A Framework for Analyzing and Constructing Hierarchical-Type A Posteriori Error Estimators

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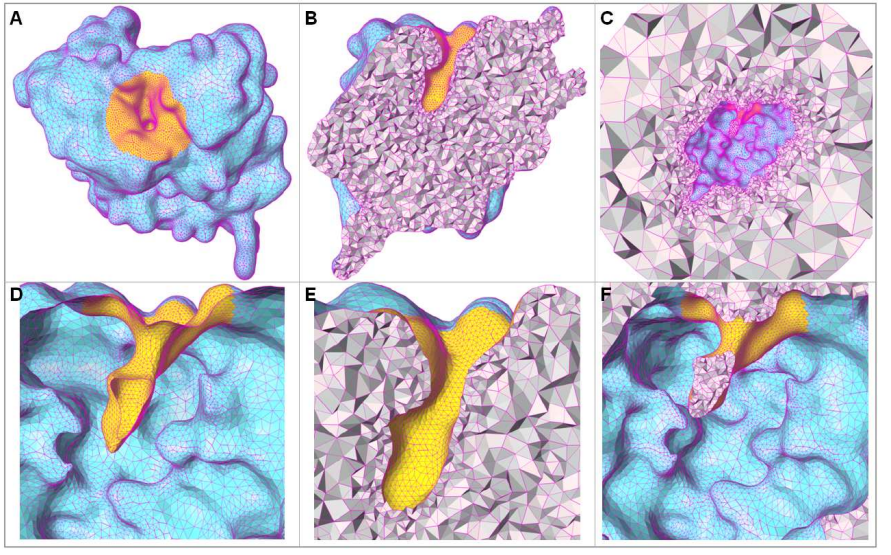
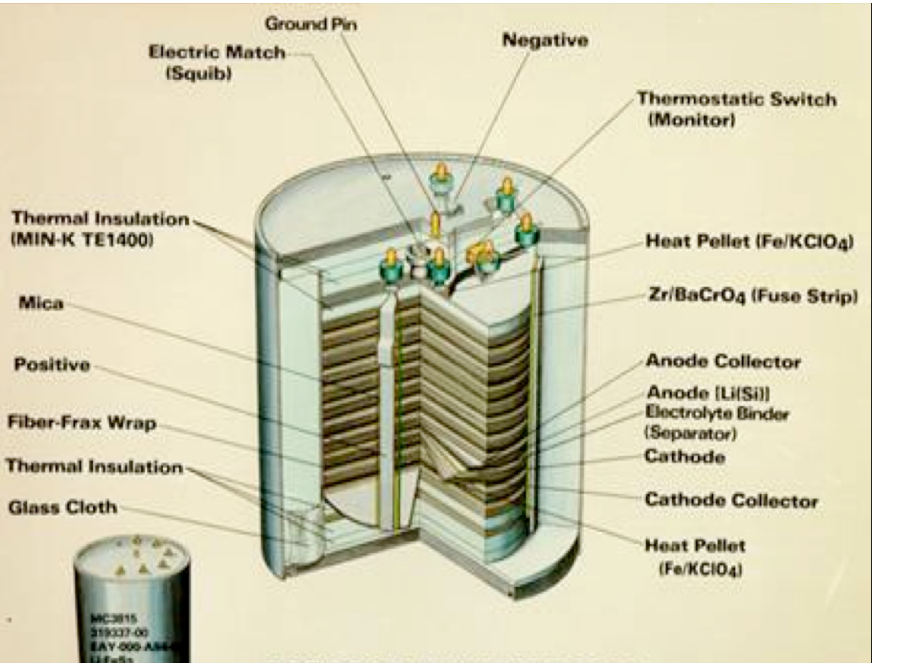
Introduction, Motivation



Mouse Acetylcholinesterase (mAChE) Monomer, 8362 Atoms



Sandia Long-life Thermal Battery

Model Problem

Setting

- $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$, bounded, polyhedral
- $\Gamma = \partial\Omega = \Gamma_D \cup \Gamma_N$, $\Gamma_D \cap \Gamma_N = \emptyset$
- $\mathcal{H} = \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_D \text{ in the trace sense}\}$

Variational Problem

Find $u \in \mathcal{H}$ such that

$$\underbrace{\int_\Omega (A\nabla u) \cdot \nabla v + (\mathbf{b} \cdot \nabla u + cu)v \, dV}_{B(u,v)} = \underbrace{\int_\Omega fv \, dV + \int_{\Gamma_N} gv \, dS}_{F(v)} \, , \; \forall v \in \mathcal{H}$$

- $|B(v,w)| \leq M\|v\|_1\|w\|_1 \quad , \quad B(v,v) \geq m\|v\|_1^2$ (can have inf-sup instead)
- $|F(v)| \leq L\|v\|_1$
- Piecewise-smooth data, $A, \mathbf{b}, c, f, g$

Finite Element Discretization

Approximation Space:

- Mesh $\mathcal{T}$: Conforming simplicial partition (triangles in $\mathbb{R}^2$, tetrahedra in $\mathbb{R}^3$)
  - **Simplices** T**:** align with discontinuities in data A, $\mathbf{b}$, c, f, g
  - **Vertices** z**:** all $\overline{\mathcal{V}}$, non-Dirichlet $\mathcal{V}$, Dirichlet $\mathcal{V}_D$
  - **Edges** E**:** all $\overline{\mathcal{E}}$, non-Dirichlet $\mathcal{E}$, Dirichlet $\mathcal{E}_D$
  - **Faces** F**:** all $\overline{\mathcal{F}}$, non-Dirichlet $\mathcal{F}$, Dirichlet $\mathcal{F}_D$
- Approximation Space V: piecewise polynomials of a fixed degree k

$$V = \mathbb{P}_k(\mathcal{T}) = \{v \in \mathcal{H} \cap C(\overline{\Omega}) : \ v|_T \in \mathbb{P}_k \text{ for all } T \in \mathcal{T}\}$$

Discrete Approximation Problem:

- $V = \text{span}\{\phi_j : 1 \leq j \leq N\}$, ϕ_j locally-supported
- Find $\hat{u} \in V$ such that $B(\hat{u}, v) = F(v)$ for all $v \in V$
- $B\mathbf{u} = \mathbf{f}$ where $B_{ij} = B(\phi_j, \phi_i)$ and $\mathbf{f}_i = F(\phi_i)$
- B large, sparse, but ill-conditioned ($\kappa(B) \sim N^{2/d} \sim h^{-2}$)

Motivation for A Posteriori Error Estimation and Adaptivity

Approximation Quality $\hat{u} \approx u$

$$B(u - \hat{u}, v) = 0 \text{ for all } v \in V \implies \|u - \hat{u}\|_1 \leq C \inf_{v \in V} \|u - v\|_1$$

- Discretization error comparable to interpolation error
- Interpolation error related to regularity/smoothness of u
- Efficiently and reliably identify problem areas and adaptively improve

$$\cdots \longrightarrow \text{solve} \longrightarrow \text{estimate error} \longrightarrow \text{mark elements} \longrightarrow \text{refine} \longrightarrow \cdots$$

Common Causes of Singularities in u

- (Re-entrant) corners and/or edges in domain
- Changes in boundary condition type (Dirichlet-Neumann interface)
- Discontinuities in problem data (abrupt changes in material properties)

Types of Error Estimators on the Market

- Residual: Appropriate weighting of volumetric and "jump" portions of strong residual
  - Oldest, most fully developed (reliablility and convergence) theory
- Gradient Recovery: Post-processing of $\nabla \hat{u}$ by local or global "averaging"
  - Problem-independent approach, popular in (some) engineering circles
  - Sometimes see (more often than is currently explainable) asymptotically exact estimation of error—super-convergence, strong smoothness assumptions
- Hierarchical Type: Approximate error function computed in an auxiliary space
  - Very robust and flexible, often see gradient recovery-type performance
  - Too expensive? I will argue "no"—certainly not for what you get
- Other Types used for Norm-Error Estimation: Equilibrated Residual, others based on solution of local Dirichlet and/or Neumann problems
- Functional Error Estimation, Goal-Oriented Adaptivity: functional error $G(u - \hat{u})$ of interest
  - Many above types can be modified to work in this setting

Abstract View of Hierarchical Error Estimators

Original Problem

$$\text{Find } u \in \mathcal{H} \text{ such that } B(u, v) = F(v) \text{ for all } v \in \mathcal{H}$$

Discrete Problem

$$\text{Find } \hat{u} \in V \text{ such that } B(\hat{u}, v) = F(v) \text{ for all } v \in V$$

Discrete Error Problem

$$\text{Find } \varepsilon \in W \text{ such that } B(\varepsilon, v) = F(v) - B(\hat{u}, v) = B(u - \hat{u}, v) \text{ for all } v \in W$$

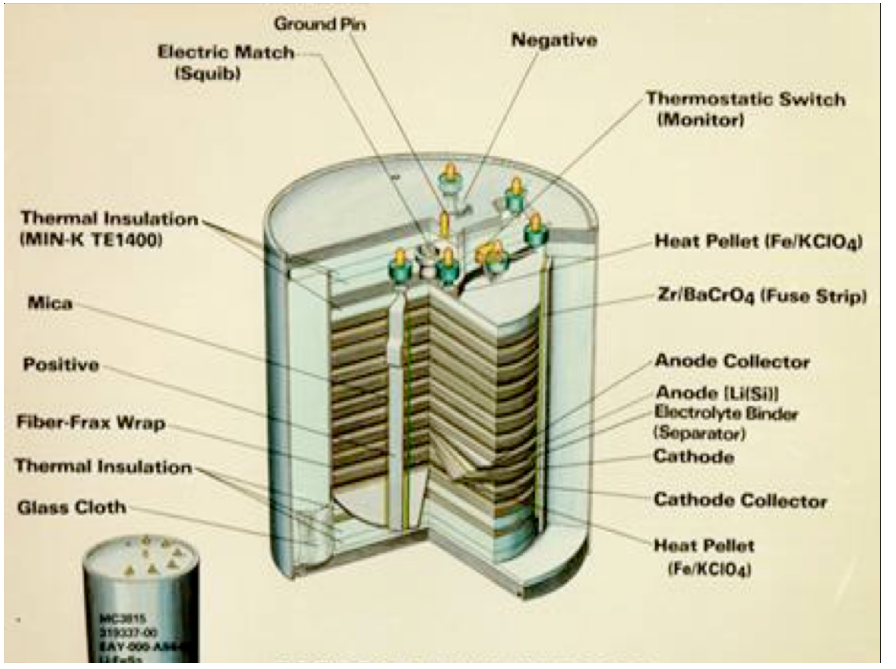
Some Common Choices for V, W:

- $V = \mathbb{P}_k(\mathcal{T})$, $W = \mathbb{P}_{k+1}(\mathcal{T}) \setminus \mathbb{P}_k(\mathcal{T})$
- $V = \mathbb{P}_k(\mathcal{T})$, $W = \mathbb{P}_k(\mathcal{T}') \setminus \mathbb{P}_k(\mathcal{T})$, $\mathcal{T}'$ from uniform refinement(s) of $\mathcal{T}$

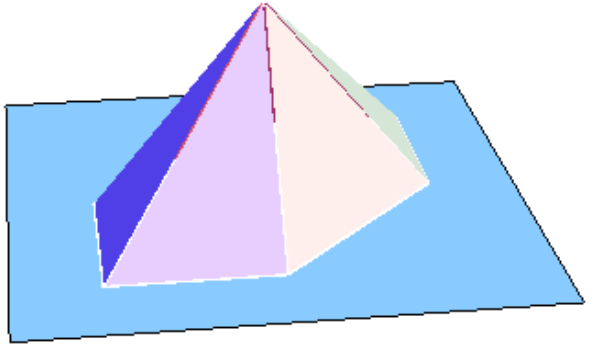
An Example in 2D—Thermal Battery Problem

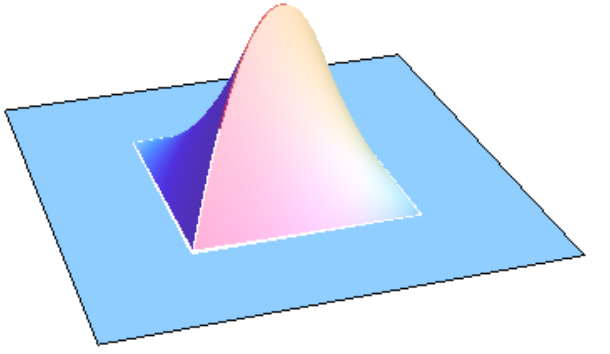
Use radial symmetry, convert to 2D

$V = \mathbb{P}_1(\mathcal{T})\ ,\ W = \mathbb{P}_2(\mathcal{T}) \setminus \mathbb{P}_1(\mathcal{T})$

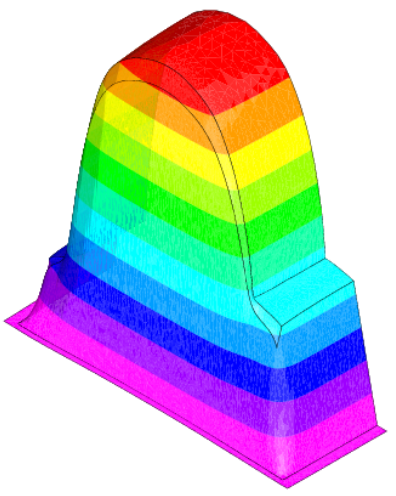


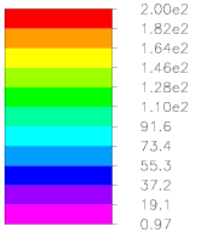
Sandia Long-life Thermal Battery

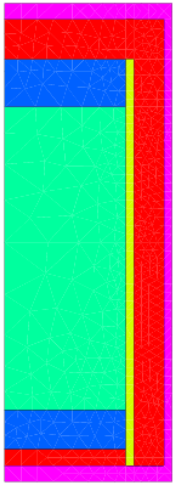


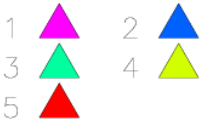


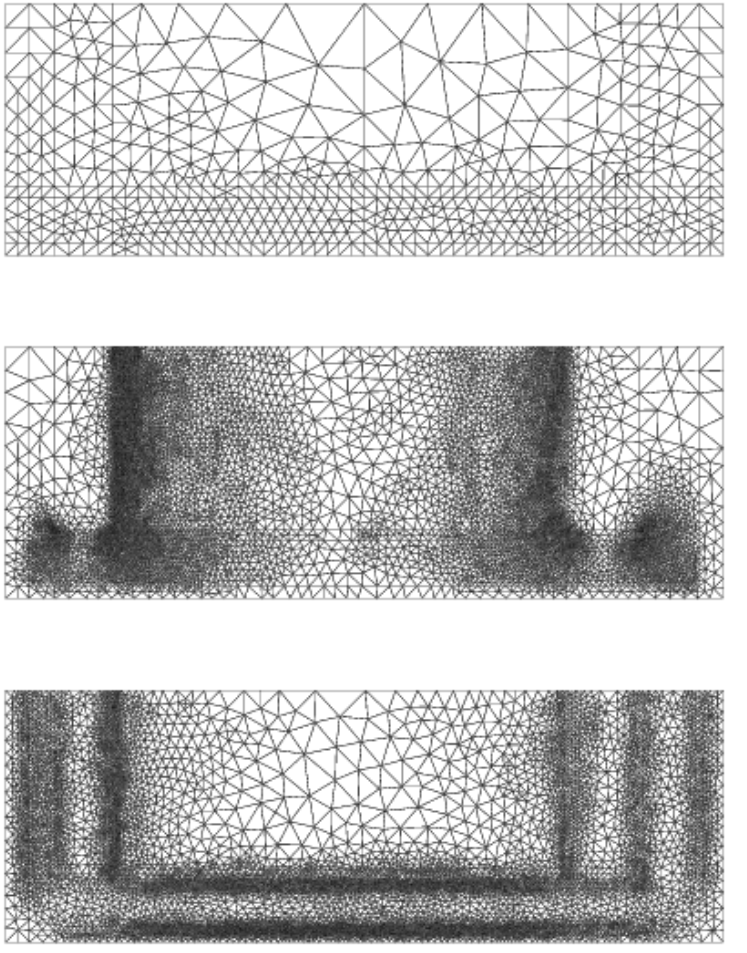
Thermal Battery Problem: HB versus GR Refinement



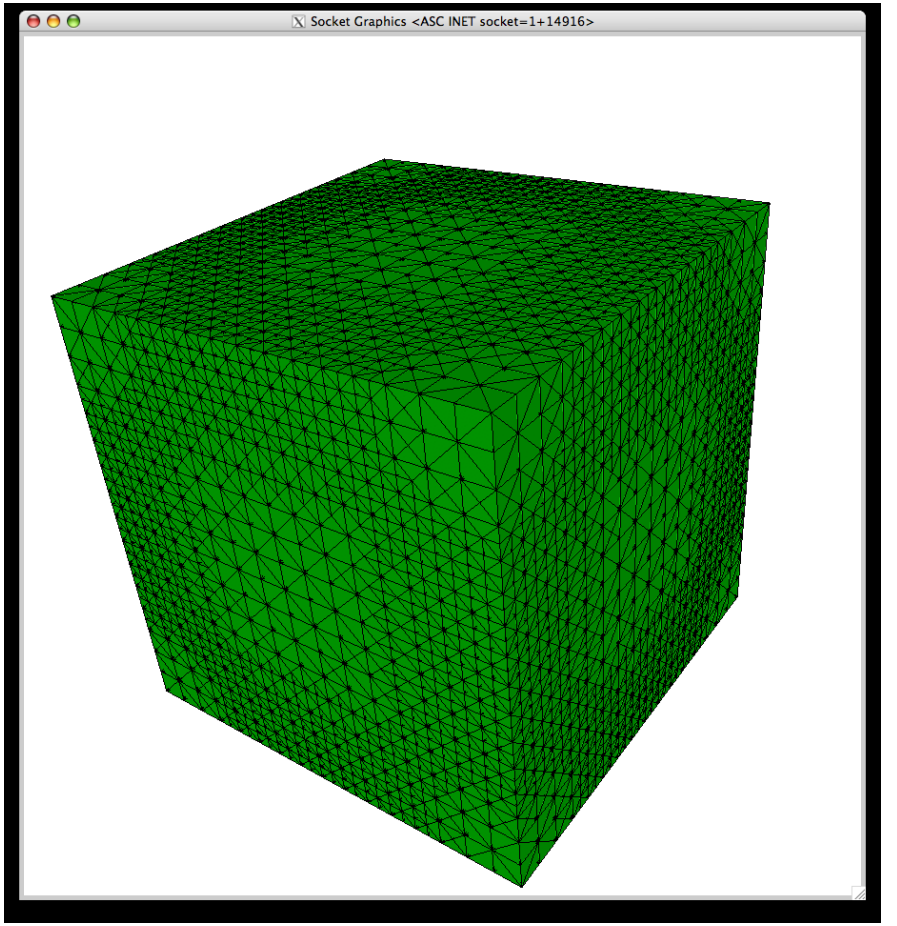


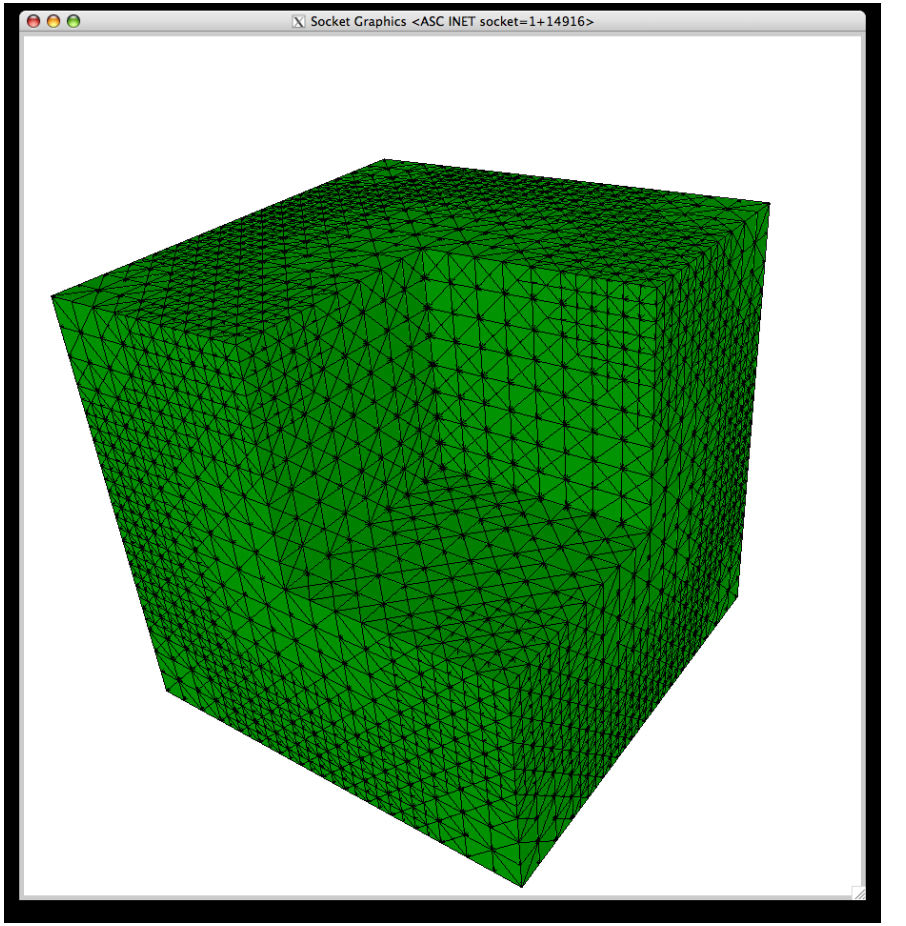






A Framework for Constructing and Analyzing Hierarchical Estimators





The Traditional Analysis

See Bank (Acta Numerica '96), or Ainsworth&Oden book

Setting/Assumptions

- B is an inner-product (no convection), energy norm $|||\cdot|||$
- $V \cap W = \{0\}$, and V contains local constants (quite sensible)
- Strong Cauchy Inquality: $|B(v,w)| \leq \gamma |||v||| |||w|||$ for $v \in V$ and $w \in W$, where $\gamma = \gamma(B,V,W) < 1$
- Saturation *Assumption*: $\inf_{v \in V \oplus W} |||u - v||| \leq \beta \inf_{v \in V} |||u - v|||$, where $\beta = \beta(B,V,W,F) < 1$
  - This assumption "compels" one to choose W so that $V \oplus W$ is a natural approximation space

$$|||\varepsilon||| \leq |||u - \hat{u}||| \leq \left((1-\gamma^2)(1-\beta^2)\right)^{-1/2} |||\varepsilon|||$$

A Different Approach to the Analysis

See Grubisic/Ovall (MC 2009), Holst/Ovall/Szypowski (APNUM 2011), Bank/Grubisic/Ovall (MC 2011??),

New Approach: For any $v \in \mathcal{H}$, $\hat{v} \in V$ and $\hat{w} \in W$,

$$\begin{aligned} B(u - \hat{u}, v) &= B(\varepsilon, \hat{w}) + B(u - \hat{u}, v - \hat{v} - \hat{w}) \\ &= B(\varepsilon, \hat{w}) + [F(v - \hat{v} - \hat{w}) - B(\hat{u}, v - \hat{v} - \hat{w})] \end{aligned}$$

$$|B(u - \hat{u}, v)| \leq [C_1 \|\varepsilon\| + C_2 \text{“residual oscillation”}] \, \|v\|$$

$$K_0 \|\varepsilon\| \leq \|u - \hat{u}\| \leq K_1 \|\varepsilon\| + K_2 \text{“residual oscillation”}$$

- Not necessarily in energy-norm setting; always true (not just asymptotic); only H^1-regularity assumption on u
- Constants scale-invariant; clear what they depend on and how—do not depend on F!!
- Choose space W, and then $\hat{v}, \hat{w}$, to make residual oscillation small
  - $\hat{v} + \hat{w}$ a well-chosen quasi-interpolant
  - Local vanishing moments for $v - (\hat{v} + \hat{w})$
- Choose space W so that computation of ε is cheap

A Realization of this Framework in $\mathbb{R}^3$

The Error Equation Revisited:

$$
\begin{aligned}
B(u-\hat{u},v) &= B(\varepsilon,w) + [F(v-\hat{v}-\hat{w}) - B(\hat{u},v-\hat{v}-\hat{w})] \\
&= B(\varepsilon,\hat{w}) + \int_\Omega (f - \mathbf{b}\cdot\nabla\hat{u} - c\hat{u})(v-\hat{v}-\hat{w}) - A\nabla\hat{u}\cdot\nabla(v-\hat{v}-\hat{w})\,dx \\
&+ \int_{\Gamma_N} (g - A\nabla\hat{u}\cdot\mathbf{n})(v-\hat{v}-\hat{w})\,ds \\
&= B(\varepsilon,\hat{w}) + \int_\Omega R(v-\hat{v}-\hat{w})\,dx + \sum_{F\in\mathcal{F}} \int_F r(v-\hat{v}-\hat{w})\,ds
\end{aligned}
$$

$$
R_{|_T} = f - (-\nabla\cdot A\nabla\hat{u} + \mathbf{b}\cdot\nabla\hat{u} + c\hat{u})
$$

$$
r_{|_F} = \begin{cases} -(A\nabla\hat{u})\cdot\mathbf{n}_T - (A\nabla\hat{u})\cdot\mathbf{n}_{T'} & , \quad F\in\mathcal{F}_I \\ g - (A\nabla\hat{u})\cdot\mathbf{n} & , \quad F\in\mathcal{F}_N \end{cases}
$$

A Realization of this Framework in $\mathbb{R}^3$

Approximation Space:

- $V = \mathbb{P}_1(\mathcal{T}) = \text{span}\{\ell_z : \ z \in \mathcal{V}\}$, $\ell_z(z') = \delta_{zz'}$ for all $z, z' \in \overline{\mathcal{V}}$
- A (non-smooth) partition-of-unity $\displaystyle\sum_{z \in \overline{\mathcal{V}}} \ell_z = 1$ on Ω
- $\omega_z \doteq \text{supp}(\ell_z)$

Error Equation (Again):

$$B(u - \hat{u}, v) = B(\varepsilon, w) + \sum_{z \in \overline{\mathcal{V}}} \int_\Omega R(v\ell_z - \hat{v}_z - \hat{w}_z)\, dx + \sum_{F \in \mathcal{F}} \int_F r(v - \hat{v} - \hat{w})\, ds$$

- $\hat{v} = \displaystyle\sum_{z \in \overline{\mathcal{V}}} v_z$, $\hat{w} = \displaystyle\sum_{z \in \overline{\mathcal{V}}} w_z$ $\qquad$ $\hat{v}_z$, $\hat{w}_z$ locally supported
- How to choose error space W? functions v_z, w_z?

A Realization of this Framework in $\mathbb{R}^3$

$$B(u-\hat{u},v) = B(\varepsilon,w) + \sum_{z\in\overline{\mathcal{V}}} \int_\Omega R(v\ell_z - \hat{v}_z - \hat{w}_z)\,dx + \sum_{F\in\mathcal{F}} \int_F r(v-\hat{v}-\hat{w})\,ds$$

A Useful Quasi-Interpolant: $\mathcal{I}v = \hat{v} + \hat{w} \in V \oplus W$

$$\int_\Omega (v\ell_z - v_z - w_z) = 0 \text{ for all } z \in \bar{\mathcal{V}} \quad , \quad \int_F (v-\hat{v}-\hat{w}) = 0 \text{ for all } F \in \mathcal{F} \qquad (1)$$

$$\text{supp}(v_z)\,,\ \text{supp}(w_z) \subset \Omega_z = \begin{cases} \omega_z & , \ z \in \mathcal{V} \\ \omega_z \cup \omega_{z'} \text{ for some } z' \in \mathcal{V} \text{ adjacent to } z & , \ z \in \mathcal{V}_D \end{cases}$$

Choosing W:

- A space W providing a single degree-of-freedom for each $F \in \mathcal{F}$ is sufficient for (1)
- We choose $W \subset \mathbb{P}_3(\mathcal{T})$ consisting of functions vanishing on every edge (cubic "face bubbles")
- $V \oplus W$ is *not* a standard approximation space

A Realization of this Framework in $\mathbb{R}^3$

$$\|u - \hat{u}\|_1 \leq K_1 \|\varepsilon\|_1 + K_2 \mathsf{osc}(R, r)$$

Reliability Argument:

$$|B(u - \hat{u}, v)| \leq M \|\varepsilon\|_1 \|\hat{w}\|_1 + \sum_{z \in \bar{\mathcal{V}}} \inf_{R_z \in \mathbb{R}} \|R - R_z\|_{0,\Omega_z} \|v\ell_z - v_z - w_z\|_{0,\Omega_z}$$

$$+ \sum_{F \in \mathcal{F}} \inf_{r_F \in \mathbb{R}} \|r - r_F\|_{0,F} \|v - \hat{v} - \hat{w}\|_{0,F}$$

$$|B(u - \hat{u}, v)| \leq C_1 \|\varepsilon\|_1 \|v\|_1 + C_{21} \sum_{z \in \bar{\mathcal{V}}} D_z \inf_{R_z \in \mathbb{R}} \|R - R_z\|_{0,\Omega_z} \|v\|_{1,\omega_z}$$

$$+ C_{22} \sum_{F \in \mathcal{F}} |F|^{1/4} \inf_{r_F \in \mathbb{R}} \|r - r_F\|_{0,F} \|v\|_{1,\Omega_F}$$

$$|B(u - \hat{u}, v)| \leq [C_1 \|\varepsilon\|_1 + C_2 \mathsf{osc}(R, r)] \|v\|_1$$

$$[\mathsf{osc}(R, r)]^2 = \sum_{z \in \bar{\mathcal{V}}} D_z^2 \inf_{R_z \in \mathbb{R}} \|R - R_z\|_{0,\Omega_z}^2 + \sum_{F \in \mathcal{F}} |F|^{1/2} \inf_{r_F \in \mathbb{R}} \|r - r_F\|_{0,F}^2$$

Reflecting on Effectivity Result and Analysis

$$K_0\|\varepsilon\|_1 \leq \|u-\hat{u}\|_1 \leq K_1\|\varepsilon\|_1 + K_2\mathsf{osc}(R,r)$$

- Argument style quite general
  - Different operators (eg. curl-curl), different elements (eg. Nédélec, Taylor-Hood)
  - Let form of residuals determine choice of error space W
  - Higher regularity: higher order elements for V, then more vanishing moments for $v-(\hat{v}+w)$
- Results hold under minimal practical assumptions (not an asymptotic or quasi-uniform analysis)
- Related notions of (data) oscillation in error analysis and AFEM convergence: Dörfler/Nochetto (2002), Nochetto/Siebert/Kreuzer/Cascon (2003,2008), Fierro/Veeser (2006), Bornemann/Erdmann/Kornhuber (1996)

Behavior of Face-Bump System

$$B_{FF'} = B(b_{F'}, b_F) \qquad D = \text{diag}(B)$$

$$\hat{B}_{FF'} = (b_{F'}, b_F)_{H^1(\Omega)} \qquad \hat{D} = \text{diag}(\hat{B})$$

- Argue that B and D are spectrally-equivalent
  1) Argue that B and $\hat{B}$ are spectrally-equivalent, and D and $\hat{D}$ are spectrally-equivalent
  2) Argue that $\hat{B}$ and $\hat{D}$ are spectrally-equivalent

1) If μ is an eigenvalue of B, then

$$m\lambda_{\text{min}}(\hat{B}) \leq \text{Re}(\mu) \leq M\lambda_{\text{max}}(\hat{B}) \quad \text{and} \quad |\text{Im}(\mu)| \leq M\lambda_{\text{max}}(\hat{B})$$

Argument for spectral equivalence of D and $\hat{D}$ is even more trivial

Behavior of Face-Bump System

Spectral Equivalence of $\hat{B}$ and $\hat{D}$

2) Let $\hat{B}_T$ = element matrix for $\hat{B}$, $\mathbf{v}_T$ = element coefficient vector for $\mathbf{v}$

$$\mathbf{v}^t \hat{B} \mathbf{v} = \sum_{T \in \mathcal{T}} \mathbf{v}_T^t \hat{B}_T \mathbf{v}_T$$

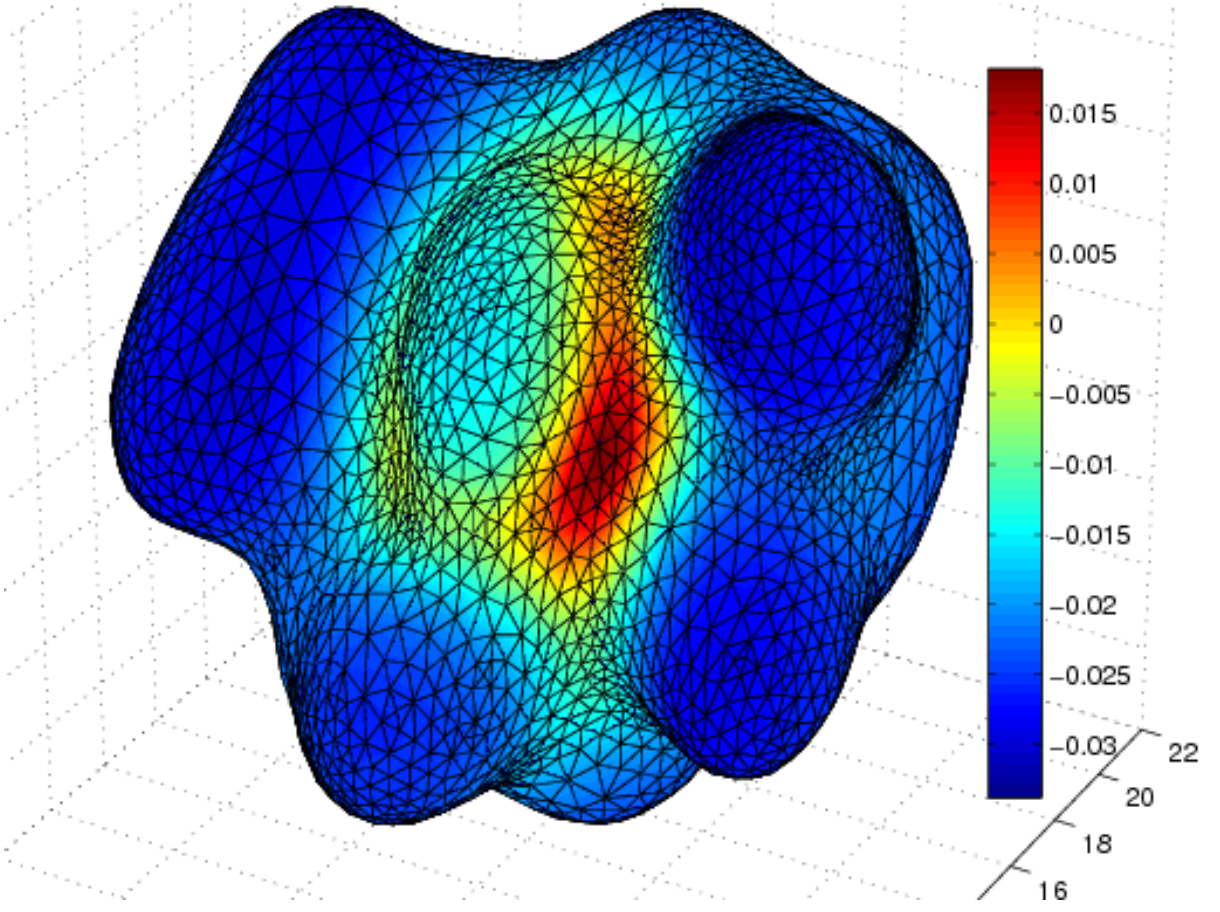
- If $k_0 \mathbf{v}_T^t \hat{D}_T \mathbf{v}_T \leq \mathbf{v}_T^t \hat{B}_T \mathbf{v}_T \leq k_1 \mathbf{v}_T^t \hat{D}_T \mathbf{v}_T$ for every T, then

$$k_0 \mathbf{v}^t \hat{D} \mathbf{v} \leq \mathbf{v}^t \hat{B} \mathbf{v} \leq k_1 \mathbf{v}^t \hat{D} \mathbf{v}$$

$$(\hat{B}_T)_{ij} = 2\frac{3!|T|}{7!} \begin{cases} \sum_{k=1}^{4} d_k^{-2} & , \quad i = j \\ \frac{\cos\theta_{kl}}{d_k d_l} - \frac{2\cos\theta_{ij}}{d_i d_j} & , \quad i \neq j \end{cases} + \frac{3!|T|}{9!} \begin{cases} 8 & , \quad i = j \\ 4 & , \quad i \neq j \end{cases}$$

- Straight-forward analysis shows that $\hat{B}_T$ is spectrally-equivalent to $\hat{D}_T$, and hence $\hat{B}$ is spectrally-equivalent to $\hat{D}$. For piecewise linears, $\hat{B}_T$ is NOT spectrally-equivalent to $\hat{D}_T$.

Illustrating the Above Assertions

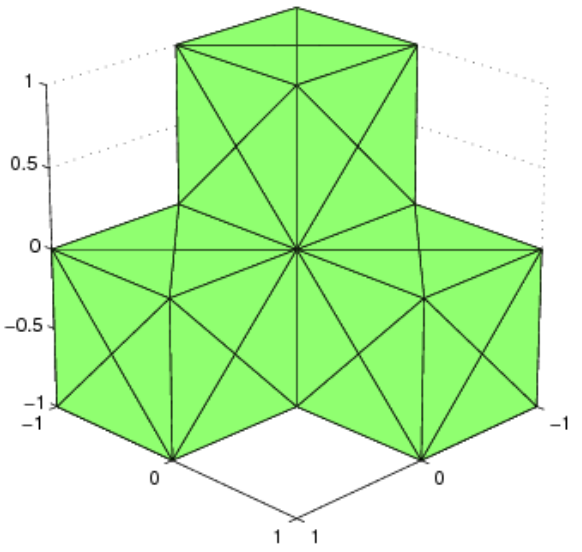


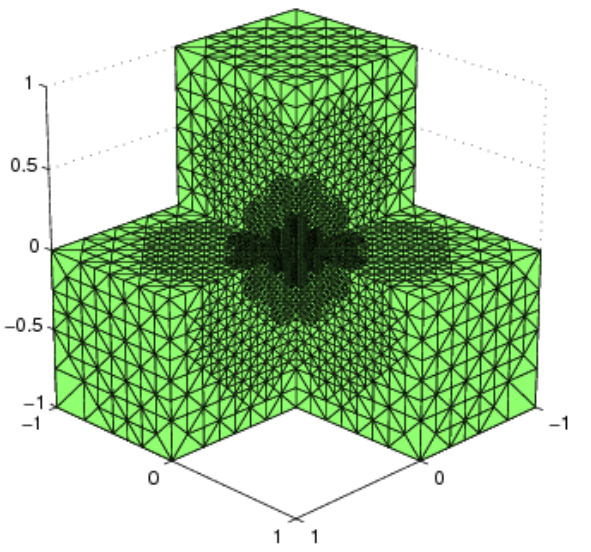
Poisson Problem with (near) Singularity

Problem:

$$-\Delta u = f \text{ in } \Omega \quad , \quad u = 0 \text{ on } \partial\Omega \quad , \quad u = \frac{\sin(\pi x)\sin(\pi y)\sin(\pi z)}{(0.001 + x^2 + y^2 + z^2)^{1.5}}$$

Initial Mesh and an Adapted Mesh

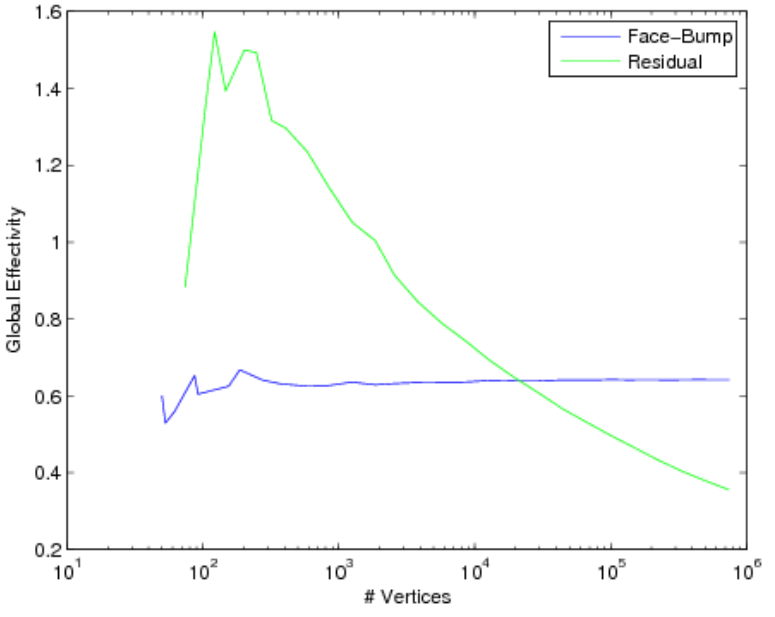


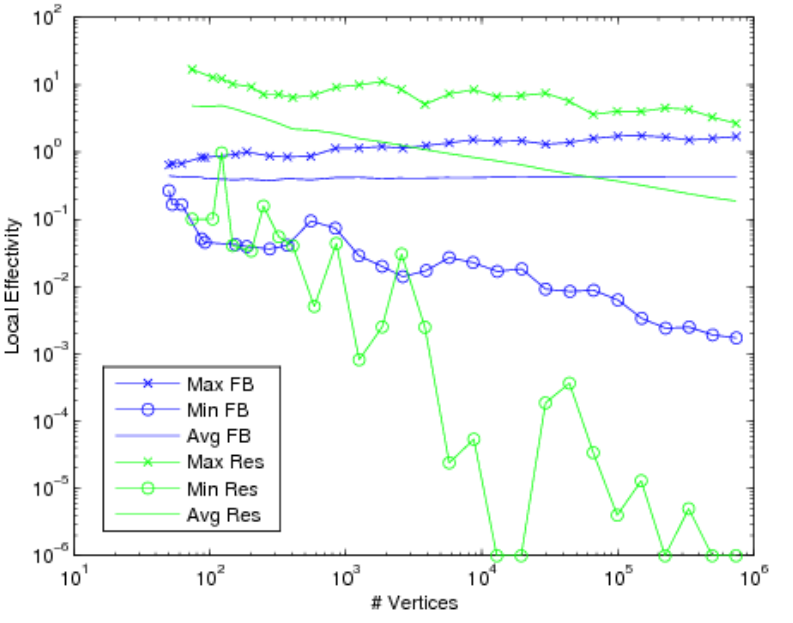


Poisson Problem with (near) Singularity

Global and Local Effectivities: $\dfrac{|||\varepsilon|||}{|||u-\hat{u}|||}$, $\dfrac{|||\varepsilon|||_T}{|||u-\hat{u}|||_T}$ Compared with standard residual indicator

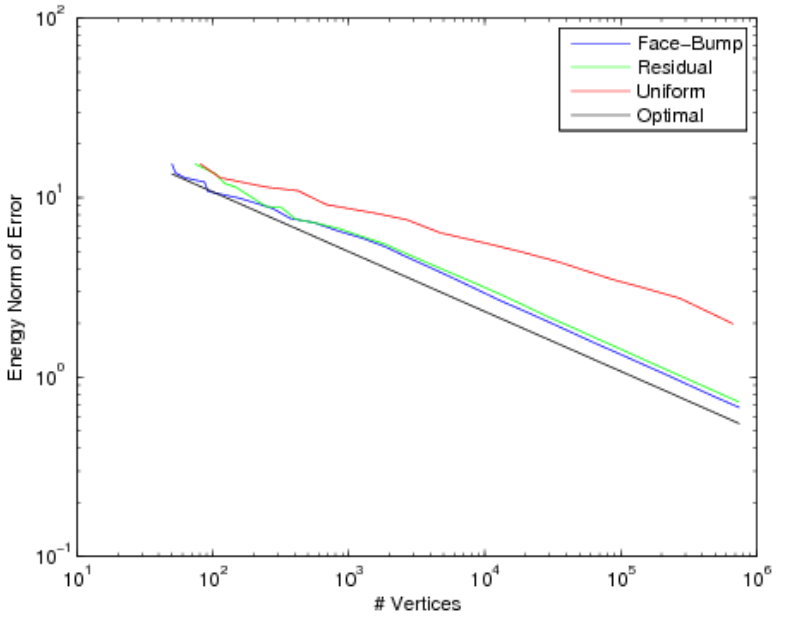
$$\eta^2 = \sum_{T\in\mathcal{T}} \eta_T^2 \quad , \quad \eta_T^2 = \frac{1}{2}\sum_{F\in\mathcal{F}_I} h_T \|r_F\|_{0,F}^2 + \sum_{F\in\partial T\cap\partial\Omega_N} h_T \|r_F\|_{0,F}^2 \ ,$$

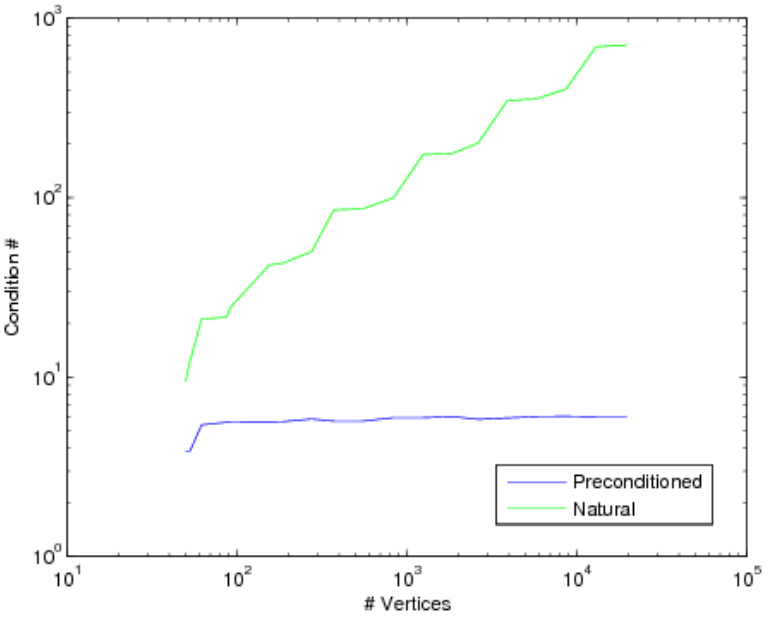




Poisson Problem with (near) Singularity

Error Convergence and Conditioning of Bump Matrix:





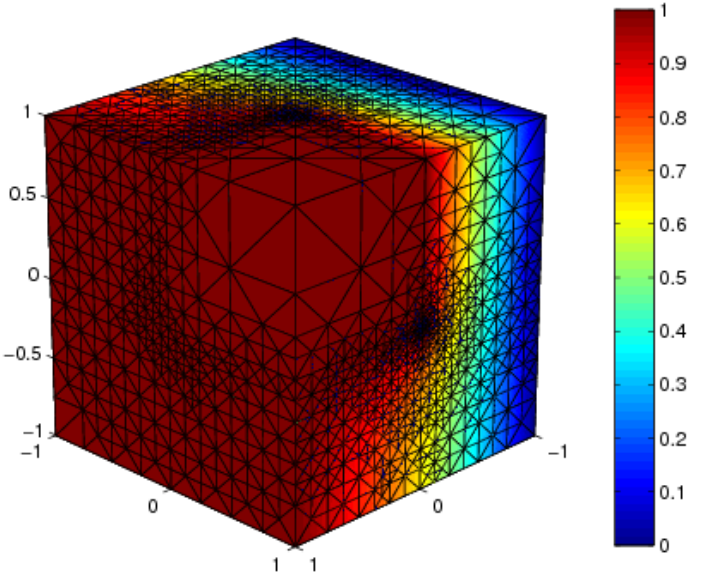
- Preconditioning (symmetric, diagonal rescaling) necessary for adapted meshes

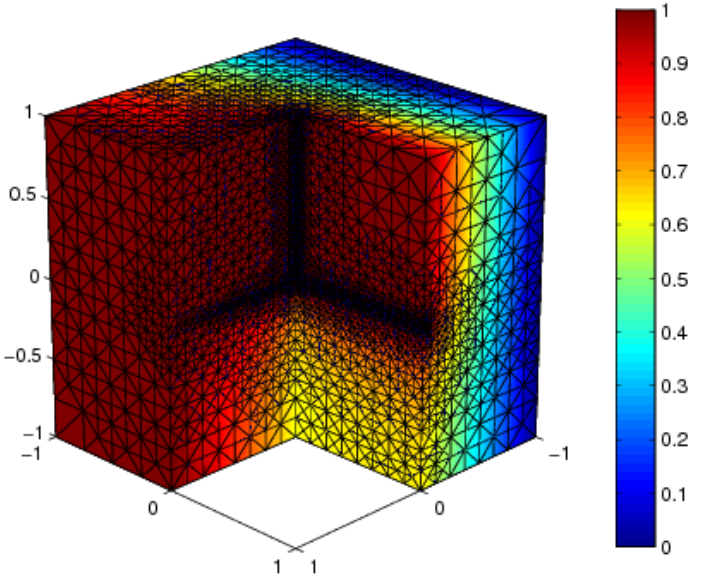
Discontinuous Diffusion Problem

Problem: $-a\Delta u = 0$ in $\Omega = (-1,1)^3$

- $a = 10^5$ in $(0,1)^3$, $a = 1$ elsewhere
- $u = 1$ at $x = 1$ and $u = 0$ at $x = -1$
- Homogeneous Neumann conditions on other four faces

An Adapted Mesh and a Look Inside

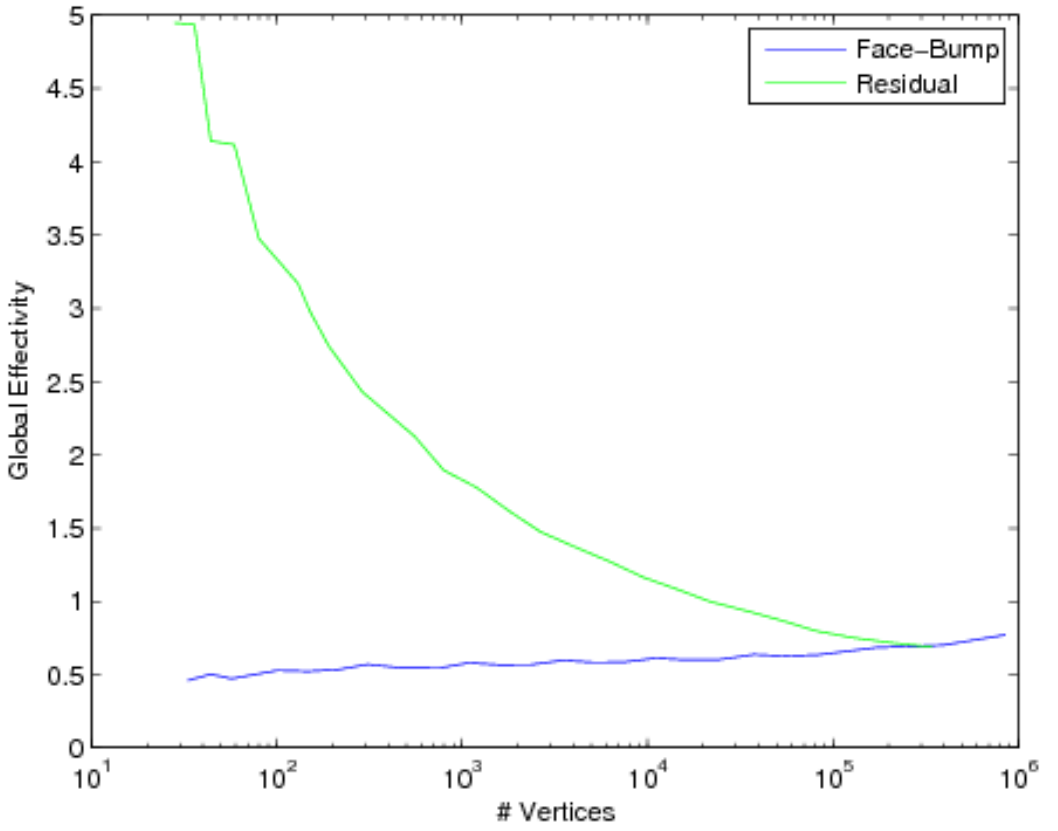




Discontinuous Diffusion Problem

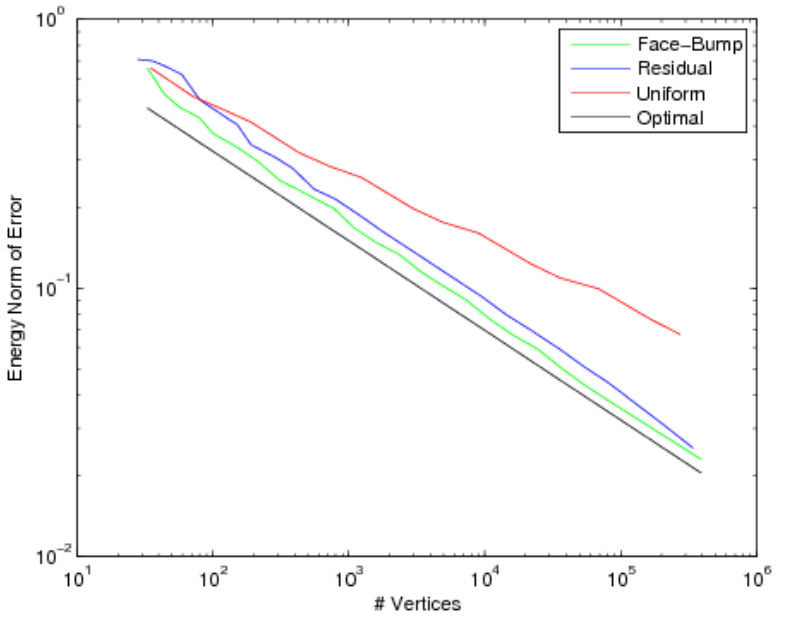
Global Effectivities: $\dfrac{\|\varepsilon\|}{\|\bar{u} - \hat{u}\|}$ $\qquad \bar{u} \in V_{>3\times10^6}$

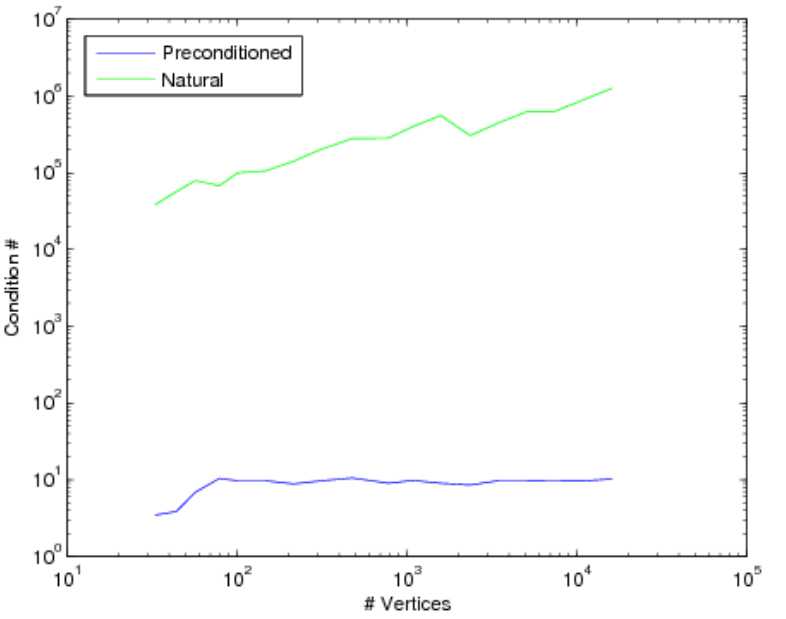
$$\|u - \hat{u}\|^2 = \|u - \bar{u}\|^2 + \|\bar{u} - \hat{u}\|^2 = \|u - \bar{u}\|^2 + (\|\bar{u}\|^2 - \|\hat{u}\|^2)$$



Discontinuous Diffusion Problem

Error Convergence and Conditioning of Bump Matrix:



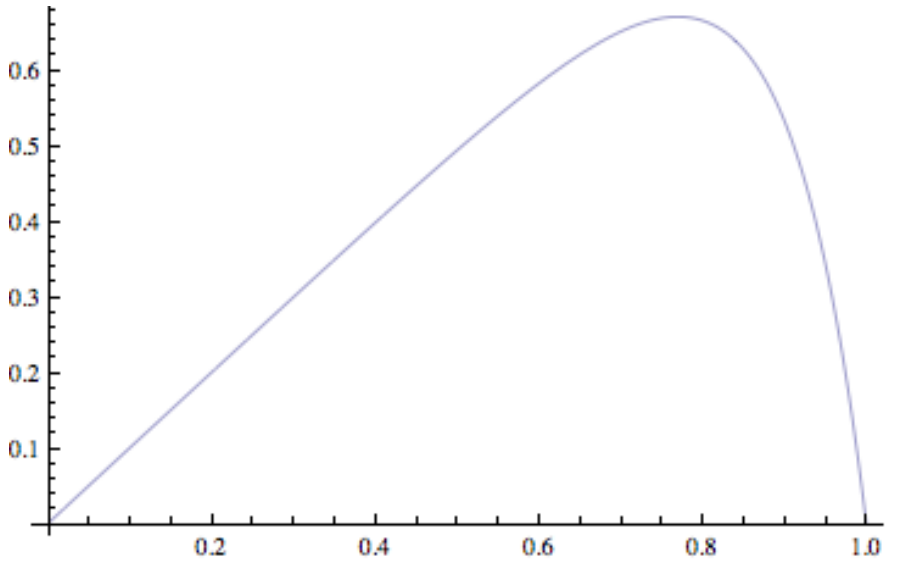


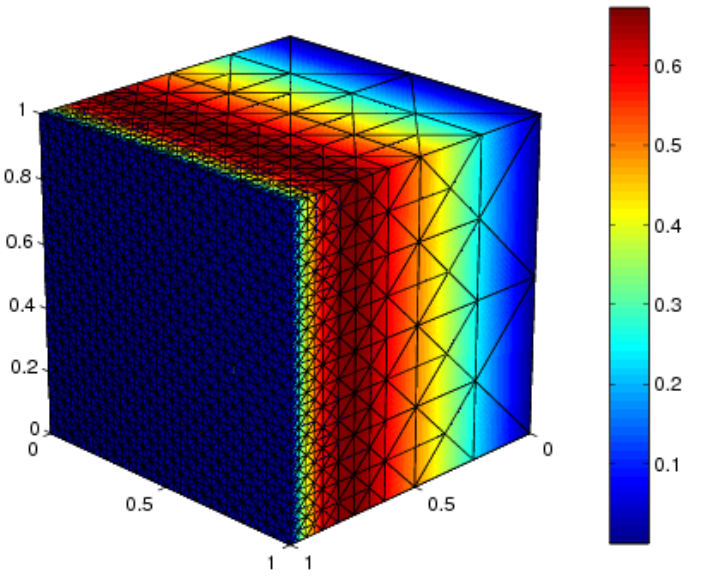
Convection-Diffusion Problem

Problem: $-\epsilon\Delta u + u_x = 1$ in $\Omega = (0,1)^3$, $u = x - \dfrac{e^{(x-1)/\epsilon} - e^{-1/\epsilon}}{1 - e^{-1/\epsilon}}$

- $\epsilon = 0.1$
- $u = 0$ at $x = 0$ and $x = -1$
- Homogeneous Neumann conditions on other four faces

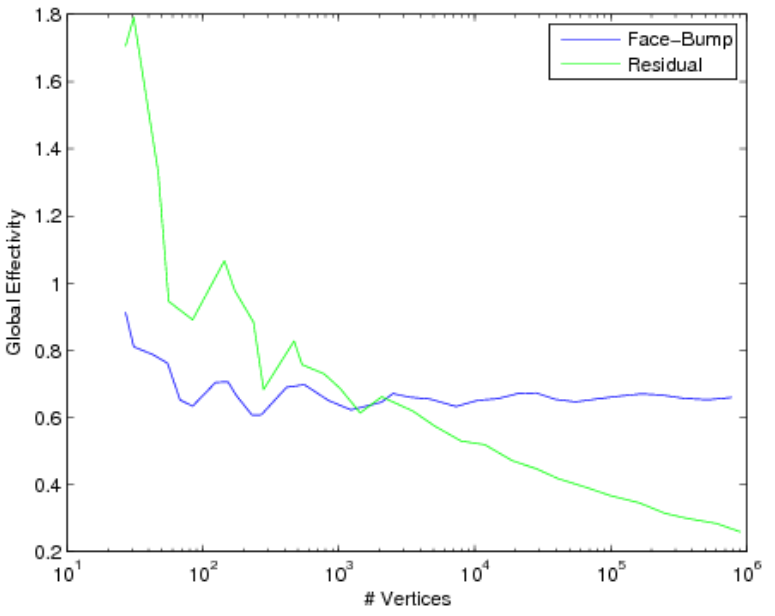
u in the x-direction and an Adapted Mesh

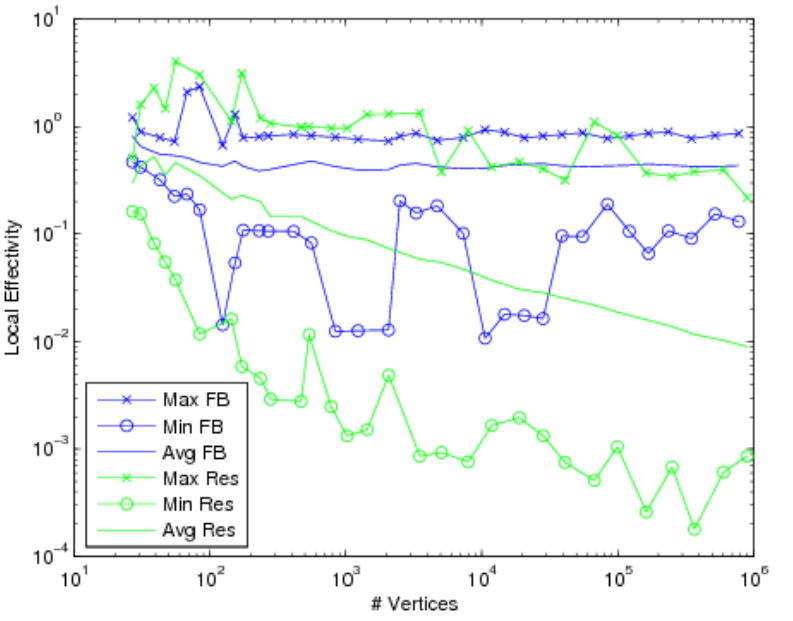




Convection-Diffusion Problem

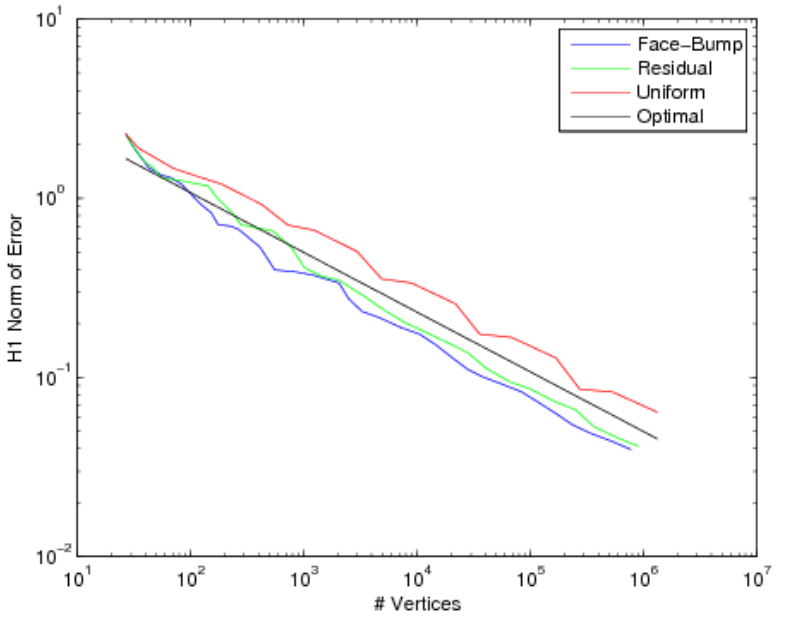
Global and Local Effectivities: $\dfrac{\|\varepsilon\|_1}{\|u-\hat{u}\|_1}$, $\dfrac{\|\varepsilon\|_{1,T}}{\|u-\hat{u}\|_{1,T}}$

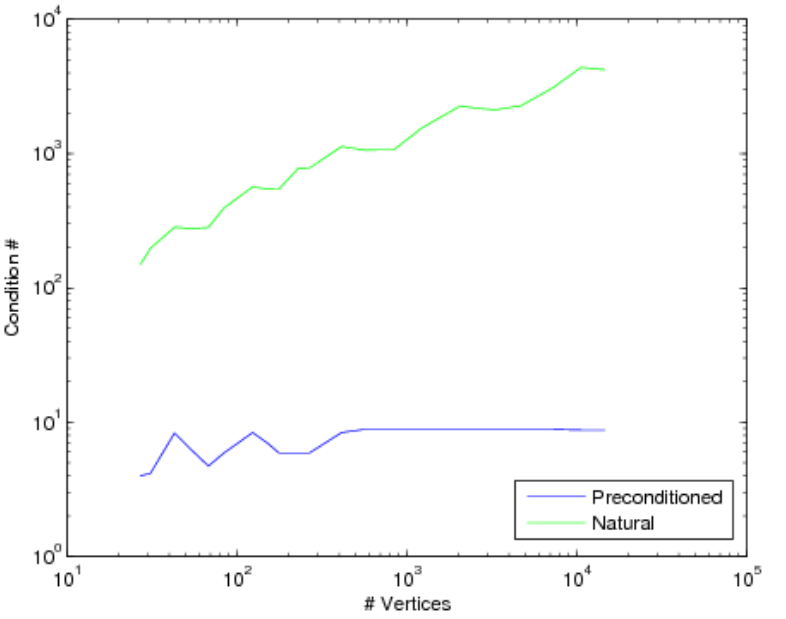




Convection-Diffusion Problem

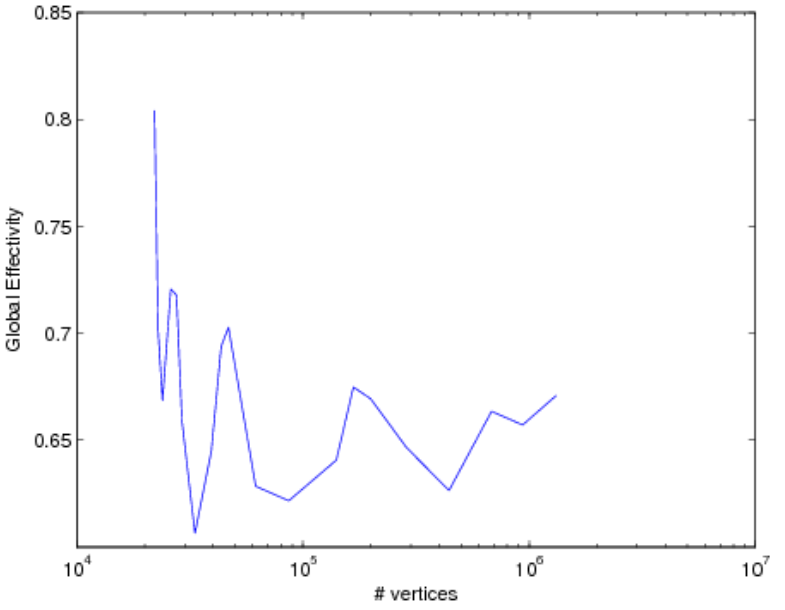
Error Convergence and Conditioning of Bump Matrix:

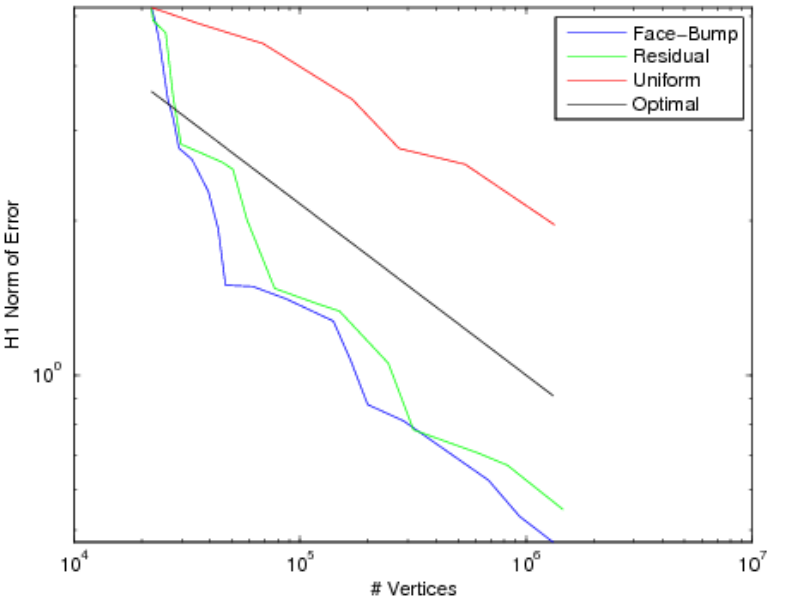




Convection-Diffusion Problem

Global Effectivity and Error Convergence for $\epsilon = 10^{-2}$:

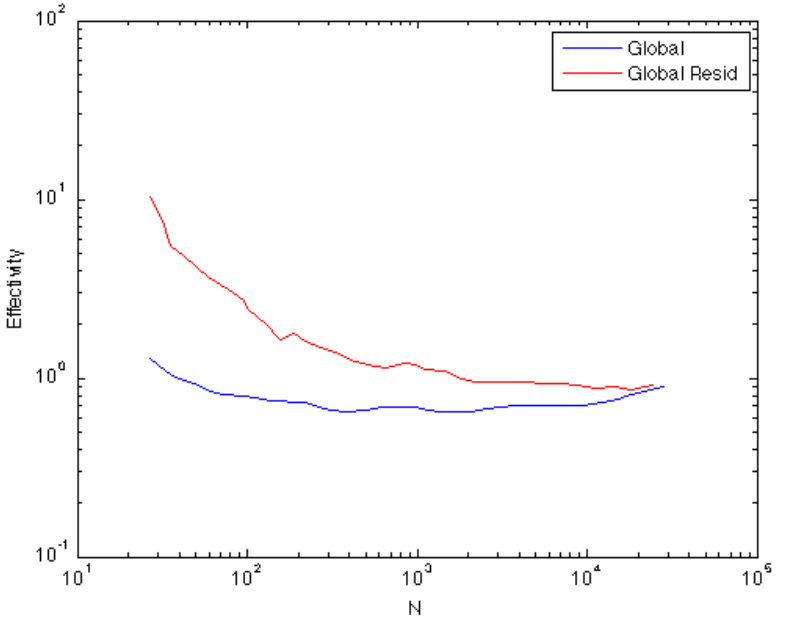


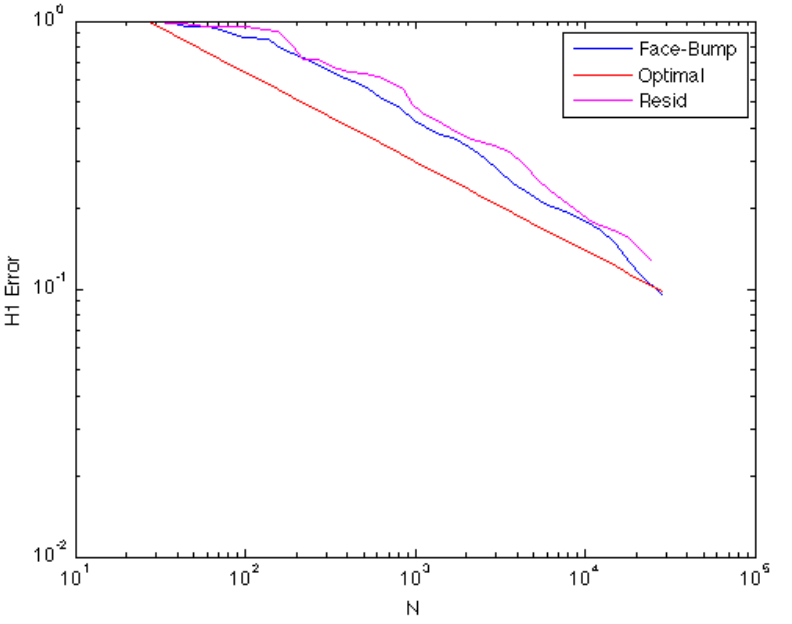


Another Convection-Diffusion Problem

Problem: $-\Delta u + \mathbf{b} \cdot \nabla u = 1$ in $\Omega = (-1,1)^3$, $u = 0$ on $\partial\Omega$, where $\mathbf{b} = (-12y, 12x, 12z)$

Global Effectivity and Error Convergence



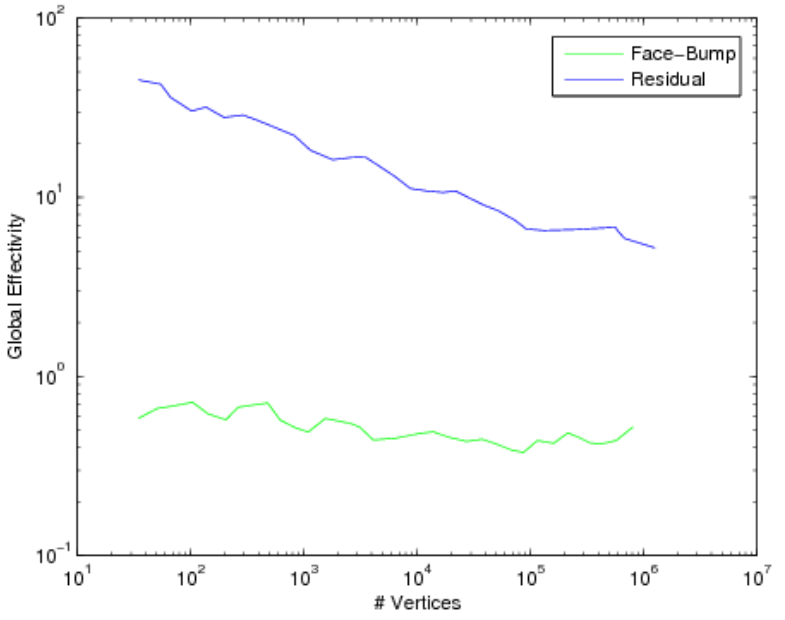


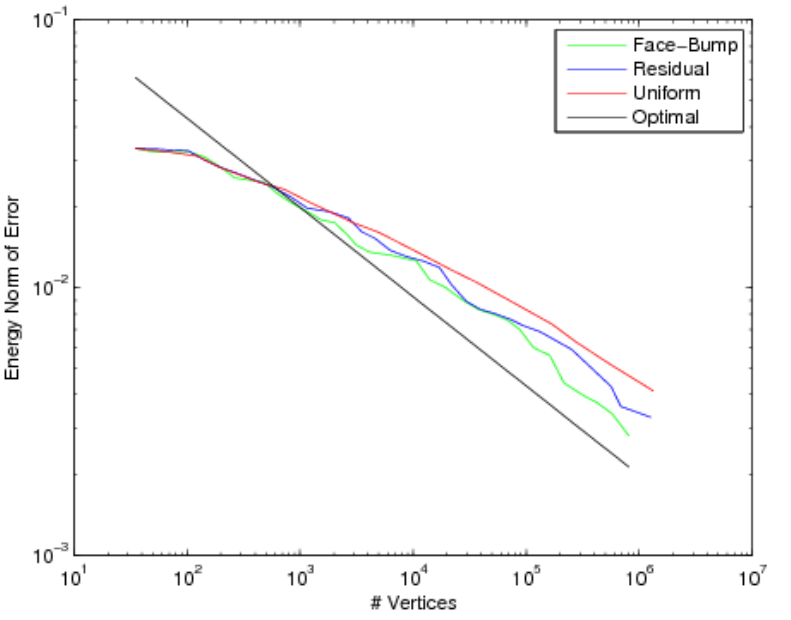
Anisotropic Diffusion Problem

Problem: $-\nabla \cdot (A\nabla u) = 1$ in $\Omega = (-1,1)^3$

- $A = \text{diag}(1, \epsilon, \epsilon^{-1})$, $\epsilon = 10^{-3}$
- Homogeneous Dirichlet conditions
- Error estimated as in Discontinuous-Diffusion problem

Global Effectivity and Error Convergence





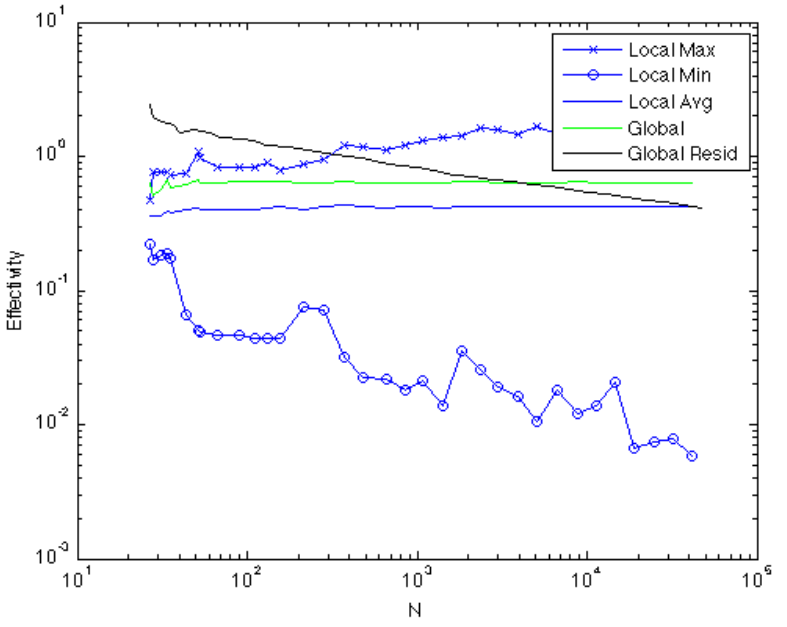
Non-Linear Reaction-Diffusion Problem

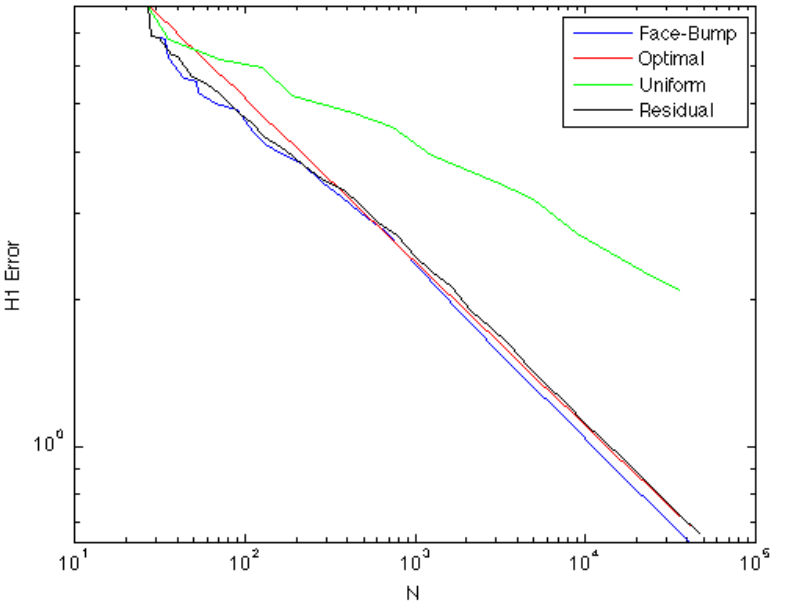
Problem: $-\Delta u + e^u = f$ in $\Omega = (0,1)^3$, $u = 0$ on $\partial\Omega$

$$u = (x^2 + y^2 + z^2 + 10^{-4})^{-3/2} \sin(\pi x)\, \sin(\pi y)\, \sin(\pi z)$$

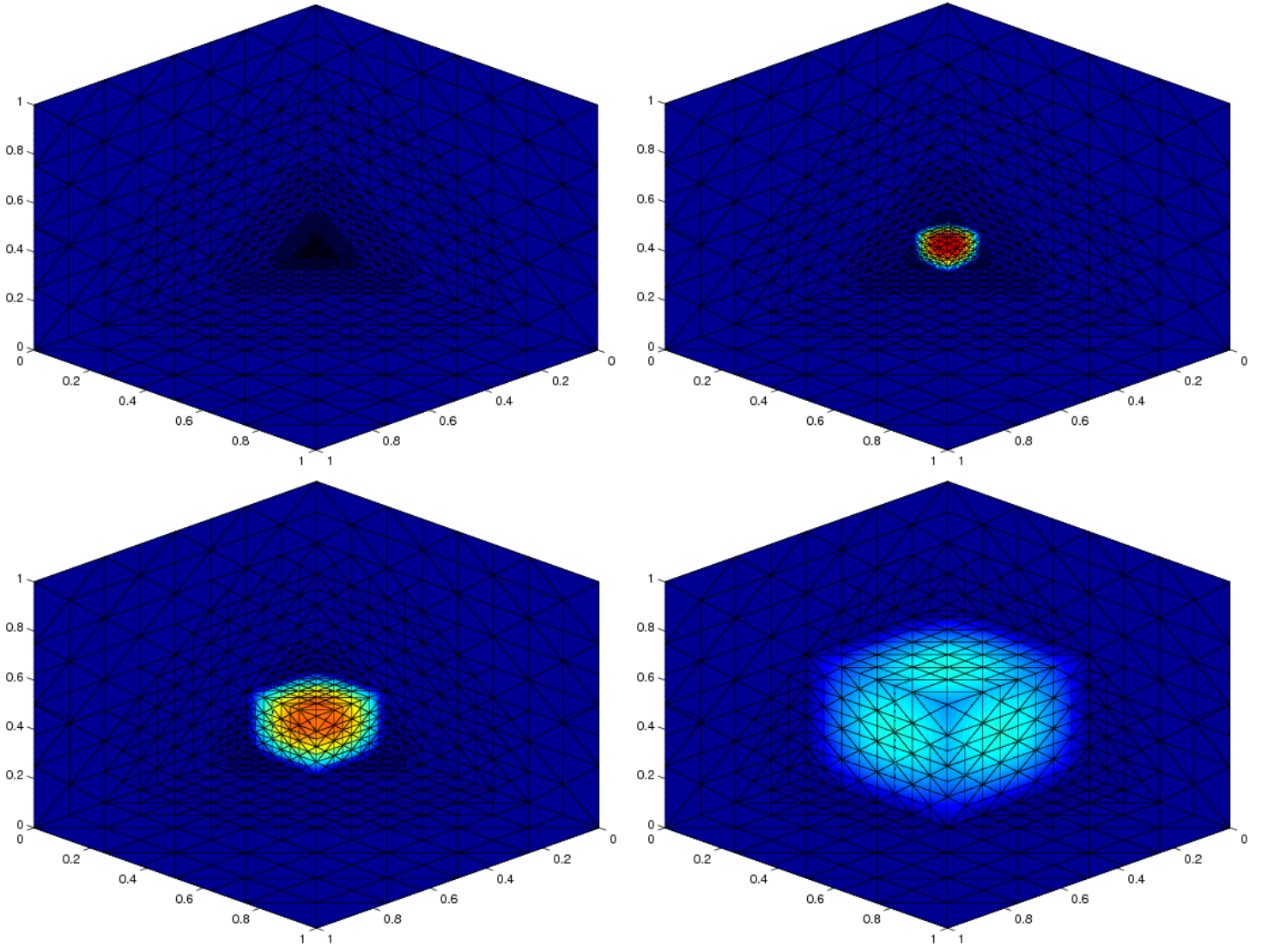
$$B(\hat{u} + \varepsilon, v) = F(v) - B(\hat{u}, v) \rightsquigarrow B(\hat{u}; \varepsilon, v) = F(v) - B(\hat{u}, v) \text{ for all } \varepsilon \in W$$

Global Effectivity and Error Convergence

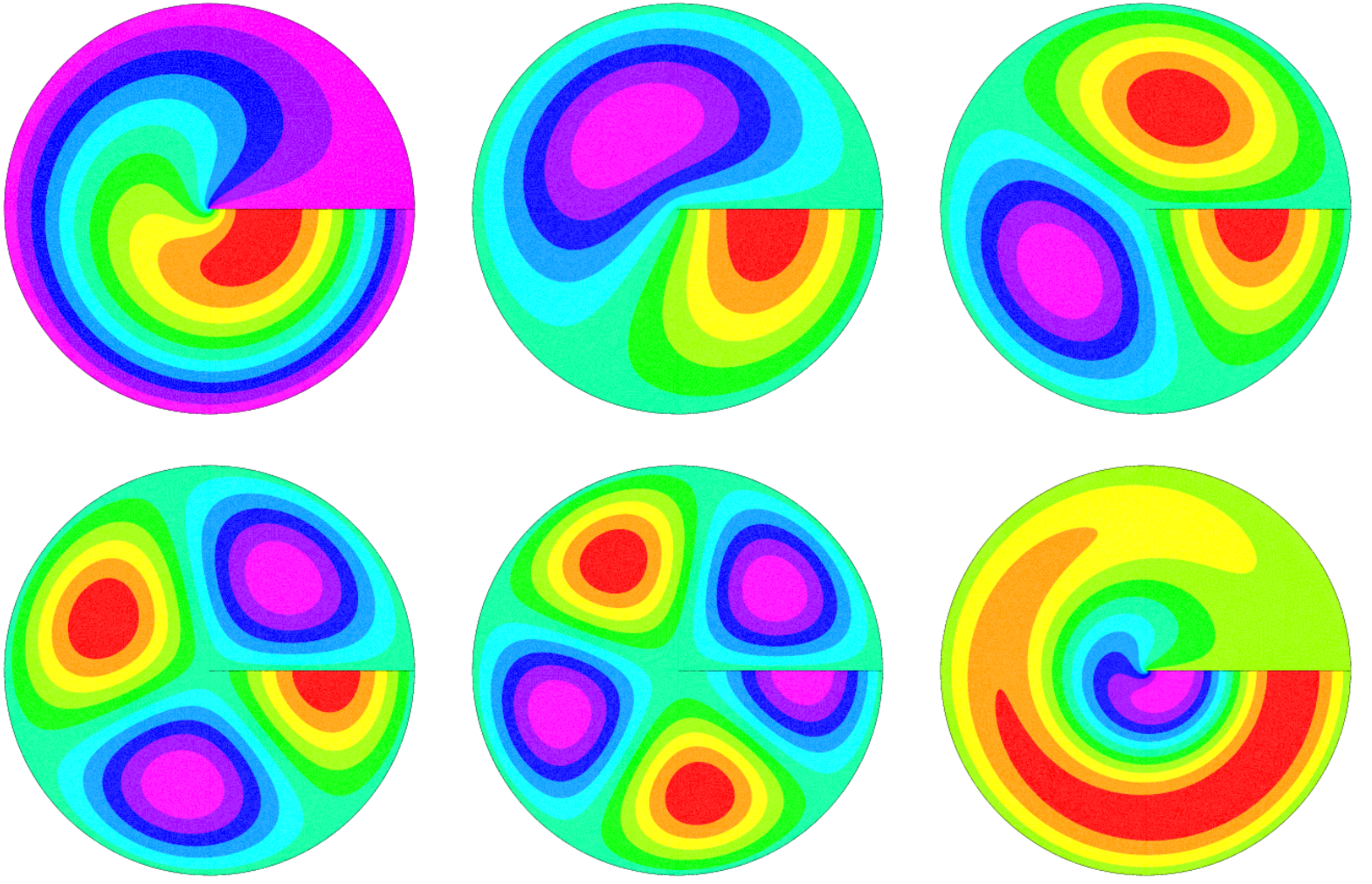




Non-Linear Reaction-Diffusion Problem

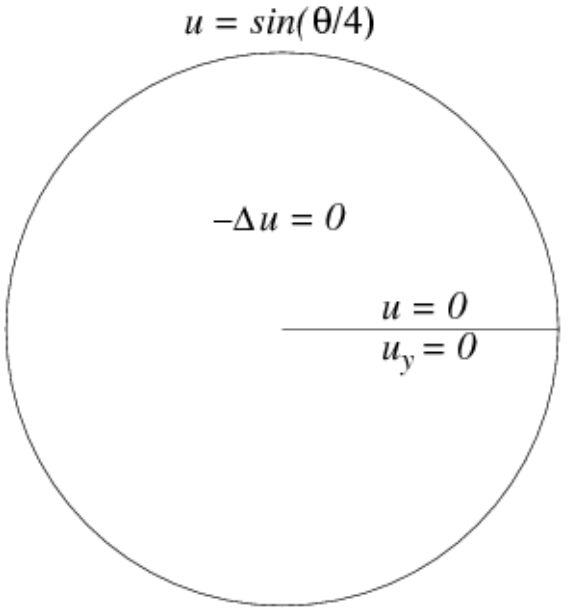


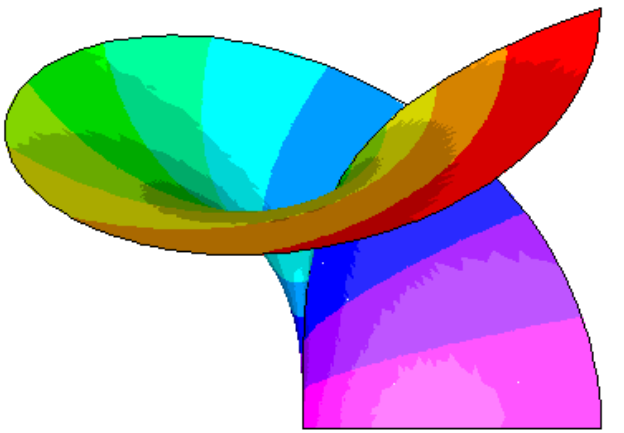
Hope for Flexibility in $\mathbb{R}^3$, Experience in $\mathbb{R}^2$



Measurements in Different Norms

$$u = r^{1/4}\sin(\theta/4) \in W^{2,1}(\Omega) \setminus H^2(\Omega)$$

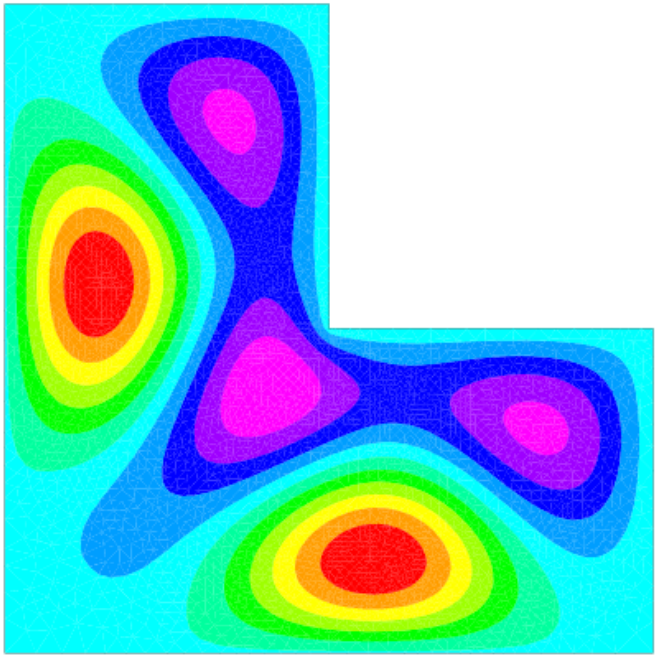


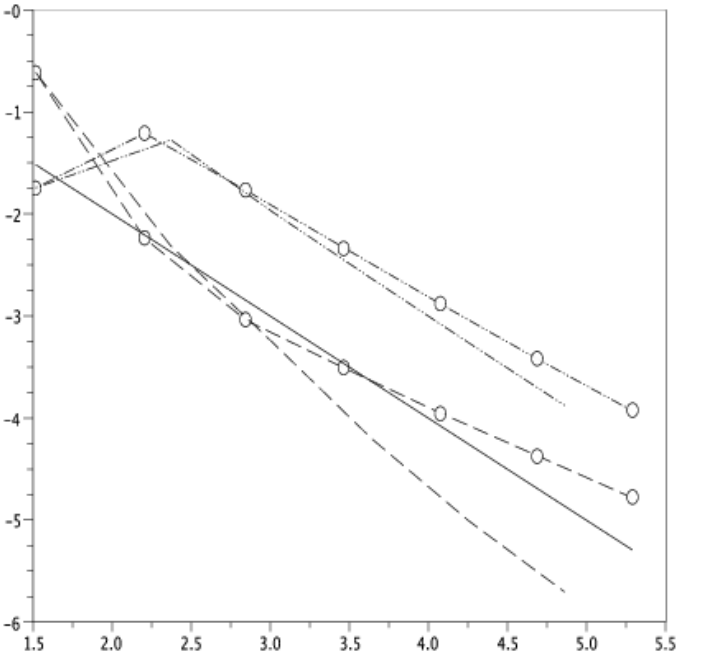


Hessian Recovery in $W^{2,1}(\Omega)$**,** $|u|_{2,1} = \int_\Omega |u_{xx}| + 2|u_{xy}| + |u_{yy}|\, dV = 12$

NT	94	481	2031	8334	33704	135632
$\lvert\varepsilon\rvert_{2,1}$	7.8728	9.3262	10.282	10.992	11.496	11.798
EFF	0.6561	0.7772	0.8568	0.9160	0.9580	0.9832

Eigenvalue Problems

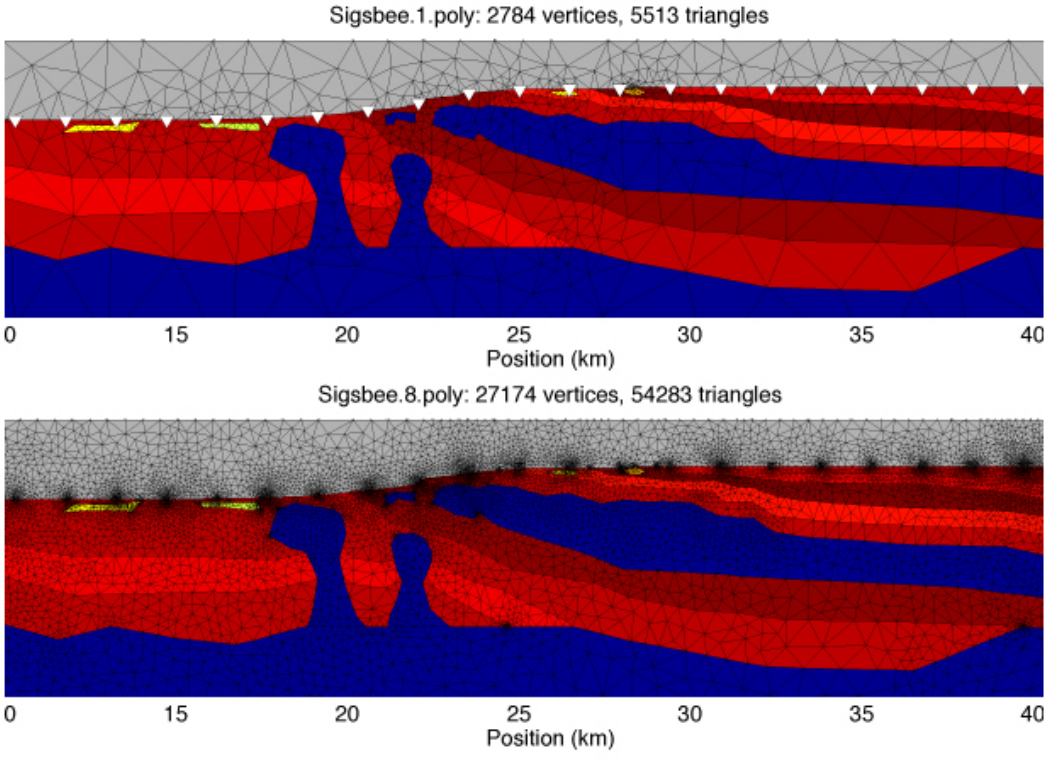




- Grubisic/Ovall 2008, Bank/Grubisic Ovall 2010, error estimates, adaptivity, covergence acceleration
- Analysis needs approximate error function(s) in $\mathcal{H}$
  - Works for clusters of eigenvalues, degenerate (multiplicity>1) eigenvalues, low-regularity eigenfunctions

Goal-Oriented Adaptivity

- Interested in driving down error in some (small) regions.
- Must be mindful of pollution effects.



- Ovall 2007, in a similar vein as Rannacher/Becker, Giles/Süli, etc.
- Some form of dual-weighting of the residual