

The Schwarz alternating method for concurrent multiscale coupling in solid mechanics

Irina Tezaur, Alejandro Mota, Coleman Alleman

Sandia National Laboratories, Livermore, CA, USA.

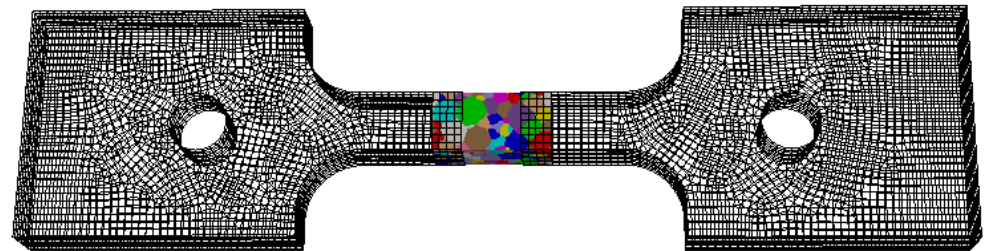
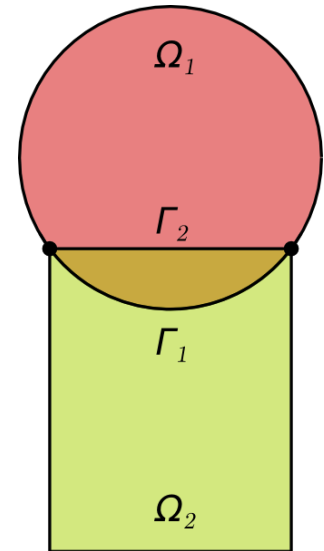
COUPLED 2017

Rhodes Island, Greece

June 12-14, 2017

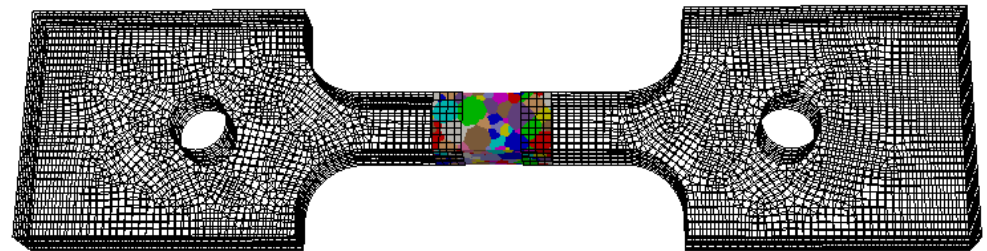
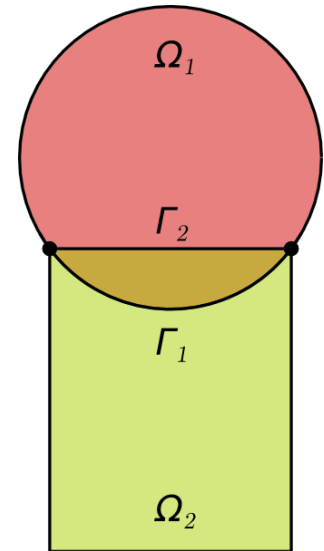
Outline

1. Motivation
2. Schwarz Alternating Method: Background & History
3. Schwarz Alternating Method for Concurrent Multiscale Coupling in Quasistatics
 - Four Variants: Full Schwarz, Inexact Schwarz, Modified Schwarz, Monolithic Schwarz
 - Implementations: MATLAB, Albany
4. Numerical Examples
5. Summary
6. Future Work
7. References
8. Appendix



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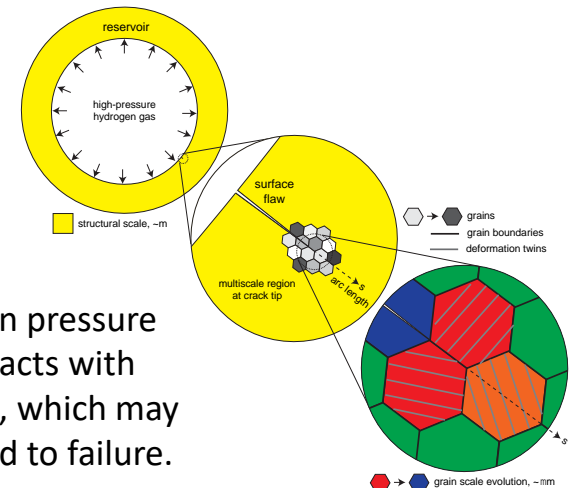
Motivation for Concurrent Multiscale Coupling

- **Large scale** structural **failure** frequently originates from **small scale** phenomena such as defects, microcracks, inhomogeneities and more, which grow quickly in unstable manner.
- Failure occurs due to **tightly coupled interaction** between small scale (stress concentrations, material instabilities, cracks, etc.) and large scale (vibration, impact, high loads and other perturbations).

Concurrent multiscale methods are **essential** for understanding and prediction of behavior of engineering systems when a **small scale failure** determines the performance of the entire system.



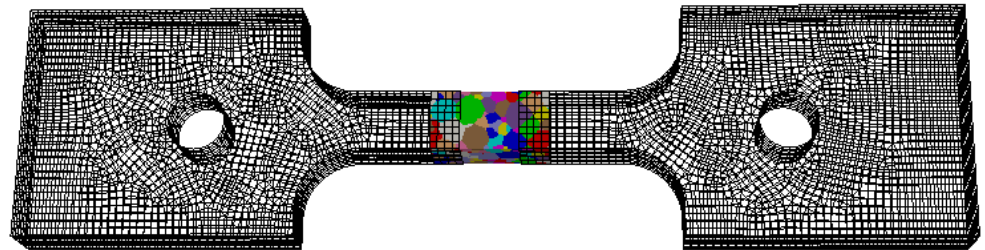
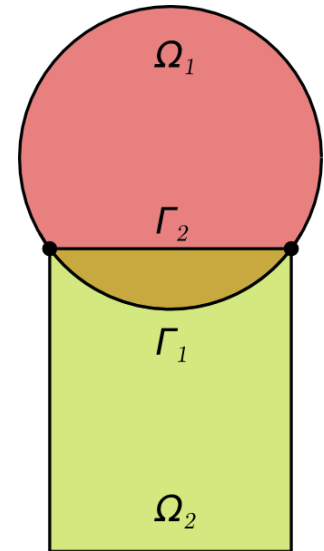
Roof failure of Boeing 737 aircraft due to fatigue cracks. From *imechanica.org*



Surface flaw in pressure vessel: interacts with microstructure, which may or may not lead to failure.

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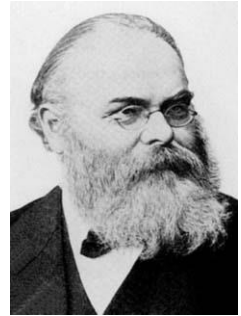
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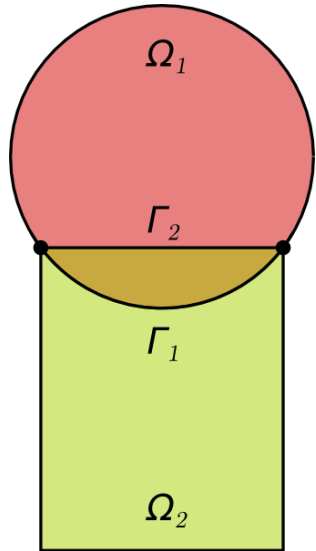
Schwarz Alternating Method for Domain Decomposition

- Proposed in 1870 by H. Schwarz for solving Laplace PDE on irregular domains.

Simple idea: if the solution is known in regularly shaped domains, use those as pieces to iteratively build a solution for the more complex domain.



H. Schwarz (1843 – 1921)



Schwarz Alternating Method

Initialize:

- Solve PDE by any method on Ω_1 w/ initial guess for Dirichlet BCs on Γ_1 .

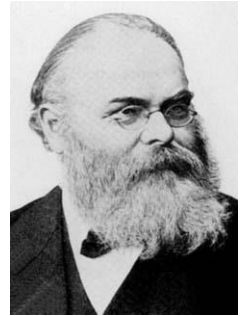
Iterate until convergence:

- Solve PDE by any method (can be different than for Ω_1) on Ω_2 w/ Dirichlet BCs on Γ_2 that are the values just obtained for Ω_1 .
- Solve PDE by any method (can be different than for Ω_2) on Ω_1 w/ Dirichlet BCs on Γ_1 that are the values just obtained for Ω_2 .

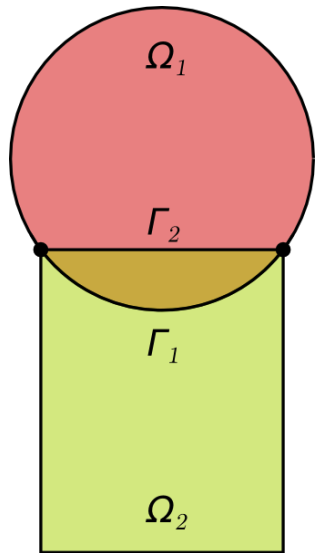
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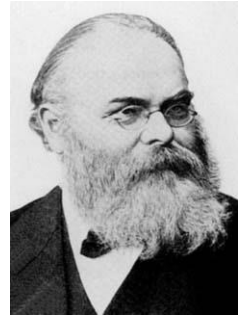
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Requirement for convergence: $\Omega_1 \cap \Omega_2 \neq \emptyset$

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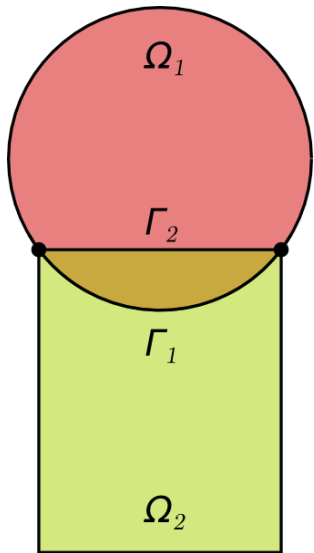
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- Schwarz alternating method most commonly used as a ***preconditioner*** for Krylov iterative methods to solve linear algebraic equations.

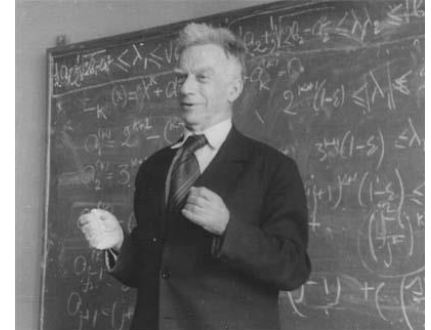
Schwarz Alternating Method after Schwarz

Using the Schwarz alternating as a *discretization method* for PDEs is natural idea with a sound *theoretical foundation*.

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- [S. L. Sobolev \(1936\)](#): posed Schwarz method for ***linear elasticity*** in variational form and ***proved method's convergence*** by proposing a convergent sequence of energy functionals.

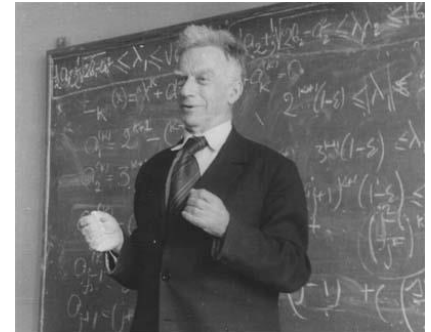


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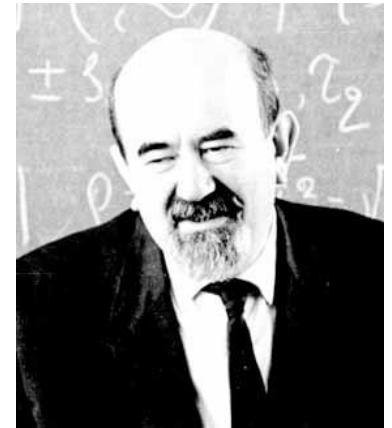
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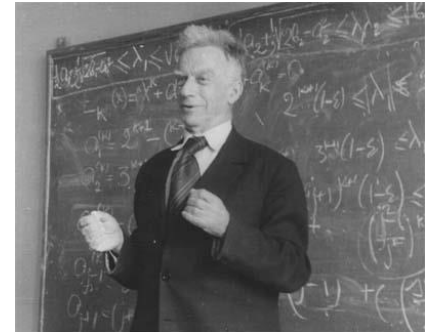
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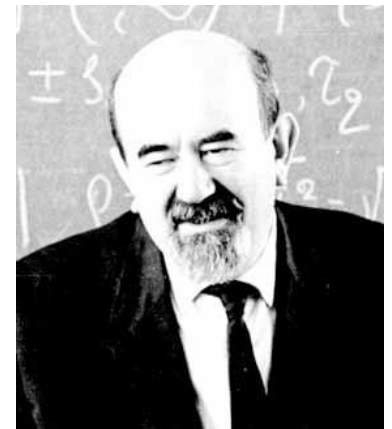
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- [A. Mota, I. Tezaur, C. Alleman \(2017\)*](#): derived a **proof of convergence** of the alternating Schwarz method for the **finite deformation quasi-static nonlinear PDEs** (with energy functional $\Phi[\varphi]$ defined below), and determined a **geometric convergence rate** for the finite deformation quasi-static problem.

$$\Phi[\varphi] = \int_B W(\mathbf{F}, \mathbf{Z}, T) dV - \int_B \mathbf{B} \cdot \boldsymbol{\varphi} dV - \int_{\partial_T B} \bar{\mathbf{T}} \cdot \boldsymbol{\varphi} dS$$
$$\nabla \cdot \mathbf{P} + \mathbf{B} = \mathbf{0}$$



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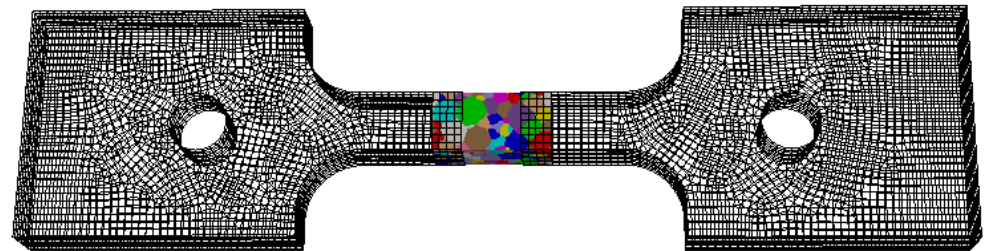
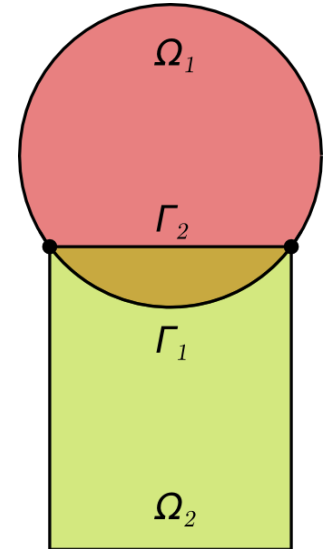


A. Mota, I. Tezaur, C. Alleman

*A. Mota, I. Tezaur, C. Alleman. "The Schwarz Alternating Method in Solid Mechanics", *CMAME* 319 (2017), 19-51.

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Schwarz Alternating Method for Multiscale Coupling in Quasistatics

1: $\varphi^{(0)} \leftarrow \text{id}_{\mathbf{X}}$ in Ω_2

2: $n \leftarrow 1$

3: **repeat**

4: $\varphi^{(n)} \leftarrow \chi$ on $\partial_{\varphi} \Omega_i$

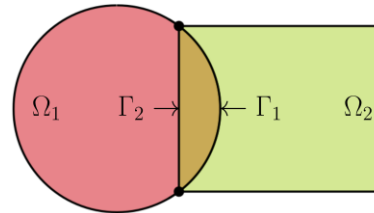
5: $\varphi^{(n)} \leftarrow P_{\Omega_j \rightarrow \Gamma_i}[\varphi^{(n-1)}]$ on Γ_i

6: $\varphi^{(n)} \leftarrow \arg \min_{\varphi \in \mathcal{S}_i} \Phi_i[\varphi]$ in Ω_i

7: $n \leftarrow n + 1$

8: **until** converged

▷ initialize to zero displacement or a better guess in Ω_2



▷ Schwarz loop

▷ Dirichlet BC for Ω_i

▷ Schwarz BC for Ω_i

▷ solve in Ω_i

Advantages:

- Conceptually very *simple*.

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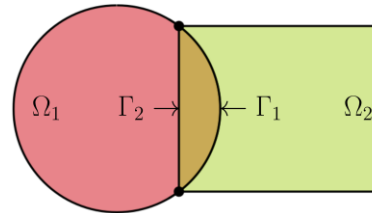
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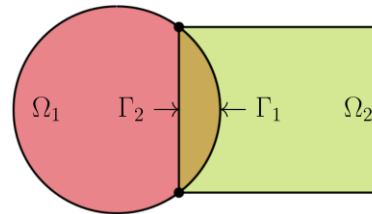
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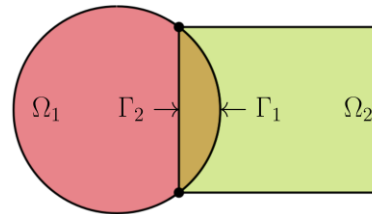
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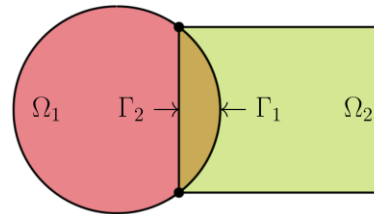
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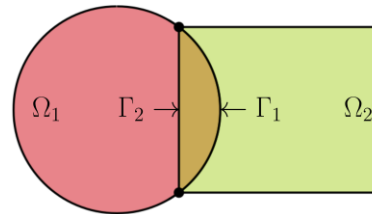
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- *Different solvers* can be used for the different regions.
- *Different material models* can be coupled provided that they are compatible in the overlap region.
- Simplifies the task of *meshing complex geometries* for the different scales.

Four Variants* of the Schwarz Alternating Method

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
6:   repeat
7:      $\Delta\mathbf{x}_B^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
8:      $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \leq \epsilon_{\text{machine}}$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_B^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \leq \epsilon_{\text{machine}}$ 
16: until  $\left[ \left( \|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Schwarz loop
 ▷ for convergence check
 ▷ project from Ω_2 to Γ_1
 ▷ Newton loop for Ω_1
 ▷ linear system
 ▷ tight tolerance
 ▷ for convergence check
 ▷ project from Ω_1 to Γ_2
 ▷ Newton loop for Ω_2
 ▷ linear system
 ▷ tight tolerance
 ▷ tight tolerance

Full Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
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9:    $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$ 
10: until  $\left[ \left( \|\Delta\mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\Delta\mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Newton-Schwarz loop
 ▷ project from Ω_2 to Γ_1
 ▷ linear system
 ▷ project from Ω_1 to Γ_2
 ▷ linear system
 ▷ tight tolerance

Modified Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
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8:      $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \leq \epsilon$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_B^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \leq \epsilon$ 
16: until  $\left[ \left( \|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Schwarz loop
 ▷ for convergence check
 ▷ project from Ω_2 to Γ_1
 ▷ Newton loop for Ω_1
 ▷ linear system
 ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
 ▷ for convergence check
 ▷ project from Ω_1 to Γ_2
 ▷ Newton loop for Ω_2
 ▷ solve linear system
 ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
 ▷ tight tolerance

Inexact Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,
3: repeat
4:    $\begin{Bmatrix} \Delta\mathbf{x}_B^{(1)} \\ \Delta\mathbf{x}_B^{(2)} \end{Bmatrix} \leftarrow \begin{pmatrix} \mathbf{K}_{AB}^{(1)} + \mathbf{K}_{A\beta}^{(1)}\mathbf{H}_{11} & \mathbf{K}_{A\beta}^{(1)}\mathbf{H}_{12} \\ \mathbf{K}_{A\beta}^{(2)}\mathbf{H}_{21} & \mathbf{K}_{AB}^{(2)} + \mathbf{K}_{A\beta}^{(2)}\mathbf{H}_{22} \end{pmatrix} \setminus \begin{Bmatrix} -\mathbf{R}_A^{(1)} \\ -\mathbf{R}_A^{(2)} \end{Bmatrix}$ 
5:    $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$ 
6:    $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$ 
7: until  $\left[ \left( \|\Delta\mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\Delta\mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Newton-Schwarz loop
 ▷ linear system
 ▷ tight tolerance

Monolithic Schwarz

Four Variants* of the Schwarz Alternating Method

Least-intrusive variant: by-passes Schwarz iteration, no need for block solver.

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
6:   repeat
7:      $\Delta\mathbf{x}_B^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \backslash \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
8:      $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \leq \epsilon_{\text{machine}}$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_B^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \backslash \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \leq \epsilon_{\text{machine}}$ 
16: until  $\left[ \left( \|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Schwarz loop
 ▷ for convergence check
 ▷ project from Ω_2 to Γ_1
 ▷ Newton loop for Ω_1
 ▷ linear system
 ▷ tight tolerance
 ▷ for convergence check
 ▷ project from Ω_1 to Γ_2
 ▷ Newton loop for Ω_2
 ▷ linear system
 ▷ tight tolerance
 ▷ tight tolerance

Full Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
5:    $\Delta\mathbf{x}_B^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \backslash \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
6:    $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$ 
7:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
8:    $\Delta\mathbf{x}_B^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \backslash \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
9:    $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$ 
10: until  $\left[ \left( \|\Delta\mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\Delta\mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Newton-Schwarz loop
 ▷ project from Ω_2 to Γ_1
 ▷ linear system
 ▷ project from Ω_1 to Γ_2
 ▷ linear system
 ▷ tight tolerance

Modified Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
6:   repeat
7:      $\Delta\mathbf{x}_B^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \backslash \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
8:      $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \leq \epsilon$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_B^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \backslash \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \leq \epsilon$ 
16: until  $\left[ \left( \|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Schwarz loop
 ▷ for convergence check
 ▷ project from Ω_2 to Γ_1
 ▷ Newton loop for Ω_1
 ▷ linear system
 ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
 ▷ for convergence check
 ▷ project from Ω_1 to Γ_2
 ▷ Newton loop for Ω_2
 ▷ solve linear system
 ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
 ▷ tight tolerance

Inexact Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,
3: repeat
4:    $\left\{ \begin{matrix} \Delta\mathbf{x}_B^{(1)} \\ \Delta\mathbf{x}_B^{(2)} \end{matrix} \right\} \leftarrow \left( \begin{matrix} \mathbf{K}_{AB}^{(1)} + \mathbf{K}_{AB}^{(1)}\mathbf{H}_{11} & \mathbf{K}_{AB}^{(1)}\mathbf{H}_{12} \\ \mathbf{K}_{AB}^{(2)}\mathbf{H}_{21} & \mathbf{K}_{AB}^{(2)} + \mathbf{K}_{AB}^{(2)}\mathbf{H}_{22} \end{matrix} \right) \backslash \left\{ \begin{matrix} -\mathbf{R}_A^{(1)} \\ -\mathbf{R}_A^{(2)} \end{matrix} \right\}$ 
5:    $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$ 
6:    $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$ 
7: until  $\left[ \left( \|\Delta\mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\Delta\mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Newton-Schwarz loop
 ▷ linear system
 ▷ tight tolerance

Monolithic Schwarz


Implementations*

- All *four variants* implemented in **3D MATLAB** code.

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
6:   repeat
7:      $\Delta\mathbf{x}_\beta^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
8:      $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \leq \epsilon_{\text{machine}}$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_\beta^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \leq \epsilon_{\text{machine}}$ 
16: until  $\left[ \left( \|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```



▷ initialize for Ω_1

▷ initialize for Ω_2

▷ Schwarz loop

▷ for convergence check

▷ project from Ω_2 to Γ_1

▷ Newton loop for Ω_1

▷ linear system

▷ tight tolerance

▷ for convergence check

▷ project from Ω_1 to Γ_2

▷ Newton loop for Ω_2

▷ linear system

▷ tight tolerance


▷ tight tolerance

Full Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
5:    $\Delta\mathbf{x}_\beta^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
6:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
7:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
8:    $\Delta\mathbf{x}_\beta^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
9:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
10: until  $\left[ \left( \|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \right)^2 + \left( \|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```



▷ initialize for Ω_1

▷ initialize for Ω_2

▷ Newton-Schwarz loop

▷ project from Ω_2 to Γ_1

▷ linear system

▷ project from Ω_1 to Γ_2

▷ linear system


▷ tight tolerance

Modified Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
6:   repeat
7:      $\Delta\mathbf{x}_\beta^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
8:      $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \leq \epsilon$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_\beta^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \leq \epsilon$ 
16: until  $\left[ \left( \|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```



▷ initialize for Ω_1

▷ initialize for Ω_2

▷ Schwarz loop

▷ for convergence check

▷ project from Ω_2 to Γ_1

▷ Newton loop for Ω_1

▷ linear system

▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$

▷ for convergence check

▷ project from Ω_1 to Γ_2

▷ Newton loop for Ω_2

▷ solve linear system

▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$


▷ tight tolerance

Inexact Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,
3: repeat
4:    $\left\{ \begin{matrix} \Delta\mathbf{x}_\beta^{(1)} \\ \Delta\mathbf{x}_\beta^{(2)} \end{matrix} \right\} \leftarrow \left( \begin{matrix} \mathbf{K}_{AB}^{(1)} + \mathbf{K}_{AB}^{(1)}\mathbf{H}_{11} & \mathbf{K}_{AB}^{(1)}\mathbf{H}_{12} \\ \mathbf{K}_{AB}^{(2)}\mathbf{H}_{21} & \mathbf{K}_{AB}^{(2)} + \mathbf{K}_{AB}^{(2)}\mathbf{H}_{22} \end{matrix} \right) \setminus \left\{ \begin{matrix} -\mathbf{R}_A^{(1)} \\ -\mathbf{R}_A^{(2)} \end{matrix} \right\}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
6:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
7: until  $\left[ \left( \|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \right)^2 + \left( \|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```



▷ initialize for Ω_1

▷ initialize for Ω_2

▷ Newton-Schwarz loop

▷ linear system

▷ tight tolerance

Monolithic Schwarz

Implementations*

- All *four variants* implemented in **3D MATLAB** code.
- **Modified & monolithic Schwarz** variants implemented in **parallel C++ Albany** code.

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
6:   repeat
7:      $\Delta\mathbf{x}_\beta^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
8:      $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \leq \epsilon_{\text{machine}}$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_\beta^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \leq \epsilon_{\text{machine}}$ 
16: until  $\left[ \left( \|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1

▷ initialize for Ω_2

▷ Schwarz loop

▷ for convergence check

▷ project from Ω_2 to Γ_1

▷ Newton loop for Ω_1

▷ linear system

▷ tight tolerance

▷ for convergence check


▷ project from Ω_1 to Γ_2

▷ Newton loop for Ω_2

▷ linear system

▷ tight tolerance

▷ tight tolerance



Full Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
5:    $\Delta\mathbf{x}_\beta^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
6:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
7:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
8:    $\Delta\mathbf{x}_\beta^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
9:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
10: until  $\left[ \left( \|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \right)^2 + \left( \|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1

▷ initialize for Ω_2

▷ Newton-Schwarz loop



▷ project from Ω_2 to Γ_1

▷ linear system

▷ project from Ω_1 to Γ_2

▷ linear system

▷ tight tolerance

Modified Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
6:   repeat
7:      $\Delta\mathbf{x}_\beta^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
8:      $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \leq \epsilon$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_\beta^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \leq \epsilon$ 
16: until  $\left[ \left( \|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1

▷ initialize for Ω_2

▷ Schwarz loop

▷ for convergence check

▷ project from Ω_2 to Γ_1

▷ Newton loop for Ω_1

▷ linear system

▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$

▷ for convergence check


▷ project from Ω_1 to Γ_2

▷ Newton loop for Ω_2

▷ solve linear system

▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$

▷ tight tolerance



Inexact Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,
3: repeat
4:    $\left\{ \begin{matrix} \Delta\mathbf{x}_\beta^{(1)} \\ \Delta\mathbf{x}_\beta^{(2)} \end{matrix} \right\} \leftarrow \left( \begin{matrix} \mathbf{K}_{AB}^{(1)} + \mathbf{K}_{AB}^{(1)}\mathbf{H}_{11} & \mathbf{K}_{AB}^{(1)}\mathbf{H}_{12} \\ \mathbf{K}_{AB}^{(2)}\mathbf{H}_{21} & \mathbf{K}_{AB}^{(2)} + \mathbf{K}_{AB}^{(2)}\mathbf{H}_{22} \end{matrix} \right) \setminus \left\{ \begin{matrix} -\mathbf{R}_A^{(1)} \\ -\mathbf{R}_A^{(2)} \end{matrix} \right\}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
6:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
7: until  $\left[ \left( \|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \right)^2 + \left( \|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```



▷ initialize for Ω_1

▷ initialize for Ω_2

▷ Newton-Schwarz loop

▷ linear system

▷ tight tolerance

Monolithic Schwarz


Implementations*

- All **four variants** implemented in **3D MATLAB** code.
- **Modified & monolithic Schwarz** variants implemented in **parallel C++ Albany** code.

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
6:   repeat
7:      $\Delta\mathbf{x}_\beta^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
8:      $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \leq \epsilon_{\text{machine}}$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_\beta^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \leq \epsilon_{\text{machine}}$ 
16: until  $\left[ (\|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\|)^2 + (\|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\|)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```





▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Schwarz loop
 ▷ for convergence check
 ▷ project from Ω_2 to Γ_1
 ▷ Newton loop for Ω_1
 ▷ linear system
 ▷ tight tolerance
 ▷ for convergence check
 ▷ project from Ω_1 to Γ_2
 ▷ Newton loop for Ω_2
 ▷ linear system
 ▷ tight tolerance
 ▷ tight tolerance

Full Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
5:    $\Delta\mathbf{x}_\beta^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
6:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
7:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
8:    $\Delta\mathbf{x}_\beta^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
9:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
10: until  $\left[ (\|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\|)^2 + (\|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\|)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```


▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Newton-Schwarz loop
 ▷ project from Ω_2 to Γ_1
 ▷ linear system
 ▷ project from Ω_1 to Γ_2
 ▷ linear system
 ▷ tight tolerance

Modified Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,  $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$  on  $\Gamma_1$ 
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,  $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$  on  $\Gamma_2$ 
3: repeat
4:    $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$ 
6:   repeat
7:      $\Delta\mathbf{x}_\beta^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$ 
8:      $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
9:   until  $\|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\| \leq \epsilon$ 
10:   $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$ 
11:   $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$ 
12:  repeat
13:     $\Delta\mathbf{x}_\beta^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$ 
14:     $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
15:  until  $\|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\| \leq \epsilon$ 
16: until  $\left[ (\|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\|/\|\mathbf{x}_B^{(1)}\|)^2 + (\|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\|/\|\mathbf{x}_B^{(2)}\|)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```





▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Schwarz loop
 ▷ for convergence check
 ▷ project from Ω_2 to Γ_1
 ▷ Newton loop for Ω_1
 ▷ linear system
 ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
 ▷ for convergence check
 ▷ project from Ω_1 to Γ_2
 ▷ Newton loop for Ω_2
 ▷ solve linear system
 ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
 ▷ tight tolerance

Inexact Schwarz

```

1:  $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$  in  $\Omega_1$ ,  $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$  on  $\partial\varphi\Omega_1$ ,
2:  $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$  in  $\Omega_2$ ,  $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$  on  $\partial\varphi\Omega_2$ ,
3: repeat
4:    $\left\{ \begin{matrix} \Delta\mathbf{x}_\beta^{(1)} \\ \Delta\mathbf{x}_\beta^{(2)} \end{matrix} \right\} \leftarrow \left( \begin{matrix} \mathbf{K}_{AB}^{(1)} + \mathbf{K}_{A\beta}^{(1)}\mathbf{H}_{11} & \mathbf{K}_{A\beta}^{(1)}\mathbf{H}_{12} \\ \mathbf{K}_{A\beta}^{(2)}\mathbf{H}_{21} & \mathbf{K}_{A\beta}^{(2)}\mathbf{H}_{22} \end{matrix} \right) \setminus \left\{ \begin{matrix} -\mathbf{R}_A^{(1)} \\ -\mathbf{R}_A^{(2)} \end{matrix} \right\}$ 
5:    $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{x}_\beta^{(1)} + \Delta\mathbf{x}_\beta^{(1)}$ 
6:    $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{x}_\beta^{(2)} + \Delta\mathbf{x}_\beta^{(2)}$ 
7: until  $\left[ (\|\Delta\mathbf{x}_\beta^{(1)}\|/\|\mathbf{x}_\beta^{(1)}\|)^2 + (\|\Delta\mathbf{x}_\beta^{(2)}\|/\|\mathbf{x}_\beta^{(2)}\|)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ 

```

▷ initialize for Ω_1
 ▷ initialize for Ω_2
 ▷ Newton-Schwarz loop
 ▷ linear system
 ▷ tight tolerance

Monolithic Schwarz

Schwarz Alternating Method in *Albany* Code

Modified & monolithic Schwarz versions have been implemented within the **LCM project** in Sandia's open-source parallel, C++, multi-physics, finite element code, **Albany**.

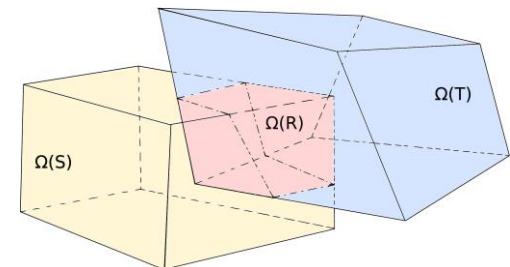


<https://github.com/gahansen/Albany>

- **Component-based** design for rapid development of capabilities.
- Extensive use of libraries from the open-source **Trilinos** project.
 - Use of the **Phalanx** package to decompose complex problem into simpler problems with managed dependencies.
 - Use of the **Sacado** package for **automatic differentiation**.
 - Use of **Teko** package for **block preconditioning**.
- **Parallel** implementation of Schwarz alternating method uses the **Data Transfer Kit (DTK)**.
- All software available on **GitHub**.



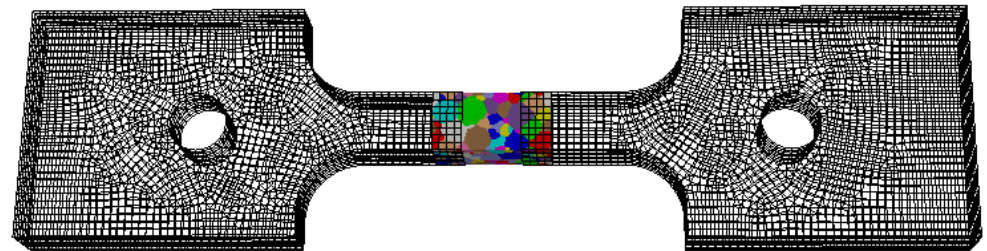
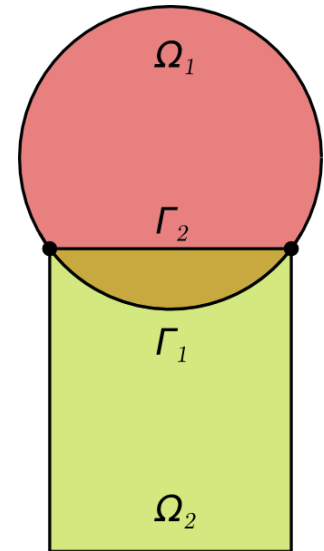
<https://github.com/trilinos/trilinos>



<https://github.com/ORNL-CEES/DataTransferKit>

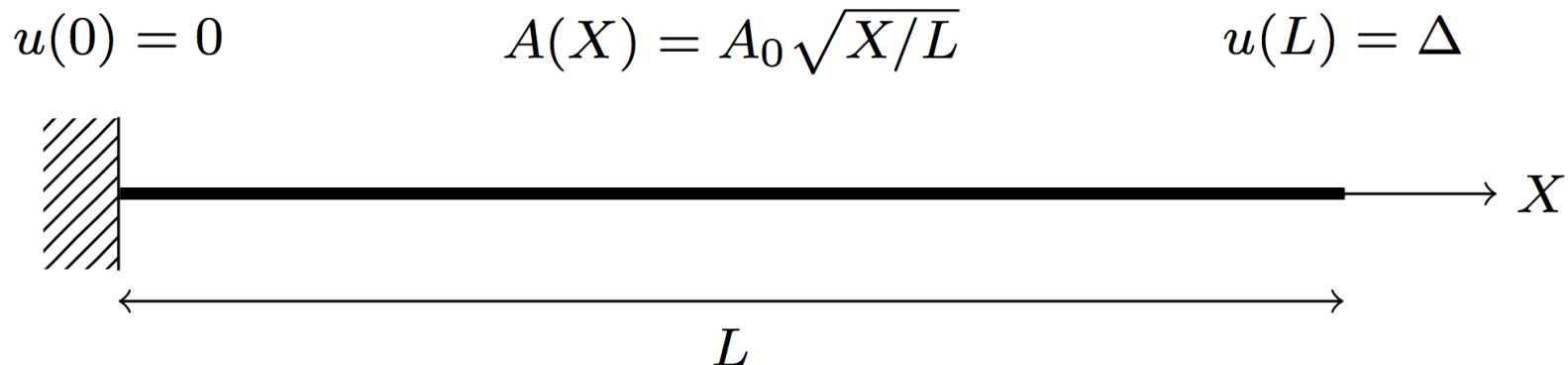
Outline

1. Motivation
2. Schwarz Alternating Method: Background & History
3. Schwarz Alternating Method for Concurrent Multiscale Coupling in Quasistatics
 - Four Variants: Full Schwarz, Inexact Schwarz, Modified Schwarz, Monolithic Schwarz
 - Implementations: MATLAB, Albany
- 4. Numerical Examples**
5. Summary
6. Future Work
7. References
8. Appendix



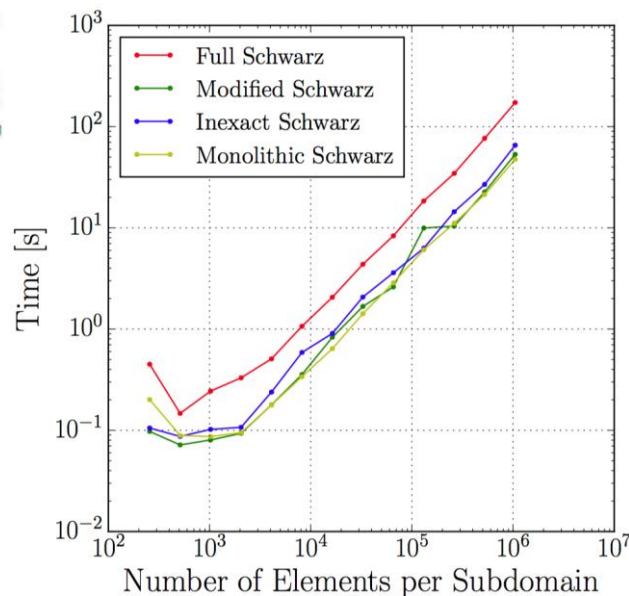
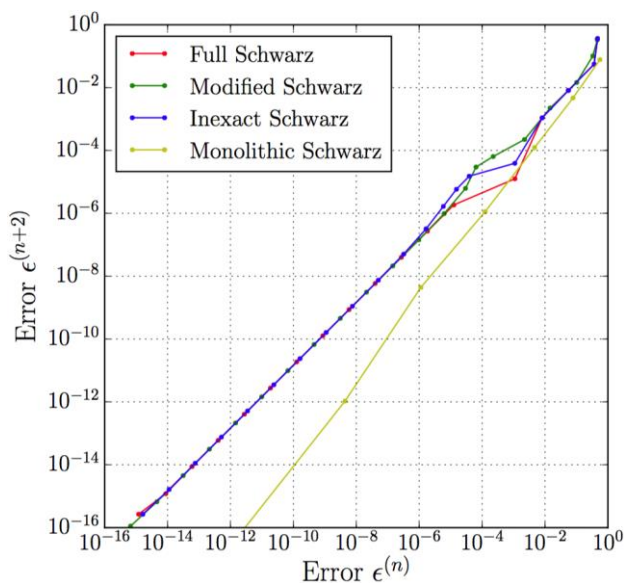
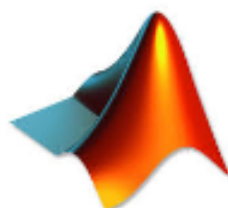
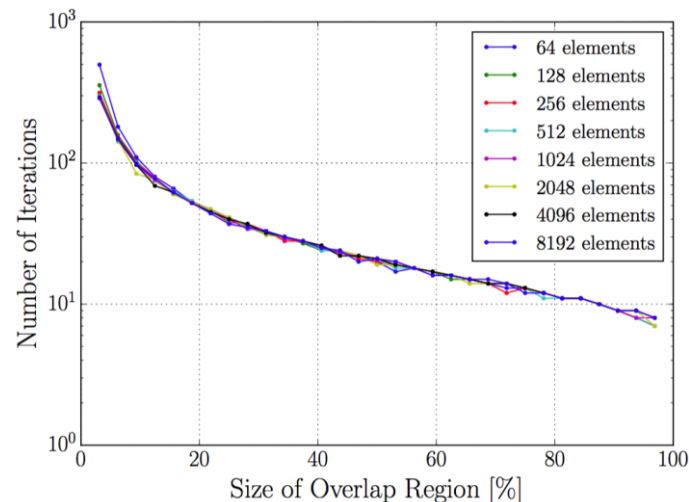
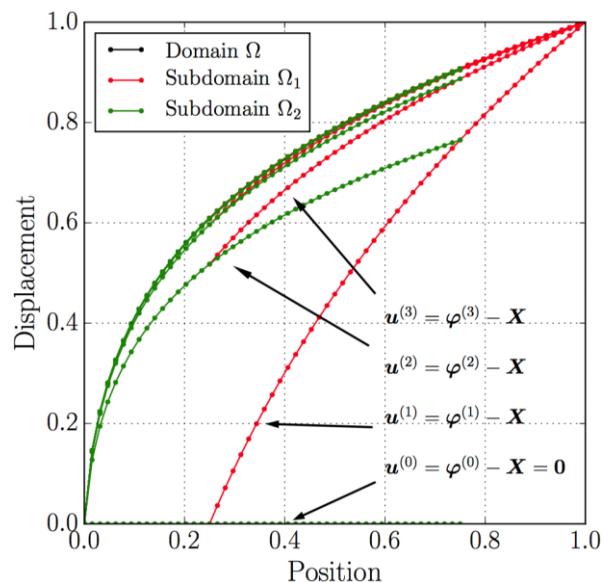
Example #1: Foulk's Singular Bar

- **1D proof of concept** problem:
 - **1D bar** with area proportional to square root of length.
 - Strong **singularity** on left end of bar.
 - Simple **hyperelastic** material model with no damage.
 - **MATLAB** implementation.

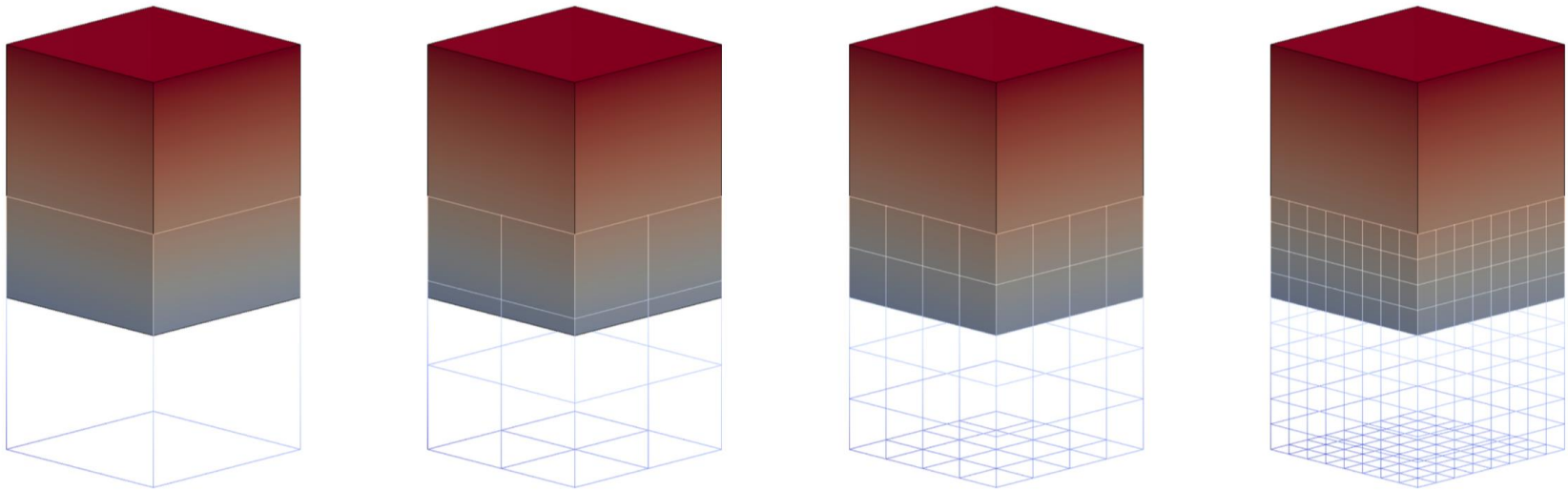


- **Problem goals:**
 - Explore **viability** of **4 variants** of the Schwarz alternating method.
 - Test **convergence** and compare with literature (Evans, 1986).
 - Expect **faster convergence** in **fewer iterations** with **increased overlap**.

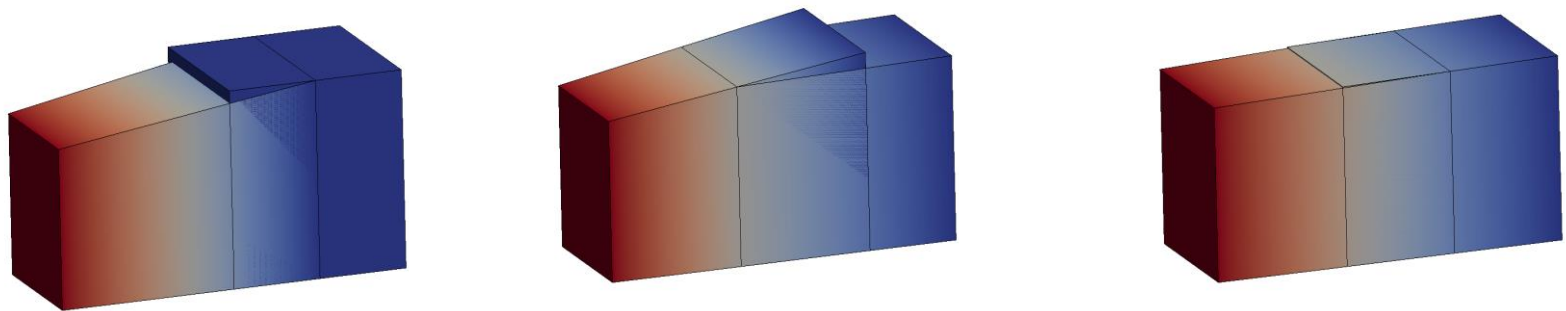
Singular Bar and Schwarz Variants



Example #2: Cuboid Problem



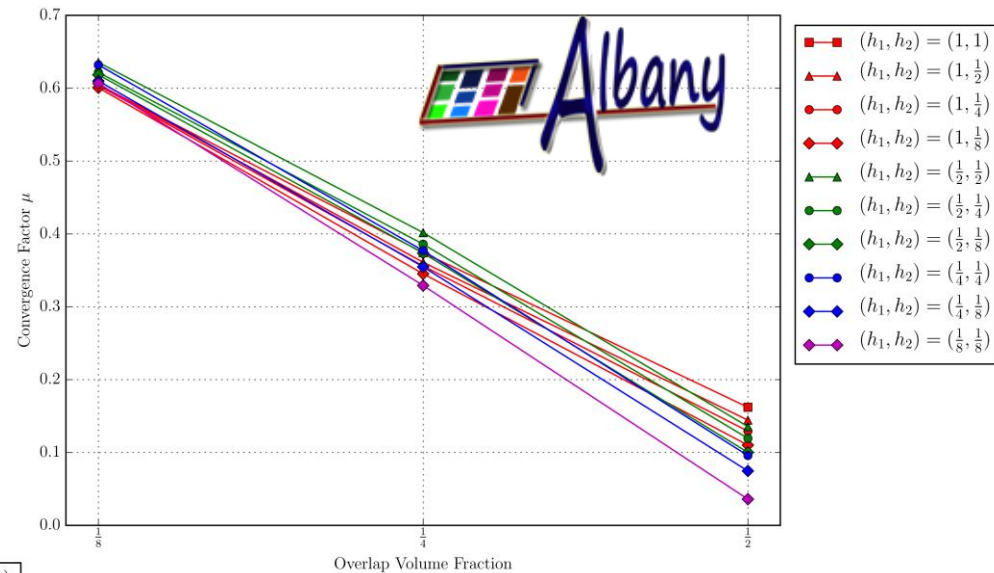
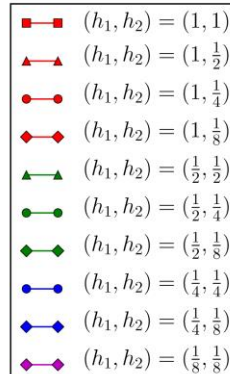
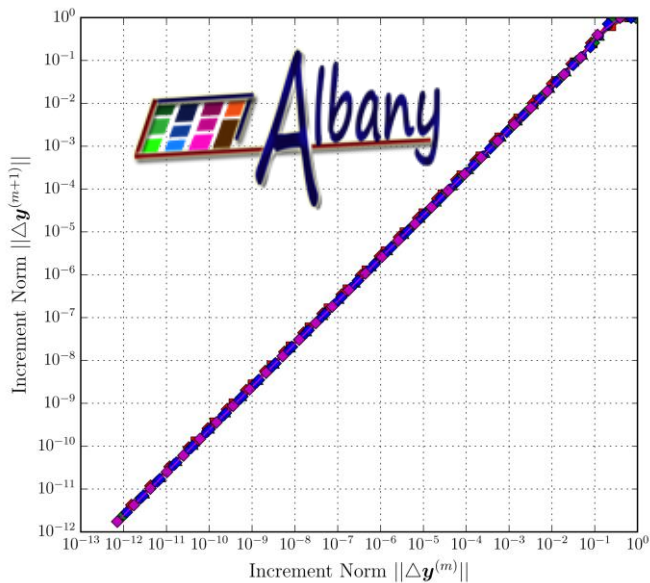
- Coupling of *two cuboids* with square base (above).
- *Neohookean*-type material model.



Combined Newton-Schwarz Iteration

Cuboid Problem: Convergence with Overlap & Refinement

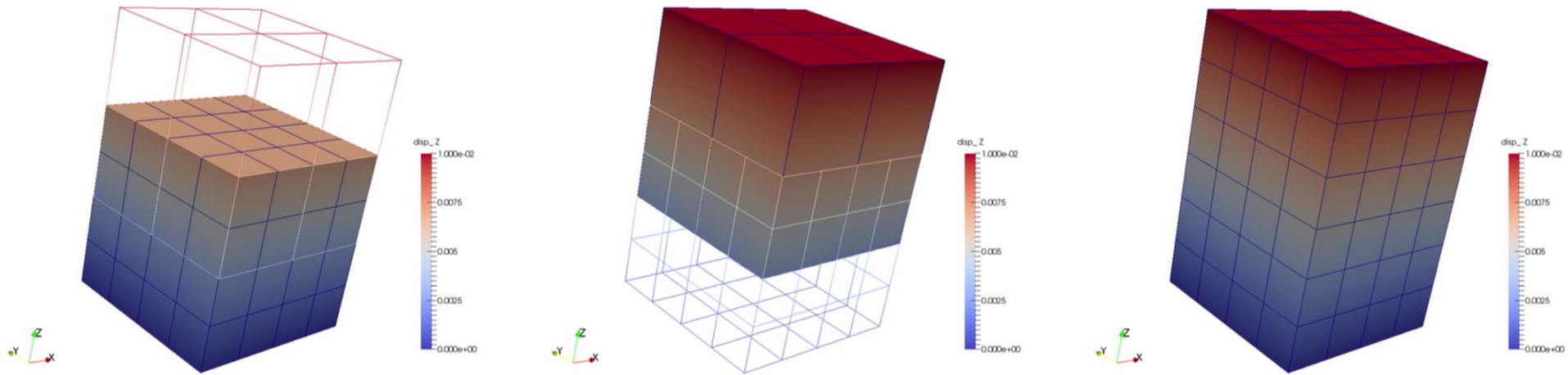
Below: Convergence of the cuboid problem for different mesh sizes and fixed overlap volume fraction. The Schwarz alternating method converges *linearly*.



Above: Convergence factor μ as a function of overlap volume and different mesh. There is *faster linear convergence* with increasing *overlap volume fraction*.

$$\Delta y^{(m+1)} \leq \mu \Delta y^{(m)}$$

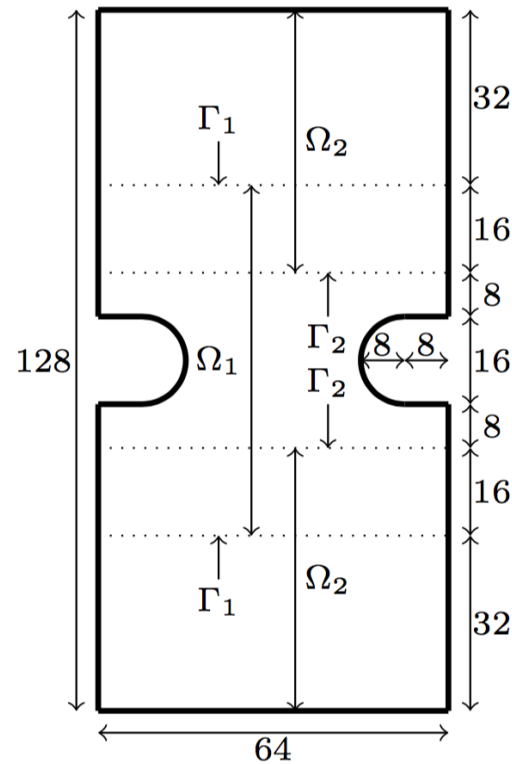
Cuboid Problem: Schwarz Error



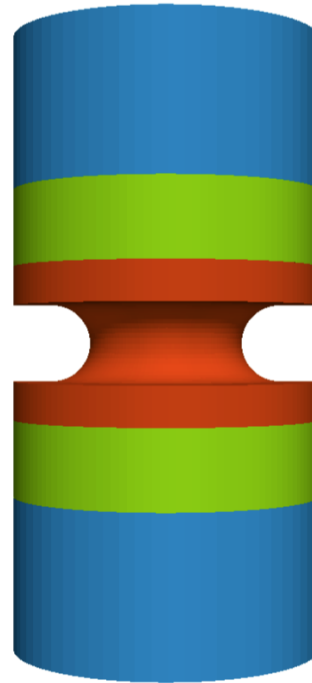
Subdomain	u_3 relative error	σ_{33} relative error
Ω_1	1.24×10^{-14}	2.31×10^{-13}
Ω_2	7.30×10^{-15}	3.06×10^{-13}



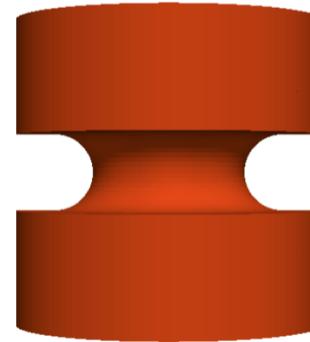
Example #3: Notched Cylinder



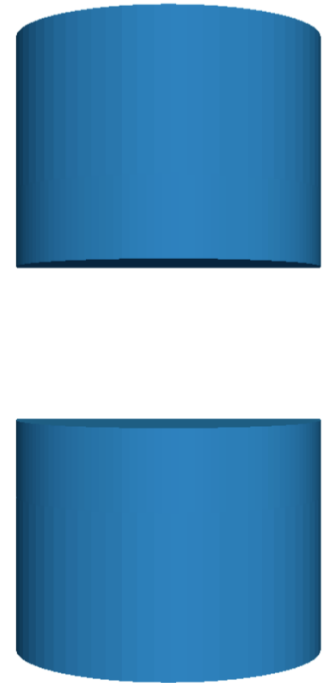
(a) Schematic



(b) Entire Domain Ω



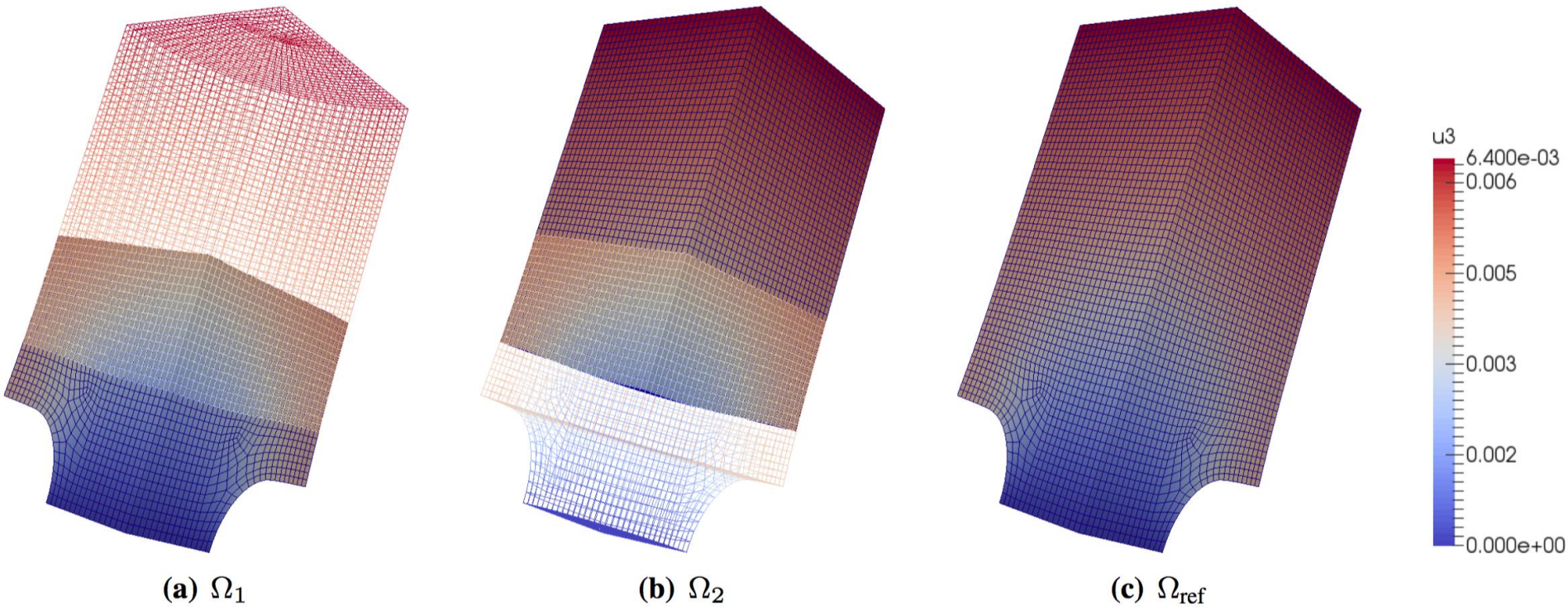
(c) Fine Region Ω_1



(d) Coarse Region Ω_2

- **Notched cylinder** that is stretched along its axial direction.
- Domain decomposed into **two subdomains**.
- **Neohookean**-type material model.

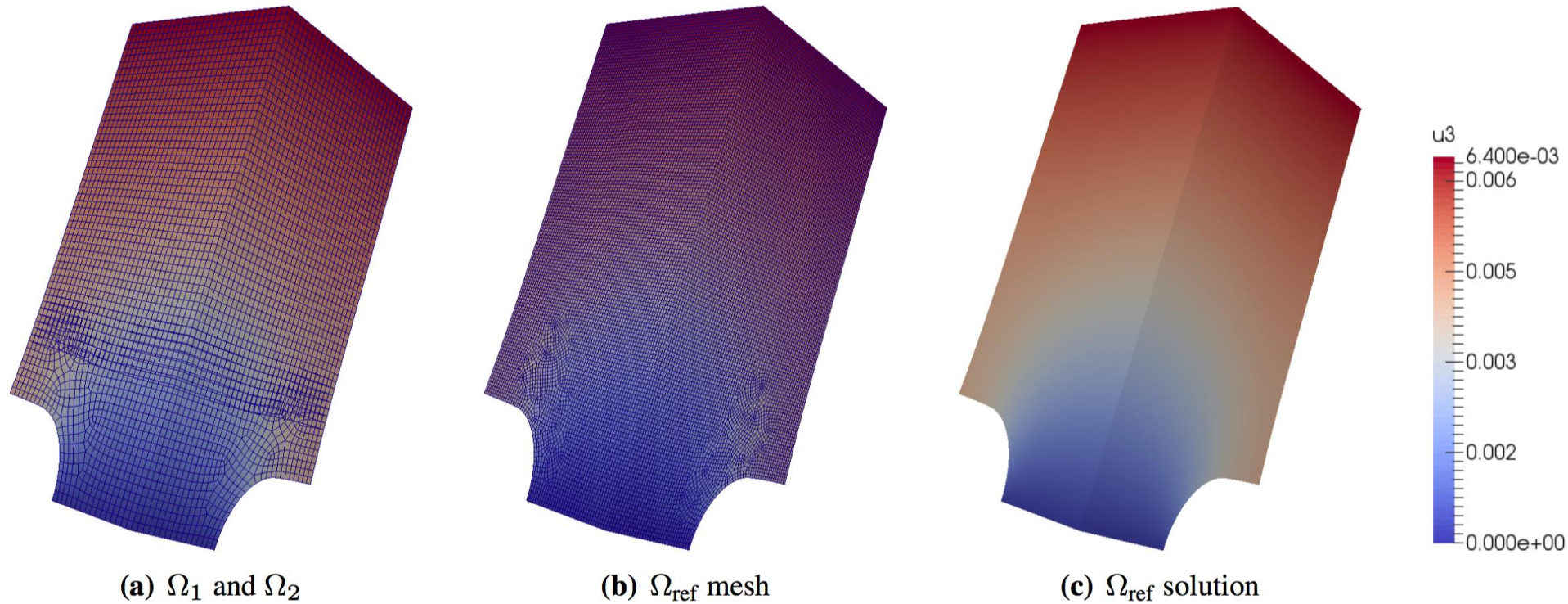
Notched Cylinder: Conformal HEX-HEX Coupling



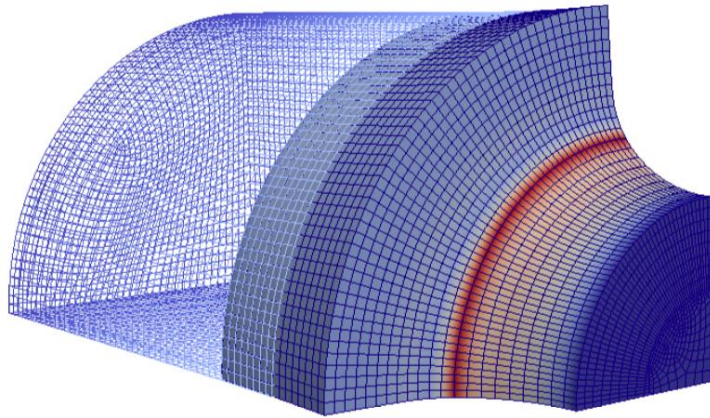
Absolute residual tolerance	u_3 relative error	
	Ω_1	Ω_2
1.0×10^{-4}	7.60×10^{-3}	3.20×10^{-3}
1.0×10^{-8}	3.10×10^{-5}	1.71×10^{-5}
1.0×10^{-12}	1.34×10^{-9}	5.10×10^{-10}
1.0×10^{-14}	1.23×10^{-11}	4.69×10^{-12}
2.5×10^{-16}	1.14×10^{-13}	8.37×10^{-14}



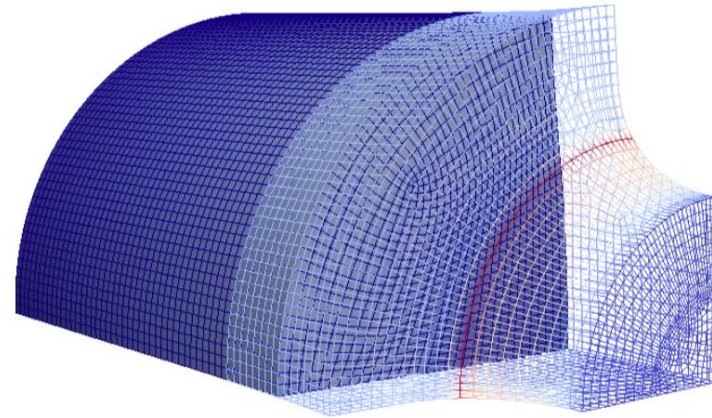
Notched Cylinder: Nonconformal HEX-HEX Coupling



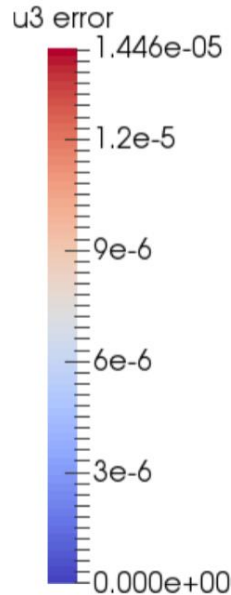
Notched Cylinder: Nonconformal HEX-HEX Coupling



(a) Ω_1



(b) Ω_2

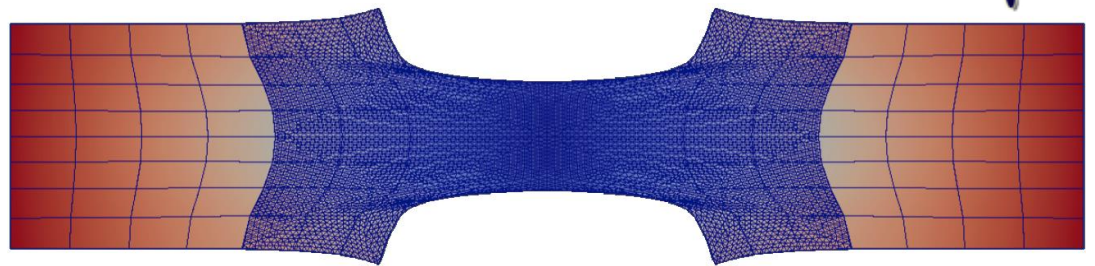
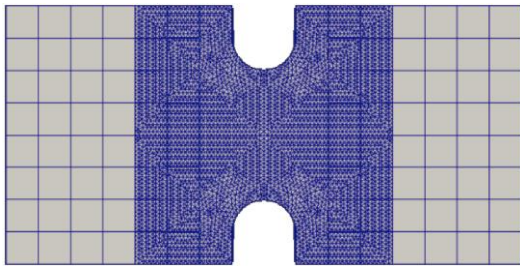
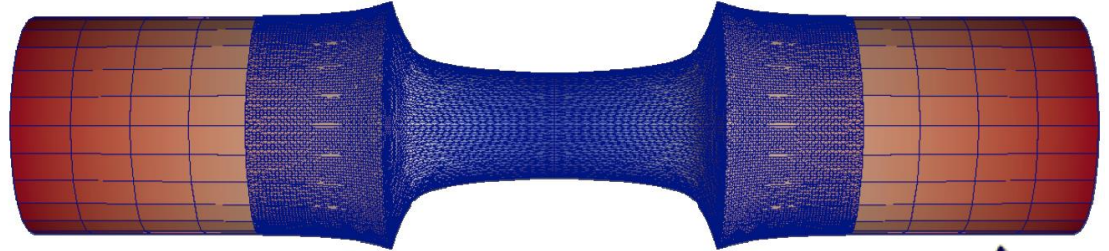
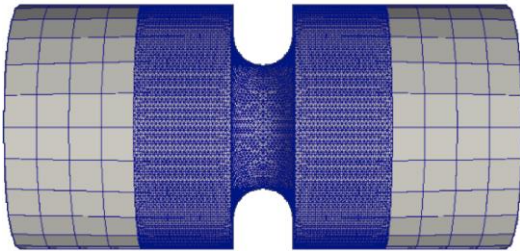


Absolute residual tolerance	u_3 relative error	
	Ω_1	Ω_2
1.0×10^{-8}	1.31×10^{-3}	4.45×10^{-4}
1.0×10^{-12}	1.30×10^{-3}	4.43×10^{-4}
1.0×10^{-14}	1.30×10^{-3}	4.43×10^{-4}
2.5×10^{-16}	1.30×10^{-3}	4.43×10^{-4}

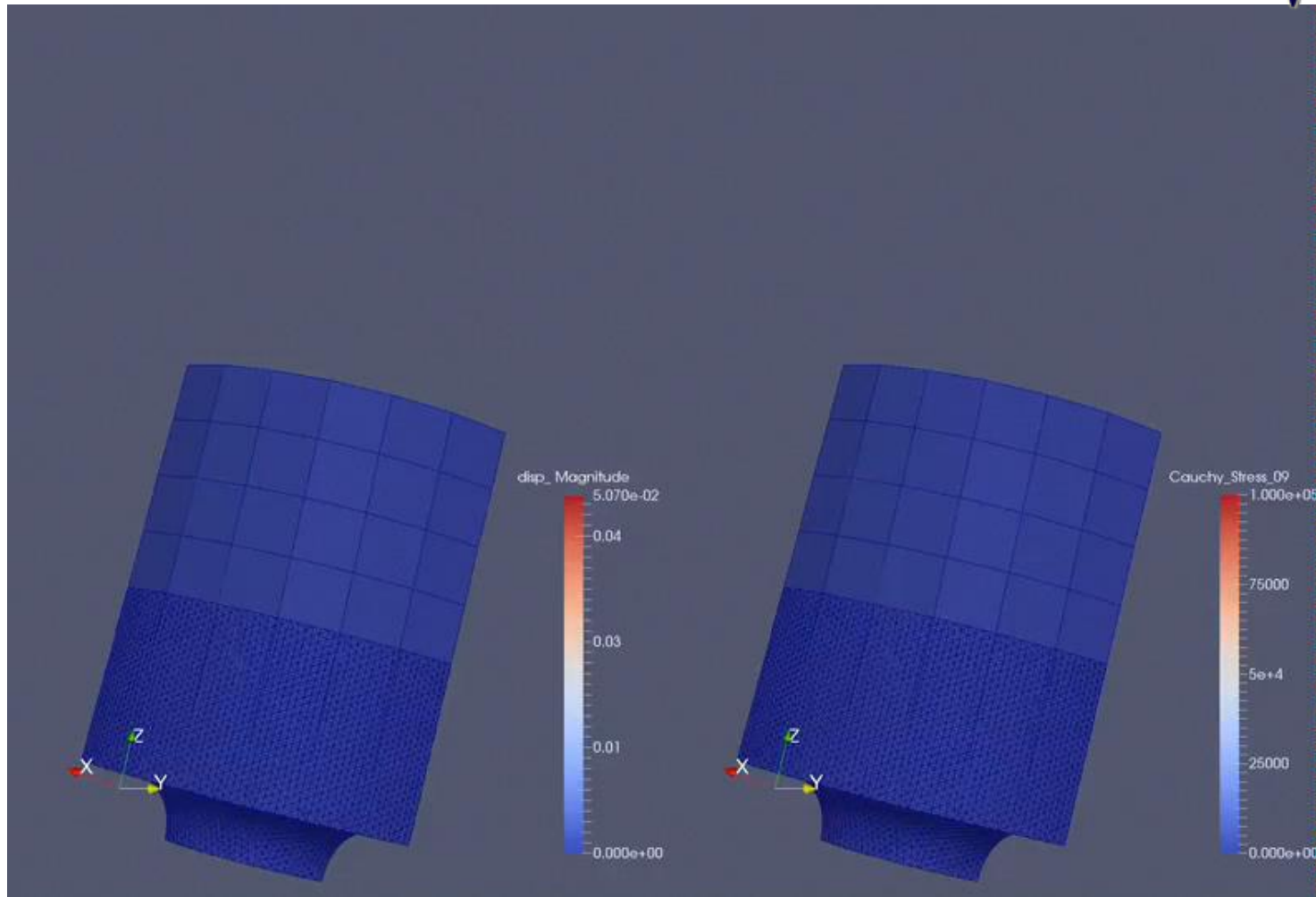


Notched Cylinder: TET-HEX Coupling

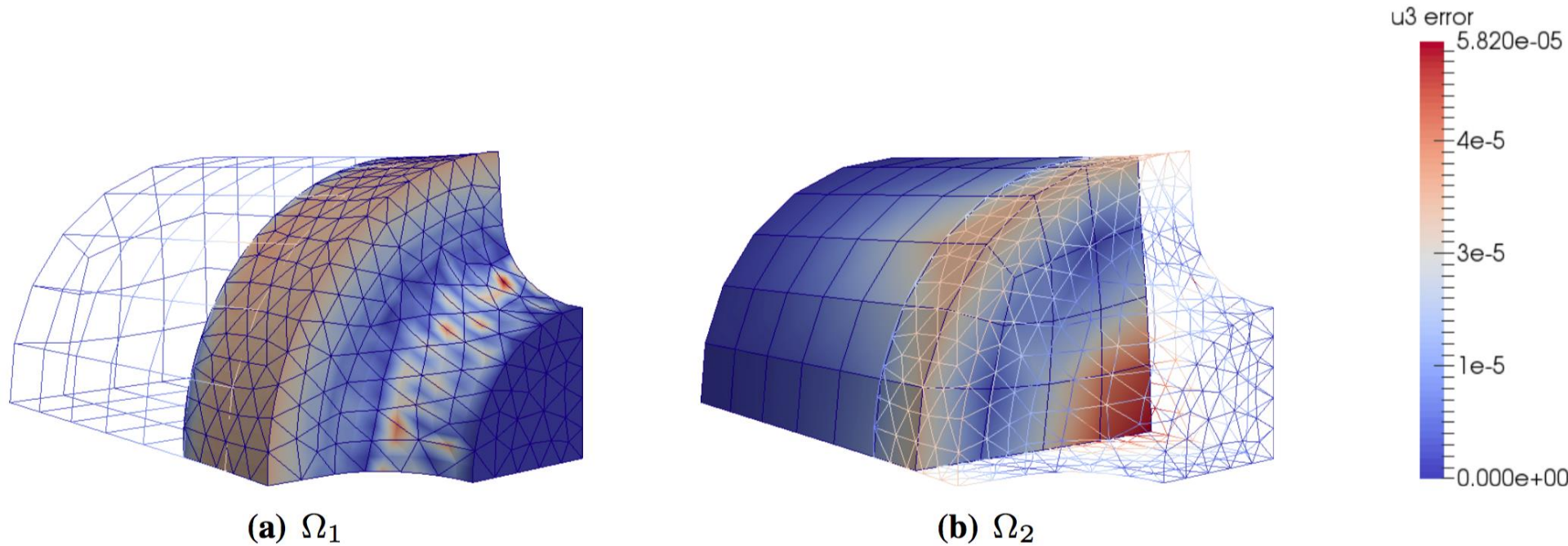
- The Schwarz alternating method is capable of coupling *different mesh topologies*.
- The notched region, where stress concentrations are expected, is *finely* meshed with *tetrahedral* elements.
- The top and bottom regions, presumably of less interest, are meshed with *coarser* *hexahedral* elements.



Notched Cylinder: TET-HEX Coupling



Notched Cylinder: Conformal TET-HEX Coupling



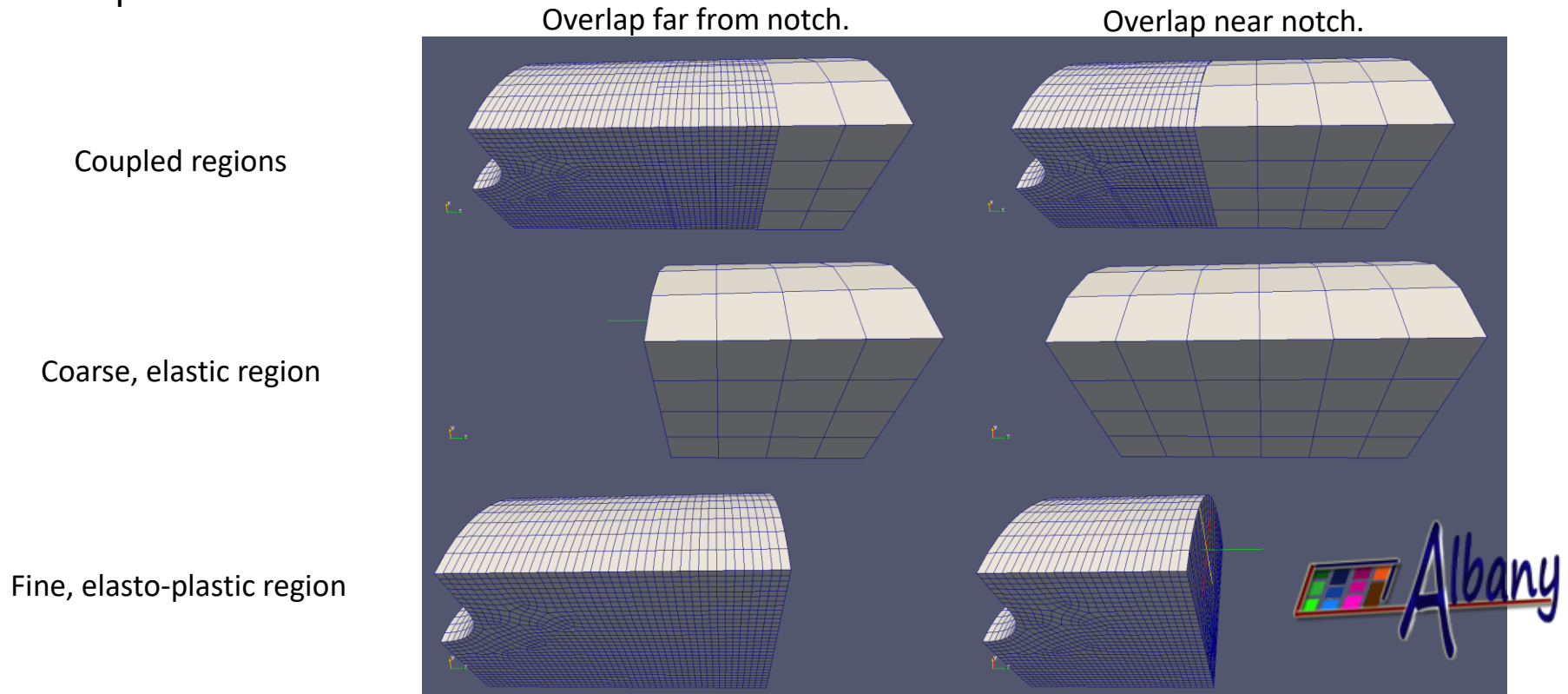
Absolute residual tolerance	u_3 relative error	
	Ω_1	Ω_2
1.0×10^{-14}	9.27×10^{-3}	3.70×10^{-3}



Notched Cylinder: Coupling Different Materials

The Schwarz method is capable of coupling regions with *different material models*.

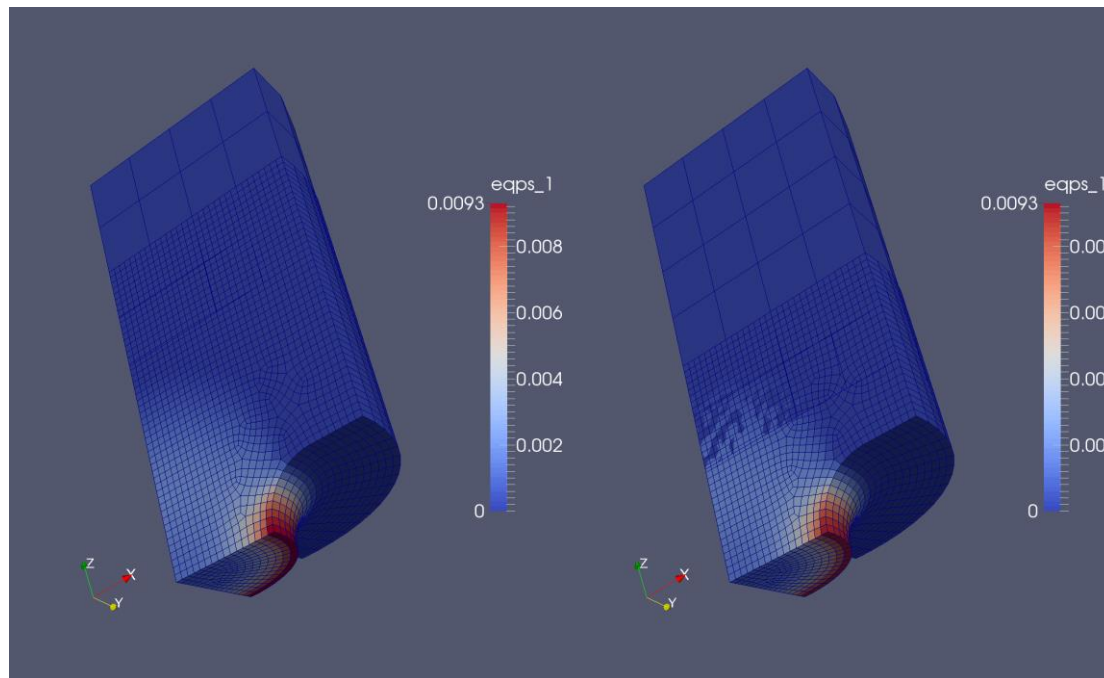
- Notched cylinder subjected to tensile load with an *elastic* and *J2 elasto-plastic* regions.
- *Coarse* region is *elastic* and *fine* region is *elasto-plastic*.
- The *overlap region* in the first mesh is nearer the notch, where plastic behavior is expected.



Notched Cylinder: Coupling Different Materials

Need to be careful to do domain decomposition so that material models are **consistent** in overlap region.

- When the **overlap** region is **far from the notch**, no plastic deformation exists in it: the coarse and fine regions predict the **same behavior**.
- When the **overlap** region is **near the notch**, plastic deformation spills onto it and the two models predict different behavior, affecting convergence **adversely**.

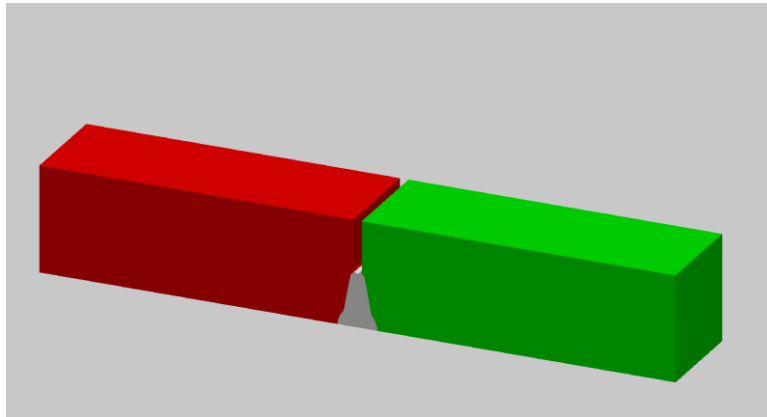


Overlap far from notch.

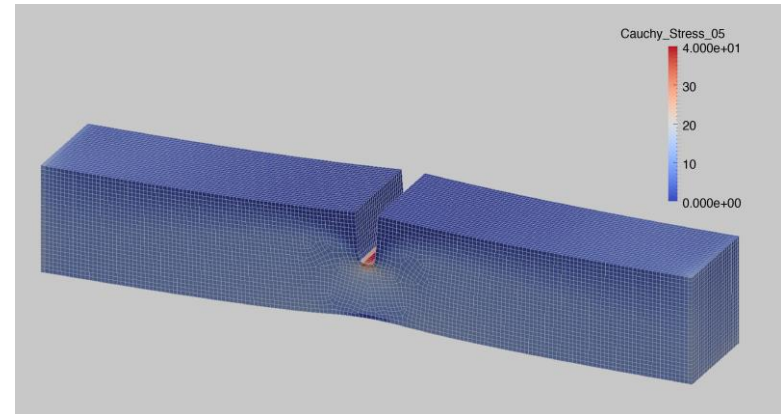
Overlap near notch.

Example #4: Laser Weld with 3 Subdomains

Laser weld specimen

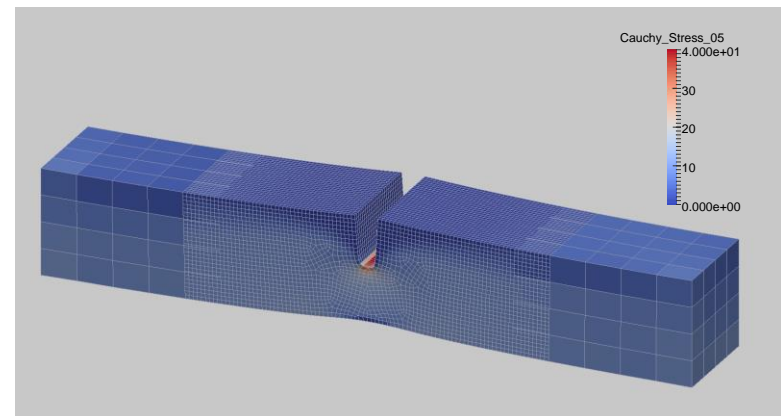


Single domain discretization

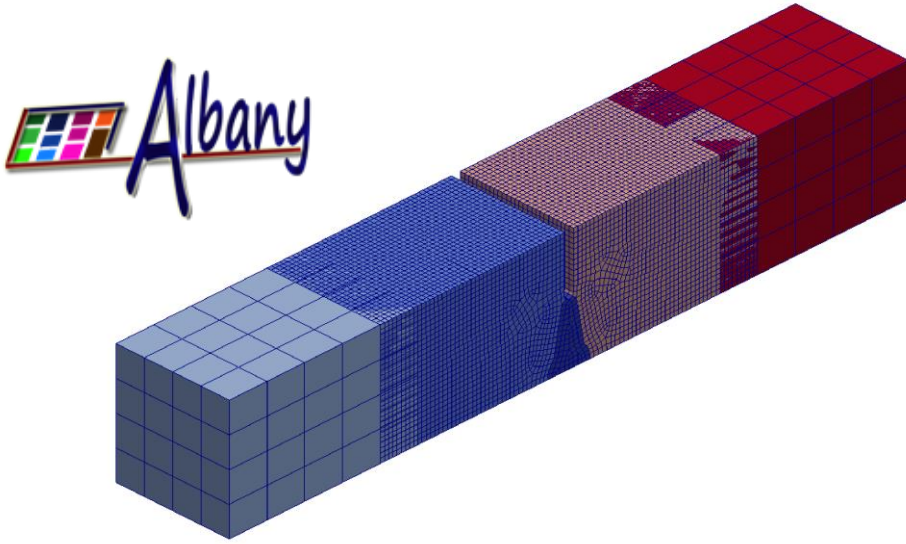


Coupled Schwarz discretization
(50% reduction in model size)

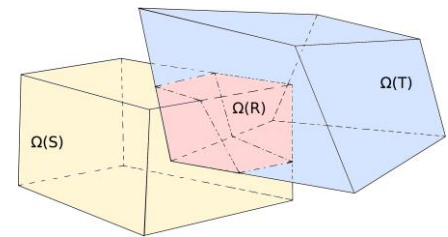
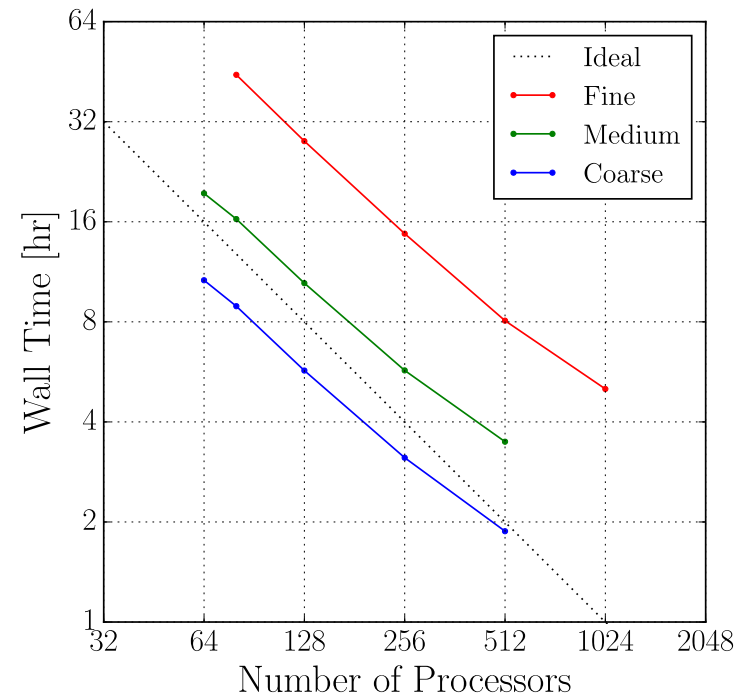
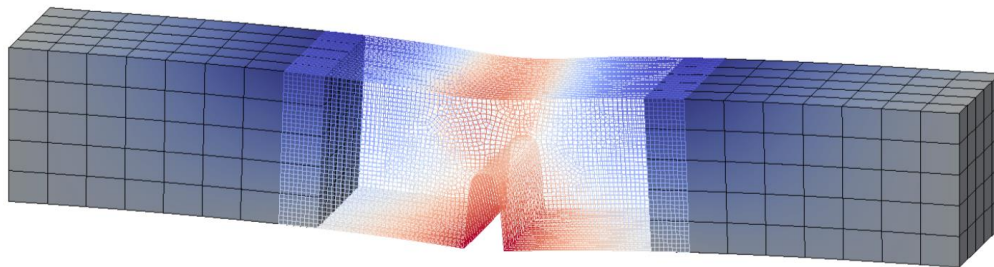
- Problem of *practical scale* (~200K dofs).
- *Isotropic elasticity* and *J2 plasticity* with linear isotropic hardening.
- *Identical parameters* for weld and base materials for proof of concept, to become independent models.



Laser Weld: Strong Scalability of Parallel Schwarz with DTK



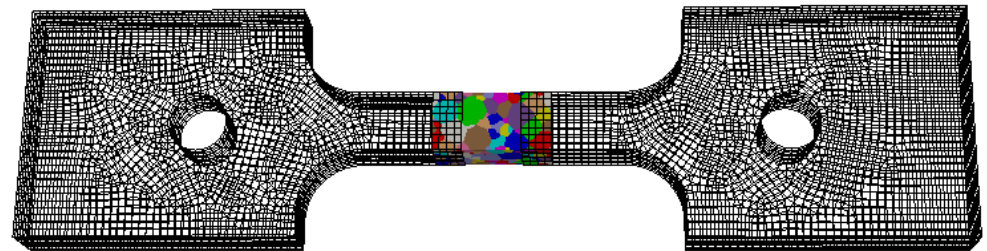
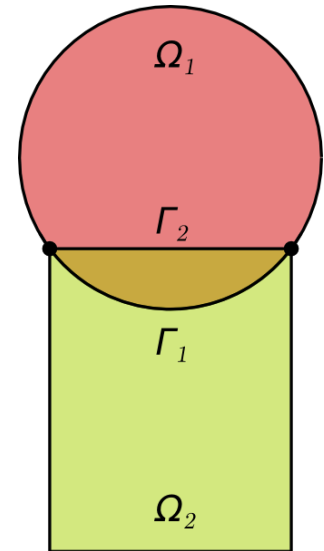
- ***Near-ideal linear speedup*** (64-1024 cores).



Data Transfer Kit (DTK)

Outline

1. Motivation
2. Schwarz Alternating Method: Background & History
3. Schwarz Alternating Method for Concurrent Multiscale Coupling in Quasistatics
 - Four Variants: Full Schwarz, Inexact Schwarz, Modified Schwarz, Monolithic Schwarz
 - Implementations: MATLAB, Albany
4. Numerical Examples
5. **Summary**
6. Future Work
7. References
8. Appendix

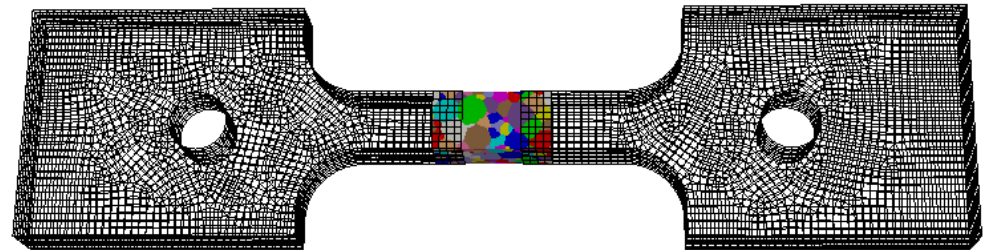
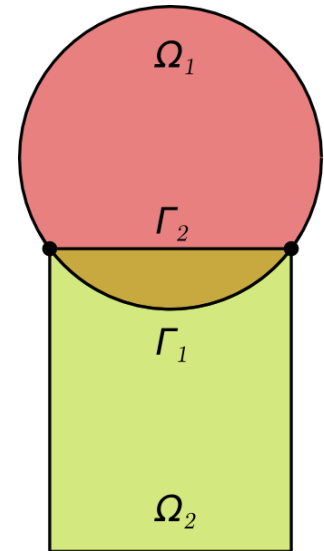


Summary

- We have proposed the ***Schwarz alternating method*** as a means of ***concurrent multiscale coupling*** in finite deformation quasistatic solid mechanics.
- We have developed ***four variants*** of the Schwarz alternating method (***Full Schwarz, Modified Schwarz, Inexact Schwarz, Monolithic Schwarz***).
- We have ***proven*** that the Full Schwarz variant converges geometrically for the solid mechanics problem.
- We have ***demonstrated numerically*** that the ***convergence*** of the Schwarz method in its four variants is ***linear***.
- We have demonstrated ***coupling*** of ***conformal*** and ***non-conformal meshes***, meshes with ***different levels of refinement***, meshes with different ***element topologies***, and ***> two subdomains*** via the proposed method.
- We have demonstrated that the ***error*** in the coupling can be decreased up to ***numerical precision*** provided that no other sources of error exist.
- We have developed a ***parallel*** implementation of the ***Modified Schwarz*** method in the ***Albany code*** and demonstrated that the ***strong scalability*** of our implementation is close to ***ideal***.

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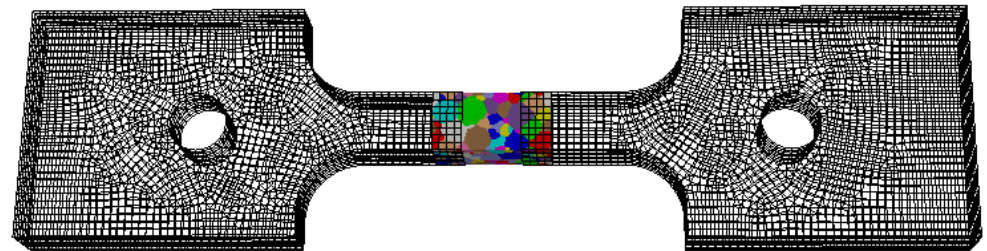
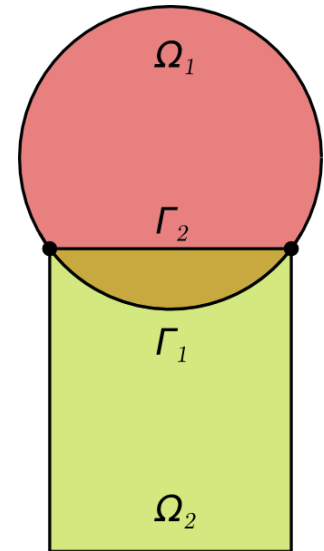


Future Work

- Extension of the methods presented herein to ***transient dynamics (hyperbolic)*** problems with the ability to use ***different time steps*** and ***time integrators*** for each subdomain.
- Development of a ***multi-physics coupling framework*** based on variational formulations and the Schwarz alternating method.
- ***Analysis*** of the convergence for the other Schwarz variants introduced herein, namely Modified Schwarz, Inexact Schwarz, and Monolithic Schwarz.
- Using the Schwarz alternating method with ***different solvers*** in different domains.
- Develop a ***hybrid FOM-ROM*** (full-order-model – reduced-order-model) framework using the Schwarz alternating method.
- Introduction of ***pervasive multi-threading*** into our *Albany* implementation of the Schwarz alternating method using the *Kokkos* framework.
- Multiscale coupling using the proposed Schwarz alternating method in ***other applications***.

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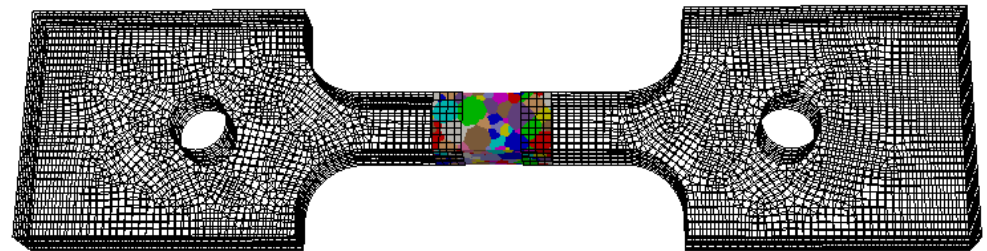
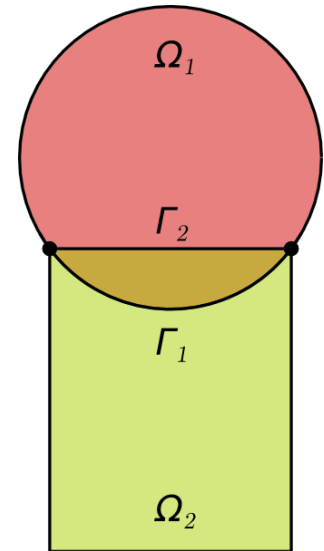


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Appendix. Previous Work

Comput Mech (2014) 54:803–820
DOI 10.1007/s00466-014-1034-0

ORIGINAL PAPER

A multiscale overlapped coupling formulation for large-deformation strain localization

WaiChing Sun · Alejandro Mota

Received: 18 September 2013 / Accepted: 7 April 2014 / Published online: 3 May 2014
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Abstract We generalize the multiscale overlapped domain framework to couple multiple rate-independent standard dissipative material models in the finite deformation regime across different length scales. We show that a fully coupled multiscale incremental boundary-value problem can be recast as the stationary point that optimizes the partitioned incremental work of a three-field energy functional. We also establish inf-sup tests to examine the numerical stability issues that arise from enforcing weak compatibility in the three-field formulation. We also devise a new block solver for the domain coupling problem and demonstrate the performance of the formulation with one-dimensional numerical examples. These simulations indicate that it is sufficient to introduce a localization limiter in a confined region of interest to regularize the partial differential equation if loss of ellipticity occurs.

strain localization may lead to the eventual failure of materials, this phenomenon is of significant importance to modern engineering applications.

The objective of this work is to introduce concurrent coupling between sub-scale and macro-scale simulations for inelastic materials that are prone to strain localization. Since it is not feasible to conduct sub-scale simulations on macroscopic problems, we use the domain coupling method such that computational resources can be efficiently allocated to regions of interest [14, 23, 24, 30]. To the best of our knowledge, this is the first work focusing on utilizing the domain coupling method to model strain localization in inelastic materials undergoing large deformation.

Nevertheless, modeling strain localization with the conventional finite element method may lead to spurious mesh-dependent results due to the loss of ellipticity at the onset of strain localization [31]. To circumvent the loss of mate-

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Three-field multiscale coupling formulation with compatibility enforced weakly using ***Lagrange multipliers***.

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Method works well, but is *difficult to implement* into existing codes.

Appendix. Full Schwarz Method

Classical algorithm originally proposed by Schwarz with **outer Schwarz loop** and **inner Newton loop**, each converged to a **tight tolerance** ($\epsilon_{\text{machine}}$).

1: $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$ in Ω_1 , $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$ on $\partial\varphi\Omega_1$, $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$ on Γ_1	▷ initialize for Ω_1
2: $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$ in Ω_2 , $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$ on $\partial\varphi\Omega_2$, $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$ on Γ_2	▷ initialize for Ω_2
3: repeat	▷ Schwarz loop
4: $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$	▷ for convergence check
5: $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$	▷ project from Ω_2 to Γ_1
6: repeat	▷ Newton loop for Ω_1
7: $\Delta\mathbf{x}_B^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$	▷ linear system
8: $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$	
9: until $\ \Delta\mathbf{x}_B^{(1)}\ /\ \mathbf{x}_B^{(1)}\ \leq \epsilon_{\text{machine}}$	▷ tight tolerance
10: $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$	▷ for convergence check
11: $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$	▷ project from Ω_1 to Γ_2
12: repeat	▷ Newton loop for Ω_2
13: $\Delta\mathbf{x}_B^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$	▷ linear system
14: $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$	
15: until $\ \Delta\mathbf{x}_B^{(2)}\ /\ \mathbf{x}_B^{(2)}\ \leq \epsilon_{\text{machine}}$	▷ tight tolerance
16: until $\left[\left(\ \mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\ /\ \mathbf{x}_B^{(1)}\ \right)^2 + \left(\ \mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\ /\ \mathbf{x}_B^{(2)}\ \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$	▷ tight tolerance

Appendix. Inexact Schwarz Method

Classical algorithm originally proposed by Schwarz with **outer Schwarz loop** and **inner Newton loop**, with Newton step converged to a **loose tolerance**.

1: $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$ in Ω_1 , $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$ on $\partial\varphi\Omega_1$, $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$ on Γ_1	▷ initialize for Ω_1
2: $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$ in Ω_2 , $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$ on $\partial\varphi\Omega_2$, $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$ on Γ_2	▷ initialize for Ω_2
3: repeat	▷ Schwarz loop
4: $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$	▷ for convergence check
5: $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$	▷ project from Ω_2 to Γ_1
6: repeat	▷ Newton loop for Ω_1
7: $\Delta\mathbf{x}_B^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$	▷ linear system
8: $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$	
9: until $\ \Delta\mathbf{x}_B^{(1)}\ /\ \mathbf{x}_B^{(1)}\ \leq \epsilon$	▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
10: $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$	▷ for convergence check
11: $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$	▷ project from Ω_1 to Γ_2
12: repeat	▷ Newton loop for Ω_2
13: $\Delta\mathbf{x}_B^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$	▷ solve linear system
14: $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$	
15: until $\ \Delta\mathbf{x}_B^{(2)}\ /\ \mathbf{x}_B^{(2)}\ \leq \epsilon$	▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
16: until $\left[\left(\ \mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\ /\ \mathbf{x}_B^{(1)}\ \right)^2 + \left(\ \mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\ /\ \mathbf{x}_B^{(2)}\ \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$	▷ tight tolerance

Appendix. Monolithic Schwarz Method

Combines Schwarz and Newton loop into *since Newton-Schwarz loop*, with *elimination of Schwarz boundary DOFs*, and tight convergence tolerance.

- 1: $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$ in Ω_1 , $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$ on $\partial_\varphi \Omega_1$, ▷ initialize for Ω_1
- 2: $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$ in Ω_2 , $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$ on $\partial_\varphi \Omega_2$, ▷ initialize for Ω_2
- 3: **repeat** ▷ Newton-Schwarz loop
- 4:
$$\begin{Bmatrix} \Delta \mathbf{x}_B^{(1)} \\ \Delta \mathbf{x}_B^{(2)} \end{Bmatrix} \leftarrow \begin{pmatrix} \mathbf{K}_{AB}^{(1)} + \mathbf{K}_{A\beta}^{(1)} \mathbf{H}_{11} & \mathbf{K}_{A\beta}^{(1)} \mathbf{H}_{12} \\ \mathbf{K}_{A\beta}^{(2)} \mathbf{H}_{21} & \mathbf{K}_{AB}^{(2)} + \mathbf{K}_{A\beta}^{(2)} \mathbf{H}_{22} \end{pmatrix} \setminus \begin{Bmatrix} -\mathbf{R}_A^{(1)} \\ -\mathbf{R}_A^{(2)} \end{Bmatrix}$$
 ▷ linear system
- 5: $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta \mathbf{x}_B^{(1)}$
- 6: $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta \mathbf{x}_B^{(2)}$
- 7: **until** $\left[\left(\|\Delta \mathbf{x}_B^{(1)}\| / \|\mathbf{x}_B^{(1)}\| \right)^2 + \left(\|\Delta \mathbf{x}_B^{(2)}\| / \|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Advantages:

- By-passes Schwarz loop.

Disadvantages:

- Off-diagonal coupling terms → block linear solver is needed.

Appendix. Modified Schwarz Method

Combines Schwarz and Newton loop into *since Newton-Schwarz loop*, with *Schwarz boundaries* at *Dirichlet boundaries* and tight convergence tolerance.

1: $\mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)}$ in Ω_1 , $\mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)})$ on $\partial\varphi\Omega_1$, $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{X}_\beta^{(1)}$ on Γ_1	▷ initialize for Ω_1
2: $\mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)}$ in Ω_2 , $\mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)})$ on $\partial\varphi\Omega_2$, $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{X}_\beta^{(2)}$ on Γ_2	▷ initialize for Ω_2
3: repeat	▷ Newton-Schwarz loop
4: $\mathbf{x}_\beta^{(1)} \leftarrow \mathbf{P}_{12}\mathbf{x}_B^{(2)} + \mathbf{Q}_{12}\mathbf{x}_b^{(2)} + \mathbf{G}_{12}\mathbf{x}_\beta^{(2)}$	▷ project from Ω_2 to Γ_1
5: $\Delta\mathbf{x}_B^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \setminus \mathbf{R}_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$	▷ linear system
6: $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta\mathbf{x}_B^{(1)}$	
7: $\mathbf{x}_\beta^{(2)} \leftarrow \mathbf{P}_{21}\mathbf{x}_B^{(1)} + \mathbf{Q}_{21}\mathbf{x}_b^{(1)} + \mathbf{G}_{21}\mathbf{x}_\beta^{(1)}$	▷ project from Ω_1 to Γ_2
8: $\Delta\mathbf{x}_B^{(2)} \leftarrow -\mathbf{K}_{AB}^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \setminus \mathbf{R}_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$	▷ linear system
9: $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta\mathbf{x}_B^{(2)}$	
10: until $\left[\left(\ \Delta\mathbf{x}_B^{(1)}\ / \ \mathbf{x}_B^{(1)}\ \right)^2 + \left(\ \Delta\mathbf{x}_B^{(2)}\ / \ \mathbf{x}_B^{(2)}\ \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$	▷ tight tolerance

Advantages:

- By-passes Schwarz loop.
- No diagonal coupling (conventional linear solver can be used in each subdomain).

Least-intrusive variant: by-passes Schwarz iteration, no need for block solver.

Appendix. Convergence Proof

2 Formulation of the Schwarz Alternating Method

We start by defining the standard finite deformation variational formulation to establish notation before presenting the formulation of the coupling method.

2.1 Variational Formulation on a Single Domain

Consider a body as the open set $\Omega \subset \mathbb{R}^2$ undergoing a motion described by the mapping $\mathbf{x} = \varphi(\mathbf{X}) : \Omega \rightarrow \mathbb{R}^2$, $\mathbf{X} \in \Omega$. Assume that the boundary of the body is $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$ with unit normal \mathbf{n} and unit tangent \mathbf{t} . $\partial\Omega_D$ is a displacement boundary, $\partial\Omega_N$ is a traction boundary, and $\partial\Omega_D \cap \partial\Omega_N = \emptyset$. The prescribed boundary displacements or Dirichlet boundary conditions are $\mathbf{u} = \mathbf{u}_D$ on $\partial\Omega_D$. The prescribed boundary tractions or Neumann boundary conditions are $\mathbf{T} \cdot \mathbf{n} = \mathbf{T}_N$ on $\partial\Omega_N$. Let $\mathbf{P} = \text{Grad } \varphi$ be the deformation gradient. Let also $\partial B \subset \Omega \rightarrow \mathbb{R}^2$ be the body force, with \mathbf{b} the mass density in the reference configuration. Furthermore, introduce the energy functional

$$\Phi[\varphi] = \int_{\Omega} A(\mathbf{F}, \mathbf{X}) dV - \int_{\Omega} \mathbf{b} \cdot \varphi dV - \int_{\partial\Omega_D} \mathbf{T}_D \cdot \varphi dS, \quad (1)$$

in which $A(\mathbf{F}, \mathbf{X})$ is the Helmholtz free-energy density and \mathbf{X} is a collection of internal variables. The weak form of the problem is obtained by minimizing the energy functional $\Phi[\varphi]$ over the Sobolev space $H^1_0(\Omega)$ that is comprised of all functions that are square-integrable and have square-integrable first derivatives. Define

$$\mathcal{S} := \{\varphi \in H^1_0(\Omega) : \varphi = \mathbf{u}_D \text{ on } \partial\Omega_D\} \quad (2)$$

and

$$Y := \{\xi \in W(\Omega) : \xi = 0 \text{ on } \partial\Omega_D\} \quad (3)$$

where $\xi \in Y$ is a test function. The potential energy is minimized if and only if $\Phi[\varphi] \leq \Phi[\varphi + \xi]$ for all $\xi \in Y$ and $\xi \in Y$. It is straightforward to show that the minimum of $\Phi[\varphi]$ is the mapping $\varphi \in \mathcal{S}$ that satisfies

$$D\Phi[\varphi](\xi) = \int_{\Omega} \mathbf{P} : \text{Grad } \xi dV - \int_{\Omega} \mathbf{b} \cdot \xi dV - \int_{\partial\Omega_D} \mathbf{T}_D \cdot \xi dS = 0, \quad (4)$$

where $\mathbf{P} = \mathbf{F}^T \mathbf{F}$. \mathbf{F} denotes the first Piola-Kirchhoff stress. The Euler-Lagrange equation corresponding to the variational statement (4) is

$$\text{Div } \mathbf{P} = \mathbf{b} \text{ in } \Omega, \quad (5)$$

$$\mathbf{P} \mathbf{n} = \mathbf{T}_N \text{ on } \partial\Omega_N, \quad (6)$$

$$\varphi = \mathbf{u}_D \text{ on } \partial\Omega_D.$$

2.2 Coupling Two or More Subdomains via the Schwarz Alternating Method

In this section, we describe the Schwarz alternating method for coupling multiple overlapping subdomains. Consider without loss of generality a partition for the domain Ω into two open subsets or subdomains Ω_1 and Ω_2 such that $\Omega = \Omega_1 \cup \Omega_2$ and $\Omega_1 \cap \Omega_2 = \Gamma$ as shown in Figure 1.

In keeping with other works on the convergence of the Schwarz alternating method, specially as we seek to prove convergence for the finite deformation solid mechanics problem (5), we introduce a set of indices that alternate between the subdomains as

$$n \in \mathbb{N}^+ = \{0, 1, 2, \dots\}, \quad i = 2 - n + 2 \left\lfloor \frac{n}{2} \right\rfloor \in \{1, 2\}, \quad j = n + 1 - 2 \left\lfloor \frac{n}{2} \right\rfloor \in \{1, 2\}, \quad (8)$$

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Figure 1: Two subdomains Ω_1 and Ω_2 and the corresponding boundaries Γ_1 and Γ_2 , and Γ_1 and Γ_2 are the interfaces between the subdomains.

that is $i = 1$ and $j = 2$ if n is odd, and $i = 2$ and $j = 1$ if n is even. Introduce the following definitions for each subdomain Ω_i :

- Closure: $\bar{\Omega}_i \supset \Omega_i \cup \partial\Omega_i$
- Dirichlet boundary: $\partial\Omega_i^D \supset \partial\Omega_i \cap \partial\Omega_D$
- Neumann boundary: $\partial\Omega_i^N \supset \partial\Omega_i \cap \partial\Omega_N$
- Schwarz boundary: $\Gamma_i \supset \partial\Omega_i \cap \Gamma$

Note that with these definitions we guarantee that $\partial\Omega_i \cap \partial\Omega_j = \emptyset$, $\partial\Omega_i \cap \Gamma_i = \emptyset$, and $\partial\Omega_i \cap \Gamma_j = \emptyset$. Now define the space

$$\mathcal{S}_i := \{\varphi \in H^1_0(\Omega_i) : \varphi = \mathbf{u}_D \text{ on } \partial\Omega_i^D, \varphi = \mathbf{P}_{\Omega_j} \cdot \mathbf{r}_i(\varphi) \text{ on } \Gamma_i\}, \quad (7)$$

and

$$Y_i := \{\varphi \in H^1_0(\Omega_i) : \varphi = 0 \text{ on } \partial\Omega_i^D, \varphi = \mathbf{P}_{\Omega_j} \cdot \mathbf{r}_i(\varphi) \text{ on } \Gamma_i\}, \quad (8)$$

where the symbol $\mathbf{P}_{\Omega_j} \cdot \mathbf{r}_i(\varphi)$ denotes the projection from the subdomain Ω_j onto the Schwarz boundary Γ_i . This projection operator plays a central role in the Schwarz alternating method. Its form and implementation are discussed in subsequent sections. For the moment it is sufficient to assume that the operator is able to project a field φ from one subdomain to the Schwarz boundary of the other subdomains. The Schwarz alternating method solves a sequence of problems on Ω_1 and Ω_2 . The solution $\varphi^{(n)}$ for the n th problem is given by

$$\varphi^{(n)} = \begin{cases} \varphi^{(n-1)} & \text{for } n = 0 \\ \arg \min_{\varphi \in \mathcal{S}_i} \Phi[\varphi] & \text{for } n > 0 \end{cases} \quad (9)$$

where $\arg \min$ is the identity map that maps X onto itself (i.e. zero displacement), and

$$\Phi[\varphi] = \int_{\Omega_i} A(\mathbf{F}, \mathbf{X}) dV - \int_{\Omega_i} \mathbf{b} \cdot \varphi dV - \int_{\partial\Omega_i^D} \mathbf{T}_D \cdot \varphi dS. \quad (10)$$

A better guess, if available, may be used to initialize $\varphi^{(0)}$ on Ω_j rather than the identity map $\varphi^{(0)} = 0$. The minimization of the functional (10) leads to a variational formulation of the form (4)–(6) for each subdomain

$$D\Phi[\varphi^{(n)}](\xi) = \int_{\Omega_i} \mathbf{P} : \text{Grad } \xi dV - \int_{\Omega_i} \mathbf{b} \cdot \xi dV - \int_{\partial\Omega_i^D} \mathbf{T}_D \cdot \xi dS = 0, \quad (11)$$

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$$\begin{aligned} & \varphi^{(n)} = \mathbf{X}^{(n)} = \mathbf{u}_D, \mathbf{X}^{(n)} = \mathbf{X}(\mathbf{X}^{(n)}) = \mathbf{u}_D, \quad \text{is valid for } \Omega_1 \\ & \varphi^{(n)} = \mathbf{X}^{(n)} = \mathbf{u}_D, \mathbf{X}^{(n)} = \mathbf{X}(\mathbf{X}^{(n)}) = \mathbf{u}_D, \quad \text{is valid for } \Omega_2 \\ & \varphi^{(n)} = \mathbf{X}^{(n)} = \mathbf{u}_D, \mathbf{X}^{(n)} = \mathbf{X}(\mathbf{X}^{(n)}) = \mathbf{u}_D, \quad \text{is true upon} \\ & \varphi^{(n)} = \mathbf{X}^{(n)} = \mathbf{u}_D, \mathbf{X}^{(n)} = \mathbf{X}(\mathbf{X}^{(n)}) = \mathbf{u}_D, \quad \text{is true upon} \\ & \varphi^{(n)} = \mathbf{X}^{(n)} = \mathbf{u}_D, \mathbf{X}^{(n)} = \mathbf{X}(\mathbf{X}^{(n)}) = \mathbf{u}_D, \quad \text{is true upon} \\ & \varphi^{(n)} = \mathbf{X}^{(n)} = \mathbf{u}_D, \mathbf{X}^{(n)} = \mathbf{X}(\mathbf{X}^{(n)}) = \mathbf{u}_D, \quad \text{is true upon} \end{aligned}$$

Appendix 5: Numerical Solution Method

[15, 34, 4]. Although we do not provide here formal convergence proofs for the remaining variants of the Schwarz method, we offer some numerical results illustrating their convergence in Section 4.

Consider the energy functional $\Phi[\varphi]$ defined in (1). We will denote by $\langle \cdot, \cdot \rangle$ the usual L^2 inner product over Ω , that is,

$$\langle \varphi, \psi \rangle = \int_{\Omega} \varphi \psi dV. \quad (12)$$

for $\varphi, \psi \in W(\Omega)$, with corresponding norm $\|\cdot\|$. The proof of the convergence of the Schwarz alternating method requires that the functional $\Phi[\varphi]$ satisfy the following properties over the space \mathcal{S} defined in (2):

1. $\Phi[\varphi]$ is coercive.
2. $\Phi[\varphi]$ is Fréchet differentiable, with $\Phi'[\varphi]$ denoting its Fréchet derivative.
3. $\Phi[\varphi]$ is strictly convex.
4. $\Phi[\varphi]$ is lower semi-continuous.
5. $\Phi[\varphi]$ is uniformly continuous on K_n , where

$$K_n = \{\varphi \in \mathcal{S} : \Phi[\varphi] < R, R \in \mathbb{R}, n \in \mathbb{N}\}. \quad (16)$$

It can be shown that the energy functional $\Phi[\varphi]$ defined in (1) is strictly convex in \mathcal{S} (property 3) provided that the Helmholtz free-energy density $A(\mathbf{F}, \mathbf{X})$ is a quasiconvex function of \mathbf{F} [33]. Properties 1, 2, 4 and 5 follow from the strict convexity of $\Phi[\varphi]$. Next, define two additional sets of spaces

$$\mathcal{S}_i = \{\varphi \in \mathcal{S} : \varphi = \mathbf{P}_{\Omega_j} \cdot \mathbf{r}_i(\varphi) \text{ on } \Gamma_i, \varphi = \mathbf{P}_{\Omega_j} \cdot \mathbf{r}_i(\varphi) \text{ on } \Gamma_j\}, \quad (17)$$

and

$$\mathcal{Y}_i = \{\xi \in \mathcal{S} : \xi = 0 \text{ on } \partial\Omega_i^D\}, \quad (18)$$

where $i = 1$ and $j = 2$ if n is odd, and $i = 2$ and $j = 1$ if n is even for $n \in \{1, 2, \dots\}$ as given by (8), with the function $\mathbf{P}_{\Omega_j} \cdot \mathbf{r}_i(\varphi)$ as initial guess. Note that the spaces \mathcal{S}_i in (17) are extensions of the spaces \mathcal{S}_i in (2) to the entire domain Ω . With this notation in place, the solution of the n -th problem (9)–(11) can be recast as

$$\varphi^{(n)} = \begin{cases} \varphi^{(n-1)} & \text{for } n = 0 \\ \arg \min_{\varphi \in \mathcal{S}_i} \Phi[\varphi] & \text{for } n > 0 \end{cases} \quad (19)$$

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Remark that [50] $\mathcal{S}_i = \mathcal{S}^{(n-1)} \cup \mathcal{Y}_i$ for $\mathcal{S}^{(n-1)} \cup \mathcal{Y}_i = \mathcal{S}^{(n-1)} \cup \mathcal{S}_i$. Consider the Schwarz alternating method of Section 2 defined by (9)–(11) and its equivalent form (19). Then

(a) $\Phi[\varphi^{(n)}] \geq \Phi[\varphi^{(n-1)}] \geq \dots \geq \Phi[\varphi^{(0)}] \geq \Phi[\varphi^{(n)}] \geq \dots \geq \Phi[\varphi^{(0)}]$, where $\varphi^{(0)}$ is the minimizer of $\Phi[\varphi]$ over \mathcal{S} .

(b) the sequence $\{\varphi^{(n)}\}$ defined in (19) converges to the minimizer φ^* of $\Phi[\varphi]$ in \mathcal{S} .

(c) the Schwarz minimum value $\Phi[\varphi^*]$ converges monotonically to the minimum value $\Phi[\varphi]$ in \mathcal{S} starting from any initial guess $\varphi^{(0)}$.

(d) $\Phi[\varphi^{(n)}]$ is a Lyapunov continuous in a neighborhood of φ^* , then the sequence $\{\varphi^{(n)}\}$ converges geometrically to the minimizer φ^* .

Proof. See Appendix A. \square

Finally, while most of works cited above present their analysis for the specific case of two subdomains, extension to multiple subdomains is a general straightforward. The case of multiple subdomains is considered specifically in Lions [53], Bales [13], Bales [13], and Lions and Evans [54].

4 Numerical Experiments

In this section, we present numerical examples of the behavior of the Schwarz alternating method for two different implementations. First, we briefly describe the two implementations, one in MATLAB and the other in the open-source ALANNA finite element code [13]. Next, we discuss the error measures used throughout the numerical examples. Then, we continue with four examples that demonstrate different features of the Schwarz alternating method and our implementations. The first example, a one-dimensional singular bar, is used to demonstrate the behavior of the four Schwarz variants of Section 2. The second example, a radial body of square bar, aims to study the effect of the size of the overlap region on the convergence of the method. The objective of the third example, a meshed cylinder, is to analyze the numerical error in the results and demonstrate the ability of the method to couple different element topologies. The last example, a half-weld geometry, is employed to demonstrate the performance and scalability of our parallel implementation of the method, as well as coupling of more than two subdomains. Throughout our numerical examples, we omit the use of units unless they are necessary for the understanding of the problem at hand.

4.1 Implementation

The four variants of the Schwarz alternating method described in Section 2.1 have been implemented in a one-dimensional MATLAB code. The objective is to determine the convergence behavior, efficiency, and performance of each variant. This code has been optimized both in terms of memory usage and execution speed.

In addition, the Modified variant of the Schwarz alternating method described in Section 2.1 has been implemented in ALANNA, an open-source multiphysics research platform developed mainly at Sandia National

See Remark 1 in the Appendix for a definition of geometric convergence.

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A Proof of Convergence of the Schwarz Alternating Method for the Finite-Deformation Inelastic Problem

In this section we give a proof of Theorem 1. The proof relies on several properties, presented below as remarks. Assume properties (i)–(v) enumerated in Section 3 hold.

Remark 1. By the coercivity of $\Phi[\varphi]$, it follows from the Lax-Milgram theorem that a unique minimizer to the functional over \mathcal{S} exists, i.e. the minimization of $\Phi[\varphi]$ is well-posed.

Remark 2. By the Stampacchia theorem, the minimization of $\Phi[\varphi]$ in \mathcal{S} is equivalent to finding $\varphi \in \mathcal{S}$ such that

$$\langle \Phi'[\varphi], \xi \rangle \geq 0 \quad (21)$$

for all $\xi \in \mathcal{S}$.

Remark 3. Recall that the strict convexity property of $\Phi[\varphi]$ can be written as

$$\Phi[\varphi_2] - \Phi[\varphi_1] - \langle \Phi'[\varphi_1], \varphi_2 - \varphi_1 \rangle > 0, \quad (22)$$

for $\varphi_1, \varphi_2 \in \mathcal{S}$. From (16), remark that if $\Phi[\varphi]$ is strictly convex over \mathcal{S} for $R < \infty$, we can find an $\alpha_R > 0$ such that $\forall \varphi_1, \varphi_2 \in K_R$ we have

$$\Phi[\varphi_2] - \Phi[\varphi_1] - \langle \Phi'[\varphi_1], \varphi_2 - \varphi_1 \rangle \geq \alpha_R \|\varphi_2 - \varphi_1\|^2. \quad (23)$$

Remark 4. By property 5, the uniform continuity of $\Phi[\varphi]$ has a modulus of continuity $\omega > 0$, with $\omega : K_R \rightarrow K_R$ such that

$$|\Phi[\varphi_2] - \Phi[\varphi_1]| \leq \omega(\|\varphi_2 - \varphi_1\|). \quad (24)$$

for $\varphi_1, \varphi_2 \in K_R$. By definition, $\omega(s) \rightarrow 0$ as $s \rightarrow 0$.

Remark 5. It was shown in [55] that in the case $\Omega_1 \cap \Omega_2 \neq \emptyset$, for \mathcal{S} , there exist C_1 and $C_2 \in \mathcal{S}$ such that

$$\varphi = C_1 + C_2, \quad (25)$$

and

$$\max(\|\mathcal{C}_1\|, \|\mathcal{C}_2\|) \leq C_0 \|\varphi\|. \quad (26)$$

for some $C_0 > 0$ independent of φ .

Remark 6. Note that (19) can be written as

$$\langle \Phi'[\varphi^{(n)}], \xi \rangle = 0, \quad \text{for } \varphi^{(n)} \in \mathcal{S}_i, \xi \in \mathcal{Y}_i, \quad (27)$$

for $i \in \{1, 2\}$ and $n \in \{0, 1, 2, \dots\}$ (recall from (8) the relation between i and n). This is due to the uniqueness of the solution to each minimization problem over \mathcal{S}_i , and the definition of \mathcal{Y}_i as the minimizer of $\Phi[\varphi]$ over \mathcal{S}_i .

Remark 7. Let $\varphi^{(n)} \in \mathcal{S}_i$, and let $\xi \in \mathcal{Y}_i$. By Remark 5, there exist $C_1 \in \mathcal{S}_1$ and $C_2 \in \mathcal{S}_2$ such that

$$\langle \Phi'[\varphi^{(n)}], \xi \rangle = \langle \Phi'[\varphi^{(n)}], C_1 \rangle. \quad (28)$$

By (27), $\langle \Phi'[\varphi^{(n)}], \xi \rangle = 0$. Hence,

$$\langle \Phi'[\varphi^{(n)}], C_1 \rangle = \langle \Phi'[\varphi^{(n)}], C_1 \rangle - \langle \Phi'[\varphi^{(n)}], C_2 \rangle = \langle \Phi'[\varphi^{(n)}], C_1 \rangle - \langle \Phi'[\varphi^{(n)}], C_2 \rangle, \quad (29)$$

since $\langle \Phi'[\varphi^{(n)}], C_2 \rangle = 0$, also by (27). By the Cauchy-Schwarz inequality,

$$\langle \Phi'[\varphi^{(n)}], C_1 \rangle = \langle \Phi'[\varphi^{(n)}], C_1 \rangle = \langle \Phi'[\varphi^{(n)}], C_1 \rangle \leq \|\Phi'[\varphi^{(n)}]\| \cdot \|C_1\|. \quad (30)$$

Again using (27) and also (30) it follows that

$$\langle \Phi'[\varphi^{(n)}], C_1 \rangle = \langle \Phi'[\varphi^{(n)}], C_1 \rangle \leq \|\Phi'[\varphi^{(n)}]\| \cdot \|C_1\|. \quad (31)$$

and substituting (30) into (31) we finally obtain that

$$\langle \Phi'[\varphi^{(n)}], C_1 \rangle \leq C_0 \|\Phi'[\varphi^{(n)}]\| \cdot \|C_1\|. \quad (32)$$

Remark 8. For part (ii) of Theorem 1, recall the definition of geometric convergence:

$$C_{n+1} \leq C_n, \quad (33)$$

for $n \in \{0, 1, 2, \dots\}$ for some $C > 0$, where

$$C_n = \|\varphi^{(n+1)} - \varphi^{(n)}\|. \quad (34)$$

Remark 9. Recall from the definition of continuity that if $\Phi'[\varphi]$ is Lipschitz continuous on $\mathcal{S}^{(n)}$ near φ , then there exists a constant $R \geq 0$ such that

$$\|\Phi'[\varphi^{(n)}] - \Phi'[\varphi]\| \leq R, \quad (35)$$

Considering that $\Phi'[\varphi] = 0$ since φ is the minimizer of $\Phi[\varphi]$, (35) is equivalent to

$$\|\Phi'[\varphi^{(n)}]\| \leq R \|\varphi^{(n)} - \varphi\|. \quad (36)$$

Proof of Theorem 1

Proof of (i). By (19), $\varphi^{(n)} = \arg \min_{\varphi \in \mathcal{S}_i} \Phi[\varphi]$. By (20), $\varphi^{(n)} \in \mathcal{S}_i$. Let φ^* be the minimizer of $\Phi[\varphi]$ over \mathcal{S} and suppose $\Phi[\varphi^*] > \Phi[\varphi^{(n)}]$. But this is a contradiction, since we can take $\varphi^* = \varphi^{(n)}$. Hence, it cannot be that $\Phi[\varphi^{(n)}] > \Phi[\varphi^{(n-1)}]$ where $\varphi^{(n-1)} = \arg \min_{\varphi \in \mathcal{S}_j} \Phi[\varphi]$. It follows by induction that

$$\Phi[\varphi^{(n)}] \leq \Phi[\varphi^{(n-1)}] \quad (37)$$

for $n \in \{1, 2, 3, \dots\}$. Now let φ^* be the minimizer of $\Phi[\varphi]$ over \mathcal{S} . Since the problem is well-posed φ^* is unique. Hence $\Phi[\varphi^*] > \Phi[\varphi^{(n)}]$ for all $n \in \{1, 2, 3, \dots\}$.

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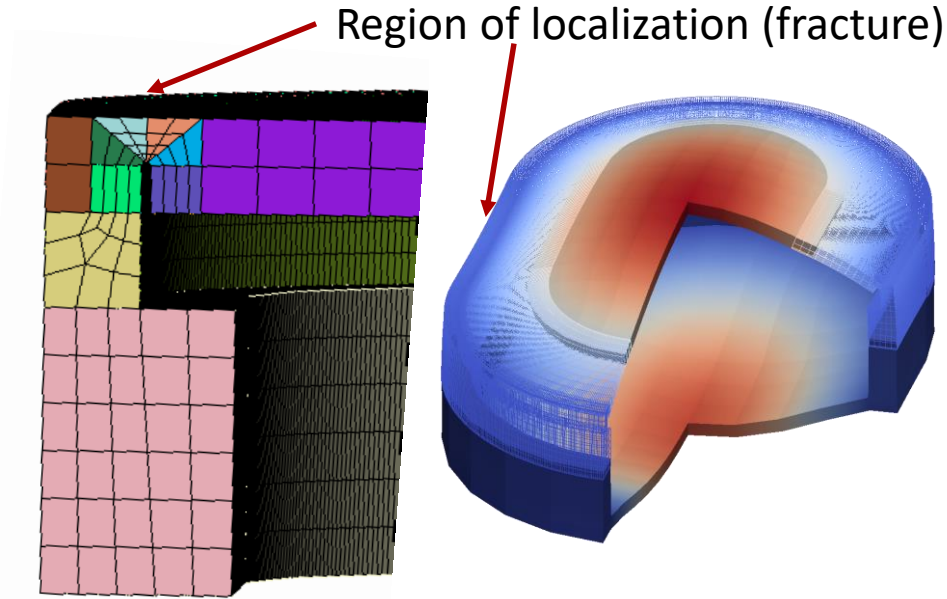
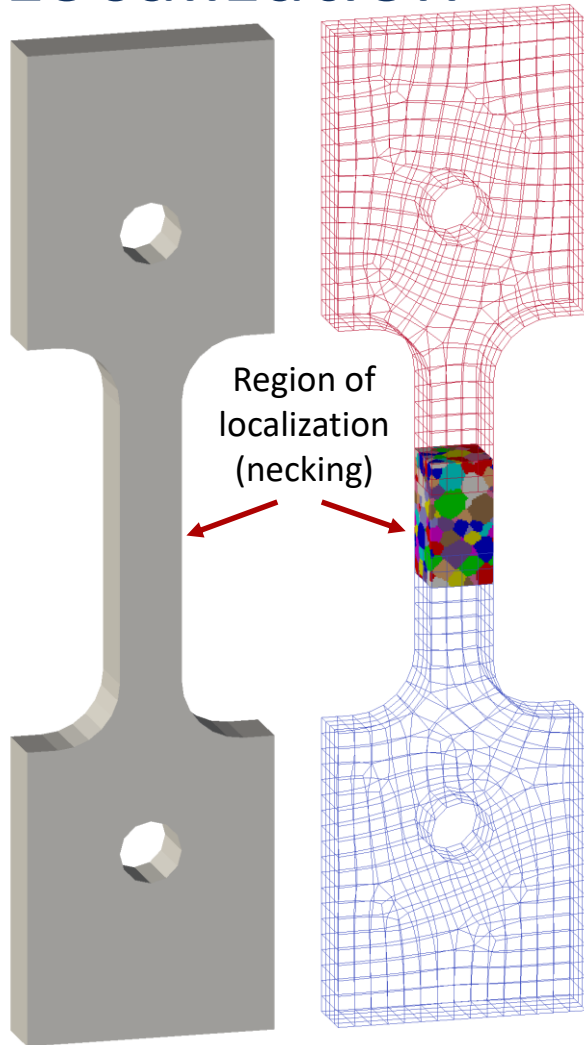
Proof of (ii). By (19), $\Phi[\varphi^{(n)}] \rightarrow J$ as $n \rightarrow \infty$ for $\varphi \in \mathcal{S}$. Now, combining (31) and (33), we have the bound

$$\Phi[\varphi^{(n)}] - \Phi[\varphi^{(n-1)}] \geq \Phi[\varphi^{(n)}] - \Phi[\varphi^{(n-1)}] - \langle \Phi'[\varphi^{(n-1)}], \varphi^{(n)} - \varphi^{(n-1)} \rangle \geq \alpha_n \|\varphi^{(n)} - \varphi^{(n-1)}\|^2, \quad (38)$$

for all $n \in \{1, 2, 3, \dots\}$. Since $\Phi[\varphi^{(n)}] \rightarrow J$ as $n \rightarrow \infty$, it follows that $\Phi[\varphi^{(n)}] - \Phi[\varphi^{(n-1)}] \rightarrow 0$ as $n \rightarrow \infty$. From (38), we have that

$$\lim_{n \rightarrow \infty}$$

Appendix. Multiscale Modeling of Localization

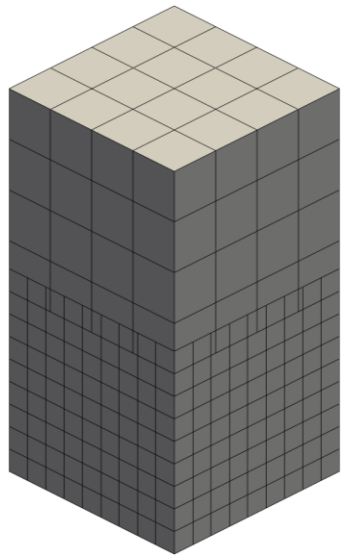


Strain localization can cause **localized necking** (left) and ultimately **fracture** (above).

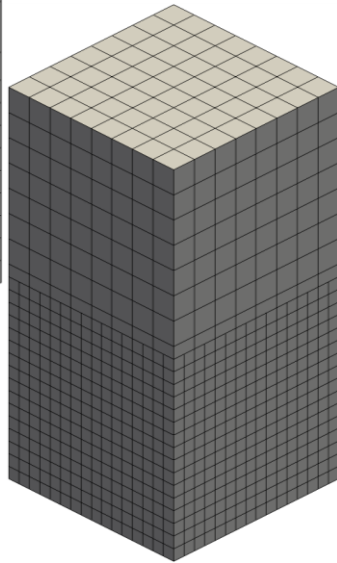
Goals:

- Connect **physical length scales** to **engineering scale models**.
- Investigate importance of **microstructural detail**.
- Develop bridging technologies for **spatial multiscale/multiphysics**.

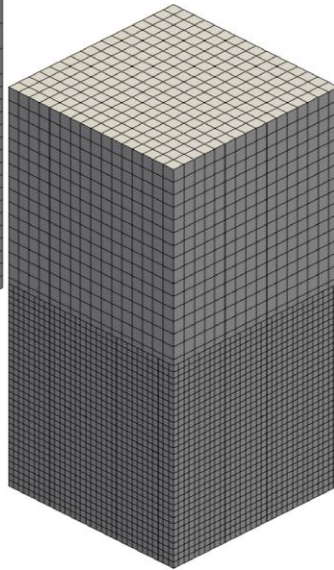
Appendix. Parallelization via DTK: Weak Scaling on Cubes Problem



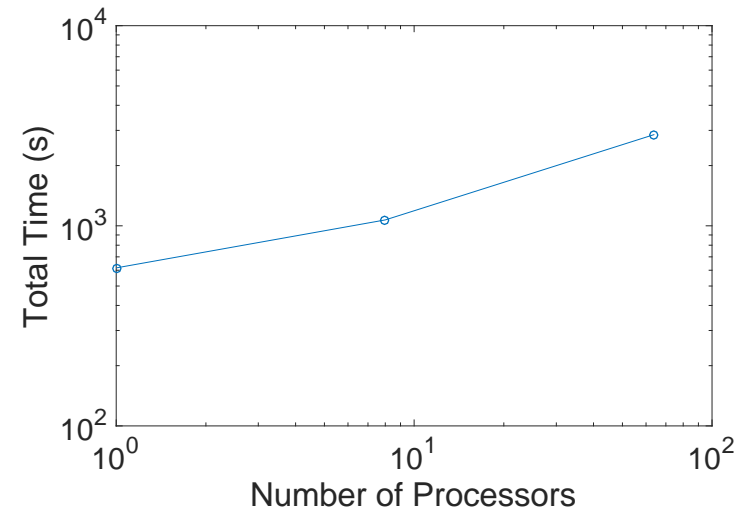
1 Processor,
 2.5×10^3 DOF / proc



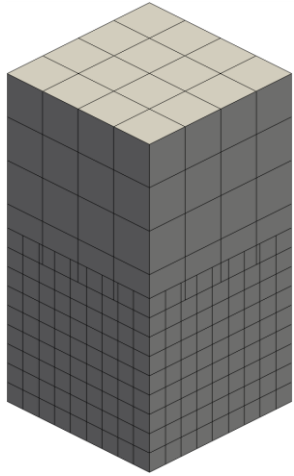
8 Processors,
 2.1×10^3 DOF / proc



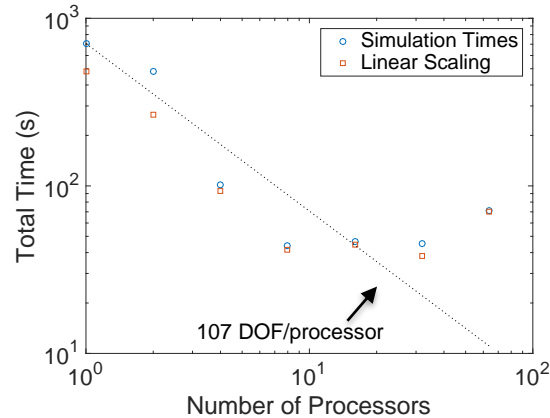
64 Processors,
 1.9×10^3 DOF / proc



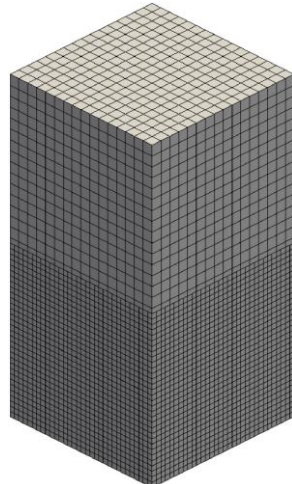
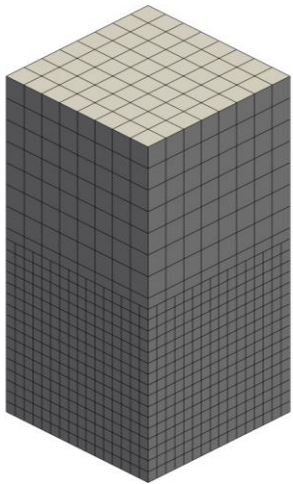
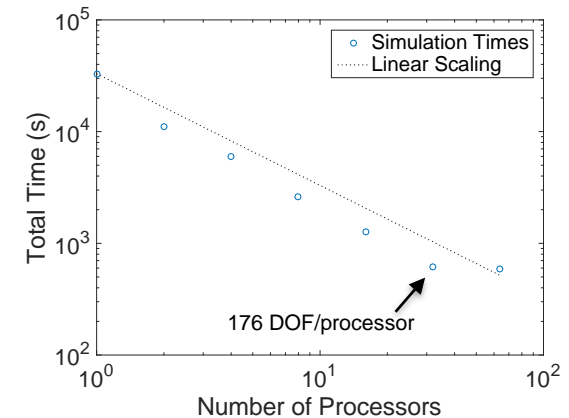
Appendix. Parallelization via DTK: Strong Scaling on Cubes Problem



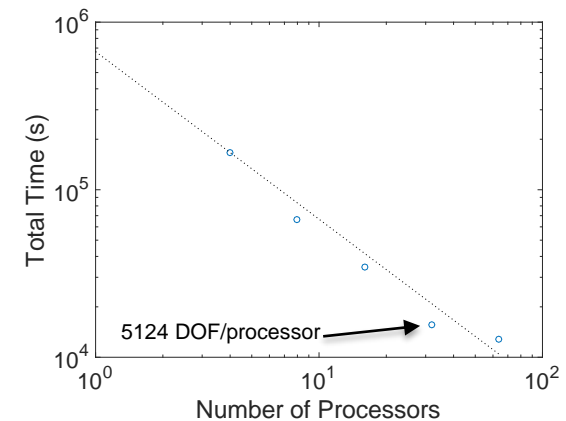
Small problem ($2.5 \cdot 10^3$ DOFs)



Medium problem ($1.7 \cdot 10^4$ DOFs)

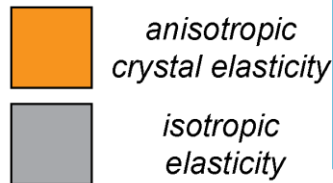


Large problem ($1.6 \cdot 10^5$ DOFs)

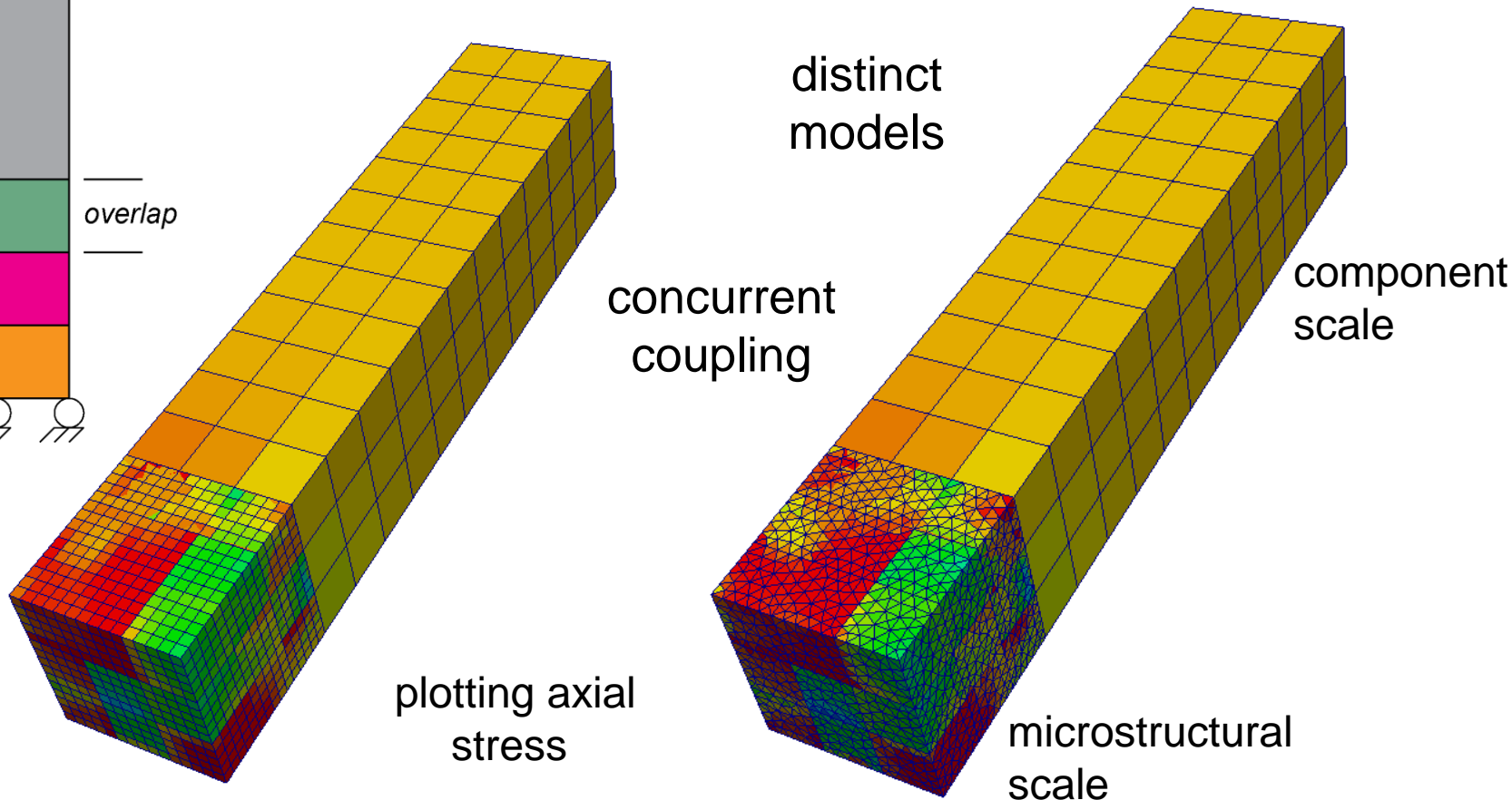


Appendix. Rubiks Cube Problem

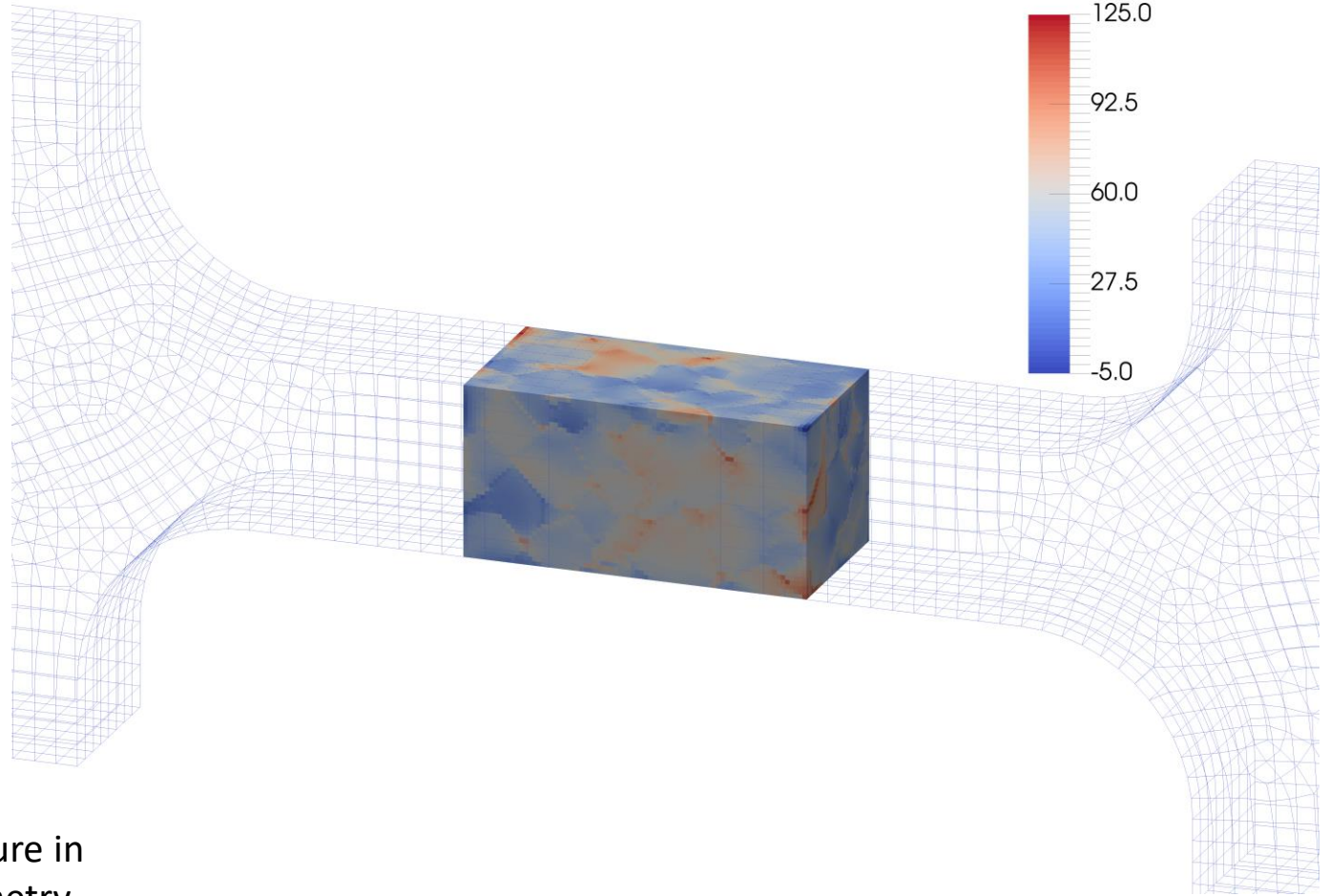
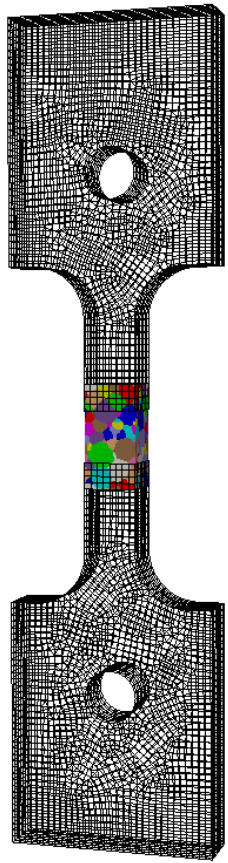
Work by J. Foulk, D. Littlewood,
C. Battaile, H. Lim



Two distinct bodies, the component scale and the microstructural scale, are coupled iteratively with alternating Schwarz



Appendix. Tensile Bar

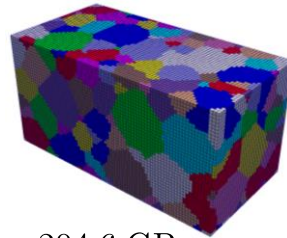


Embed microstructure in
ASTM tensile geometry

Appendix. Tensile Bar: Meso-Macroscale Coupling

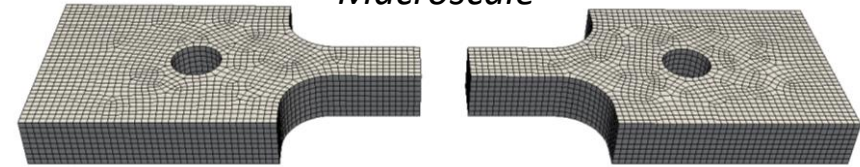
Mesoscale

SPARKS-generated
microstructure (F. Abdeljawad)



+

Macroscale



cubic elastic constant : $C_{11} = 204.6$ GPa

cubic elastic constant : $C_{12} = 137.7$ GPa

cubic elastic constant : $C_{44} = 126.2$ GPa

reference shear rate : $\dot{\gamma}_0 = 1.0$ 1/s

rate sensitivity factor : $m = 20$

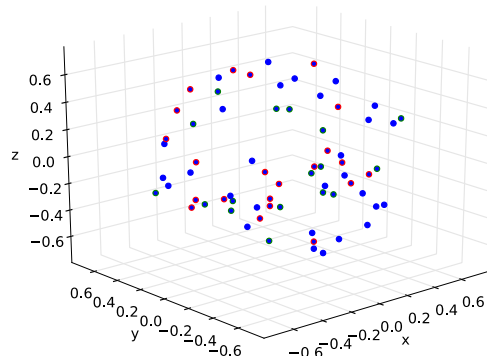
hardening rate parameter : $\dot{g}_0 = 2.0 \times 10^4$ 1/s

initial hardness : $g_0 = 90$ MPa

saturation hardness : $g_s = 202$ MPa

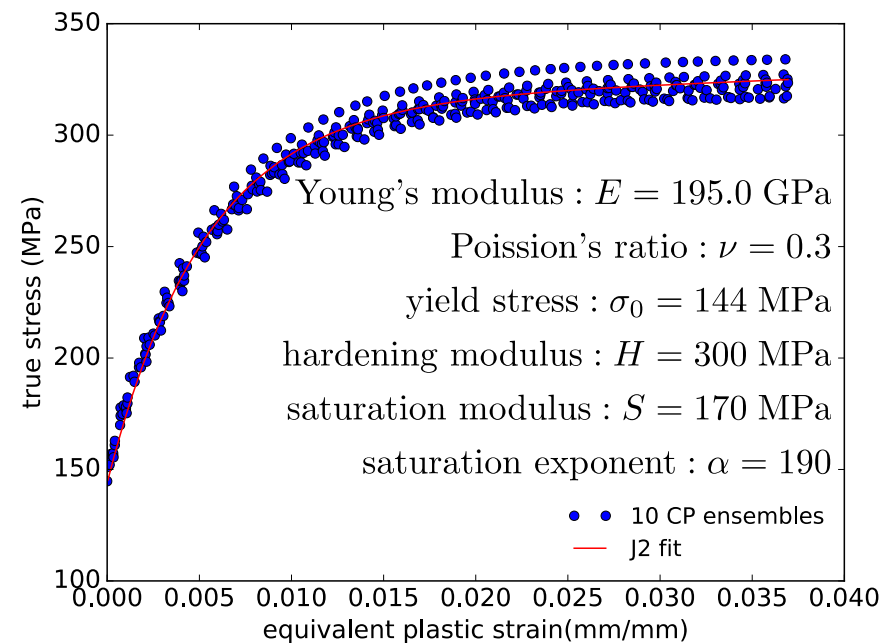
saturation exponent : $\omega = 0.01$

Fix microstructure, investigate ensembles



151 axial vectors
from 3 of the 10
ensembles of
random rotations
(blue, green, red)

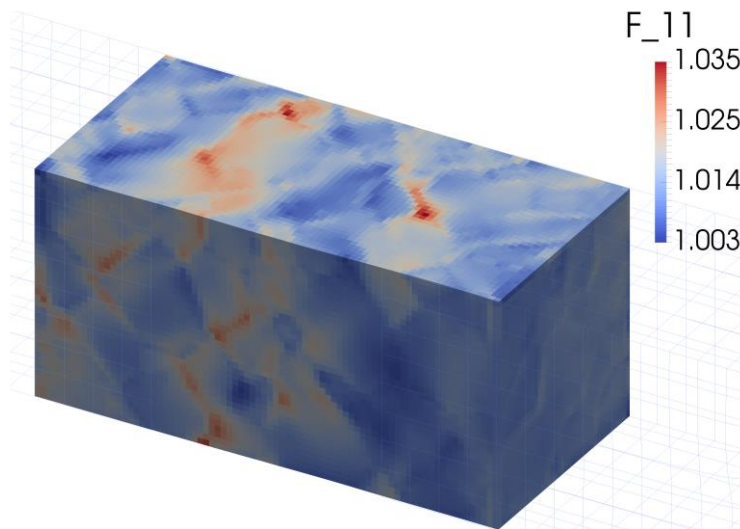
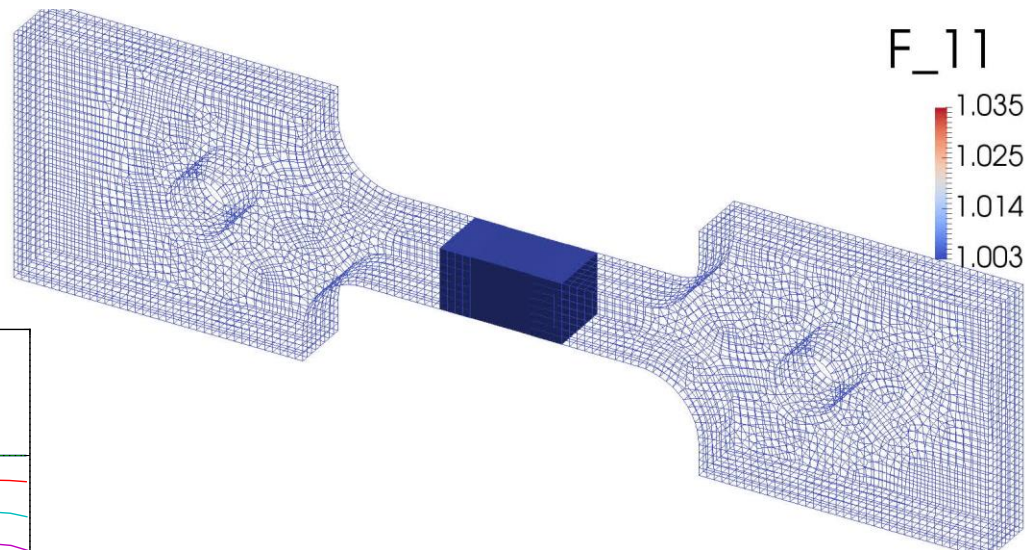
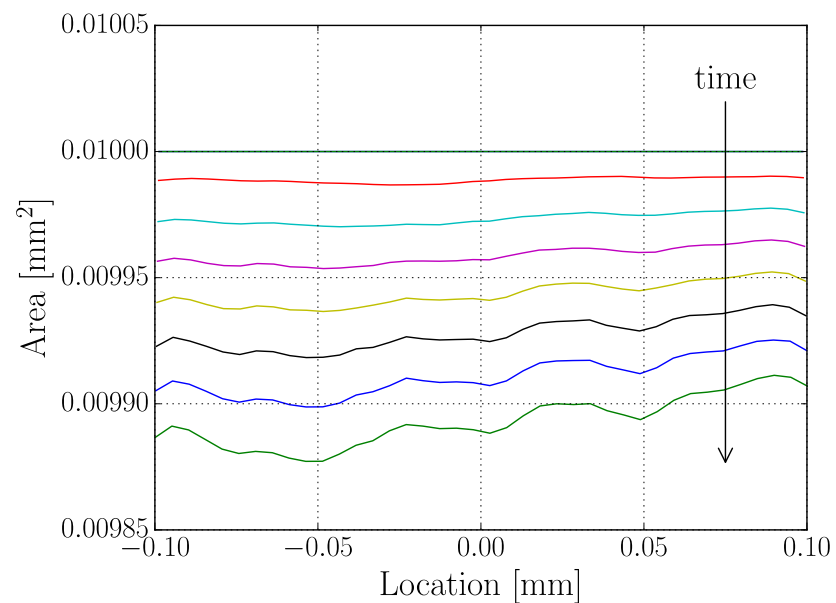
- Load microstructural ensembles in uniaxial stress
- Fit flow curves with a macroscale J_2 plasticity model



$$\sigma_y = \sigma_0 + H\epsilon_p + S(1 - e^{-\alpha\epsilon_p})$$

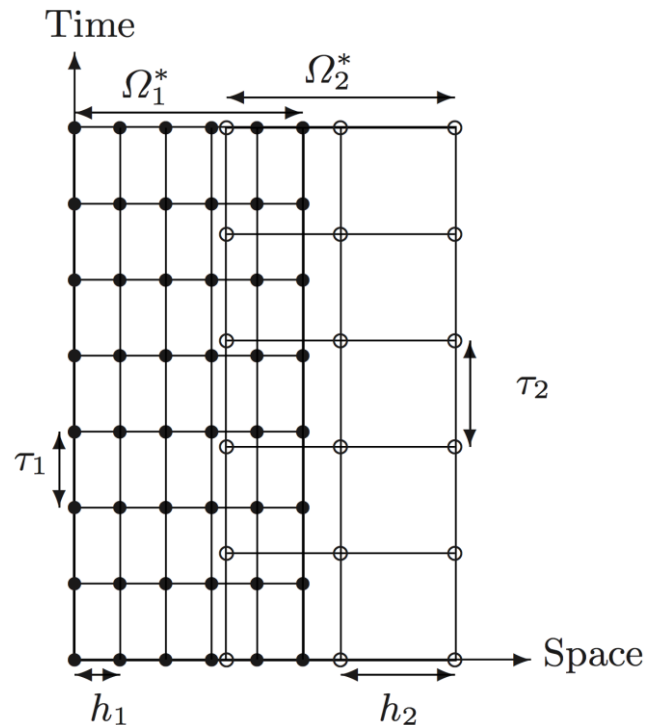
Appendix. Tensile Bar: Results

Reduction in cross-sectional
area over time



Appendix. Schwarz Alternating Method for Dynamics

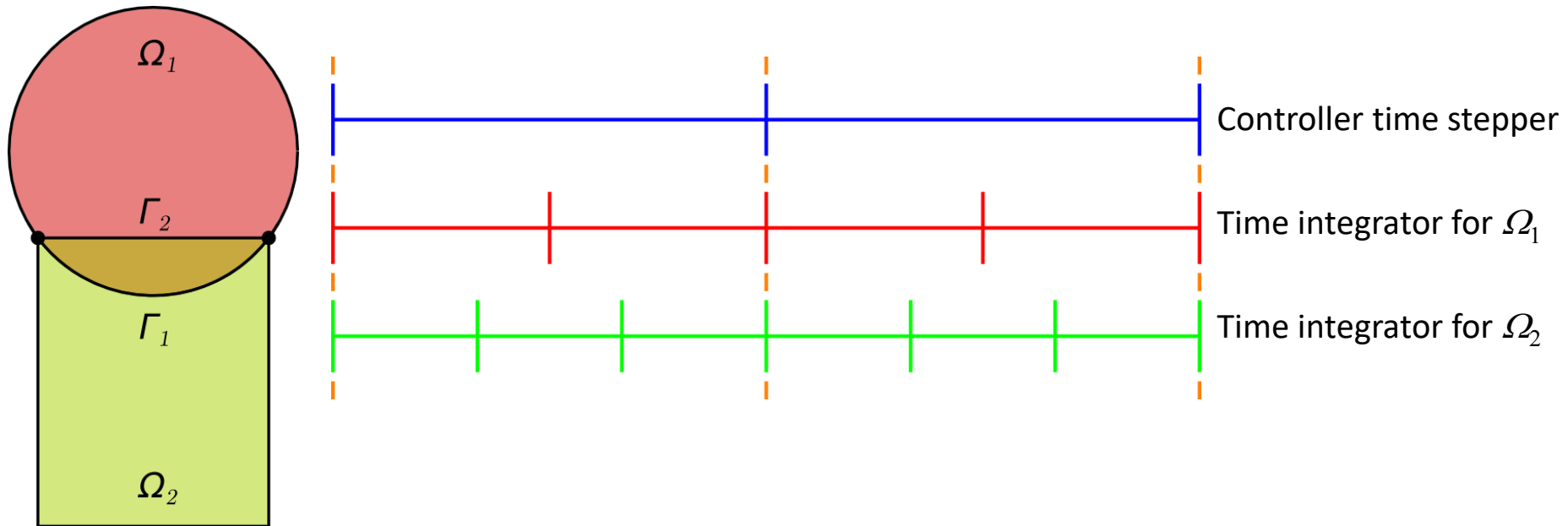
- In the literature the Schwarz method is applied to dynamics by using ***space-time discretizations***.
- This was deemed ***unfeasible*** given the design of our current codes and size of simulations.



Overlapping non-matching meshes and time steps in dynamics.

Appendix. A Schwarz-like Time Integrator

- We developed an ***extension of Schwarz coupling*** to ***dynamics*** using a governing time stepping algorithm that controls time integrators within each domain.
- Can use ***different integrators*** with ***different time steps*** within each domain.
- 1D results show ***smooth coupling without numerical artifacts*** such as spurious wave reflections at boundaries of coupled domains.



Appendix. Dynamic Singular Bar

- Inelasticity masks problems by introducing **energy dissipation**.
- Schwarz does **not** introduce **numerical artifacts**.
- Can couple domains with **different time integration schemes** (**Explicit-Implicit** below).

