A Least-Squares Finite Element formulation of the Geometrically-Nonlinear Elasticity Equations

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Outline

- Introduction
  - First-Order System Least Squares (FOSLS) methodology
- Elasticity
  - Elasticity notation, definitions and FOSLS formulation
  - Theory overview
  - Computational results: Smooth solutions
  - Regularity, what (not) to expect
- FOSLS in Nonsmooth Domains
  - Weighted spaces and the weighted-norm approach
  - Theory and error bounds
  - Computational results: Nonsmooth solutions
- Concluding remarks and questions
Consider solving the first-order system \( Lu = f \) by minimizing

\[
G(u; f) = \| Lu - f \|^2
\]

over all \( u \in \mathcal{V} \). This leads to the weak problem: find \( u \in \mathcal{V} \) such that

\[
(Lu, Lv) = (f, Lv) \quad \forall v \in \mathcal{V}.
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$$(Lu, Lv) = (f, Lv) \quad \forall v \in \mathcal{V}.$$ 

**$\mathcal{V}$ ellipticity:** If $G(u; 0)^{\frac{1}{2}} = \|Lu\|$ is equivalent to the norm on $\mathcal{V}$:

$$c_0\|u\|_{\mathcal{V}} \leq \|Lu\| \leq c_1\|u\|_{\mathcal{V}},$$

then the weak problem is well-posed in $\mathcal{V}$. 
Consider the FE space $\mathcal{V}^h \subseteq \mathcal{V}$. The discrete weak problem is: find $u^h \in \mathcal{V}^h$ such that

$$(Lu^h, Lv^h) = (f, Lv^h) \quad \forall v^h \in \mathcal{V}^h.$$ 

When $\mathcal{V}^h \subseteq H^1(\Omega)$ and $\| \cdot \|_{\mathcal{V}} = \| \cdot \|_1$, $H^1$ elliptic functionals result in:

- Existence and uniqueness of $u^h \in \mathcal{V}^h$
- Optimal order FE discretization accuracy (given regularity of $Lu = f$)
- $O(h^{-2})$ conditioned linear systems solved with standard multigrid methods
- Local functional values a free $H^1 a posteriori$ error bound
Elasticity Notation and Definitions

Displacement
Deformation
Strain Tensor
Stress Tensor
Elasticity Notation and Definitions

\[ \phi(x) = x + u(x) \]

\[ E = \frac{1}{2} (I - \nabla \phi^t \nabla \phi) \]
\[ = \frac{1}{2} (\nabla u + \nabla u^t + \nabla u^t \nabla u) \]

\[ \Sigma = \lambda tr(E) I + 2\mu E + o(E) \]

- \( \phi \)  Displacement
- \( \phi \)  Deformation
- \( E \)  Strain Tensor
- \( \Sigma \)  Stress Tensor

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Elasticity Notation and Definitions

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\( u \) Displacement
\( \phi \) Deformation
\( E \) Strain Tensor
\( \Sigma \) Stress Tensor
Nonlinear Elasticity Equations

\begin{equation}
\begin{cases}
\nabla \cdot [(I + \nabla u)\Sigma(\nabla u)] = f \quad \text{in} \quad \Omega \\
\mathbf{n} \cdot (I + \nabla u)\Sigma(\nabla u) = g \quad \text{on} \quad \Gamma_T \\
u = 0 \quad \text{on} \quad \Gamma_D
\end{cases}
\end{equation}

Accurate for deformations of "large-displacement and small-strain." May scale with $\nu = 1$, and let $\nu$ determine incompressibility.
Nonlinear Elasticity Equations

\[ \nabla \cdot [(I + \nabla \mathbf{u}) \Sigma(\nabla \mathbf{u})] = \mathbf{f} \quad \text{in} \quad \Omega \]
\[ \mathbf{n} \cdot (I + \nabla \mathbf{u}) \Sigma(\nabla \mathbf{u}) = \mathbf{g} \quad \text{on} \quad \Gamma_T \]
\[ \mathbf{u} = 0 \quad \text{on} \quad \Gamma_D \]

The equilibrium equation may be written as

\[ \mu \Delta \mathbf{u} + (\lambda + \mu) \nabla \nabla \cdot \mathbf{u} + \nabla \cdot P_3(\nabla \mathbf{u}) = \mathbf{f} \]

- **Accurate for deformations of “large-displacement and small-strain”**
- **May scale with \( \mu = 1 \), and let \( \lambda \) determine incompressibility**
Pose in terms of $U = \nabla u$  (First-Order System)
- $\Phi = I + U$ is the Jacobian of the mapping
- $\det(\Phi) \approx 1$, $\|\Phi\|^2_{l_2} \approx 2$

2-Stage Solution Algorithm
- Solve for $U$
- Recover $u$ from: $\nabla u = U$

Linearize around a current approximation by Newton’s method
- Initial guess: $U_0 = 0$ ... the reference configuration
- General Newton Step: $\nabla \cdot A_n U = F_n$
- $1^{st}$ step is linear elasticity
Problem Modification

- **Problem**: System matrix $A_n = A(\Phi_n)$ is generally indefinite
- Can modify $A_n$ without changing the solution

Choose $B$ to be such that $\nabla \cdot B = \nabla \times$,

$$\implies \nabla \cdot B \nabla p = 0 \text{ for any } p,$$

Choose $\tilde{A}_n = A_n + B$ then,

$$\nabla \cdot \tilde{A}_n U = \nabla \cdot A_n U$$

- Choose $B$ to shift the spectrum of $A_n$ positive...
Properties of $\tilde{A}_n$

- The geometrically-nonlinear model assumes $o(E) \approx 0$. Thus we may also impose an assumption on the size of $E = \frac{1}{2}(\Phi^t \Phi - I)$.

- The $\ell^2$ norm of the strains and the full spectrum of $\tilde{A}_n$ can be written in terms of $\delta = det(\Phi)$, $\sigma = \|\Phi\|^2_{\ell^2}$.

- We show $\tilde{A}_n$ positive definite under the small strains assumption:

  $$\|\Phi^t \Phi - I\|_{\ell^2} < \frac{\sqrt{2}}{\lambda + 3} \implies \tilde{A}_n \text{ is positive definite.}$$
Define the FOSLS functional for each step:

\[
G(U; U_n, F_n) = \| \nabla \cdot \tilde{A}_n U - F_n \|^2_0 + \| \nabla \times U \|^2_0,
\]

for \( U \) in the space

\[
\mathcal{V} = \{ \mathbf{V} \in H^1(\Omega)^4 : \tau \cdot \mathbf{V} = 0 \text{ on } \Gamma_D \}.
\]

Solve by minimization principle: Choose \( U \in \mathcal{V} \) so that

\[
G(U; U_n, F_n) = \inf_{\mathbf{V} \in \mathcal{V}} G(\mathbf{V}; U_n, F_n).
\]

We show a well-posed Newton minimization, converging by an inexact nested iteration-Newton-FOSLS-multigrid process (cf. Codd, Manteuffel and McCormick).
Elasticity Theory

- Pure Dirichlet boundary conditions
- Boundary is $C^{4+\delta}$ smooth
- $f \in H^{2+\delta}$ and near the origin
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\[ \exists ! \text{ solution to the nonlinear problem, } U^* \in H^{\delta+\delta} \text{ near the origin} \]
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$\tilde{A}$ pos def on $\Omega$
Elasticity Theory

Pure Dirichlet boundary conditions

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$H^k$ functional is $H^{1+k}$ elliptic for $k = 0, 1$

Newton iterates converge
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- $H^k$ functional is $H^{1+k}$ elliptic for $k = 0, 1$
- Bounded MG Convergence Factors
- Well posed Newton step ...
- next iterate remains in $H^{1+\delta}$ using $L^2$ functional
- Next iterate is bounded
- Newton iterates converge
Elasticity Theory

- Pure Dirichlet boundary conditions
- Boundary is $C^{4+\delta}$ smooth
- $f \in H^{2+\delta}$ and near the origin
- $U_n$ has "small strains"
- $U_n \in H^{1+\delta}$
- $A$ pos def on $\Omega$
- $H^k$ functional is $H^{1+k}$ elliptic for $k = 0, 1$
- New iterate remains in $H^{1+\delta}$
- Newton iterates converge
- Next iterate is bounded

Well posed Newton step ... next iterate remains in $H^{1+\delta}$ using $L^2$ functional

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Elasticity Theory

- Pure Dirichlet boundary conditions
- Boundary is $C^{4+\delta}$ smooth
- $f \in H^{2+\delta}$ and near the origin

$U_n$ has "small strains"

$U_n \in H^{1+\delta}$

$H^k$ functional is $H^{1+k}$ elliptic for $k = 0, 1$

Well posed Newton step ... next iterate remains in $H^{1+\delta}$ using $L^2$ functional

Bounded MG Convergence Factors

Newton iterates converge

Next iterate is bounded

$\exists!$ solution to the nonlinear problem, $U^* \in H^{4+\delta}$ near the origin

$\tilde{A}$ pos def on $\Omega$
Main Assumptions

- Pure displacement boundary conditions...
  - Mixed and pure traction cases perform similarly in practice.
  - Most likely a sufficient but not necessary condition.
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- The solution has small strains...
  - We seek to show that "small strains" reasonably corresponds to the limits of the model.
  - Most likely a sufficient but not necessary condition.

- The domain is sufficiently smooth...
  - We seek a method for LS problems in nonsmooth domains.
  - A necessary and sufficient condition for most problems.
Small Strains: Pure Shear and Pure Tensile Strain

Pure shear strain:

"Small strain" limit of pure shear strain versus $\lambda$
Pure tensile strain:

"Small strain" limit of pure tensile strain versus $\lambda$
Small strains example

For this configuration our theory holds for $\lambda < 3.25$ ($\nu < 0.38$).

$$\max_\Omega \| \Phi^t \Phi - I \|_{L^2} = 0.241$$

<table>
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<tr>
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<th>$^*\nu$</th>
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<tr>
<td>Nickel</td>
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<td>0.30</td>
</tr>
<tr>
<td>Aluminum</td>
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<td>0.34</td>
</tr>
<tr>
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<td>0.38</td>
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<tr>
<td>Lead</td>
<td>7.30</td>
<td>0.44</td>
</tr>
<tr>
<td>Rubber</td>
<td>33.3</td>
<td>0.49</td>
</tr>
</tbody>
</table>

*The Poisson ratio, $\nu = \frac{\lambda}{2(\lambda+1)}$, is another measure of incompressibility.
Numerical Results: Smooth Solutions

- Displacement boundary conditions on $\Omega = [0, 1]^2$
- Known smooth solution $U \in H^2(\Omega)$
- Bilinear finite elements on uniform meshes, $h^{-1} = 8, 16, ..., 128$
- Computations done using FOSPACK, by J. Ruge
- Lamé constants $\lambda = 2.15$, $\mu = 1.0$ (i.e., $\nu = 0.34$)

- Convergence of Newton's method
- Finite Element approximation rates
- Multigrid performance
- Nested Iteration efficiency
FE Discretization Accuracy

Nonlinear Functional: \( g(U; f) = \| \nabla \cdot [(I + U) \Sigma(U)] - f \|^2 + \| \nabla \times U \|^2 \)

- Optimal \( O(h) \) convergence in \( H^1 \) and functional norms
- Optimal \( O(h^2) \) convergence in \( L^2 \) norm
### Computational Cost

**Nested Iteration, 3 V(1,1)-pcg cycles per level**

<table>
<thead>
<tr>
<th>$h^{-1}$</th>
<th>m</th>
<th>$G(U^h; f)^{\frac{1}{2}}$</th>
<th>Ratio</th>
<th>$\bar{\rho}$</th>
<th>$W_T$</th>
<th>time (s)</th>
</tr>
</thead>
<tbody>
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<td>2.64e-02</td>
<td></td>
<td>0.29</td>
<td>12.3</td>
<td>1</td>
</tr>
<tr>
<td>16</td>
<td>2</td>
<td>1.31e-02</td>
<td>2.01</td>
<td>0.25</td>
<td>16.0</td>
<td>4</td>
</tr>
<tr>
<td>32</td>
<td>3</td>
<td>6.61e-03</td>
<td>1.98</td>
<td>0.24</td>
<td>19.0</td>
<td>15</td>
</tr>
<tr>
<td>64</td>
<td>4</td>
<td>3.32e-03</td>
<td>1.99</td>
<td>0.24</td>
<td>20.8</td>
<td>60</td>
</tr>
<tr>
<td>128</td>
<td>5</td>
<td>1.66e-03</td>
<td>2.00</td>
<td>0.23</td>
<td>21.6</td>
<td>242</td>
</tr>
</tbody>
</table>

- **m** Newton step
- **$G^{\frac{1}{2}}$** Nonlinear functional norm
- **$\bar{\rho}$** Average V(1,1)-pcg convergence factor
- **$W_T$** Total Cumulative Work: in # of Jacobi sweeps relative to current grid
Loss of smoothness at corners in polygonal domains is well understood (Kondrat’ev, Grisvard, Maz’ya, et. al.)

\[ u = u_0 + S(r, \theta) \]

\[ u_0 \in H^2(\Omega) \]

\[ S(r, \theta) = r^\alpha \Theta(\theta) \in H^{\alpha+1}(\Omega) \]

The value of \( \alpha \) is determined by

- Boundary Condition Type: displacement, traction, mixed
- Geometry: interior angle at the corner
- Lamé Constants: \( \lambda, \mu \)

This difficulty occurs in many second-order problems and is especially problematic for FOSLS discretizations!
Consider the FOSLS two-stage solution of Poisson’s equation:

\[
\begin{aligned}
\begin{cases}
\Delta p = f, & \Omega \\
p = 0, & \partial \Omega
\end{cases} & \implies \\
\begin{cases}
\nabla p - \mathbf{u} = 0, & \Omega \\
\nabla \cdot \mathbf{u} = f, & \Omega \\
\nabla \times \mathbf{u} = 0, & \Omega \\
p = 0, & \partial \Omega \\
\tau \cdot \mathbf{u} = 0, & \partial \Omega
\end{cases}
\end{aligned}
\]
Consider the FOSLS two-stage solution of Poisson’s equation:

\[
\begin{cases}
\nabla p - u = 0, & \Omega \\
\nabla \cdot u = f, & \Omega \\
\nabla \times u = 0, & \Omega \\
p = 0, & \partial \Omega \\
\mathbf{\tau} \cdot u = 0, & \partial \Omega \\
\end{cases}
\]

\[
G_1(u; f) = \|\nabla \cdot u - f\|^2 + \|\nabla \times u\|^2
\]

\[
G_2(p; u) = \|\nabla p - u\|^2
\]

\[
\mathcal{V} = \{ u \in H^1(\Omega) : \mathbf{\tau} \cdot u = 0 \text{ on } \partial \Omega \}
\]

\[
\mathcal{W} = \{ p \in H^1(\Omega) : p = 0 \text{ on } \partial \Omega \}
\]
Consider the FOSLS two-stage solution of Poisson’s equation:

\[
\begin{aligned}
\nabla p - \mathbf{u} &= 0, \quad \Omega \\
\nabla \cdot \mathbf{u} &= f, \quad \Omega \\
\nabla \times \mathbf{u} &= 0, \quad \Omega \\
p &= 0, \quad \partial \Omega \\
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\]

\[
G_1(\mathbf{u}; f) = \|\nabla \cdot \mathbf{u} - f\|^2 + \|\nabla \times \mathbf{u}\|^2
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G_2(p; \mathbf{u}) = \|\nabla p - \mathbf{u}\|^2
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\]

(1) Given \(f \in L^2(\Omega)\), choose \(\mathbf{u} = \arg\min_{\mathbf{v} \in \mathcal{V}} G_1(\mathbf{v}; f)\)
Consider the FOSLS two-stage solution of Poisson’s equation:

\[
\begin{align*}
\nabla p - \mathbf{u} &= 0, \quad \Omega \\
\nabla \cdot \mathbf{u} &= f, \quad \Omega \\
\nabla \times \mathbf{u} &= 0, \quad \Omega \\
p &= 0, \quad \partial \Omega \\
\mathbf{\tau} \cdot \mathbf{u} &= 0, \quad \partial \Omega
\end{align*}
\]

\[
G_1(\mathbf{u}; f) = \|\nabla \cdot \mathbf{u} - f\|^2 + \|\nabla \times \mathbf{u}\|^2
\]

\[
G_2(p; \mathbf{u}) = \|\nabla p - \mathbf{u}\|^2
\]

\[
\mathcal{V} = \{ \mathbf{u} \in H^1(\Omega) : \mathbf{\tau} \cdot \mathbf{u} = 0 \text{ on } \partial \Omega \}
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\[
\mathcal{W} = \{ p \in H^1(\Omega) : p = 0 \text{ on } \partial \Omega \}
\]

1. Given \( f \in L^2(\Omega) \), choose \( \mathbf{u} = \arg\min_{\mathbf{v} \in \mathcal{V}} G_1(\mathbf{v}; f) \)

2. Given \( \mathbf{u} \in \mathcal{V} \), choose \( p = \arg\min_{q \in \mathcal{W}} G_2(q; \mathbf{u}) \)
Each corner has a singularity of power $\alpha$.

Away from irregular boundary points, the solution is sufficiently smooth.
The solution to Poisson’s equation near the corner may have a component of the form:

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

\((r, \theta)\) a local polar coordinate system
The solution to Poisson’s equation near the corner may have a component of the form:

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

\((r, \theta)\) a local polar coordinate system

\[
\begin{aligned}
  p &= p_0 + s \\
  u &= u_0 + S
\end{aligned}
\]

\[
\begin{aligned}
  p_0 &\in H^2(\Omega), \quad s \in H^{1+\alpha}(\Omega) \\
  u_0 &\in H^1(\Omega), \quad S \in H^\alpha(\Omega)
\end{aligned}
\]

\[ \omega > \pi \implies \alpha < 1 \implies u \notin H^1(\Omega) \]

- Using standard FE subspaces of \(H^1\) results in stalling convergence and a global loss of accuracy!
The Pollution Effect

Exact component \( u_1 \)

\( u_1^h \) computed by standard FOSLS
Even away from the singularity the solution is not accurate!
Existing Methods

- Add singular functions to finite element space
- Inverse-norm methods: $H^{-1}$ least-squares, FOSLL$^*$
- $H(div)$-conforming finite element spaces
- Weighted-norm FOSLS
Weighted-Norm FOSLS

Replace the $L^2$ norm functionals with locally weighted $L^2$ norms:

$$G_w(u; f) = \| w(\nabla \cdot u - f) \|^2 + \| w \nabla \times u \|^2, \quad w = r^\beta$$

Let $V^h \subset V$ be the FE space. The discrete problem now becomes:

Given $f \in L^2(\Omega)$, choose

$$u^h = \arg\min_{v^h \in V^h} G_w(v^h; f)$$

Choose the weight parameter $\beta$ in order to

- make $H^1$ dense in $H(div) \cap H(curl)$ in the weighted functional norm
- recover the best possible convergence throughout $\Omega$
Define the weighted Sobolev norm and space:

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

\[ H^k_\beta(\Omega) = \{ u : \| u \|_{k, \beta} < \infty \}. \]

for example:

\[ \| u \|_{1, \beta}^2 = \| r^\beta \nabla u \|^2 + \| r^{\beta - 1} u \|^2 \]
Define the weighted Sobolev norm and space:

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

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

Also define

$$L = \begin{pmatrix} \nabla \cdot \\ \nabla \times \end{pmatrix}, \quad f = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$  \implies Lu = f \quad \text{and}$$

$$G_w(u^h; f) = \| Lu^h - f \|^2_{0,\beta} = \| L(u^h - u) \|^2_{0,\beta}.$$
Let $\Omega$ be a polygonal domain with one reentrant corner of interior angle $\omega$ and assume $f \in L^2(\Omega)$. Let $u \in H^\alpha(\Omega)$ satisfy $Lu = f$. If $u^h \in VH$ is chosen to minimize the weighted functional,

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

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

1. $\|u - u^h\|_{1,\beta} \leq Ch^{\alpha + \beta - 1} \|u\|_{\alpha + \beta, \beta}, \quad O(h^{\alpha + \beta - 1})$
2. $G_w(u - u^h; 0)^{\frac{1}{2}} \leq Ch^{\alpha + \beta - 1} \|u\|_{\alpha + \beta, \beta}, \quad O(h^{\alpha + \beta - 1})$
3. $\|u - u^h\|_{0,\beta} \leq Ch^{\alpha + \beta} \|u\|_{\alpha + \beta, \beta}, \quad O(h^{\alpha + \beta})$
4. $\|u - u^h\|_0 \leq Ch^\alpha (\|u\|_\alpha + \|u\|_{\alpha + \beta, \beta}), \quad O(h^\alpha)$
Reduction of the Pollution Effect

\[ u_1 - u_1^h \]

Standard FOSLS, No weighting

\[ u_1 - u_1^h \]

Weighted-norm FOSLS, \( \beta = 4/3 \)
Each plot is the power of the singularity $\alpha$ vs. interior angle $\omega$ for linear elasticity with Lamé constants $\lambda = 2.15$, $\mu = 1$.

- Pure Displacement $\omega \geq \pi \implies U \notin H^1(\Omega)$
- Mixed Boundaries $\omega \gtrsim 0.3\pi \implies U \notin H^1(\Omega)$
Mixed boundary conditions on $\Omega$

Interior body force $\Rightarrow U \in L^2(\Omega) \setminus H^1(\Omega)$

Use weighted functional:

$$G_w(U; U_n, F_n) = \| \nabla \cdot \tilde{A}_n U - F_n \|^2_{0,\beta} + \| \nabla \times U \|^2_{0,\beta}$$

Use weight of $\beta = 2 - \alpha$ near each corner
Domain and Boundary Conditions

\[ U \sim r^{\alpha - 1} \in H^\alpha (\Omega) \]
Numerical Results: Singular Solutions

Nested Iteration, 5 V(1,1)-pcg cycles per level

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- $m$ Newton step
- $G_w^{\frac{1}{2}}$ Weighted nonlinear functional norm
- $\bar{\rho}$ Average V(1,1)-pcg convergence factor
- $W_T$ Total Cumulative Work: in # of Jacobi sweeps relative to current grid
Concluding Remarks and Open Questions

Summary

- Robust solution strategy for geometrically-nonlinear elasticity problems in both smooth and nonsmooth domains.
- Corner singularities for many problems can be treated with weighted norms, restoring (nearly) optimal discretization convergence rates.

Open Questions

- Elasticity theory for pure traction, mixed boundary conditions
- Elasticity in the incompressible limit, $\lambda \to \infty$
- Improved multigrid solvers for weighted problems