Accuracy Control of Simulations and Self-Adaptive Numerical Methods

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Grand Computational Challenges

- **complex systems**

  multi-scales, multi-physics, etc.

- **computational difficulties**
  - **oscillations**
  - **interior/boundary layers, discontinuities**
  - **interface singularities**
  - **...**
- **new challenges** those information are **not** *a priori* **available**

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open problems:
- accurate/guaranteed error control on pre-asymptotic meshes
- efficient *a posteriori* error indicators
- efficient design of self-adaptive numerical method

- **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
- Estimators (explicit residual, ZZ, hybrid, dual)
- Discretization-Accurate Stopping Criterion
- Efficient AMR Algorithms

Acknowledgement

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Motivations of A Posteriori Error Estimation

- **Accuracy Control or Solution Verification**
- **Adaptive Control of Numerical Algorithms**

Accuracy Control in Numerical PDEs

- **continuous problem**

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

- **discrete problem**

$$\mathcal{L}_h\, u_h = f_h \qquad\qquad \text{find } u_h \in V_h \text{ s.t. } a(u_h,v) = f(v) \quad \forall\, v \in V_h$$

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

$$|\!|\!| u - \tilde{u}_h |\!|\!| \le \epsilon$$

A Priori Error Estimation

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

$$\|u - u_h\| \le C(u)\, h^\alpha \to 0 \qquad \text{as } h \to 0$$

- **error control** Given a tolerance ϵ

$$C(u)\, h^\alpha \le \epsilon \quad \Longrightarrow \quad h \le \left(\frac{\epsilon}{C(u)}\right)^{1/\alpha} \quad \Longrightarrow \quad \|u - u_h\| \le \epsilon$$

- **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 $\eta(\tilde{u}_h)$, estimator, such that

$$\|u - \tilde{u}_h\| \le C_r\, \eta(\tilde{u}_h) \qquad \text{(reliability bound)}$$

where C_r is a constant independent of the solution

- **error control** Given a tolerance ϵ

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

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

stability

Adaptive Control of Numerical Algorithms

If the current approximation $\tilde{u}_h$ is not good enough

- **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

$$\eta_K \le C_e \, \|u - \tilde{u}_h\|_{\omega_K} \qquad \text{(efficiency bound)}$$

- **estimator**

$$\eta = \left(\sum_{K \in \mathcal{T}} \eta_K^2 \right)^{1/2}$$

Adaptive Local 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 $\rightarrow$ **Estimate** $\rightarrow$ **Mark** $\rightarrow$ **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**

$$|\!|\!| u - \tilde{u}_h |\!|\!| \le C_r \eta$$

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

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

Construction of Error Estimators

- **a difficult task**

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

- **possible avenues**
  - **residual estimator**

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

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

$$\|G(\nabla \tilde{u}_h) - \nabla \tilde{u}_h\|$$

  - **.......**

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 $u_h \in V^h \subset V = H^1_D(\Omega)$ such that

$$a(u_h, v) = f(v) \quad \forall\, v \in V^h$$

- **residual functional**

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

where $v_I \in V^h$

Explicit Residual Estimator

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

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

- **global reliability bound**

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

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

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

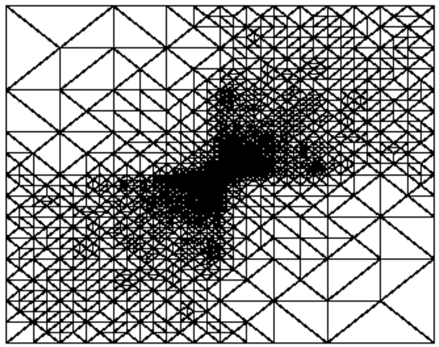
Explicit Residual Estimators – Types of Discretization Error

- **types of discretization error**
  - **element residuals:**

    measuring violation of the original equation
  - **flux edge jumps:**

    measuring violation of the continuity of the normal component of the numerical flux $\boldsymbol{\sigma} = -\alpha \nabla u_h$

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**

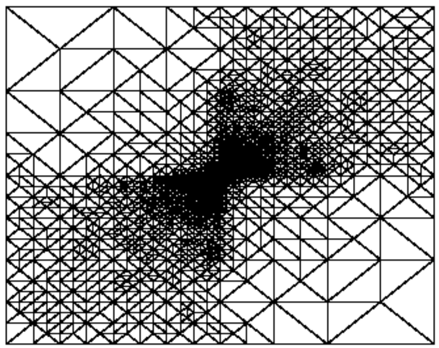
$$\|u - u_h\| \le C \sup_{0 \ne v \in (V, \|\cdot\|)} \frac{|r(v)|}{\|v\|} \le C \left(\sum_{K \in \mathcal{T}} \eta_K^2 \right)^{1/2}$$

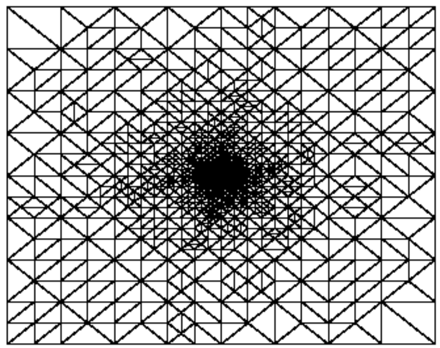
- **examples of the explicit residual indicator**
  - Babuska & Rheinboldt 79 (1D), Babuska & Miller 87 (2D)

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

  - Bernardi & Verfürth 2000, Petzoldt 2002

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





meshes generated by BM and BV indicators

Robust Efficiency and Reliability Bounds

(Bernardi & Verfürth 2000, Petzoldt 2002)

- **robust efficiency bound**

$$\eta_K \le C\, \|\alpha^{1/2}\nabla(u-u_h)\|_{0,\omega_K}$$

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

$$\|\alpha^{1/2}\nabla(u-u_h)\|_{0,\Omega} \le C\,\eta$$

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

(Cai-He-Zhang 2017, MathComp and SINUM)

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

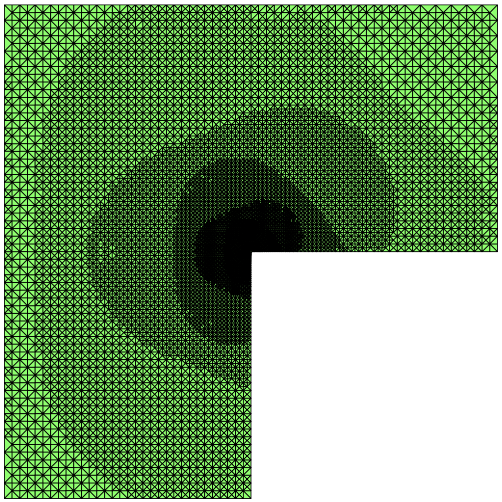
- **indicator and estimator**

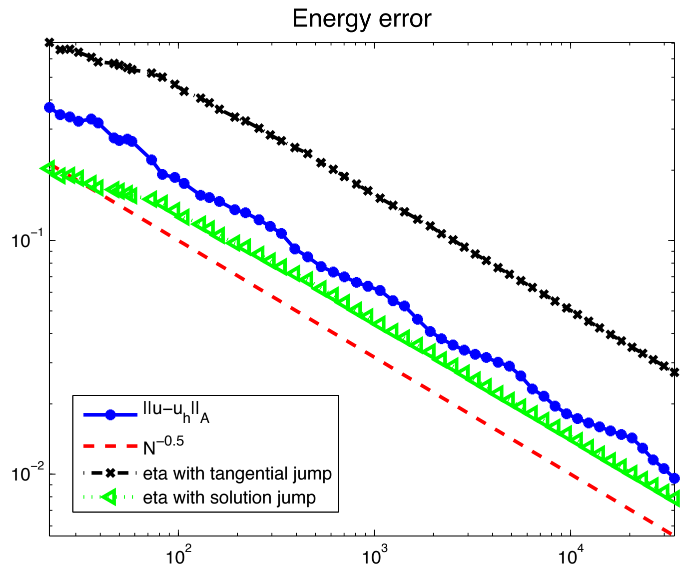
$$\eta^2 = \sum_{K\in\mathcal{T}} \eta_K^2 \quad \text{with} \quad \eta_K^2 = \eta_{r,K}^2 + \frac{1}{2}\sum_{F\in\mathcal{E}} \left(\eta_{j,n,F}^2 + \eta_{j,u,F}^2\right)$$

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

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

Estimators for Nonconforming Elements





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

for discontinuous elements, let $e = u - u_h$ and let

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

- **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**

$$\|\alpha^{1/2} \nabla_h e\|^2 = \sum_{K \in \mathcal{T}} (f_{k-1} + \nabla \cdot (\alpha \nabla u_h), e - \bar{e}_K)_K - \sum_{F \in \mathcal{E}_I} \int_F j_{n,F} \{e - \bar{e}_K\}^w ds$$

$$- \sum_{F \in \mathcal{E}} \int_F \{\alpha \nabla e \cdot \mathbf{n}\}_w [\![u_h]\!] ds - \sum_{F \in \mathcal{E}} \int_F \gamma \frac{\alpha_{F,H}}{h_F} [\![u_h]\!] \, [\![\bar{e}_K]\!] ds$$

where $\bar{e}_K$ is the average of e over K.

Zienkiewicz-Zhu (ZZ) Error Estimators

- **ZZ estimators**

$$\xi_G = \|G(\nabla \tilde{u}_h) - \nabla \tilde{u}_h\|$$

where $G: L^2(\Omega)^d \to U^h \subset C^0(\Omega)^d$ is gradient recovery operator

- **recovery operators**
  - **Zienkiewicz & Zhu estimator** (87, cited 2800 times)

$$G(\nabla \tilde{u}_h)(z) = \frac{1}{|\omega_z|} \int_{\omega_z} \nabla \tilde{u}_h \, dx \quad \forall\, z \in \mathcal{N}$$

  - L^2**-projection** find $G(\nabla \tilde{u}_h) \in U^h$ such that

$$\|G(\nabla \tilde{u}_h) - \nabla \tilde{u}_h\| = \min_{\boldsymbol{\rho} \in U^h} \|\boldsymbol{\rho} - \nabla \tilde{u}_h\|$$

  - **other recovery techniques**

    Bank-Xu, Carstensen, Schatz-Wahlbin, Z. Zhang, ...

Zienkiewicz-Zhu (ZZ) Error Estimators

- **recovery-based estimators**

$$\xi_G = \|G(\nabla \tilde{u}_h) - \nabla \tilde{u}_h\|$$

where $G: L^2(\Omega)^d \to U^h \subset C^0(\Omega)^d$ is gradient recovery operator

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

  $$\|\nabla u - G(\nabla \tilde{u}_h)\| \le \beta \|\nabla u - \nabla \tilde{u}_h\| \Longrightarrow 1 - \beta \le \frac{\xi_G}{\|G(\nabla \tilde{u}_h) - \nabla u\|} \le 1 + \beta$$

  - efficiency and reliability bounds

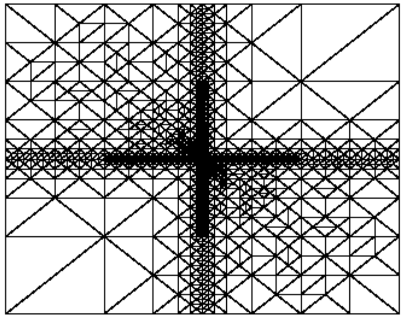
    Carstensen, Zhou, etc.

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

$$\nabla u \notin C^0(\Omega)^d \quad \text{and} \quad \boldsymbol{\sigma} = -\alpha \nabla u \notin C^0(\Omega)^d$$

- **recovery spaces**

$$G(\nabla \tilde{u}_h) \in C^0(\Omega)^d \quad \text{and} \quad G(-\alpha \nabla \tilde{u}_h) \in C^0(\Omega)^d$$

- **the reason of the failure**

approximating discontinuous functions by continuous functions

How to Fix It?

- **true gradient and flux**

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

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

- **conforming elements**

$$\left.\begin{aligned} \tilde{u}_h \in H^1(\Omega) \Longrightarrow \nabla \tilde{u}_h \in H(\mathsf{curl}, \Omega) \\ \tilde{\boldsymbol{\sigma}}_h = -\alpha \nabla \tilde{u}_h \notin H(\mathsf{div}, \Omega) \end{aligned}\right\} \quad \Longrightarrow \quad G(\boldsymbol{\sigma}_h) \in RT_0 \text{ or } BDM_1$$

- **mixed elements** gradient $\nabla\, u = -\alpha^{-1} \boldsymbol{\sigma}$

$$\left.\begin{aligned} \tilde{u}_h \in L^2(\Omega), \quad \tilde{\boldsymbol{\sigma}}_h \in H(\mathsf{div}, \Omega) \\ \tilde{\boldsymbol{\rho}} = -\alpha^{-1} \tilde{\boldsymbol{\sigma}}_h \notin H(\mathsf{curl}, \Omega) \end{aligned}\right\} \quad \Longrightarrow \quad G(-\alpha^{-1} \tilde{\boldsymbol{\sigma}}_h) \in \mathbb{D}_1 \text{ or } \mathbb{N}_1$$

Improved ZZ Estimator for Continuous Linear Elements

(Cai-Zhang 09, SINUM)

- **numerical flux** $\tilde{\boldsymbol{\sigma}}_h = -\alpha\nabla\tilde{u}_h \notin H(\text{div};\,\Omega)$

- **implicit flux recovery** find $\hat{\boldsymbol{\sigma}}_h \in \mathcal{V} = RT_0$ or $BDM_1 \in H(\text{div};\Omega)$

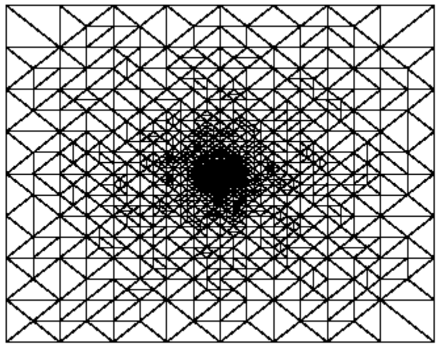
$$\|\alpha^{-1/2}(\hat{\boldsymbol{\sigma}}_h - \tilde{\boldsymbol{\sigma}}_h)\| = \min_{\boldsymbol{\tau}\in\mathcal{V}} \|\alpha^{-1/2}(\boldsymbol{\tau} - \tilde{\boldsymbol{\sigma}}_h)\|$$

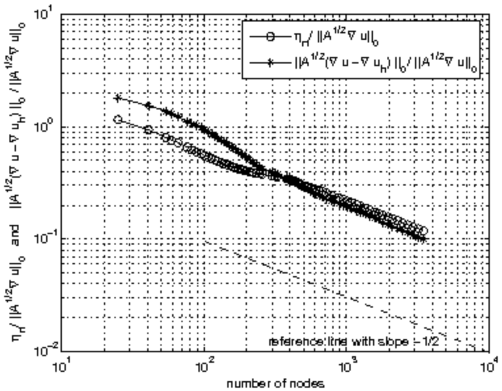
- **explicit flux recovery**

$$\hat{\boldsymbol{\sigma}}_h = \sum_{F\in\mathcal{E}_h} \sigma_F\,\boldsymbol{\psi}_F^{rt}(x) \quad \text{with} \quad \sigma_F = \frac{\alpha_F^+}{\alpha_F^- + \alpha_F^+}\bar{\sigma}_F^- + \frac{\alpha_F^-}{\alpha_F^- + \alpha_F^+}\bar{\sigma}_F^+$$

- **indicator and estimator**

$$\xi_K = \|\alpha^{-1/2}(\hat{\boldsymbol{\sigma}}_h - \tilde{\boldsymbol{\sigma}}_h)\|_{0,K} \quad \text{and} \quad \xi = \|\alpha^{-1/2}(\hat{\boldsymbol{\sigma}}_h - \tilde{\boldsymbol{\sigma}}_h)\|_{0,\Omega}$$





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

Explicit Flux Recovery for Conforming Linear Element
(Cai-He-Zhang 17, CMAME)

Diffusion tensor A is full tenser. Let $\boldsymbol{\psi}_{F}^{rt}$ be the nodal basis function on edge F and let

$$a_{rt,F} = \frac{\beta_{rt,F}^{-}}{\beta_{rt,F}^{-} + \beta_{rt,F}^{+}} \quad \text{with} \quad \beta_{rt,F}^{\pm} = \left(A^{-1}\boldsymbol{\psi}_{F}^{rt}, \boldsymbol{\psi}_{F}^{rt}\right)_{K_F^{\pm}}.$$

- **explicit flux recovery in RT_0** Let $\hat{\sigma}_F^{\pm}$ be numerical fluxes, then

$$\hat{\boldsymbol{\sigma}}_h^{rt} = \sum_{F\in\mathcal{E}} \sigma_F^{rt}\, \boldsymbol{\psi}_F^{rt}$$

where the nodal value is given by

$$\sigma_F^{rt} = a_{rt,F}\,\hat{\sigma}_F^{-} + (1 - a_{rt,F})\,\hat{\sigma}_F^{+}$$

Explicit Flux Recovery for Conforming Linear Element
(Cai-He-Zhang 17, CMAME)

Let $\boldsymbol{\psi}_{i,F}^{bdm}$, $i = 0, 1$, be the nodal basis function on edge F and let

$$a_{bdm,F} = \frac{\beta_{00,F}^{-}\beta_{11,F} - \beta_{01,F}^{-}\beta_{01,F}}{\beta_{00,F}\beta_{11,F} - \beta_{01,F}^{2}} \quad \text{and} \quad b_{bdm,F} = \frac{\beta_{01,F}^{-}\beta_{00,F}^{+} - \beta_{00,F}^{-}\beta_{01,F}^{+}}{\beta_{00,F}\beta_{11,F} - \beta_{01,F}^{2}}$$

where

$$\beta_{ij,F}^{\pm} = \left(A^{-1}\boldsymbol{\psi}_{i,F}^{bdm}, \boldsymbol{\psi}_{j,F}^{bdm}\right)_{K_F^{\pm}} \quad \text{and} \quad \beta_{ij,F} = \beta_{ij,F}^{-} + \beta_{ij,F}^{+}$$

- **explicit flux recovery in BDM_1** Let $\hat{\sigma}_F^{\pm}$ be numerical fluxes,

then

$$\hat{\boldsymbol{\sigma}}_h^{bdm} = \sum_{F\in\mathcal{E}} \sigma_F^{bdm}\, \boldsymbol{\psi}_{0,F}^{bdm} + \sum_{F\in\mathcal{E}_I} b_{bdm,F}\, j_{f,F}\, \boldsymbol{\psi}_{1,F}^{bdm}$$

where

$$\sigma_F^{bdm} = a_{bdm,F}\,\hat{\sigma}_F^{-} + (1 - a_{bdm,F})\,\hat{\sigma}_F^{+} \quad \text{and} \quad j_{f,F} = \hat{\sigma}_F^{-} - \hat{\sigma}_F^{+}$$

Hybrid A Posteriori Error Estimators

(Cai-Zhang 10, SINUM and D.Cai-Cai 18, CMAME)

- **general elliptic problems**

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

- **hybrid estimator**

$$\eta_K = \left(\|\alpha^{-\frac{1}{2}}(\hat{\boldsymbol{\sigma}}_h - \tilde{\boldsymbol{\sigma}}_h)\|_K^2 + \gamma_K h_K^2 \alpha_K^{-1} \|\hat{r}_K\|_K^2 \right)^{1/2}$$

where the numerical flux $\tilde{\boldsymbol{\sigma}}_h = -\alpha\nabla u_h$, the recovered flux $\hat{\boldsymbol{\sigma}}_h$, the modified element residual $\hat{r}_K = \bar{f} - \text{div}\,\hat{\boldsymbol{\sigma}}_h - \mathbf{a}\cdot\nabla u_h + bu_h$, and the weight for the convection/reaction-dominant diffusion problem $(\alpha = \epsilon)$ is given by

$$\gamma_K = \min\{1,\, h_K^{-1}\epsilon^{1/2}\beta^{-1/2}\}.$$

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**
  - Ainsworth-Oden, ...
  - Ainsworth, Repin, Vejchodsky, Ern, Vohralik, ...
  - Braess-Schöberl (08), ...
  - Cai-Zhang (12), Cai-Cao-Falgout (6), with He, Starke, ...

Estimators through Duality

- **minimization problem:**

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

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

- **dual problem:**

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

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

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

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

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

Estimators through Duality

(Hlavacek-Haslinger-Necas-Lovišek 82, Demkowicz et al 87)

- **guaranteed reliable estimator** for $\tilde{u}_h \in H^1_D(\Omega)$

$$
\begin{aligned}
\|A^{1/2}\nabla(u-\tilde{u}_h)\|^2 &= 2\Big(J(\tilde{u}_h)-J(u)\Big) = \min_{v\in H^1_D(\Omega)} 2\Big(J(\tilde{u}_h)-J(v)\Big)\\
&= 2\Big(J(\tilde{u}_h)-J^*(\boldsymbol{\sigma})\Big) = \min_{\boldsymbol{\tau}\in\Sigma_N(f)} 2\Big(J(\tilde{u}_h)-J^*(\boldsymbol{\tau})\Big)\\
&\le 2\Big(J(\tilde{u}_h)-J^*(\boldsymbol{\sigma}_h)\Big) = \min_{\boldsymbol{\tau}\in\Sigma_N(f)\cap RT_{p-1}} 2\Big(J(\tilde{u}_h)-J^*(\boldsymbol{\tau})\Big)\\
&\le \eta(\boldsymbol{\tau}) := 2\Big(J(\tilde{u}_h)-J^*(\boldsymbol{\tau})\Big), \quad \forall\, \boldsymbol{\tau}\in\Sigma_N(f)\cap RT_{p-1}\\
&= \|A^{-1/2}(\boldsymbol{\tau}-\tilde{\boldsymbol{\sigma}}_h)\|^2, \quad \text{numerical flux } \tilde{\boldsymbol{\sigma}}_h = -A\nabla\tilde{u}_h
\end{aligned}
$$

- **concerns:**

(1) construction of $\hat{\boldsymbol{\sigma}}_h$ and its computational cost

(2) local efficiency bound $\eta_K(\hat{\boldsymbol{\sigma}}_h) \le C\,\|A^{1/2}\nabla(u-\tilde{u}_h)\|_{\Delta_K}$

Estimators through Duality

(Equilibrated Residual Error Estimator)

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

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

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

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

$$(\nabla(\tilde{u}_h - u),\ A\nabla u + \boldsymbol{\tau})) = -(\tilde{u}_h - u,\ \nabla\cdot(A\nabla u) + \nabla\cdot\boldsymbol{\tau})) = 0$$

- **guaranteed reliable estimator** $\tilde{\boldsymbol{\sigma}}_h = -A^{-1}\nabla\tilde{u}_h$

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

Equilibrated Residual Error Estimator

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

- explicit calculation of numerical flux for linear element (Braess-Schöberl 08 for 2D, Ern-Vohralik 2018 for 3D)

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

- 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**

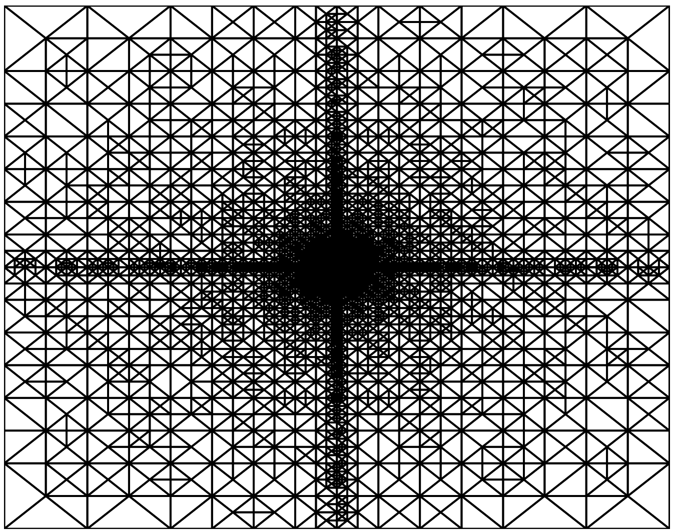
$$\eta_K(\hat{\boldsymbol{\sigma}}_{BPS}) \le C_e \, \|A^{1/2}\nabla(u - \tilde{u}_h)\|_{\omega_K}$$

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 (Cai-Zhang 12, SINUM)



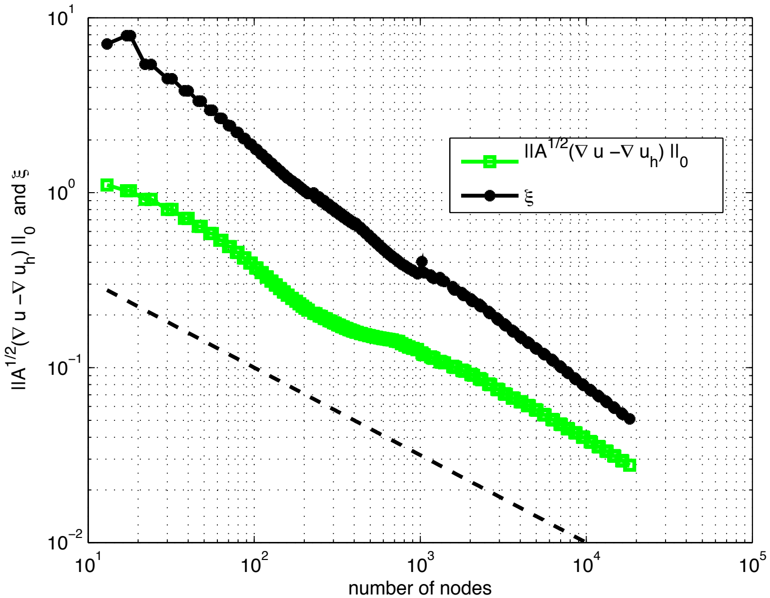


Figure 1: mesh generated by η_{BS} Figure 2: error and estimator η_{BS}

Equilibrated Residual Error Estimator
(Cai-Zhang 12, SINUM, Cai-Cai-Zhang, 2017)

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

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

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

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

- **α and p-robust efficiency**

$$\eta_K(\hat{\boldsymbol{\sigma}}_{CCZ}) \le C_e \, \|A^{1/2}\nabla(u - \tilde{u}_h)\|_{\omega_K}$$

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

Equilibrated Residual Error Estimator

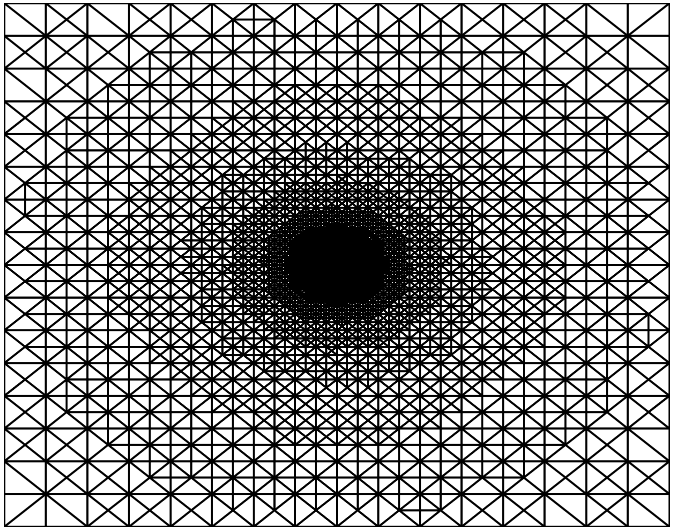


Figure 3: mesh generated by η_{CZ}

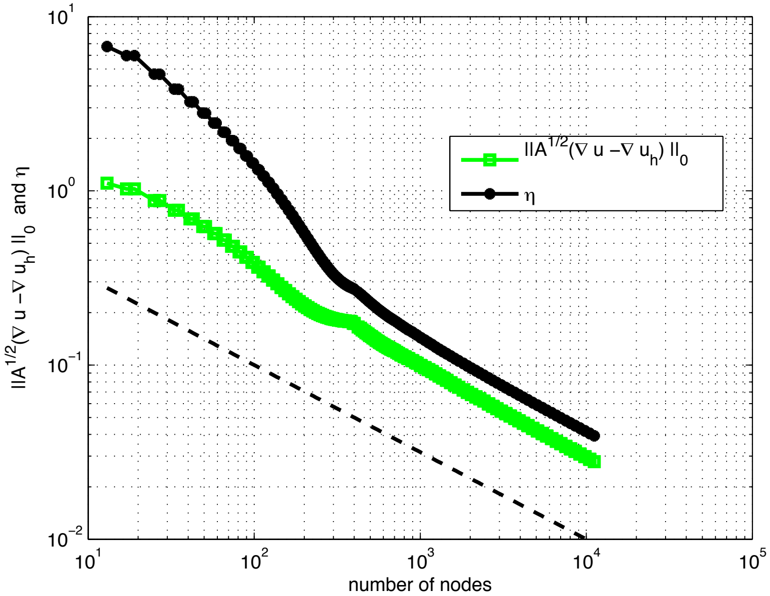


Figure 4: error and estimator η_{CZ}

H(curl) Problems

- **H(curl) problem**

$$\begin{cases} \nabla\times(\mu^{-1}\nabla\times\mathbf{u}) + \beta\,\mathbf{u} = \mathbf{f}, & \text{in } \Omega \subset R^3, \\ \mathbf{u}\times\mathbf{n} = \mathbf{g}_{_D}, \quad \text{on } \Gamma_D \quad \text{and} \quad (\mu^{-1}\nabla\times\mathbf{u})\times\mathbf{n} = \mathbf{g}_{_N}, & \text{on } \Gamma_N. \end{cases}$$

where $0 < \mu_0^{-1} \le \mu^{-1}(\mathbf{x})$ and $0 < \beta_0 \le \beta(\mathbf{x})$.

- **variational formulation** (primal problem) find $\mathbf{u} \in \mathbf{H_D}(\mathbf{curl};\boldsymbol{\Omega})$ such that

$$A_{\mu,\beta}(\mathbf{u},\,\mathbf{v}) = f_{_N}(\mathbf{v}), \quad \forall\,\mathbf{v} \in \mathring{\mathbf{H}}_D(\mathbf{curl};\Omega),$$

where the bilinear and linear forms are given by

$$A_{\mu,\beta}(\mathbf{u},\mathbf{v}) = (\mu^{-1}\nabla\times\mathbf{u},\nabla\times\mathbf{v}) + (\beta\,\mathbf{u},\mathbf{v}) \quad \text{and} \quad f_{_N}(\mathbf{v}) = (\mathbf{f},\mathbf{v}) + \langle \mathbf{g}_{_N},\mathbf{v}\rangle_{\Gamma_N}.$$

Residual Estimator for H(curl) Problems (Beck-Hiptmair-Hoppe-Wohlmuth, 00)

- **H(curl) problem**

$$\begin{cases} \nabla\times(\mu^{-1}\nabla\times\mathbf{u}) + \beta\,\mathbf{u} = \mathbf{f}, \quad \text{in } \Omega\subset R^3, \\ \mathbf{u}\times\mathbf{n} = \mathbf{g}_{_D}, \quad \text{on } \Gamma_D \quad \text{and} \quad (\mu^{-1}\nabla\times\mathbf{u})\times\mathbf{n} = \mathbf{g}_{_N}, \quad \text{on } \Gamma_N. \end{cases}$$

- **finite element approximation**

find $\mathbf{u}_h \in \mathbf{H_D}(\mathbf{curl};\boldsymbol{\Omega})\cap\mathbf{NE_p}$ such that

$$A_{\mu,\beta}(\mathbf{u}_h,\,\mathbf{v}) = f_{_N}(\mathbf{v}), \quad \forall\,\mathbf{v}\in\mathring{\mathbf{H}}_D(\mathbf{curl};\Omega)\cap NE_p$$

- **residual estimator** if $\mathbf{f}\in H(\text{div};\Omega)$

$$\eta_K^2 = h_K^2\|\mathbf{f} - (\nabla\times(\mu^{-1}\nabla\times\mathbf{u}_h) + \beta\,\mathbf{u}_h)\|_{0,K}^2 + h_K^2\|\nabla\cdot(\mathbf{f} - \beta\,\mathbf{u}_h)\|_{0,K}^2$$

$$+\frac{1}{2}\sum_{F\in\partial K} h_F\left(\|[\![(\mu^{-1}\nabla\times\mathbf{u}_h)\times\mathbf{n}]\!]\|_{0,F}^2 + \|[\![(\beta\mathbf{u}_h)\cdot\mathbf{n}]\!]\|_{0,F}^2\right)$$

Residual Error Estimator (BHHW, 00)

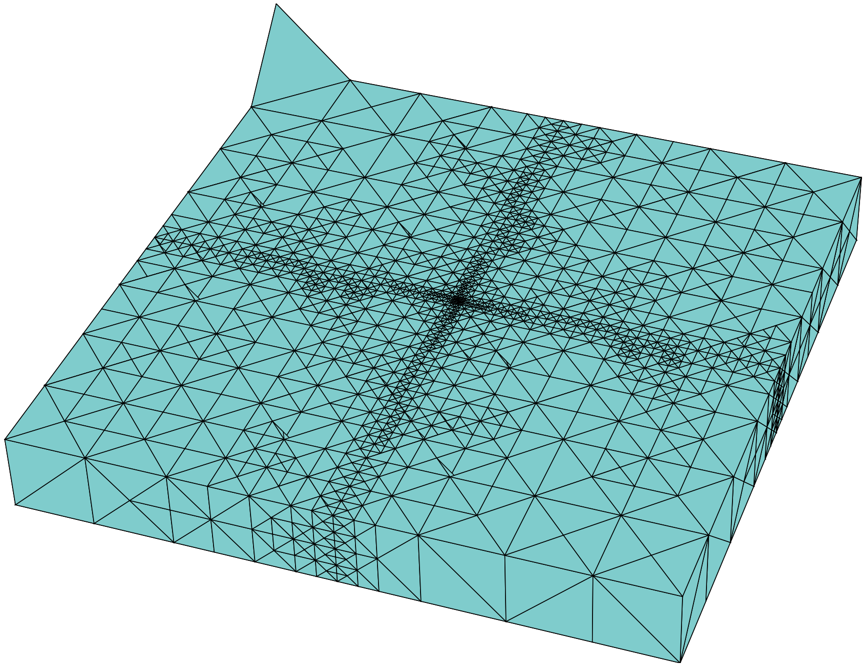


Figure 5: mesh by η_{Res}

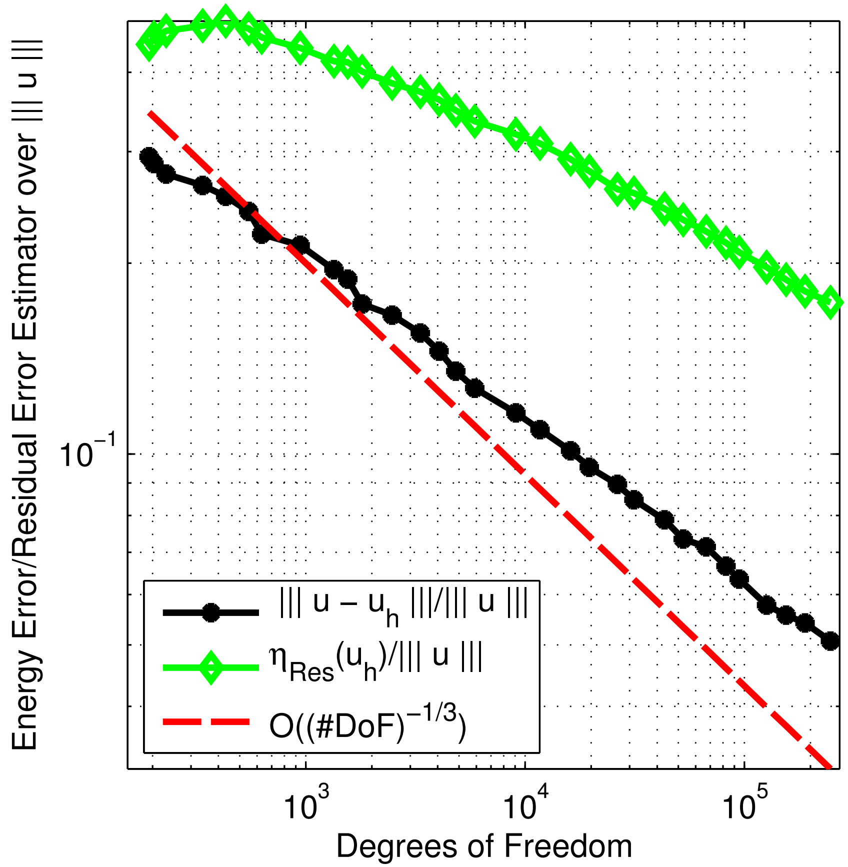


Figure 6: convergence of η_{Res}

Duality Estimator for H(Curl) Problem
(Cai-Cao-Falgout 16, CMAME)

- **dual problem** find $\boldsymbol{\sigma} \in \mathbf{H_N}(\mathbf{curl};\boldsymbol{\Omega})$ such that

$$A_{\beta,\mu}(\boldsymbol{\sigma},\boldsymbol{\tau}) = f_{_D}(\boldsymbol{\tau}), \quad \forall\, \boldsymbol{\tau} \in \mathring{\mathbf{H}}_N(\mathbf{curl};\Omega),$$

where the bilinear and linear forms are given by

$A_{\beta,\mu}(\boldsymbol{\sigma},\boldsymbol{\tau}) = (\beta^{-1}\nabla\times\boldsymbol{\sigma},\nabla\times\boldsymbol{\tau})+(\mu\,\boldsymbol{\sigma},\boldsymbol{\tau})$ and $f_{_D}(\boldsymbol{\tau}) = (\beta^{-1}\mathbf{f},\nabla\times\boldsymbol{\tau})-\langle \mathbf{g}_{_D},\boldsymbol{\tau}\rangle_{\boldsymbol{\Gamma}_D}$

- **duality estimator**

$$\eta_K = \left(\|\mu^{-1/2}\,(\mu\,\boldsymbol{\sigma}_{\mathcal{T}} - \nabla\times\mathbf{u}_{\mathcal{T}})\,\|_K^2 + \|\beta^{-1/2}\,(\nabla\times\boldsymbol{\sigma}_{\mathcal{T}} + \beta\,\mathbf{u}_{\mathcal{T}} - \mathbf{f})\,\|_K^2\right)^{1/2}$$

- **efficiency and reliability**

$$\eta_{_K} \le \sqrt{2}\,\left(\|\mathbf{u}-\mathbf{u}_{\mathcal{T}}\|^2_{\mu,\beta,K} + \|\boldsymbol{\sigma}-\boldsymbol{\sigma}_{\mathcal{T}}\|^2_{\beta,\mu,K}\right)^{1/2}$$

$$\eta = \left(\|\mathbf{u}-\mathbf{u}_{\mathcal{T}}\|^2_{\mu,\beta} + \|\boldsymbol{\sigma}-\boldsymbol{\sigma}_{\mathcal{T}}\|^2_{\beta,\mu}\right)^{1/2}$$

Residual Error Estimator (CCF, 16)

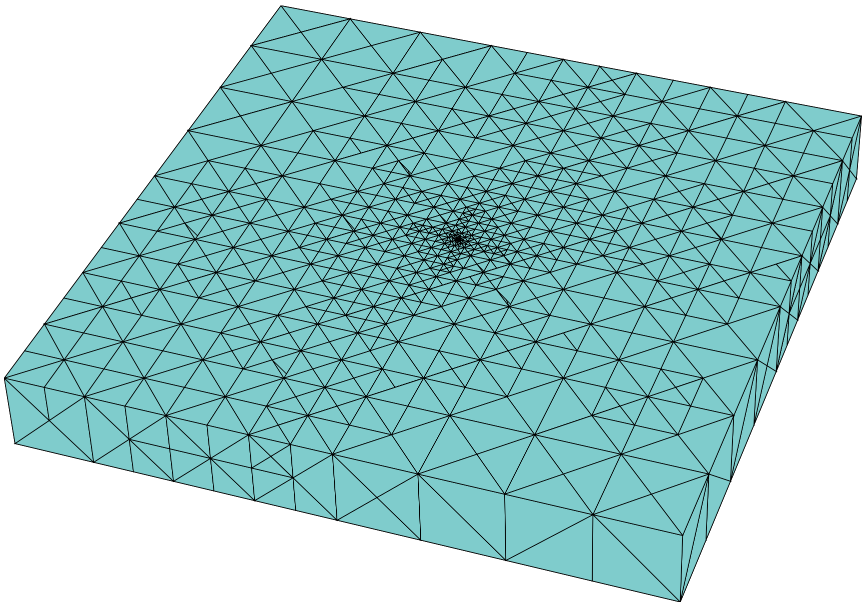


Figure 7: mesh by η_{Dual}

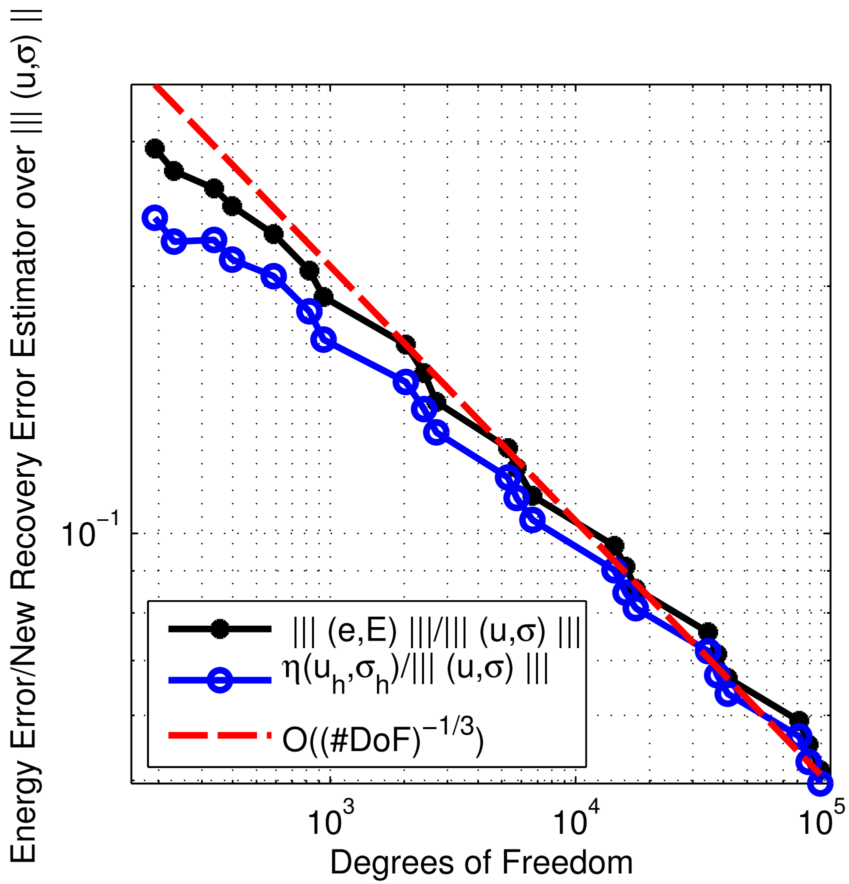


Figure 8: convergence of η_{Dual}

Estimators Comparison

Table 1: Estimators Comparison, $\mathbf{f} \notin \mathbf{H}(\mathrm{div}; \mathbf{\Omega})$

	# Iter	# DoF	error	rel-error	η	eff-index
η_{Res}	31	247003	0.0337	0.0507	0.115	3.420
η_{Rec}	24	218497	0.0355	0.0534	0.0559	1.577
η_{Dual}	22	99215	0.0342	0.0514	0.0329	0.964

Estimators through Duality for Discontinuous Elements

- **guaranteed reliable estimator** for $\tilde{u}_h \in H^1(\mathcal{T})$

(Braess-Fraunholz-Hoppe, SINUM 14)

$$\|\nabla_h(u-\tilde{u}_h)\|^2 \le \min_{\boldsymbol{\tau}\in\Sigma_N(f)} \|\boldsymbol{\tau}-\tilde{\boldsymbol{\sigma}}_h\|^2 + 2 \min_{v\in H^1_D(\Omega)} \|\nabla_h(v-\tilde{u}_h)\|^2$$

$$\le \|\boldsymbol{\tau}-\tilde{\boldsymbol{\sigma}}_h\|^2 + 2\,\|\nabla_h(v-\tilde{u}_h)\|^2 =: \eta^2(\boldsymbol{\tau},v)$$

for any $\boldsymbol{\tau}\in\Sigma_N(f)\cap RT_{p-1}$ and any $v\in V_h\subset H^1_D(\Omega)$

- **guaranteed reliable estimator** for $\tilde{u}_h \in H^1_D(\Omega)$

$$\|A^{1/2}\nabla(u-\tilde{u}_h)\| = \min_{\boldsymbol{\tau}\in\Sigma_N(f)} \|A^{-1/2}(\boldsymbol{\tau}-\tilde{\boldsymbol{\sigma}}_h)\|$$

$$\le \|A^{-1/2}(\boldsymbol{\tau}-\tilde{\boldsymbol{\sigma}}_h)\|, \qquad \forall\,\boldsymbol{\tau}\in\Sigma_N(f)\cap RT_{p-1}$$

where $\tilde{\boldsymbol{\sigma}}_h = -A\nabla\tilde{u}_h$ is the numerical flux.

Estimators through Duality for Discontinuous Elements

- **guaranteed reliable estimator** for $\tilde{u}_h \in H^1(\mathcal{T})$

(Braess-Fraunholz-Hoppe, SINUM 14)

$$\begin{aligned} \|\nabla_h(u-\tilde{u}_h)\|^2 &\le \min_{\boldsymbol{\tau}\in\Sigma_N(f)} \|\boldsymbol{\tau}-\tilde{\boldsymbol{\sigma}}_h\|^2 + 2 \min_{v\in H^1_D(\Omega)} \|\nabla_h(v-\tilde{u}_h)\|^2 \\ &\le \|\boldsymbol{\tau}-\tilde{\boldsymbol{\sigma}}_h\|^2 + 2\,\|\nabla_h(v-\tilde{u}_h)\|^2 =: \eta^2(\boldsymbol{\tau}, v) \end{aligned}$$

for any $\boldsymbol{\tau} \in \Sigma_N(f) \cap RT_{p-1}$ and any $v \in V_h \subset H^1_D(\Omega)$

- **guaranteed reliable estimator** for $\tilde{u}_h \in H^1(\mathcal{T})$

(Cai-He-Starke-Zhang, 2017)

$$\begin{aligned} \|A^{\frac{1}{2}}\nabla_h(u-\tilde{u}_h)\|^2 &= \min_{\boldsymbol{\tau}\in\Sigma_N(f)} \|A^{-\frac{1}{2}}(\boldsymbol{\tau}-\tilde{\boldsymbol{\sigma}}_h)\|^2 + \min_{v\in H^1_D(\Omega)} \|A^{-\frac{1}{2}}\nabla_h(v-\tilde{u}_h)\|^2 \\ &\le \eta^2(\boldsymbol{\tau}, v) := \|A^{-\frac{1}{2}}(\boldsymbol{\tau}-\tilde{\boldsymbol{\sigma}}_h)\|^2 + \|A^{-\frac{1}{2}}\nabla_h(v-\tilde{u}_h)\|^2 \end{aligned}$$

for any $\boldsymbol{\tau} \in \Sigma_N(f) \cap RT_{p-1}$ and any $v \in V_h \subset H^1_D(\Omega)$

Discretization-Accurate Stopping Criterion

- **total error** $\|u - u_{\mathcal{T}}^k\| \le \|u - u_{\mathcal{T}}\| + \|u_{\mathcal{T}} - u_{\mathcal{T}}^k\|.$
- **discretization error:** compute the dual estimator $\eta_d(u_{\mathcal{T}}^k)$, then

$$\|u - u_{\mathcal{T}}^k\| \le \eta_d(u_{\mathcal{T}}^k) + C_a\|u_{\mathcal{T}} - u_{\mathcal{T}}^k\|$$

- **algebraic error:** Let ρ be the (unknown) spectral radius of the iterative matrix

$$\|u_{\mathcal{T}} - u_{\mathcal{T}}^k\| \le \frac{\rho}{1-\rho}\|u_{\mathcal{T}}^k - u_{\mathcal{T}}^{k-1}\|,$$

Let $\rho_k = \|\mathbf{r}_k\|_{l^2}/\|\mathbf{r}_{k-1}\|_{l^2}$, then $\dfrac{\rho_k}{1-\rho_k} \uparrow \dfrac{\rho}{1-\rho}$ as $k \to \infty$

- **algebraic error estimator:**

$$\eta_a = \frac{\rho_k}{1-\rho_k}\|u_{\mathcal{T}}^k - u_{\mathcal{T}}^{k-1}\|$$

Comparison of Stopping Criterions

	Stopping	# Iter	total error	alg error
MG-V(1,1)	$\eta_a \leq 0.67\,\eta_d$	2	0.0821	3.5×10^{-2}
MG	$\\|\mathbf{r}_k\\|_{l^2}/\\|\mathbf{r}_0\\|_{l^2} \leq 10^{-7}$	15	0.0741	3.4×10^{-8}
Sym GS	$\eta_a \leq 0.67\,\eta_d$	31	0.1051	7.5×10^{-2}
Sym GS	$\\|\mathbf{r}_k\\|_{l^2}/\\|\mathbf{r}_0\\|_{l^2} \leq 10^{-5}$	289	0.0741	2.7×10^{-4}

Table 2: Comparison of stopping criterions

Efficient AMR Algorithm

- **AMR algorithm**

$$\text{Solve} \rightarrow \text{Estimate} \rightarrow \text{Mark} \rightarrow \text{Refine}$$

- **AMR convergence** There exist constants $C_0 > 0$ and $\delta \in (0, 1)$ such that

$$|||u - u_{\mathcal{T}}^k||| \leq C_0 \delta^k |||u - u_{\mathcal{T}}^0|||$$

- **efficient AMR algorithm**

$$\text{Solve} \rightarrow \text{Estimate} \rightarrow \text{Mark} \rightarrow \text{Refine}$$

$$\rightarrow \text{Estimate} \rightarrow \cdots \rightarrow \text{Refine}$$

Comparison of Stopping Criterions

# Iterations	# Nodes	Effectivity Indices	# Refinements
136	3238	0.9242	once
63	3060	0.9214	twice
42	3164	0.9196	three times

Table 3: Comparison of the number of refinements for each "Solve"

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