A Posteriori Error Estimation Techniques for Finite Element Methods

Zhiqiang Cai
Purdue University

- **Books**
  - Ainsworth & Oden, *A posteriori error estimation in finite element analysis*, John Wiley & Sons, Inc., 2000.
  - Babŭska & Strouboulis, *Finite element method and its reliability*, Oxford Science Publication, New York, 2001.
  - Demkowicz, *Computing with hp-adaptive finite elements*, Chapman & Hall/CRC, New York, 2007.
  - Verfürth, *A review of a posteriori error estimation and adaptive mesh refinement techniques*, John Wiley, 1996.
  - Verfürth, *A posteriori error estimation techniques for finite element methods*, Oxford University Press, 2013.
- **Oberwolfach Workshop** September 4-9, 2016

Self-adaptive numerical methods for comput. challenging problems

Outline

- Introduction
- Explicit Residual Estimators
- Zienkiewicz-Zhu (ZZ) Estimators
- Estimators through Duality
- Estimators through Least-Squares Principle

Acknowledgement

This work is supported in part by the National Science Foundation and by Lawrence Livermore National Laboratory.

Motivations of A Posteriori Error Estimation

- **Error Control or Solution Verification**

- **Adaptive Control of Numerical Algorithms**

Error Control in Numerical PDEs

- **continuous problem**

$\mathcal{L}\, u = f \quad \text{in } \Omega$ find $u \in V$ s.t. $a(u, v) = f(v) \quad \forall\, v \in V$

- **discrete problem**

$\mathcal{L}_{\mathcal{T}}\, u_{\mathcal{T}} = f_{\mathcal{T}}$ find $u_{\mathcal{T}} \in V_{\mathcal{T}}$ s.t. $a(u_{\mathcal{T}}, v) = f(v) \quad \forall\, v \in V_{\mathcal{T}}$

- **error control or solution verification** Given a tolerance ϵ

$$\|u - u_{\mathcal{T}}\| \le \epsilon$$

A Priori Error Estimation

- **a priori error estimation (convergence)**

$$\|u - u_{\mathcal{T}}\| \le C(u)\, h_{\mathcal{T}}^{\alpha} \to 0 \qquad \text{as } h_{\mathcal{T}} \to 0$$

- **error control** Given a tolerance ϵ

$$C(u)\, h_{\mathcal{T}}^{\alpha} \le \epsilon \quad \Longrightarrow \quad h_{\mathcal{T}} \le \left(\frac{\epsilon}{C(u)}\right)^{1/\alpha} \quad \Longrightarrow \quad \|u - u_{\mathcal{T}}\| \le \epsilon$$

- **how to get the a priori error estimation?**

discrete stability $+$ **consistency (smoothness)**

$\Longrightarrow$ **convergence**

A Posteriori Error Estimation

- **a posteriori error estimation**

compute a quantity $\eta(u_{\mathcal{T}})$, estimator, such that

$$\|u - u_{\mathcal{T}}\| \le C_r \, \eta(u_{\mathcal{T}}) \qquad \text{(reliability bound)}$$

where C_r is a constant independent of the solution

- **error control** Given a tolerance ϵ

$$\text{for known } C_r, \quad \eta(u_{\mathcal{T}}) \le \epsilon / C_r \quad \Longrightarrow \quad \|u - u_{\mathcal{T}}\| \le \epsilon$$

- **how to get the reliability bound?**

stability

Adaptive Control of Numerical Algorithms

If the current approximation $u_{\mathcal{T}}$ is not good enough

- **adaptive global mesh or degree refinement**

- **adaptive local mesh or degree refinement**

compute quantities $\eta_K(u_{\mathcal{T}})$, indicators, for all $K \in \mathcal{T}$ such that

$$\eta_K \leq C_e \, \| u - u_{\mathcal{T}} \|_{\omega_K} \qquad \text{(efficiency bound)}$$

Adaptive Mesh Refinement (AMR) Algorithm

- **AMR algorithm**

Given the data of the underlying PDEs and a tolerance ϵ, compute a numerical soltuion with an error less than ϵ.

(1) Construct an initial coarse mesh $\mathcal{T}_0$ representing sufficiently well the geometry and the data of the problem. Set $k = 0$.

(2) Solve the discrete problem on $\mathcal{T}_k$.

(3) For each element $K \in \mathcal{T}_k$,

compute an error indicator η_K.

(4) If the global estimate η is less than ϵ, then stop.

Otherwise, locally refine the mesh $\mathcal{T}_k$ to construct the next mesh $\mathcal{T}_{k+1}$. Replace k by $k + 1$ and return to Step (2).

Adaptive Mesh Refinement (AMR) Algorithm

- **AMR algorithm**

Solve $\to$ Estimate $\to$ Mark $\to$ Refine

A Posteriori Error Estimation

- **computation of the a posteriori error estimation**
  - **indicator** η_K – a computable quantity for each $K \in \mathcal{T}$
  - **estimator** $\eta = \left(\sum_{K\in\mathcal{T}} \eta_K^2\right)^{1/2}$
- **theory of the a posteriori error estimation**
  - **reliability bound for error control**

$$\|u - u_{\mathcal{T}}\| \le C_r \eta$$

  - **efficiency bound for efficiency of AMR algorithms**

$$\eta_K \le C_e \|u - u_{\mathcal{T}}\|_{\omega_K} \quad \forall\, K \in \mathcal{T}$$

Construction of Error Estimators

- **a difficult task**

$$u = ? \quad \Rightarrow \quad \begin{cases} e = u - u_{\mathcal{T}} = ? & \text{impossible} \\ \|e\| = \left(\sum_{K \in \mathcal{T}} \|e\|_K^2 \right)^{1/2} = ? & \text{doable} \end{cases}$$

- **possible avenues**

  - **residual estimator**

$$r = \mathcal{L}e = \mathcal{L}(u - u_{\mathcal{T}}) = f - \mathcal{L}u_{\mathcal{T}}$$

  - **Zienkiewicz-Zhu (ZZ) estimator**

$$\|\boldsymbol{\rho}_{\mathcal{T}} - \nabla u_{\mathcal{T}}\|$$

  - **duality estimator**

$$\|\alpha^{-1/2}(\boldsymbol{\sigma}_{\mathcal{T}} + \alpha \nabla u_{\mathcal{T}})\| \quad \text{with} \quad \nabla \cdot \boldsymbol{\sigma}_{\mathcal{T}} = f$$

Interface Problems

- **elliptic interface problems**

$$\begin{cases} -\nabla \cdot (\alpha(x)\nabla u) = f \quad \text{in } \Omega \subset \mathcal{R}^d \\ u = g \quad \text{on } \Gamma_D \quad \text{and} \quad \mathbf{n} \cdot (\alpha(x)\nabla u) = h \quad \text{on } \Gamma_N \end{cases}$$

where $\alpha(x)$ is positive piecewise constant w.r.t $\bar{\Omega} = \cup_{i=1}^n \bar{\Omega}_i$:

$$\alpha(x) = \alpha_i > 0 \quad \text{in } \Omega_i$$

- **smoothness**

$$u \in H^{1+\beta}(\Omega)$$

where $\beta > 0$ could be very small.

A Test Problem with Intersecting Interfaces

- **the Kellogg test problem**

$$\Omega = (-1,\,1)^2, \quad \Gamma_D = \partial\Omega, \quad f = 0$$

$$\text{and} \quad \alpha(x) = \begin{cases} 161.448 & \text{in } (0,1)^2 \cup (-1,0)^2 \\ 1 & \text{in } \Omega \setminus ([0,1]^2 \cup [-1,0]^2) \end{cases}$$

- **exact solution**

$$u(r,\theta) = r^{0.1}\mu(\theta) \in H^{1.1-\epsilon}(\Omega)$$

with $\mu(\theta)$ being smooth

Explicit Residual Estimator

- **conforming finite element approximation**

  find $u_{\mathcal{T}} \in V_{\mathcal{T}} \subset V = H^1_D(\Omega)$ such that

$$a(u_{\mathcal{T}}, v) = f(v) \quad \forall\, v \in V_{\mathcal{T}}$$

- **residual functional**

$$\begin{aligned} r(v) &= f(v) - a(u_{\mathcal{T}},\, v) = a(u - u_{\mathcal{T}}, v) \qquad\qquad \forall\, v \in V \\ &= a(u - u_{\mathcal{T}}, v - v_I) = \sum_{K \in \mathcal{T}} \int_K \alpha \nabla (u - u_{\mathcal{T}}) \cdot \nabla (v - v_I)\, dx \\ &= \sum_{K \in \mathcal{T}} \int_K (f + \mathrm{div}\,(\alpha \nabla u_{\mathcal{T}}))(v - v_I)\, dx + \sum_{e \in \mathcal{E}} \int_e [\![\mathbf{n}_e \cdot (\alpha \nabla u_{\mathcal{T}})]\!]_e (v - v_I)\, ds \end{aligned}$$

Explicit Residual Estimator

- L^2 **representation of the residual functional**

$$r(v) \;=\; \sum_{K\in\mathcal{T}}\int_K (f + \mathrm{div}\,(\alpha\nabla u_{\mathcal{T}}))(v - v_I)\,dx + \sum_{e\in\mathcal{E}}\int_e [\![\mathbf{n}_e \cdot (\alpha\nabla u_{\mathcal{T}})]\!]_e (v - v_I)\,ds$$

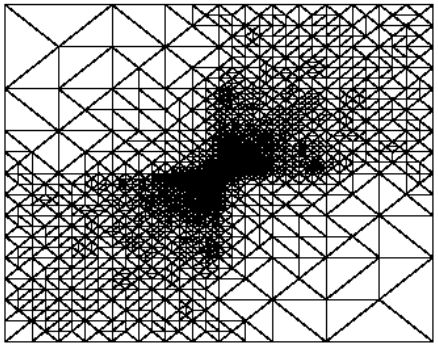
- **global reliability bound**

$$\|u - u_{\mathcal{T}}\| \le C \sup_{0\ne v\in(V,\|\cdot\|)} \frac{|r(v)|}{\|v\|} \le C\left(\sum_{K\in\mathcal{T}} \eta_K^2\right)^{1/2}$$

- **examples of the explicit residual indicator**
  - Babuska & Rheinboldt 79 (1D), Babuska & Miller 87 (2D)

$$\eta_K^2 \;=\; h_K^2\|f + \mathrm{div}\,(\alpha\nabla u_{\mathcal{T}})\|_K^2 + \frac{1}{2}\sum_{e\in\partial K} h_e \|[\![\mathbf{n}_e\cdot(\alpha\nabla u_{\mathcal{T}})]\!]\|_e^2$$

interface test problem



exact solution

$$u(r,\theta) = r^{0.1}\mu(\theta) \in H^{1.1-\epsilon}(\Omega)$$

Explicit Residual Estimator

- **global reliability bound**

$$\|u - u_{\mathcal{T}}\| \le C \sup_{0 \ne v \in (V, \|\cdot\|)} \frac{|r(v)|}{\|v\|} \le C \left(\sum_{K \in \mathcal{T}} \eta_K^2 \right)^{1/2}$$

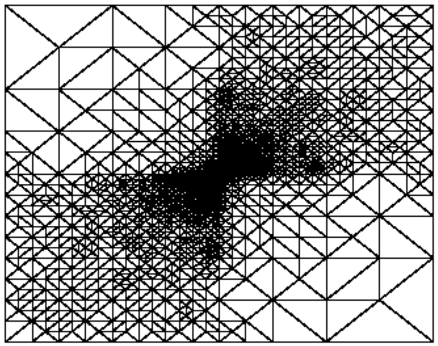
- **examples of the explicit residual indicator**

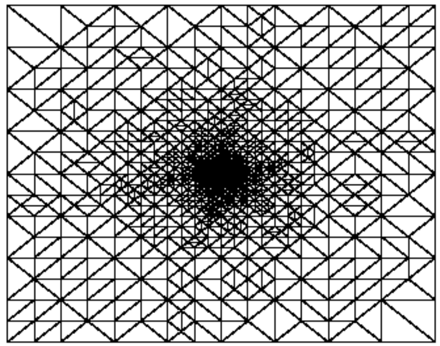
  - Babuska & Rheinboldt 79 (1D), Babuska & Miller 87 (2D)

$$\eta_K^2 \quad = \quad h_K^2 \|f + \mathrm{div}\,(\alpha \nabla u_{\mathcal{T}})\|_K^2 + \frac{1}{2} \sum_{e \in \partial K} h_e \|[\![\mathbf{n}_e \cdot (\alpha \nabla u_{\mathcal{T}})]\!]\|_e^2$$

  - Bernardi & Verfürth 2000, Petzoldt 2002

$$\eta_K^2 = h_K^2 \|\alpha^{-\frac{1}{2}} (f + \mathrm{div}\,(\alpha \nabla u_{\mathcal{T}}))\|_K^2 + \frac{1}{2} \sum_{e \in \partial K} h_e \|\alpha_e^{-\frac{1}{2}} [\![\mathbf{n}_e \cdot (\alpha \nabla u_{\mathcal{T}})]\!]\|_e^2$$





meshes generated by BM and BV indicators

Robust Efficiency and Reliability Bounds

(Bernardi & Verfürth 2000, Petzoldt 2002)

- **robust efficiency bound**

$$\eta_K \leq C \,\|\alpha^{1/2}\nabla(u-u_{\mathcal{T}})\|_{0,\omega_K}$$

where C is independent of the jump of α

- **Quasi-Monotonicity Assumption (QMA):**

any two different subdomains $\bar{\Omega}_i$ and $\bar{\Omega}_j$, which share at least one point, have a connected path passing from $\bar{\Omega}_i$ to $\bar{\Omega}_j$ through adjacent subdomains such that the diffusion coefficient $\alpha(x)$ is monotone along this path.

- **robust reliability bound** under the QMA, there exists a constant C independent of the jump of α such that

$$\|\alpha^{1/2}\nabla(u-u_{\mathcal{T}})\|_{0,\Omega} \leq C\,\eta$$

Robust Estimator for Nonconforming Elements without QMA in both Two and Three Dimensions

(C.-He-Zhang, Math Comp 2017 and SINUM 2017)

for nonconforming linear elements, let $e = u - u_{\mathcal{T}}$ and let

$$\eta_{r,K} = \frac{h_K}{\sqrt{\alpha_K}}\|f_0\|_{0,K}, \qquad \eta_{j,n,F} = \sqrt{\frac{h_F}{\alpha_{F,A}}}\,\|j_{n,F}\|_{0,F},$$

and $$\eta_{j,u,F} = \sqrt{\frac{\alpha_{F,H}}{h_F}}\,\|[\![u_h]\!]\|_{0,F} \quad \text{with} \quad j_{n,F} = [\![\alpha\nabla_h u_h \cdot \mathbf{n}]\!]_F$$

- **indicator and estimator**

$$\eta^2 = \sum_{K\in\mathcal{T}} \eta_K^2 \quad \text{with} \quad \eta_K^2 = \eta_{r,K}^2 + \frac{1}{2}\sum_{F\in\mathcal{E}}\left(\eta_{j,n,F}^2 + \eta_{j,u,F}^2\right)$$

- **L^2 representation of the error in the energy norm**

$$\|\alpha^{1/2}\nabla_h e\|^2 = \sum_{K\in\mathcal{T}}(f, e - e_I)_K - \sum_{F\in\mathcal{E}_I}\int_F j_{n,F}\{e - e_I\}^w ds - \sum_{F\in\mathcal{E}}\int_F \{\alpha\nabla e\cdot\mathbf{n}\}_w[\![u_{\mathcal{T}}]\!]ds$$

Robust Estimator for Discontinunous Elements without QMA in both Two and Three Dimensions

(C.-He-Zhang, SINUM 2017)

for discontinuous elements, let $e = u - u_{\mathcal{T}}$ and let

$$\eta_{r,K} = \frac{h_K}{\sqrt{\alpha_K}} \|f_{k-1} + \nabla \cdot (\alpha \nabla u_{\mathcal{T}})\|_{0,K},$$

- **indicator and estimator**

$$\eta^2 = \sum_{K \in \mathcal{T}} \eta_K^2 \quad \text{with} \quad \eta_K^2 = \eta_{r,K}^2 + \frac{1}{2} \sum_{F \in \mathcal{E}} \left(\eta_{j,n,F}^2 + \eta_{j,u,F}^2\right)$$

- **L^2 representation of the error in the energy norm**

$$\|\alpha^{1/2} \nabla_h e\|^2 = \sum_{K \in \mathcal{T}} (f_{k-1} + \nabla \cdot (\alpha \nabla u_{\mathcal{T}}), e - \bar{e}_K)_K - \sum_{F \in \mathcal{E}_I} \int_F j_{n,F} \{e - \bar{e}_K\}^w ds$$
$$- \sum_{F \in \mathcal{E}} \int_F \{\alpha \nabla e \cdot \mathbf{n}\}_w [\![u_{\mathcal{T}}]\!] ds - \sum_{F \in \mathcal{E}} \int_F \gamma \frac{\alpha_{F,H}}{h_F} [\![u_{\mathcal{T}}]\!] [\![\bar{e}_K]\!] ds$$

Zienkiewicz-Zhu (ZZ) Error Estimators

- **ZZ estimators**

$$\xi_G = \|\boldsymbol{\rho}_{\mathcal{T}} - \nabla u_{\mathcal{T}}\|$$

where $\boldsymbol{\rho}_{\mathcal{T}} \in U_{\mathcal{T}} \subset C^0(\Omega)^d$ is a recovered gradient

- **recovery operators**

  - **Zienkiewicz & Zhu estimator** (87, cited 2600 times)

$$\boldsymbol{\rho}_{\mathcal{T}}(z) = \frac{1}{|\omega_z|} \int_{\omega_z} \nabla u_{\mathcal{T}} \, dx \quad \forall\, z \in \mathcal{N}$$

  - L^2-**projection** find $\boldsymbol{\rho}_{\mathcal{T}} \in U^h$ such that

$$\|\boldsymbol{\rho}_{\mathcal{T}} - \nabla u_{\mathcal{T}}\| = \min_{\boldsymbol{\gamma} \in U_{\mathcal{T}}} \|\boldsymbol{\gamma} - \nabla u_{\mathcal{T}}\|$$

  - **other recovery techniques**
    Bank-Xu, Carstensen, Schatz-Wahlbin, Z. Zhang, ...

Zienkiewicz-Zhu (ZZ) Error Estimators

- **recovery-based estimators**

$$\xi_{zz} = \|\boldsymbol{\rho}_{\mathcal{T}} - \nabla\, u_{\mathcal{T}}\|$$

- **theory**

  - saturation assumption: there exists a constant $\beta \in [0, 1)$ s.t.

$$\|\nabla\, u - \boldsymbol{\rho}_{\mathcal{T}})\| \le \beta \|\nabla u - \nabla\, u_{\mathcal{T}}\| \Longrightarrow 1 - \beta \le \frac{\xi_{zz}}{\|\boldsymbol{\rho}_{\mathcal{T}} - \nabla\, u\|} \le 1 + \beta$$

  - efficiency and reliability bounds

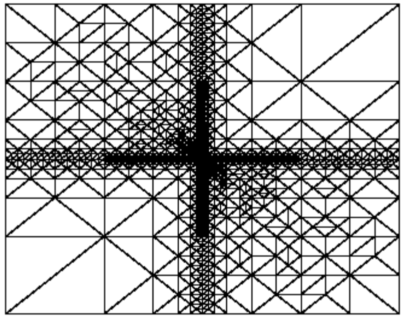
    Carstensen, Zhou, etc.

Zienkiewicz-Zhu (ZZ) Error Estimators

- **Pro and Con**

  + simple
    universal
    asymptotically exact

  – inefficiency for nonsmooth problems
    unreliable on coarse meshes
    higher-order finite elements, complex systems, etc.



3443 nodes mesh generated by η_{ZZ}

Why Does It Fail?

- **true gradient and flux** for interface problems

$$\nabla u \notin C^0(\Omega)^d$$

- **recovery space**

$$\boldsymbol{\rho}_{\mathcal{T}} \in C^0(\Omega)^d$$

- **the reason of the failure**

approximating discontinuous functions by continuous functions

How to Fix It?

(C.-Zhang, SINUM (09, 10, 11), C.-He-Zhang, CMAME 17)

- **true gradient and flux**

$$u \in H^1(\Omega) \quad \Longrightarrow \quad \nabla u \in H(\mathrm{curl}, \Omega)$$

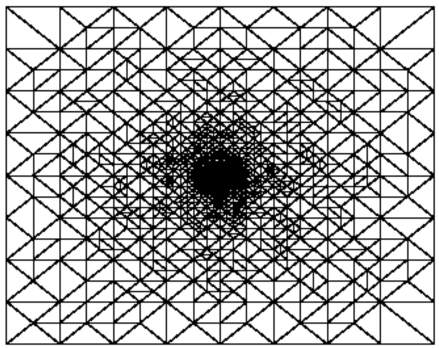
$$\boldsymbol{\sigma} = -\alpha \nabla u \in H(\mathrm{div}, \Omega)$$

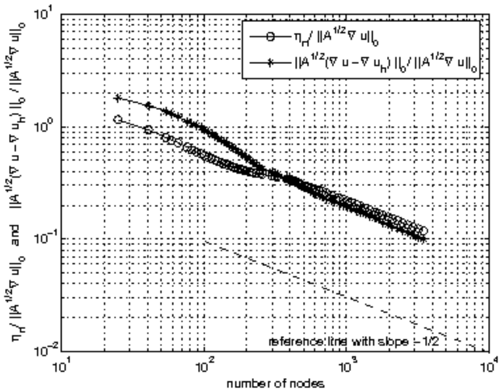
- **conforming elements**

$$\left.\begin{aligned} u_{\mathcal{T}} \in H^1(\Omega) \Longrightarrow \nabla u_{\mathcal{T}} \in H(\mathrm{curl}, \Omega) \\ \tilde{\boldsymbol{\sigma}}_{\mathcal{T}} = -\alpha \nabla u_{\mathcal{T}} \notin H(\mathrm{div}, \Omega) \end{aligned}\right\} \quad \Longrightarrow \quad \hat{\boldsymbol{\sigma}}_{\mathcal{T}} \in RT_0 \text{ or } BDM_1$$

- **mixed elements** gradient $\nabla u = -\alpha^{-1} \boldsymbol{\sigma} \in H(\mathrm{div}, \Omega)$

$$\left.\begin{aligned} u_{\mathcal{T}} \in L^2(\Omega), \boldsymbol{\sigma}_{\mathcal{T}} \in H(\mathrm{div}, \Omega) \\ \tilde{\boldsymbol{\rho}}_{\mathcal{T}} = -\alpha^{-1} \boldsymbol{\sigma}_{\mathcal{T}} \notin H(\mathrm{curl}, \Omega) \end{aligned}\right\} \quad \Longrightarrow \quad \hat{\boldsymbol{\rho}}_{\mathcal{T}} \in \mathbb{D}_1 \text{ or } \mathbb{N}_1$$





3557 nodes mesh generated by ξ_{RT} with $\alpha = 0.1$

Summary of Improved ZZ Error Estimators

- **Pro and Con**

  + simple
    universal
    asymptotically exact

  – inefficiency for nonsmooth problems
    unreliable on coarse meshes
    higher-order finite elements, complex systems, etc.

Estimators through Duality

- **early work**
  - Hlaváček, Haslinger, Nećas, and Lovišek,
    Solution of Vatiational Inequality in Mechanics,
    Springer-Verlag, New York, 1989. (Translation of 1982 book.)
  - Ladevéze-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

(Equilibrated Residual Error Estimator)

(Ladevéze-Leguillon 83, Vejchodsky 04, Braess-Schöberl 08)

- **Prager-Synge identity** for $u,\ u_{\mathcal{T}} \in H^1_D(\Omega)$

$$\|A^{1/2}\nabla(u_{\mathcal{T}} - u)\|^2 + \|A^{1/2}(\nabla u + A^{-1}\boldsymbol{\tau})\|^2 = \|A^{1/2}(\nabla u_{\mathcal{T}} + A^{-1}\boldsymbol{\tau})\|^2$$

for all $\boldsymbol{\tau} \in \Sigma_N(f) \equiv \{\boldsymbol{\tau} \in H_N(\text{div};\,\Omega) \,\big|\, \nabla\cdot\boldsymbol{\tau} = f\}$

$$(\nabla(u_{\mathcal{T}} - u),\ A\nabla u + \boldsymbol{\tau})) = -(u_{\mathcal{T}} - u,\ \nabla\cdot(A\nabla u) + \nabla\cdot\boldsymbol{\tau})) = 0$$

- **guaranteed reliable estimator** $\tilde{\boldsymbol{\sigma}}_{\mathcal{T}} = -A^{-1}\nabla u_{\mathcal{T}}$

$$\|A^{1/2}\nabla(u - u_{\mathcal{T}})\| \le \eta(\boldsymbol{\tau}) \equiv \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\| \quad \forall\ \boldsymbol{\tau} \in \Sigma_N(f)$$

Equilibrated Residual Error Estimator

- **explicit/local calculation of numerical flux** Assume that f is piecewise polynomial of degree $p-1$ w.r.t. $\mathcal{T}$
  - explicit calculation of numerical flux for linear element (Braess-Schöberl 08)

$$\hat{\boldsymbol{\sigma}}_{BS} \in \Sigma_N(f) \cap RT_0$$

  - solving a vertex patch mixed problem for p-th order element (Braess-Pillwein-Schöberl 09)

$$\hat{\boldsymbol{\sigma}}_{BPS} \in \Sigma_N(f) \cap RT_{p-1}$$

- **p-robust efficiency**

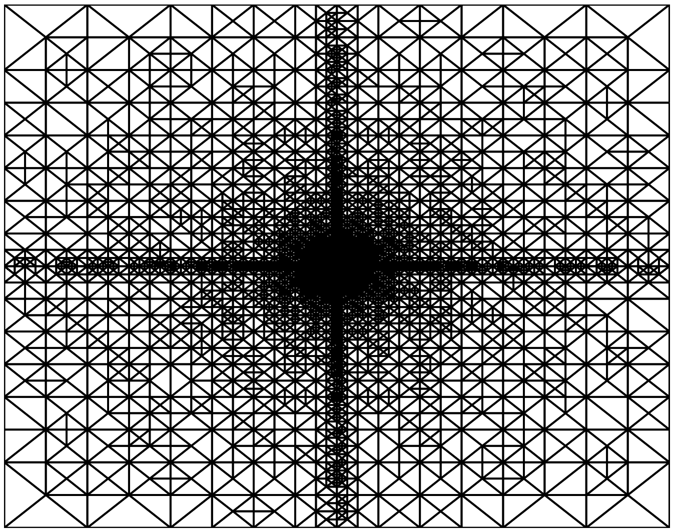
$$\eta_K(\hat{\boldsymbol{\sigma}}_{BPS}) \le C_e \, \|A^{1/2}\nabla(u - u_{\mathcal{T}})\|_{\omega_K}$$

where $C_e > 0$ is a constant independent of p

• Non-robustness on constant-free estimator

for singular-perturbed reaction- or convection-diffusion problems (Verfürth 09, SINUM)

for interface problems (C.-Zhang, SINUM 2012)



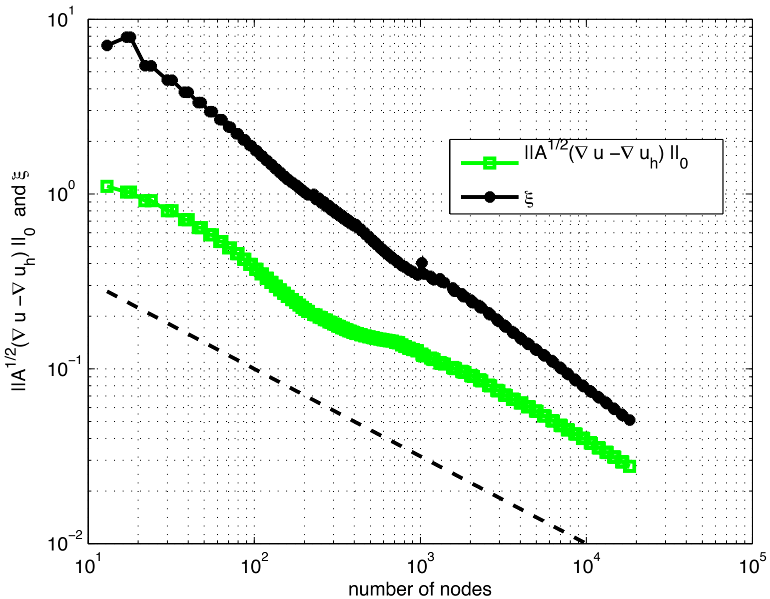


Figure 1: mesh generated by η_{BS} Figure 2: error and estimator η_{BS}

Robust Equilibrated Residual Error Estimator

- **Prager-Synge identity** for all $\boldsymbol{\tau} \in \Sigma_N(f)$

$$\|A^{1/2}\nabla(u - u_{\mathcal{T}})\|^2 + \|A^{1/2}(\nabla u + A^{-1}\boldsymbol{\tau})\|^2 = \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_h)\|^2$$

- **guaranteed reliable estimator**

$$\begin{aligned}\|A^{1/2}\nabla(u - u_{\mathcal{T}})\| &\le \eta(\boldsymbol{\tau}) \equiv \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\| \quad \forall\, \boldsymbol{\tau} \in \Sigma_N(f)\\ &\le \inf_{\boldsymbol{\tau} \in \Sigma_N(f)} \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|\end{aligned}$$

- **discrete equilibrated flux**

$$\|A^{-1/2}(\hat{\boldsymbol{\sigma}}_{\mathcal{T}} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\| = \min_{\boldsymbol{\tau} \in \Sigma_N(f) \cap RT_{p-1}} \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|$$

For improved ZZ flux, the minimization is over RT_0 or BDM_1

Equilibrated Residual Error Estimator
(C.-Zhang, SINUM 2012)

- **explicit/local calculation of numerical flux** Assume that f is piecewise polynomial of degree $p-1$ w.r.t. $\mathcal{T}$

  - explicit calculation of numerical flux for linear element

$$\hat{\boldsymbol{\sigma}}_{CZ} \in \Sigma_N(f) \cap RT_0$$

  - solving a vertex patch problem for p-th order element

$$\hat{\boldsymbol{\sigma}}_{CZ} \in \Sigma_N(f) \cap RT_{p-1}$$

- **α and p-robust efficiency**

$$\eta_K(\hat{\boldsymbol{\sigma}}_{CZ}) \le C_e \, \|A^{1/2}\nabla(u-u_{\mathcal{T}})\|_{\omega_K}$$

where $C_e > 0$ is a constant independent of α and p

Equilibrated Residual Error Estimator

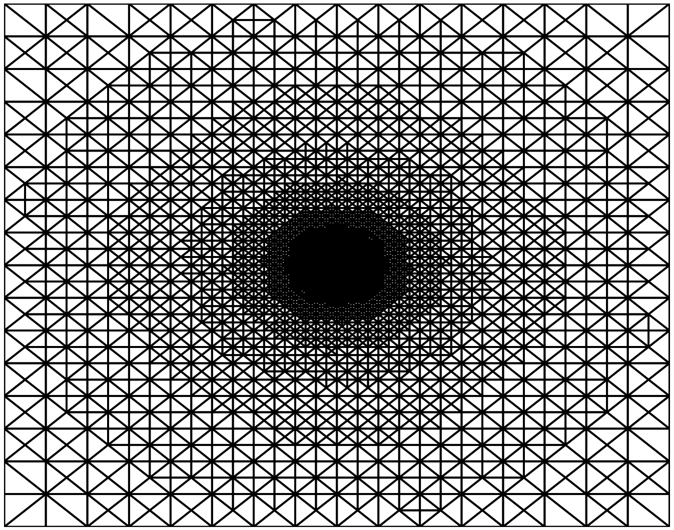


Figure 3: mesh generated by η_{CZ}

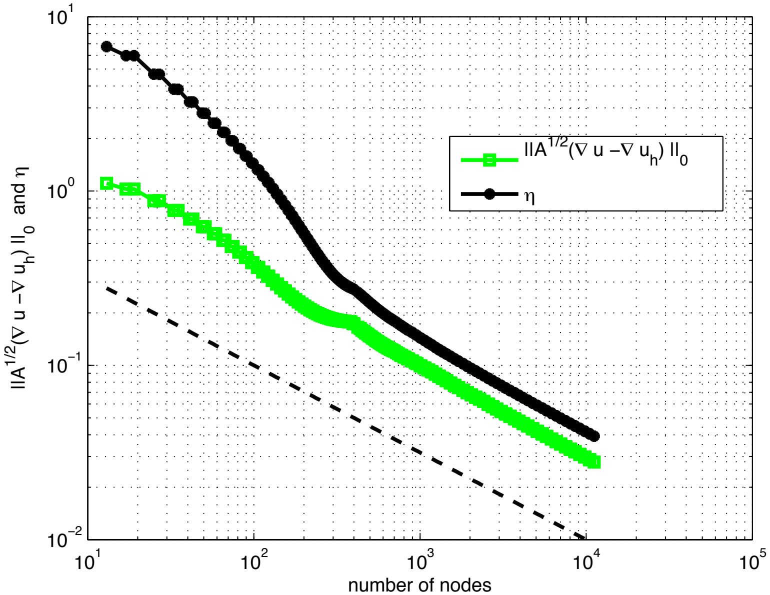


Figure 4: error and estimator η_{CZ}

Estimators through Duality

- **minimization problem:**

$$J(u) = \min_{v \in H^1_D(\Omega)} J(v)$$

where $J(v) = \frac{1}{2}\left(A\nabla v,\, \nabla v\right) - f(v)$ is the energy functional

- **dual problem:**

$$J^*(\boldsymbol{\sigma}) = \max_{\boldsymbol{\tau} \in \Sigma_N(f)} J^*(\boldsymbol{\tau})$$

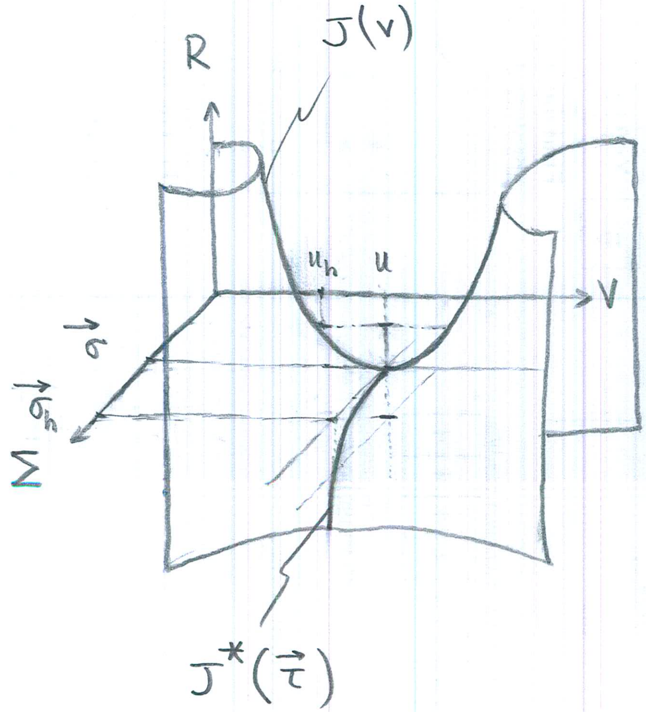
where $J^*(\boldsymbol{\tau}) = -\frac{1}{2}\left(A^{-1}\boldsymbol{\tau},\, \boldsymbol{\tau}\right)$ is the complimentary functional and

$$\Sigma_N(f) \equiv \{\boldsymbol{\tau} \in H_N(\text{div};\, \Omega) \,\big|\, \nabla \cdot \boldsymbol{\tau} = f\}$$

- **duality theory:** (Ekeland-Temam 76)

$$J(u) = J^*(\boldsymbol{\sigma}) \quad \text{and} \quad \boldsymbol{\sigma} = -A\nabla u$$

duality gap



the error

$$= J(u_h) - J(u)$$

$$= J(u_h) - J^*(\vec{\sigma})$$

$$\leq J(u_h) - J^*(\vec{\sigma}_h)$$

Summery on Estimators through Duality

- **guaranteed reliability bound**

$$\|A^{1/2}\nabla(u-u_{\mathcal{T}})\| \le \eta(\boldsymbol{\sigma}_{CZ})$$

where $\eta(\boldsymbol{\sigma}_{CZ}) = \left(J(u_{\mathcal{T}}) - J^*(\boldsymbol{\sigma}_{CZ})\right)^{1/2}$

- **robust local efficiency bound** for $A = \alpha\, I$

$$\eta_K(\boldsymbol{\sigma}_{CZ}) \le C_e\, \|\alpha^{1/2}\nabla(u-u_{\mathcal{T}})\|_{0,\omega_K}$$

Equilibrated Error Estimator for Discontinuous Elements (C.-He-Starke-Zhang)

- **continuous elements** let $u^c_{\mathcal{T}} \in H^1_D(\Omega)$ be an approximation

$$\|A^{1/2}\nabla(u - u^c_{\mathcal{T}})\| \le \inf_{\boldsymbol{\tau} \in \Sigma_N(f)} \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_h)\|$$

where $\tilde{\boldsymbol{\sigma}}_{\mathcal{T}} = -A\nabla u^c_{\mathcal{T}}$ is the numerical flux

- **discontinuous elements** let $u_{\mathcal{T}} \in H^1_D(\mathcal{T})$ be an approximation

$$\begin{aligned}
&\|A^{1/2}\nabla_h(u - u_{\mathcal{T}})\|^2 \\
\le\ & \inf_{\boldsymbol{\tau}\in\Sigma_N(f)} \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|^2 + \inf_{v\in H^1_D(\Omega)} \|A^{1/2}(\nabla v - \tilde{\boldsymbol{\rho}}_{\mathcal{T}})\|^2 \\
=\ & \inf_{\boldsymbol{\tau}\in\Sigma_N(f)} \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|^2 + \inf_{\boldsymbol{\gamma}\in \mathring{H}_D(\text{curl},\Omega)} \|A^{1/2}(\boldsymbol{\gamma} - \tilde{\boldsymbol{\rho}}_{\mathcal{T}})\|
\end{aligned}$$

where $\tilde{\boldsymbol{\sigma}}_{\mathcal{T}} = -A\nabla u_{\mathcal{T}}$ and $\tilde{\boldsymbol{\rho}}_{\mathcal{T}} = \nabla u_{\mathcal{T}}$ are the numerical flux and gradient, respectively.

Equilibrated Error Estimator for Non-conforming Elements of Odd Order

- **discontinuous elements** let $e = u - u_{\mathcal{T}}^{nc}$

$$\|A^{1/2}\nabla_h e\|^2 \le \inf_{\boldsymbol{\tau}\in\Sigma_N(f)} \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|^2 + \inf_{v\in H_D^1(\Omega)} \|A^{1/2}(\nabla v - \tilde{\boldsymbol{\rho}}_{\mathcal{T}})\|^2$$

$$= \inf_{\boldsymbol{\tau}\in\Sigma_N(f)} \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|^2 + \inf_{\boldsymbol{\gamma}\in \mathring{H}_D(\text{curl},\Omega)} \|A^{1/2}(\boldsymbol{\gamma} - \tilde{\boldsymbol{\rho}}_{\mathcal{T}})\|$$

- **explicit calculation of an equilibrated flux for odd order**

$$\hat{\boldsymbol{\sigma}}_{\mathcal{T}} \in \Sigma_N(f) \cap RT_{p-1}$$

- **explicit calculation of a gradient**

$$\hat{\boldsymbol{\rho}}_{\mathcal{T}} \in H_D(\text{curl},\Omega) \cap NE_{p-1}$$

Equilibrated Error Estimator for Non-conforming Elements of Odd Order

- **discontinuous elements** let $e = u - u_{\mathcal{T}}^{nc}$

$$\|A^{1/2}\nabla_h e\|^2 \le \inf_{\boldsymbol{\tau}\in\Sigma_N(f)} \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|^2 + \inf_{v\in H_D^1(\Omega)} \|A^{1/2}(\nabla v - \tilde{\boldsymbol{\rho}}_{\mathcal{T}})\|^2$$

$$= \inf_{\boldsymbol{\tau}\in\Sigma_N(f)} \|A^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|^2 + \inf_{\boldsymbol{\gamma}\in \mathring{H}_D(\text{curl},\Omega)} \|A^{1/2}(\boldsymbol{\gamma} - \tilde{\boldsymbol{\rho}}_{\mathcal{T}})\|$$

- **indicator and estimator**

$$\eta^2 = \sum_{K\in\mathcal{T}} \eta_K^2 \quad \text{with} \quad \eta_K^2 = \eta_{\sigma,K}^2 + \eta_{\rho,K}^2$$

where $\eta_{\sigma,K}$ and $\eta_{\rho,K}$ are given by

$$\eta_{\sigma,K} = \|A^{-1/2}(\hat{\boldsymbol{\sigma}}_{\mathcal{T}} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|_{0,K} \quad \text{and} \quad \eta_{\rho,K} = \|A^{1/2}(\hat{\boldsymbol{\rho}}_{\mathcal{T}} - \tilde{\boldsymbol{\rho}}_{\mathcal{T}})\|_{0,K}$$

Equilibrated Error Estimator for Non-conforming Elements of Odd Order

- **indicator and estimator**

$$\eta^2 = \sum_{K \in \mathcal{T}} \eta_K^2 \quad \text{with} \quad \eta_K^2 = \eta_{\sigma,K}^2 + \eta_{\rho,K}^2$$

where $\eta_{\sigma,K}$ and $\eta_{\rho,K}$ are given by

$$\eta_{\sigma,K} = \|A^{-1/2}(\hat{\boldsymbol{\sigma}}_{\mathcal{T}} - \tilde{\boldsymbol{\sigma}}_{\mathcal{T}})\|_{0,K} \quad \text{and} \quad \eta_{\rho,K} = \|A^{1/2}(\hat{\boldsymbol{\rho}}_{\mathcal{T}} - \tilde{\boldsymbol{\rho}}_{\mathcal{T}})\|_{0,K}$$

- **α-robust efficiency without QMA**

$$\eta_K \le C_e \left(\|A^{1/2}\nabla(u - u_{\mathcal{T}}^c)\|_{\omega_K} + \operatorname{osc}(f, \omega_K) \right)$$

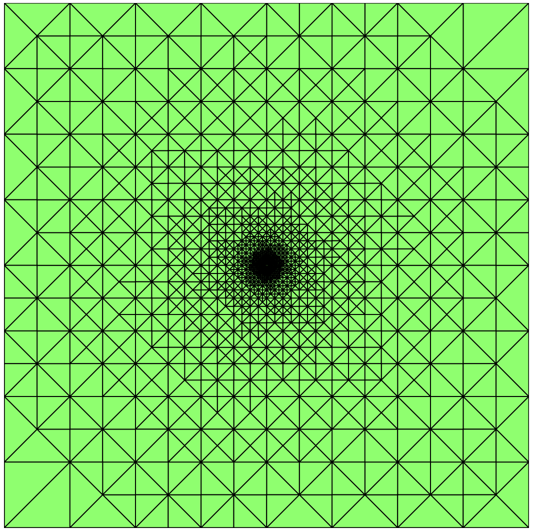
where $C_e > 0$ is a constant independent of α

- **α-robust reliability without QMA**

$$\|A^{1/2}\nabla(u - u_{\mathcal{T}}^{nc})\| \le C_r \left(\eta + \operatorname{osc}(f, \mathcal{T})\right)$$

where $C_r > 0$ is a constant independent of α

Kellogg's Problem for Crouzeix-Raviart Element conforming error $\eta_\sigma = 0$



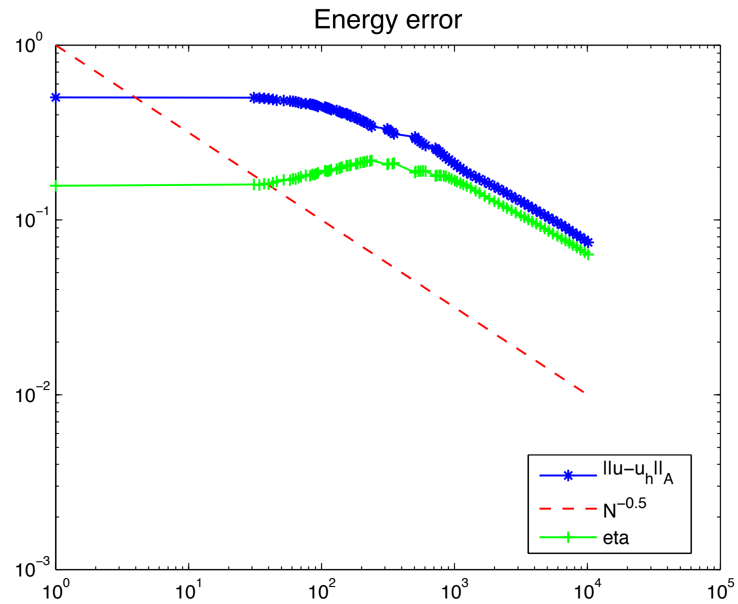
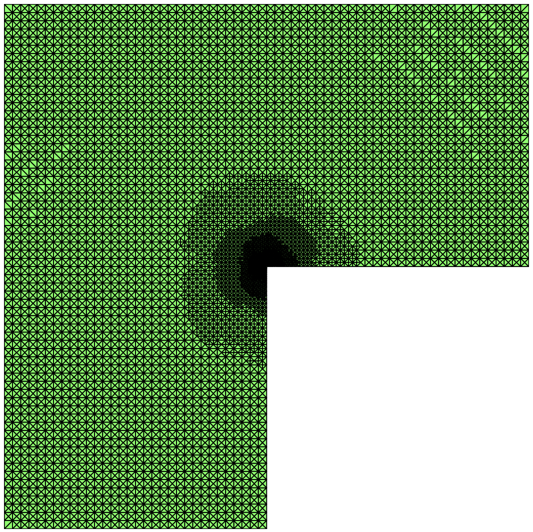


Figure 5: mesh generated by η_K

Figure 6: error and estimator η

Poisson's Equation on L-Shape Domain for Crouzeix-Raviart Element



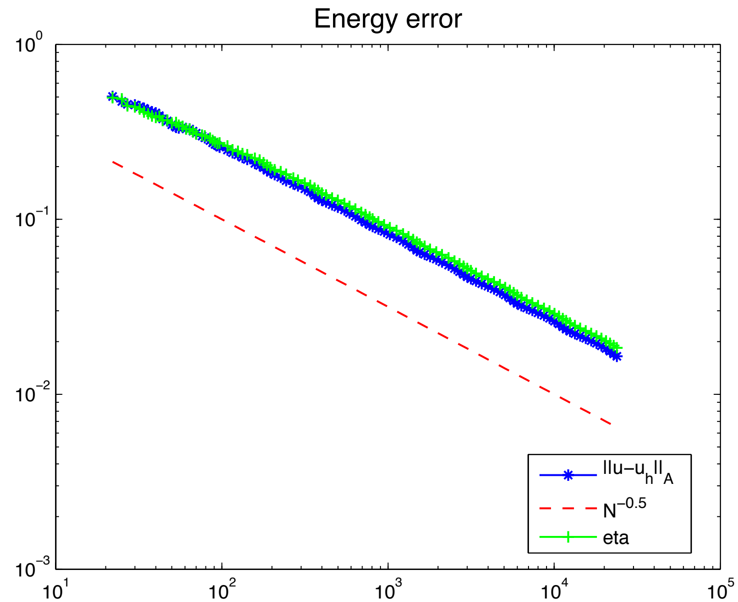


Figure 7: mesh generated by η_K

Figure 8: error and estimator η

Summary

- **estimators**
  - explicit residual: reasonable mesh, not efficient error control
  - improved ZZ: ignoring equilibrium equation
  - dual: the method of choice
- **adaptive control of meshing (AMR)**
  - some “nice” problems: many viable estimators
  - challenging problems (layers, oscillations, etc) : a few
- **error control**
  - asymptotic meshes: some smooth problems
  - non-asymptotic meshes: ???
  - challenging problems : ???

Grand Computational Challenges

- complex systems

multi-scales, multi-physics, etc.

- computational difficulties
  - 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