

LEAST-SQUARES FINITE ELEMENT METHODS FOR PDES IN NONSMOOTH DOMAINS

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- Haris Amin
- Sam Calisch

Broad Overview

Partial differential equations (PDEs) on polygonal/polyhedral domains may have nonsmooth solutions and, as a consequence, many numerical methods have difficulties. We address this problem in a least-squares finite element context.

Target Applications:

- Elasticity
 - Linear
 - Geometrically Nonlinear (soft tissue, e.g.)
- Incompressible Fluid Flow
 - Navier-Stokes
 - Non-Newtonian (biological fluids, e.g.)

Outline

- Regularity of 2nd order problems
- Prototypical div-curl and $H(\text{div})$ least-squares methods
- Weighted-norm minimization
- Theoretical results
- Numerical results
- Example in viscoelasticity
- Conclusions / open questions / current projects

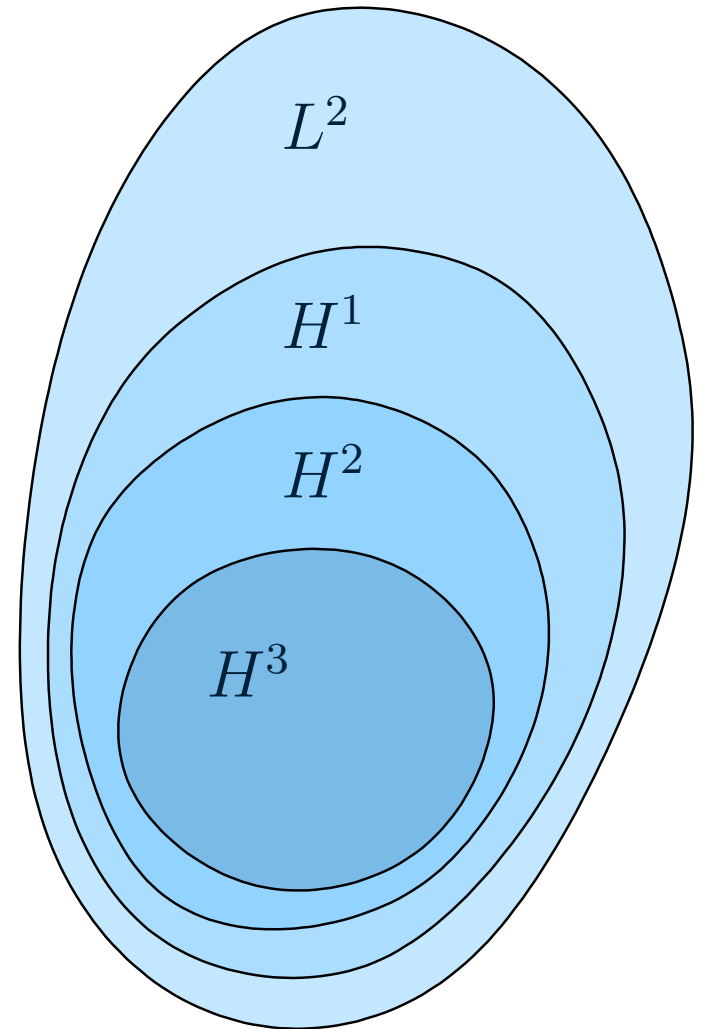
Standard Sobolev Norms and Spaces

The $L^2(\Omega)$ norm of u is

$$\|u\| = \left(\int_{\Omega} |u|^2 dx \right)^{1/2}$$

The $H^k(\Omega)$ norm is

$$\|u\|_k = \left(\sum_{|\alpha| \leq k} \int_{\Omega} |D^{\alpha} u|^2 dx \right)^{1/2}$$



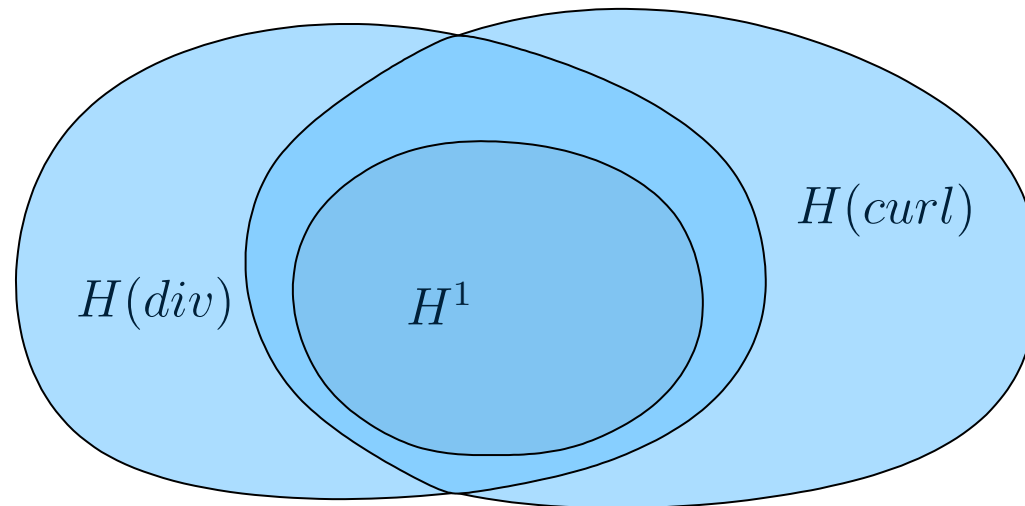
Spaces for Vector Functions

for vector functions, $\mathbf{u} \in L^2(\Omega)^2$

$$\|\mathbf{u}\|_1 = (\|\mathbf{u}\|^2 + \|\nabla \mathbf{u}\|^2)^{1/2}$$

$$\|\mathbf{u}\|_{H(div)} = (\|\mathbf{u}\|^2 + \|\nabla \cdot \mathbf{u}\|^2)^{1/2} \quad H^1 \subseteq H(div) \cap H(curl)$$

$$\|\mathbf{u}\|_{H(curl)} = (\|\mathbf{u}\|^2 + \|\nabla \times \mathbf{u}\|^2)^{1/2}$$



but when is $H(div) \cap H(curl) = H^1$?

PDEs and Regularity in Nonsmooth Domains

Let Ω be a polygonal domain in \mathbb{R}^2 .

Consider the Dirichlet problem for Poisson's equation

$$\Delta p = f, \text{ in } \Omega$$

$$p = 0, \text{ on } \partial\Omega$$

Q: If $f \in L^2(\Omega)$ when can we expect $p \in H^2(\Omega)$?

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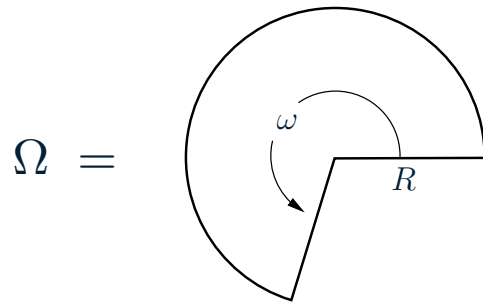
$$p = 0, \text{ on } \partial\Omega$$

Q: If $f \in L^2(\Omega)$ when can we expect $p \in H^2(\Omega)$?

A: It depends on Ω . If Ω is convex then the problem has full regularity and

$$f \in L^2(\Omega) \implies p \in H^2(\Omega).$$

Nonsmooth Domains

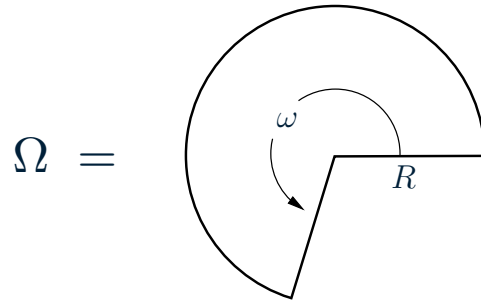


The solution to Poisson's equation near the corner may have a component of the form:

$$s(r, \theta) = r^\alpha \sin(\alpha\theta), \quad \alpha = \frac{\pi}{\omega}$$

(r, θ) a local polar coordinate system

Nonsmooth Domains



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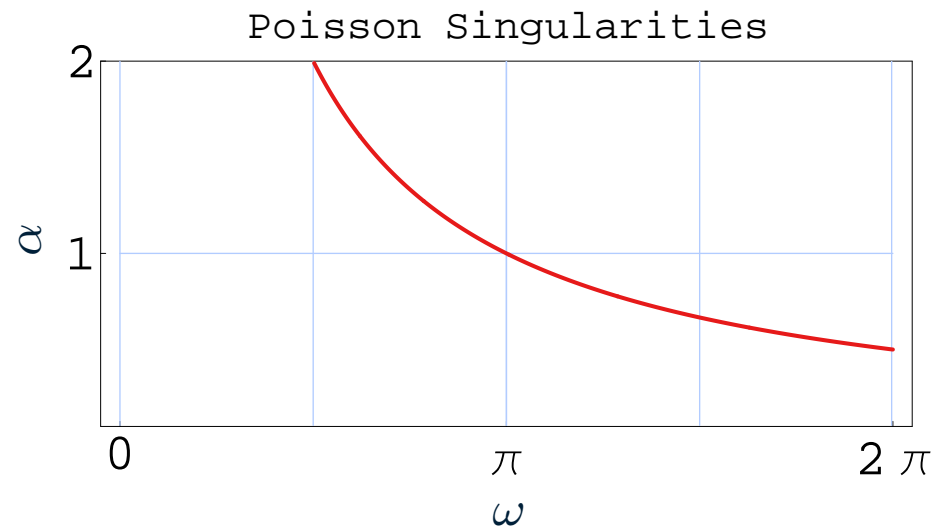
(r, θ) a local polar coordinate system

$$p = p_0 + s \quad p_0 \in H^2(\Omega), \quad s \in H^{1+\alpha}(\Omega)$$

$$\omega > \pi \quad \implies \quad \alpha < 1 \quad \implies \quad p \notin H^2(\Omega)$$

Singular Functions for 2nd Order PDEs

$$\alpha = \pi/\omega$$
$$p \in H^{1+\alpha}(\Omega)$$

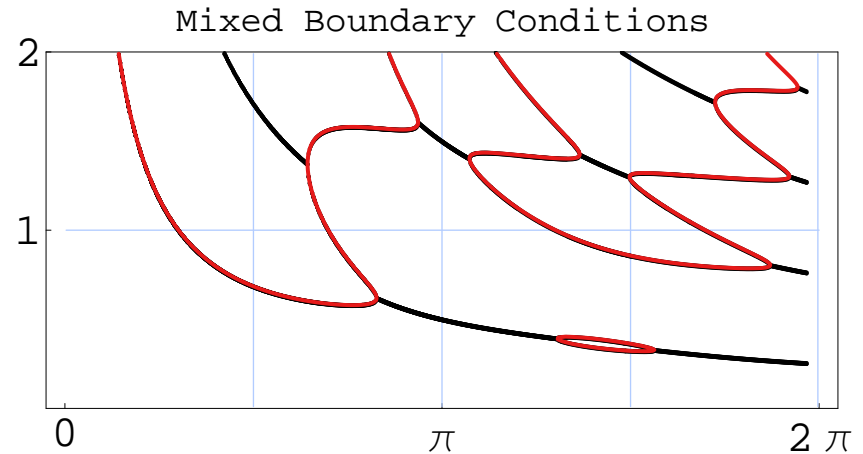
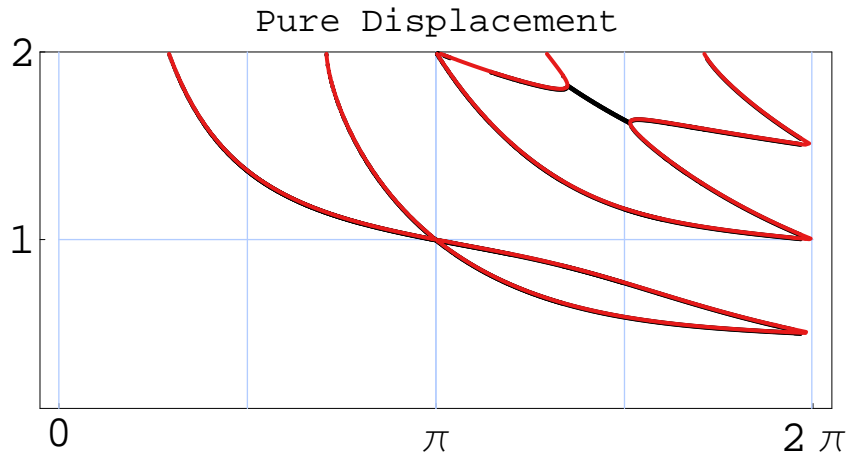


$\alpha < 1 \implies$ Loss of regularity for the PDE

This singular behavior is known for many 2nd order PDEs. (Grisvard et. al.)

Other PDEs: 2-d Linear Elasticity

α vs. ω for linear elasticity with Lamé constants $\lambda = 2.15$, $\mu = 1$.



In general, the singular solutions may depend on

- Corner angle, ω
- Boundary condition type
- PDE coefficients
- Nonlinearities

Implications for Numerical Methods

Convergence of standard methods is limited by the smoothness of the solution.

example:

P_k = degree k piecewise polynomial functions on a mesh of size h .

The interpolant onto P_k gives

$$\|p - I^h p\| \leq ch^\alpha \|p\|_\alpha \quad \text{for } \alpha \leq k + 1.$$

\implies convergence is limited by both the FE space and α .

Pollution Effect:

Reduced rates are seen globally even though the singularity is local.

Numerical Solutions to PDEs

Let

$$Lu = f$$

be a first-order PDE on a bounded $\Omega \subset \mathbb{R}^d$.

- L first-order differential operator
- $u \in \mathcal{V}$ unknowns
- \mathcal{V} some appropriate function space
- $\mathcal{V}^h \subset \mathcal{V}$ a finite element space
- $f \in L^2(\Omega)$ given data function

Least-Squares Methods

Define the least-squares functional

$$G(u; f) = \|Lu - f\|_X^2$$

Minimizing G over \mathcal{V}^h is equivalent to the weak problem:

$$\text{Find } u^h \in \mathcal{V}^h \text{ such that } \langle Lu^h - f, Lv^h \rangle_X = 0 \quad \forall v^h \in \mathcal{V}^h.$$

Here, a variational problem is formed by minimizing the residual of the problem in the norm $\|\cdot\|_X$. This leads to a s.p.d. linear problem of the form

$$A_{ij} = \langle L\phi_j, L\phi_i \rangle.$$

(Here, $\{\phi_i\}$ is the basis of the approximation space.)

If the approximation error is $e^h = u^h - u$ then

$$\begin{aligned} G(u^h; f) &= \|Lu^h - f\|_X^2 \\ &= \|Lu^h - Lu\|_X^2 \\ &= \|L(u^h - u)\|_X^2 \\ &= \|Le^h\|_X^2 \\ &= G(e^h; 0) \end{aligned}$$

and we seek to show \mathcal{V} -ellipticity: $\exists c_0, c_1 > 0$ where

$$c_0 \|u\|_{\mathcal{V}} \leq \|Lu\|_X \leq c_1 \|u\|_{\mathcal{V}} \quad \text{for all } u \in \mathcal{V}.$$

\implies minimizing $G(u^h, f)$ minimizes the error in the \mathcal{V} norm.

The design of a least-squares finite element method involves...

- formulating an appropriate first-order system, $Lu = f$
- finding the right norm, $\|\cdot\|_X$, to minimize over
- proving equivalence of LS functional to a meaningful norm on \mathcal{V}
- choosing good FE spaces, $\mathcal{V}^h \subset \mathcal{V}$

2 Specific Examples for Poisson

$$\begin{cases} \Delta p = f, & \Omega \\ p = 0, & \partial\Omega \end{cases}$$

$$(1) \begin{cases} \nabla p - \mathbf{u} = 0, & \Omega \\ \nabla \cdot \mathbf{u} = f, & \Omega \\ \nabla \times \mathbf{u} = 0, & \Omega \\ p = 0, & \partial\Omega \\ \boldsymbol{\tau} \cdot \mathbf{u} = 0, & \partial\Omega \end{cases}$$

div-curl method

$$(2) \begin{cases} \nabla p - \boldsymbol{\sigma} = 0, & \Omega \\ \nabla \cdot \boldsymbol{\sigma} = f, & \Omega \\ p = 0, & \partial\Omega \\ \boldsymbol{\tau} \cdot \boldsymbol{\sigma} = 0, & \partial\Omega \end{cases}$$

H(div) method

div-curl Method

$$\left\{ \begin{array}{ll} \nabla p - \mathbf{u} = 0, & \Omega \\ \nabla \cdot \mathbf{u} = f, & \Omega \\ \nabla \times \mathbf{u} = 0, & \Omega \\ p = 0, & \partial\Omega \\ \boldsymbol{\tau} \cdot \mathbf{u} = 0, & \partial\Omega \end{array} \right. \quad \begin{array}{l} G_1(\mathbf{u}; f) = \|\nabla \cdot \mathbf{u} - f\|^2 + \|\nabla \times \mathbf{u}\|^2 \\ G_2(p; \mathbf{u}) = \|\nabla p - \mathbf{u}\|^2 \\ \mathcal{V} = \{\mathbf{v} \in H^1(\Omega) : \boldsymbol{\tau} \cdot \mathbf{v} = 0 \text{ on } \partial\Omega\} \\ \mathcal{W} = \{q \in H^1(\Omega) : q = 0 \text{ on } \partial\Omega\} \end{array}$$

(1) Given $f \in L^2(\Omega)$, choose \mathbf{u} so that

$$G_1(\mathbf{u}; f) = \min_{\mathbf{v} \in \mathcal{V}} G_1(\mathbf{v}; f)$$

(2) Given $\mathbf{u} \in \mathcal{V}$, choose u so that

$$G_2(p; \mathbf{u}) = \min_{q \in \mathcal{W}} G_2(q; \mathbf{u})$$

First stage functional, G_1

We would like to solve

$$\begin{cases} \nabla \cdot \mathbf{u} = f, & \Omega \\ \nabla \times \mathbf{u} = 0, & \Omega \end{cases}$$

over a subspace of $H^1(\Omega)$. Naturally,

$$f \in L^2(\Omega) \implies \mathbf{u} \in H(\operatorname{div}) \cap H(\operatorname{curl}).$$

Full regularity would give

$$f \in L^2(\Omega) \implies p \in H^2(\Omega) \implies \mathbf{u} \in H^1(\Omega).$$

For polygonal domains $H^1(\Omega) = H(\operatorname{div}) \cap H(\operatorname{curl}) \iff \Omega$ is convex.

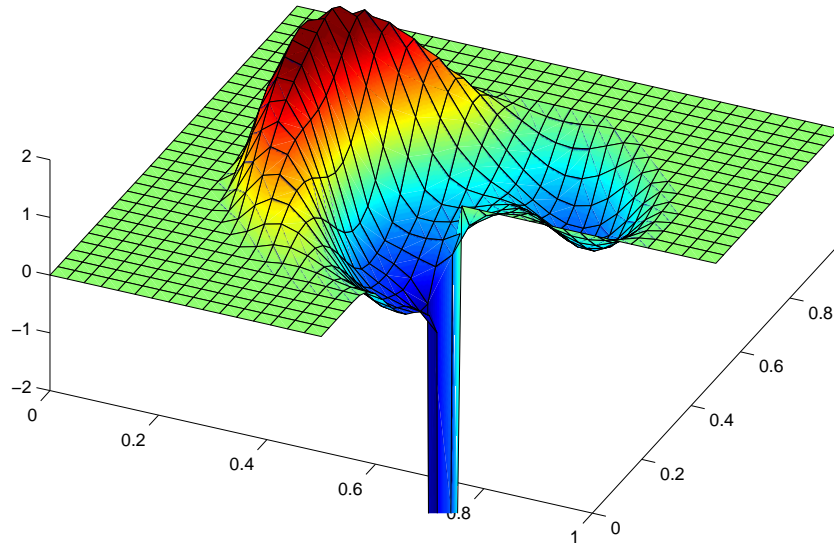
Numerical Approximations and Convergence

Let \mathcal{T}^h be a regular triangulation of Ω of elements, K , of size $O(h)$, and $P_1(K)$ be the space of linear polynomials on K .

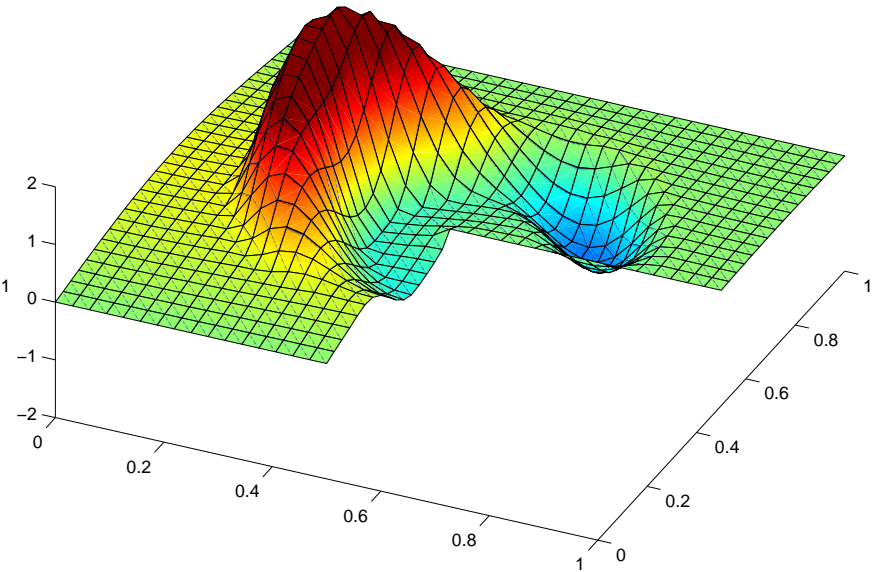
$$\mathbf{u}^h \in \mathcal{V}^h = \underbrace{\{\mathbf{v} \in H^1(\Omega) : \boldsymbol{\tau} \cdot \mathbf{v}|_{\partial\Omega} = 0, \mathbf{v}|_K \in P_1(K) \forall K \in \mathcal{T}^h\}}_{\text{continuous piecewise linears}}$$

- if $\alpha < 1$ then $\mathbf{u} \in H(\text{div}) \cap H(\text{curl}) \setminus H^1(\Omega)$, and the method will not converge to the right solution.
- if $\alpha \in [1, 2)$ then $\mathbf{u} \in H^1(\Omega) \setminus H^2(\Omega)$, and the method will converge slowly.
- if $\alpha \geq 2$ then $\mathbf{u} \in H^2(\Omega)$, and the method will converge at optimal $O(h)$.

The Pollution Effect, $\alpha = 2/3$

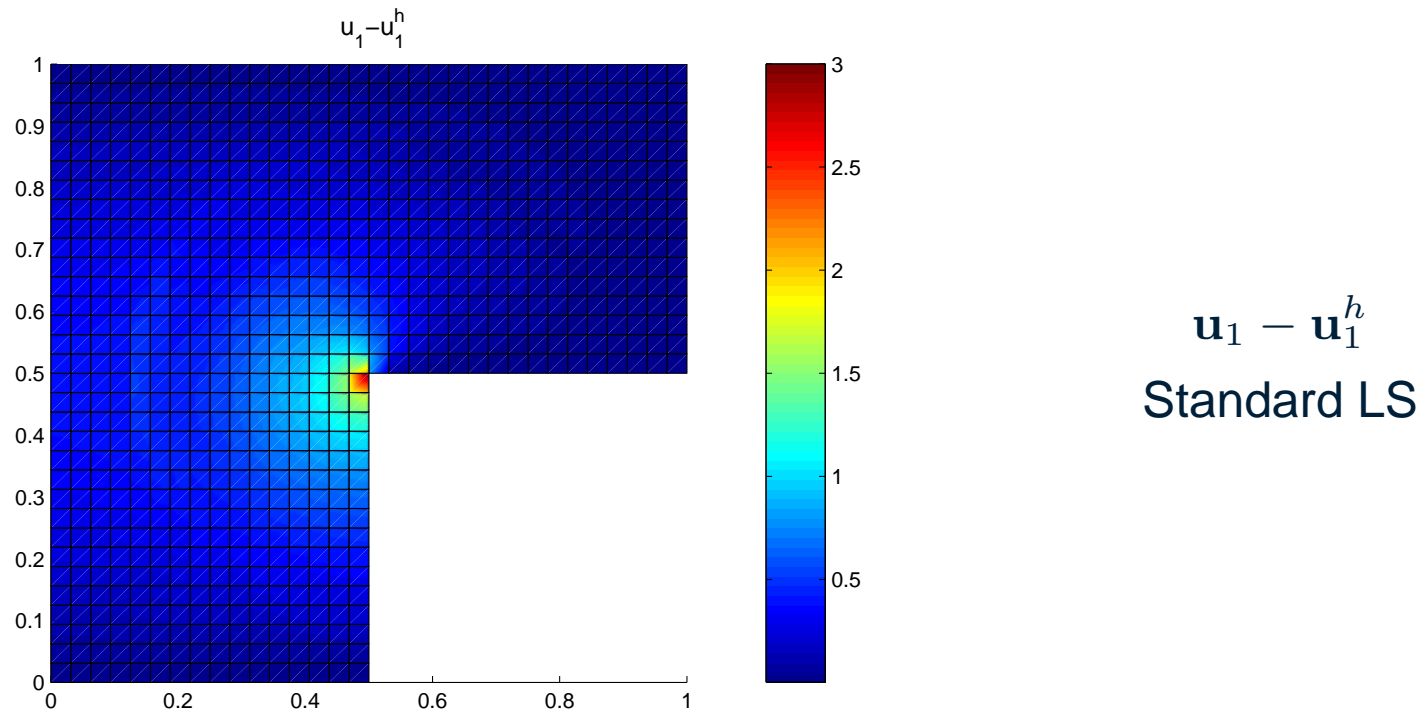


Exact component u_1



u_1^h computed by standard LS

The Pollution Effect, $\alpha = 2/3$



- Significant global errors persist due to gap between solution space and approximation space.

H(div) Formulation of Poisson

$$\left\{ \begin{array}{ll} \nabla p - \boldsymbol{\sigma} = 0, & \Omega \\ \nabla \cdot \boldsymbol{\sigma} = f, & \Omega \\ p = 0, & \partial\Omega \\ \boldsymbol{\tau} \cdot \boldsymbol{\sigma} = 0, & \partial\Omega \end{array} \right. \quad G(p, \boldsymbol{\sigma}; f) = \|\nabla p - \boldsymbol{\sigma}\|^2 + \|\nabla \cdot \boldsymbol{\sigma} - f\|^2$$

$p \in H^1(\Omega)$ and $\boldsymbol{\sigma} \in H(\text{div})$ naturally

\implies use FE spaces that conform to these...

Raviart-Thomas space of order 0: $RT_0(K) = P_0(K)^d + \mathbf{x}P_0(K)$.

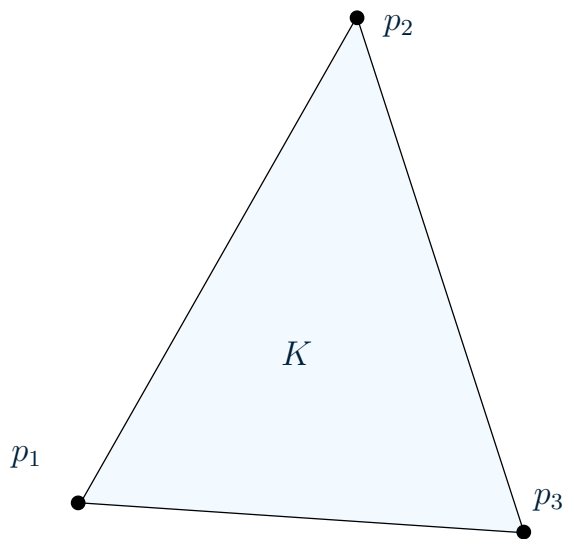
$$p^h \in \mathcal{V}^h = \{q \in H^1(\Omega) : q|_{\partial\Omega} = 0, q|_K \in P_1(K) \forall K \in \mathcal{T}^h\}$$

$$\boldsymbol{\sigma}^h \in \mathcal{W}^h = \{\boldsymbol{\tau} \in H(\text{div}) : \boldsymbol{\tau}|_K \in RT_0(K) \forall K \in \mathcal{T}^h\}$$

Mixed Finite Element Spaces

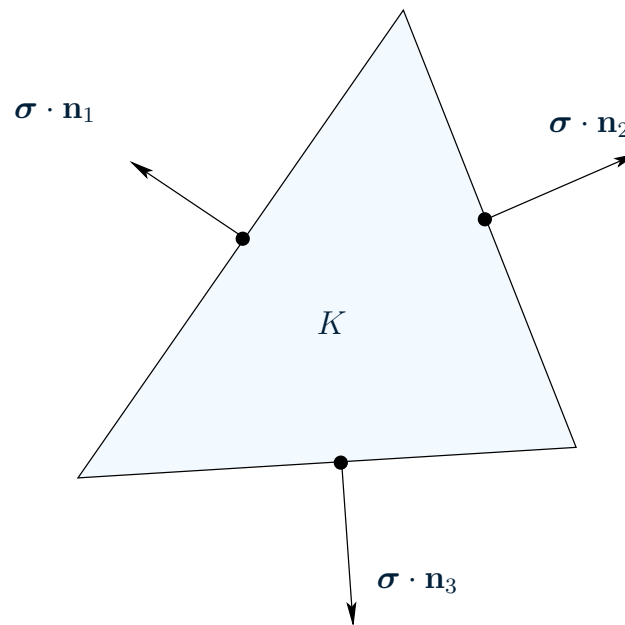
P_1 is the space of continuous, piecewise linear functions. RT_0 is also linear on each element, but instead of enforcing continuity we conserve a vector flux across the edges.

$$p^h|_K \in P_1(K)$$



degrees of freedom at corners

$$\boldsymbol{\sigma}^h|_K \in RT_0(K) = P_0(K)^d + \mathbf{x}P_0(K)$$



degrees of freedom on edges

This formulation leads to

$$\|p - p^h\|_1 + \|\sigma - \sigma^h\| + \|\nabla \cdot (\sigma - \sigma^h)\| \sim O(h^\alpha)$$

- $\alpha \geq 1 \implies$ globally optimal convergence
- $\alpha < 1 \implies$ globally slow convergence

Summary so far...

Least-squares methods work well when full regularity can be guaranteed...

- div-curl methods in H^1 spaces require $\alpha \geq 2$
- H(div) methods in $H^1 \times H(\text{div})$ spaces require $\alpha \geq 1$

Least-Squares Methods

Main Advantages

- s.p.d. linear systems often solved scalably with multigrid methods
- Accurate simultaneous approximations to meaningful physical quantities
- Well-posed minimization principles by design
- No need for artificial stabilization
- Freedom in choice of FE spaces (no LBB condition as in mixed methods)
- Free *a posteriori* error estimator in natural norm

Main Disadvantages

- Often more unknowns to approximate
- Often higher regularity requirements
- Not always strongly conservative

Intuition: The pollution effect is caused by the method paying too much attention to the solution where it is difficult to approximate. By shifting more attention away from the singularity we can recover optimal convergence away from the singularity. Near the singularity we can expect no better than the FE space will allow.

Our Approach: Weighted norm minimization

Again consider solving $Lu = f$ in some nonsmooth Ω , but minimize

$$G(u; f) = \|w(Lu - f)\|^2$$

where w is some weight function of the form $w = r^\beta$ near each singular point.

Define the weighted Sobolev norm and space:

$$\|\mathbf{u}\|_{k,\beta} = \left(\sum_{|j| \leq k} \|r^{\beta+j-k} D^j \mathbf{u}\|^2 \right)^{\frac{1}{2}},$$

$$H_{\beta}^k(\Omega) = \{\mathbf{u} : \|\mathbf{u}\|_{k,\beta} < \infty\}.$$

For example:

$$\|\mathbf{u}\|_{1,\beta}^2 = \|r^{\beta} \nabla \mathbf{u}\|^2 + \|r^{\beta-1} \mathbf{u}\|^2$$

These norms induce homogenous weighted spaces, or “Babuška-Kondratiev” spaces, as opposed to nonhomogenous norms which have the same weight for each term. These spaces are natural for our analysis.

Example 1: div-curl Formulation of Poisson

$$\text{Let } L = \begin{pmatrix} \nabla \cdot \\ \nabla \times \end{pmatrix}, \text{ and } \mathbf{f} = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$

$$\begin{aligned} G(\mathbf{u}; \mathbf{f}) &= \|r^\beta (\nabla \cdot \mathbf{u} - f)\|^2 + \|r^\beta \nabla \times \mathbf{u}\|^2 \\ &= \|r^\beta (\nabla \cdot \mathbf{u} - f)\|_{0,\beta}^2 + \|r^\beta \nabla \times \mathbf{u}\|_{0,\beta}^2 \\ &= \|L\mathbf{u} - \mathbf{f}\|_{0,\beta}^2 \end{aligned}$$

We (Lee, Manteuffel, Westphal) show the equivalence

$$G(\mathbf{u}; \mathbf{0})^{1/2} \sim \|\mathbf{u}\|_{1,\beta} \text{ for } \beta < |1 - \alpha|.$$

div-curl Theory

Theorem (Lee, Manteuffel, Westphal) Let Ω be a polygonal domain with one corner admitting a singularity of power α and assume $\mathbf{f} \in L^2(\Omega)$. Let $\mathbf{u} \in H^\alpha(\Omega)$ satisfy $L\mathbf{u} = \mathbf{f}$. If $\mathbf{u}^h \in \mathcal{V}^h$ is chosen to minimize the weighted functional,

$$G_w(\mathbf{u}^h; \mathbf{f}) = \min_{\mathbf{v}^h \in \mathcal{V}^h} \|L\mathbf{v}^h - \mathbf{f}\|_{0,\beta}^2,$$

for $1 - \alpha < \beta < \min(1 + \alpha, 2 - \alpha)$, then the approximation error, $\mathbf{u} - \mathbf{u}^h$, satisfies the following bounds:

$$(1) \quad \|\mathbf{u} - \mathbf{u}^h\|_{1,\beta} \leq Ch^{\alpha+\beta-1} \|\mathbf{u}\|_{\alpha+\beta,\beta}, \quad O(h^{\alpha+\beta-1})$$

$$(2) \quad G_w(\mathbf{u} - \mathbf{u}^h; \mathbf{0})^{\frac{1}{2}} \leq Ch^{\alpha+\beta-1} \|\mathbf{u}\|_{\alpha+\beta,\beta}, \quad O(h^{\alpha+\beta-1})$$

$$(3) \quad \|\mathbf{u} - \mathbf{u}^h\|_{0,\beta} \leq Ch^{\alpha+\beta} \|\mathbf{u}\|_{\alpha+\beta,\beta}, \quad O(h^{\alpha+\beta})$$

$$(4) \quad \|\mathbf{u} - \mathbf{u}^h\|_0 \leq Ch^\alpha (\|\mathbf{u}\|_\alpha + \|\mathbf{u}\|_{\alpha+\beta,\beta}). \quad O(h^\alpha)$$

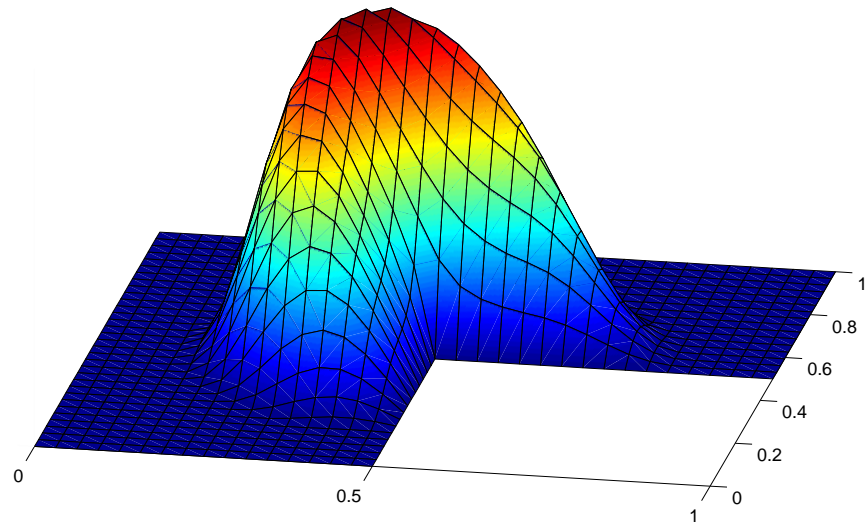
div-curl Numerical Test Problem

Let

$$p(r, \theta) = \delta(r)r^{\frac{2}{3}} \sin(2\theta/3),$$
$$\Omega = (0, 1)^2 \setminus (0.5, 1) \times (0, 0.5).$$

Define $f = \Delta p$.

$$f \in L^2(\Omega), \quad p \notin H^2(\Omega)$$



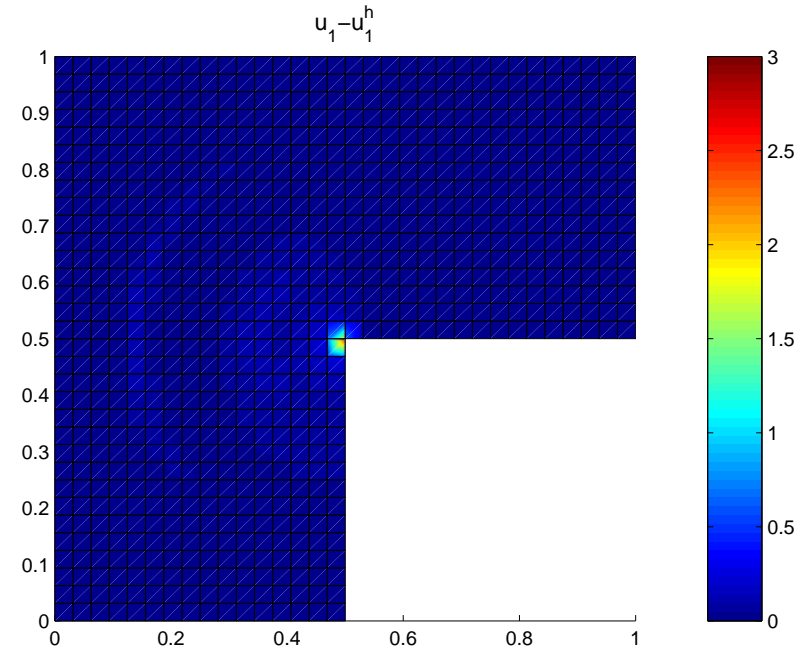
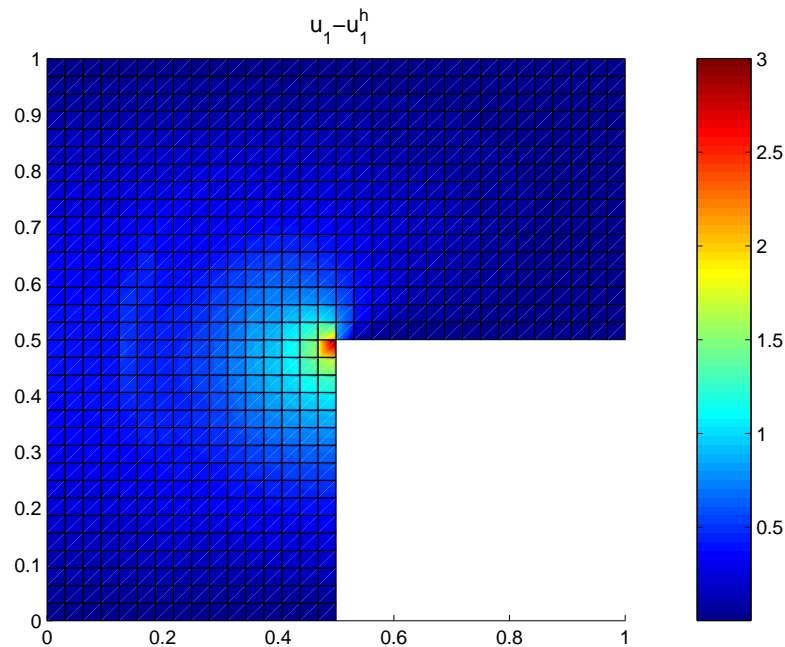
$p(r, \theta)$

We consider minimizing

$$G_w(\mathbf{u}^h; \mathbf{f}) = \|\mathbf{L}\mathbf{u}^h - \mathbf{f}\|_{0,\beta}^2$$

over the space of bilinear finite elements of uniform meshsize h .

Reduction of the Pollution Effect



$u_1 - u_1^h$
Standard LS, No weighting

$u_1 - u_1^h$
Weighted-norm LS, $\beta = 4/3$

Example 2: H(div) Formulation for Scalar Elliptic Problems

$$\begin{cases} -\nabla \cdot A\nabla p + \mathbf{b} \cdot \nabla p + cp = f, & \Omega \\ p = 0, & \partial\Omega \end{cases}$$

Assume A s.p.d. and denote $Xp := \mathbf{b} \cdot \nabla p + cp$. Define $\boldsymbol{\sigma} = -A\nabla p$ and

$$G(p, \boldsymbol{\sigma}; f) = \|A^{-1/2}(\boldsymbol{\sigma} + A\nabla p)\|_{0,\beta_1}^2 + \|\nabla \cdot \boldsymbol{\sigma} + Xp - f\|_{0,\beta_2}^2$$

for

$$p \in \{q \in H_{\beta_1}^1(\Omega) : q|_{\partial\Omega} = 0\}$$

$$\boldsymbol{\sigma} \in \{\boldsymbol{\tau} \in H_{\beta_1}^0(\Omega) : \nabla \cdot \boldsymbol{\tau} \in H_{\beta_2}^0(\Omega)\}$$

H(div) Approach: Weighted Norms

Define

$$\| (p, \boldsymbol{\sigma}) \|_{\beta_1, \beta_2} := \left(\|p\|_{1, \beta_1}^2 + \|\boldsymbol{\sigma}\|_{0, \beta_1}^2 + \|\nabla \cdot \boldsymbol{\sigma}\|_{0, \beta_2}^2 \right)^{1/2}$$

For $\beta_1 \leq \beta_2 \leq \beta_1 + 1$ and $\beta_1 \leq |\alpha|$ we (Cai, Westphal) show that

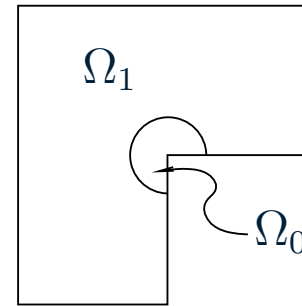
$$G(p, \boldsymbol{\sigma}; 0)^{1/2} \sim \| (p, \boldsymbol{\sigma}) \|_{\beta_1, \beta_2}$$

and minimizing over the mixed $H^1 \times H(\text{div})$ spaces leads to:

$$\| (p - p^h, \boldsymbol{\sigma} - \boldsymbol{\sigma}^h) \|_{\beta_1, \beta_2} \leq ch^{\alpha + \beta_1},$$

$$\| \boldsymbol{\sigma} - \boldsymbol{\sigma}^h \| \leq ch^\alpha.$$

Numerical Results: Dirichlet on L-shaped Domain



Convergence rates* for $\alpha = 2/3$, $\beta_2 = 0.3$

β_1	$G(p, \sigma; f)^{1/2}$			β_1	$\ \sigma - \sigma^h\ $		
	Ω	Ω_0	Ω_1		Ω	Ω_0	Ω_1
0.0	0.67	0.65	1.02	0.0	0.65	0.64	1.27
0.1	0.76	0.75	1.01	0.1	0.64	0.64	1.25
0.2	0.85	0.83	1.00	0.2	0.63	0.63	1.19
0.3	0.92	0.90	1.00	0.3	0.62	0.62	1.14

*Work with Grinnell student Sam Calisch, summer 2006; based on $h^{-1} = 256, 512$.

Target Application: Blood Flow

Many biological models assume a Newtonian model for blood flow. A more realistic model involves

- Characterization of the elastic nature of the fluid (viscoelastic behavior)
- A shear-dependent viscosity (shear thinning behavior)

Blood can be modeled as an elastic polymer (red blood cells) dissolved in a viscous solvent (blood plasma). This can be modeled by the Oldroyd-B equations (a generalization of Navier-Stokes' equations).

Oldroyd-B Viscoelasticity

The steady state equations are

$$\left\{ \begin{array}{l} \nabla \cdot \mathbf{u} = 0, \\ -\mu_s \Delta \mathbf{u} + \mathcal{R}e \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nabla \cdot \boldsymbol{\tau} = \mathbf{f}, \\ \boldsymbol{\tau} + \mathcal{W}e (\mathbf{u} \cdot \nabla \boldsymbol{\tau} - (\nabla \mathbf{u}) \boldsymbol{\tau} - \boldsymbol{\tau} (\nabla \mathbf{u})^t) - 2\mu_e \boldsymbol{\epsilon}(\mathbf{u}) = \mathbf{0}. \end{array} \right.$$

velocity \mathbf{u}

pressure p

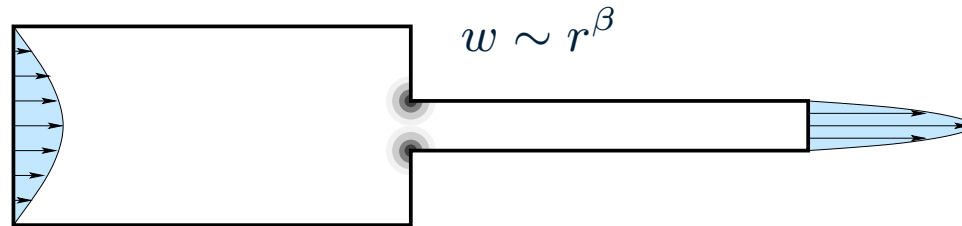
elastic stress $\boldsymbol{\tau}$

and one more...

H(div) method : total stress $\boldsymbol{\sigma} = \boldsymbol{\tau} + 2\mu_s \boldsymbol{\epsilon}(\mathbf{u}) - p\mathbf{I}$ (Cai, Westphal)

div-curl method : velocity gradient $\mathbf{U} = \nabla \mathbf{u}$ (Westphal)

Numerical Results 4:1 Contraction



Alves et al. (2003) shows $\mathbf{u} \sim r^{5/9}$, $\boldsymbol{\tau} \sim r^{-2/3}$

$$\implies \boldsymbol{\tau} \notin H^1(\Omega)$$

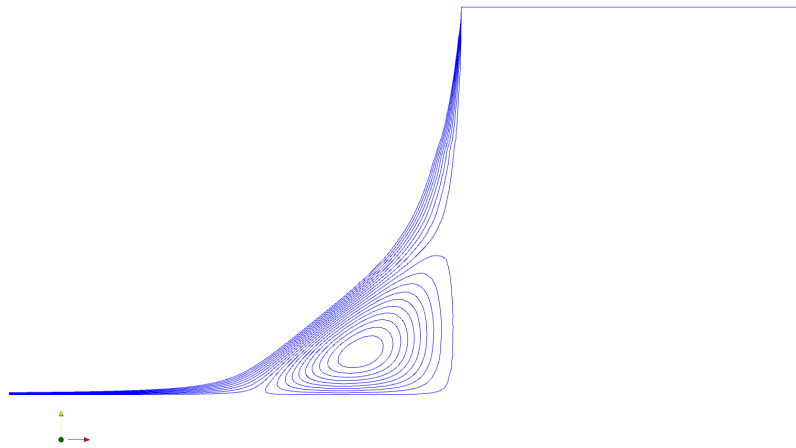
It's also clear that $\boldsymbol{\tau}$ is not necessarily in $H(\text{div})$.

We choose $w = r^\beta$ to make $\boldsymbol{\tau} \in H_\beta^2(\Omega) \implies \beta \approx 1.7$

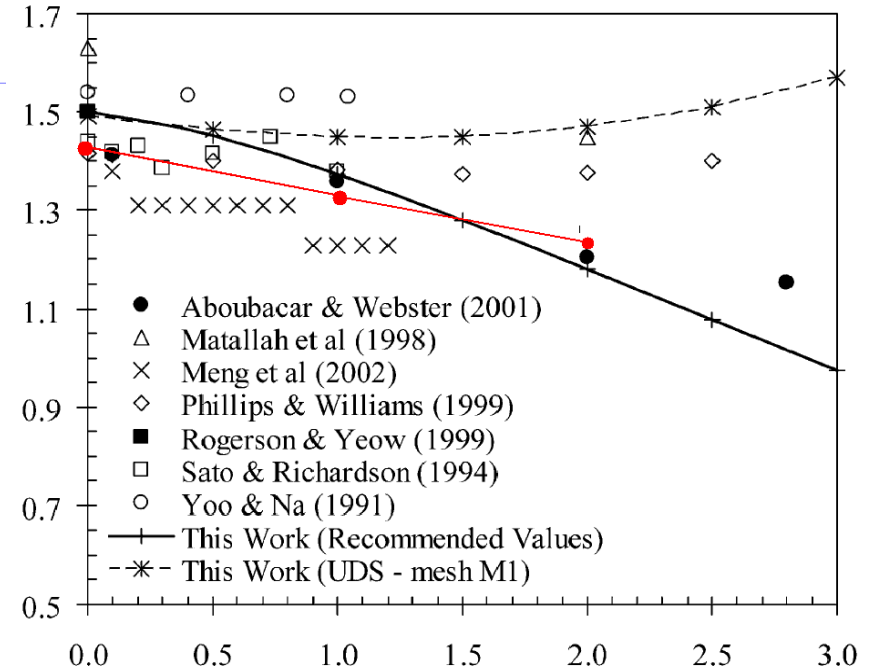
Thus, in both div-curl and $H(\text{div})$ approaches, aggressive weighting is necessary for terms associated with $\boldsymbol{\tau}$.

Numerical Results 4:1 Contraction

χ_r = horizontal reattachment length



χ_r vs. We



With $\beta = 1.7$, our results* (in red) track well with the current benchmark of highest resolution. Ignoring the singularity, our computations show the wrong trend: increasing χ_r with We .

* Numerical computations done with Wabash student, Haris Amin, summer 2006.

Conclusions

- Least-squares methods work well, but often have higher regularity requirements than other methods. A weighted-norm least-squares approach is one way to recover from this.
- The method is flexible and trivially implemented into existing LS code.
- It doesn't require specific knowledge of the singular functions, only an estimate of the severity.
- Theory and computation both generalize to 3-d.
- It can be used in conjunction with adaptive refinement.
- It is a good time to be in numerical analysis / scientific computation!