A Posteriori Error Estimation

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• Issues to be addressed:
  • reliability of computer simulations
  • self-adaptive numerical method

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Applied Mathematics

• **Mathematical Modeling**

\[ \begin{align*}
-\nabla \cdot (\alpha(x) \nabla u) &= f & \text{in } \Omega \subset \mathbb{R}^d \\
u &= g & \text{on } \Gamma_D \\
\mathbf{n} \cdot (\alpha(x) \nabla u) &= h & \text{on } \Gamma_N
\end{align*} \]

• **Theory of PDEs**

• **Numerical PDEs**

  • discretization \(\Rightarrow\) system of algebraic equations
  
  • fast algebraic solver
  
  • a posteriori error estimation
    
    – reliability of computer simulations
    
    – self-adaptive numerical method
Figure 6.1. The first column displays the final mesh and the second column is the numerical solutions on the final mesh. The first row is the result of (4.3.27) with $i = 1$. The second row corresponds to $i = 2$ and the third row to $i = 3$. 
Numerical PDEs

- **continuous problem**

\[ \mathcal{L} u = f \quad \text{in} \; \Omega \]

- **discrete problem**

\[ \mathcal{L}_h u_h = f_h \]

- **reliability of computer simulations**

Given a tolerance \( \epsilon \)

\[ \| u - \tilde{u}_h \| \leq \epsilon \]
A Posteriori Error Estimation

- **a posteriori error estimation**
  
  compute a quantity \( \eta(\tilde{u}_h) \), estimator, such that

  \[
  \| u - \tilde{u}_h \| \leq \eta(\tilde{u}_h) \quad \text{(reliability bound)}
  \]

- **reliability of computer simulation**
  
  Given a tolerance \( \epsilon \)

  \[
  \eta(\tilde{u}_h) \leq \epsilon \quad \implies \quad \| u - \tilde{u}_h \| \leq \epsilon
  \]
A Posteriori Error Estimation

assume that the current simulation $\tilde{u}_h$ is not good enough

- **self-adaptive numerical method**
  - adaptive **global** mesh or degree refinement
  - adaptive **local** mesh or degree refinement:
    - compute quantities $\eta_K(\tilde{u}_h)$, indicators, for all $K \in \mathcal{T}$ such that
    \[
    \eta_K \leq C_e \|u - \tilde{u}_h\|_{\omega_K} \quad \text{(efficiency bound)}
    \]
Construction of Error Estimators

• a difficult task

\[ e = u - \tilde{u}_h =? \]

\[ \|e\| = \left( \sum_{K \in T} \|e\|_K^2 \right)^{1/2} =? \]

impossible

\[ \|e\| = \left( \sum_{K \in T} \|e\|_K^2 \right)^{1/2} =? \]

doable

• possible avenues

(books by Babuška-Strouboulis (01) and by Verfürth (13))

• residual estimator

\[ r = \mathcal{L}e = \mathcal{L}(u - \tilde{u}_h) = f - \mathcal{L}\tilde{u}_h \]

• estimators of recovery type
A Posteriori Error Estimators of Recovery Type

- **Zienkiewicz-Zhu estimator** (87, cited by 2400)

\[
\min_{\rho \in P_1^d \subset C^0(\Omega)^d} \| \rho - \nabla \tilde{u}_h \|
\]

- **improved ZZ estimator** (Cai-Zhang 09, 16)

\[
\min_{\tau \in RT_0 \subset H(\text{div};\Omega)} \| \alpha^{-1/2} (\tau - \tilde{\sigma}_h) \| \quad \text{with} \quad \tilde{\sigma}_h = -\alpha \nabla \tilde{u}_h
\]

- **duality estimator** (Cai-Zhang 12, ...)

\[
\min_{\tau \in RT_{p-1} \cap \{\nabla \cdot \tau = f\}} \| \alpha^{-1/2} (\tau - \tilde{\sigma}_h) \|
\]
3443 nodes mesh generated by $\eta_{ZZ}$
3557 nodes mesh generated by $\xi_{RT}$ with $\alpha = 0.1$
Estimators through Duality

**early work**


- Ladevèze-Leguillon (83), Demkowicz and Swierczek (85), Oden, Demkowicz, Rachowicz, and Westermann (89)

**recent work**

- Vejchodsky (04)

- Braess-Schöberl (08), ...

- Cai-Zhang (12), with Cao, Falgout, He, Starke, ...
Estimators through Duality

- **minimization problem:**
  \[ J(u) = \min_{v \in H^1_D(\Omega)} J(v) \]
  where \( J(v) \) is the energy functional

- **dual problem:**
  \[ J^*(\sigma) = \max_{\tau \in \Sigma_N(f)} J^*(\tau) \]
  where \( J^*(\tau) \) is the complimentary functional and

- **duality theory:**  (Ekeland-Temam 76)
  \[ J(u) = J^*(\sigma) \quad \text{and} \quad \sigma = -A\nabla u \]
duality gap

\[ \text{the error:} \]
\[ = J(u_h) - J(u) \]
\[ = J(u_h) - J^*(\vec{\sigma}) \]
\[ \leq J(u_h) - J^*(\vec{\sigma_h}) \]
A Posteriori Error Estimator through Duality
(Cai-Zhang 12, SINUM)

the current simulation $\tilde{u}_h$
explicitly calculating an equilibrated flux $\sigma_{CZ}$ such that

$$\|A^{1/2}\nabla(u - \tilde{u}_h)\| \leq \eta(\sigma_{CZ})$$

and

$$\eta_K(\sigma_{CZ}) \leq C_e \|A^{1/2}\nabla(u - \tilde{u}_h)\|_{\omega_K}$$
Duality Error Estimator
(Cai-Zhang 12, SINUM)

Figure 1: mesh generated by $\eta_{CZ}$

Figure 2: error and estimator $\eta_{CZ}$
Grand Computational Challenges

- complex systems
  multi-scales, multi-physics, etc.
- computational difficulties (no a priori knowledge)
  - oscillations
  - interior/boundary layers
  - interface singularities
  - nonlinearity
  - ???
- a general and viable approach
  adaptive method + accurate, robust error estimation
Adaptive Control of Numerical Algorithms

“If error is corrected whenever it is recognized as such, the path to error is the path of truth”

by Hans Reichenbach, the renowned philosopher of science, in his 1951 treatise, The Rise of Scientific Philosophy