y}\|_0 + \|\mathbf{y} - \nabla u_h\|_0 \quad \forall \mathbf{y} \in \mathbf{H}(\operatorname{div}, \Omega)$$

[Aubin, Burchard, 1971], [Hlaváček et al. 1970s], [Repin 2000–]

Upper bounds

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Theorem: Let $u_h \in V$ be arbitrary. Then

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Proof: $v \in V$

$$\begin{aligned} a(u - u_h, v) &= (f, v) - (\nabla u_h, \nabla v) = (f + \operatorname{div}\mathbf{y}, v) + (\mathbf{y} - \nabla u_h, \nabla v) \\ &\leq \|f + \operatorname{div}\mathbf{y}\|_0 \|v\|_0 + \|\mathbf{y} - \nabla u_h\|_0 \|\nabla v\|_0 \\ &\leq \left(C_{\mathrm{F}} \|f + \operatorname{div}\mathbf{y}\|_0 + \|\mathbf{y} - \nabla u_h\|_0\right) |||v||| \end{aligned}$$

Set $v = u - u_h$. $\square$

[Aubin, Burchard, 1971], [Hlaváček et al. 1970s], [Repin 2000–]

Upper bounds

(F) Complementary

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$$|||u - u_h||| \leq C_{\mathrm{F}} \|f + \operatorname{div} \mathbf{y}\|_0 + \|\mathbf{y} - \nabla u_h\|_0 \quad \forall \mathbf{y} \in \mathbf{H}(\operatorname{div}, \Omega)$$

Remarks:

- $\mathbf{y} = \nabla u$ gives exact estimate
- Complementary problem $\Leftrightarrow$ optimal $\mathbf{y}$
- Unknown value of C_{F}:
  - avoid by exact equilibration: $\mathbf{y} \in \mathbf{H}(\operatorname{div}, \Omega) : f + \operatorname{div} \mathbf{y} = 0$
  - compute upper bound on C_{F}

[Aubin, Burchard, 1971], [Hlaváček et al. 1970s], [Repin 2000–]

(G) Quantity of interest

Quantity of interest: $\Phi \in V^*$

Adjoint problem: $z \in V: \quad a(v,z) = \Phi(v) \quad \forall v \in V$

Approx. adjoint prob.: $z_h \in V_h: \quad a(v_h,z_h) = \Phi(v_h) \quad \forall v_h \in V_h$

Error representation formula:

$$\Phi(u-u_h) = a(u-u_h,z) = \mathcal{R}(z) = \mathcal{R}(z-z_h) = a(u-u_h,z-z_h)$$

where
- $\mathcal{R}(v) = \mathcal{F}(v) - a(u_h,v)$
- $\mathcal{R}(v_h) = 0 \quad \forall v_h \in V_h$

Error estimate: $|\Phi(u-u_h)| \le \|u-u_h\| \|z-z_h\| \le \eta^{\mathrm{pri}}\eta^{\mathrm{adj}}$

$$\Rightarrow \quad \Phi(u_h) - \eta^{\mathrm{pri}}\eta^{\mathrm{adj}} \le \Phi(u) \le \Phi(u_h) + \eta^{\mathrm{pri}}\eta^{\mathrm{adj}}$$

[Bangerth, Rannacher, 2003]

Adaptive algorithm

1. Initialize: Construct the initial mesh $\mathcal{T}_h$.
2. Solve: Find u_h on $\mathcal{T}_h$.
3. Error indicator: Compute η_K for all $K \in \mathcal{T}_h$.
4. Error estimator: E.g. $\eta^2 = \sum_{K \in \mathcal{T}_h} \eta_K^2$.
5. Stopping criterion: If $\quad \eta \leq \text{TOL} \quad \Rightarrow \quad$ STOP.
6. Mark: If $\quad \eta_K \geq \Theta \max_{K \in \mathcal{T}_h} \eta_K \quad \Rightarrow \quad$ mark K. $\qquad 0 < \Theta < 1$
7. Refine: Refine marked elements and build the new mesh $\mathcal{T}_h$.
8. Go to 2.

Summary

- Introduction – reference solution
- Good error indicators
  - Explicit residual estimators
  - Postprocessing
- Lower bounds
  - Hierarchic
  - Implicit residual – Dirichlet
- Upper bounds
  - Implicit residual – Neumann
  - Complementary
- Quantity of interest
- Adaptive algorithm

Recommended books

- I. Babuška, J.R. Whiteman, T. Strouboulis, Finite elements: an introduction to the method and error estimation, Oxford University Press, Oxford, 2011.
- M. Ainsworth, J.T. Oden, A posteriori error estimation in finite element analysis, Wiley, New York, 2000.
- I. Babuška, T. Strouboulis, The finite element method and its reliability, Clarendon Press, Oxford University Press, New York, 2001.
- P. Neittaanmäki, S. Repin, Reliable methods for computer simulation, error control and a posteriori estimates, Elsevier, Amsterdam, 2004.
- S. Repin, A posteriori estimates for partial differential equations, de Gruyter, Berlin, 2008.
- R. Verfürth, A review of a posteriori error estimation and adaptive mesh-refinement techniques., Wiley-Teubner, Chichester/Stuttgart, 1996.

Thank you for your attention

Part I – Overview

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April 17, 2012, Technical University of Ostrava