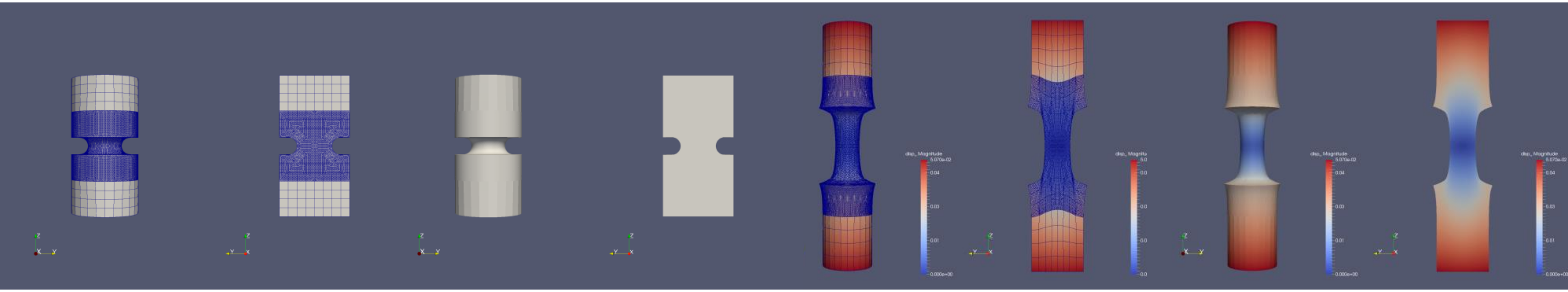

The Schwarz alternating method for concurrent multiscale coupling in solid mechanics

Irina Tezaur, Alejandro Mota, Coleman Alleman

Sandia National Laboratories, Livermore, CA, USA.

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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
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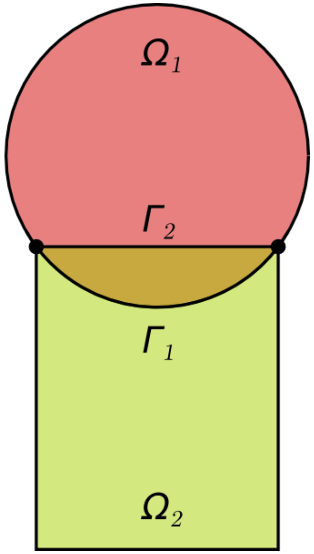

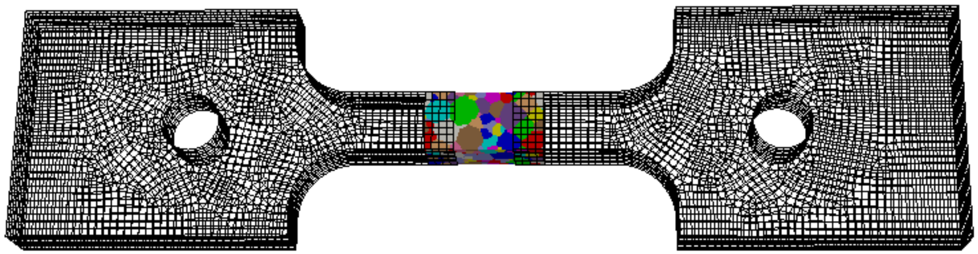

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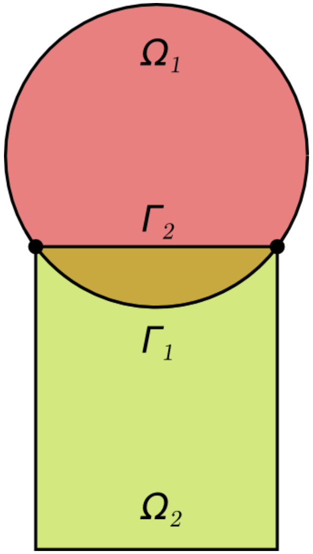
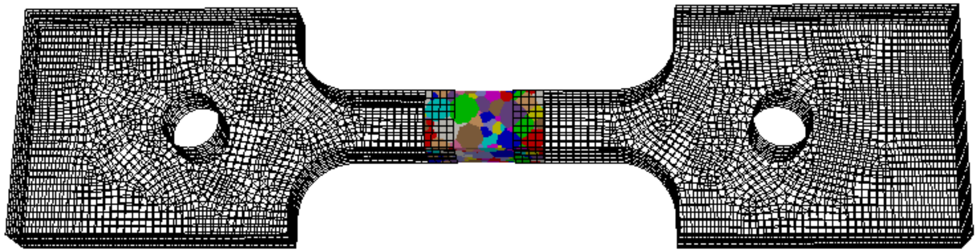




Motivation for Concurrent Multiscale Coupling

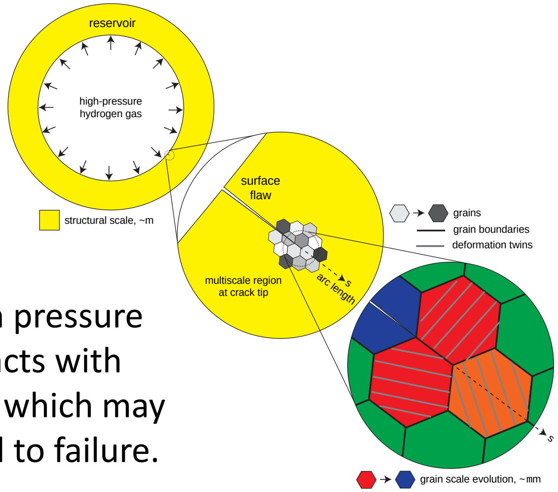
Sandia National Laboratories

- ***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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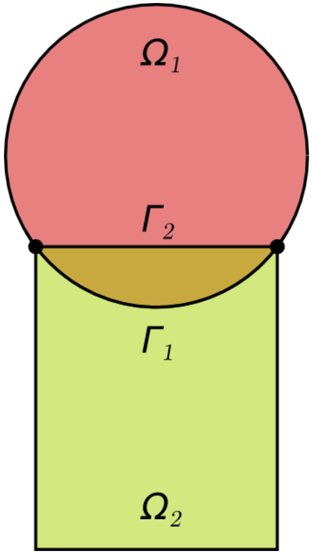
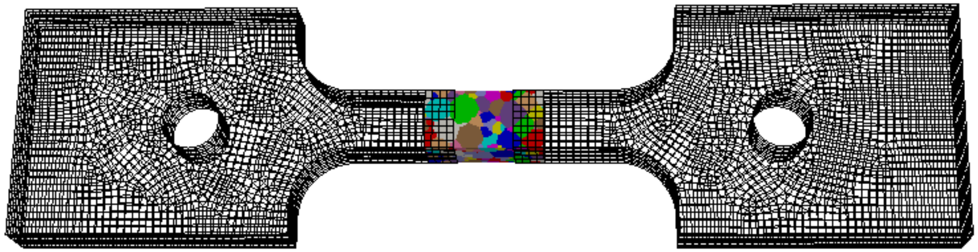
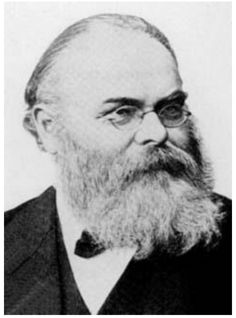




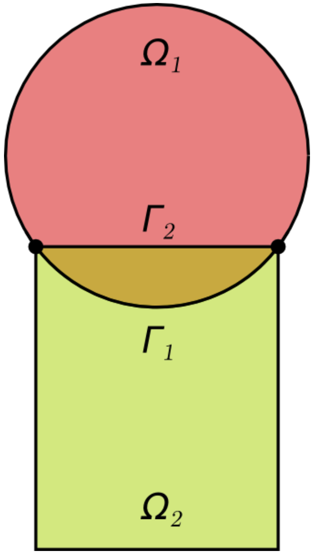
Schwarz Alternating Method for Domain Decomposition

- 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.
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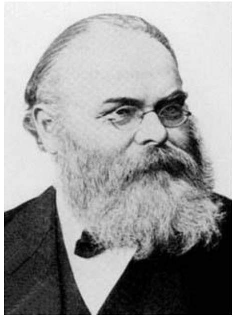

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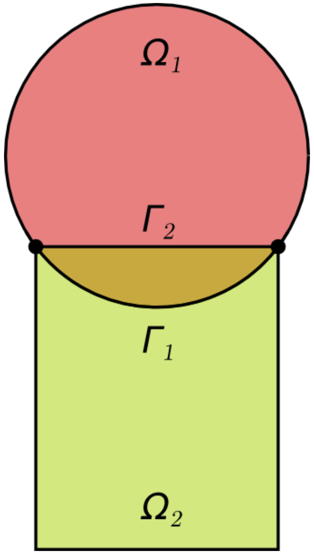

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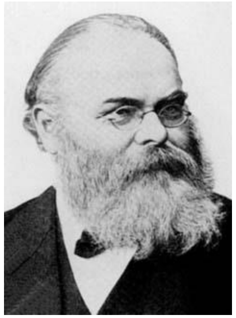

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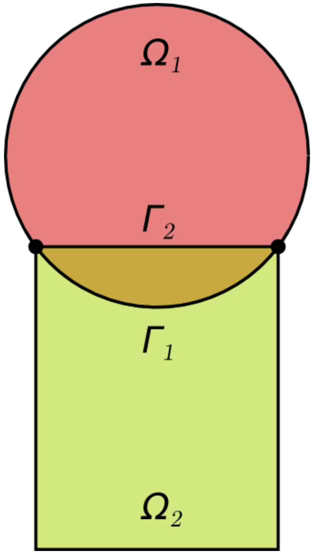

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- Schwarz alternating method most commonly used as a ***preconditioner*** for Krylov iterative methods to solve linear algebraic equations.

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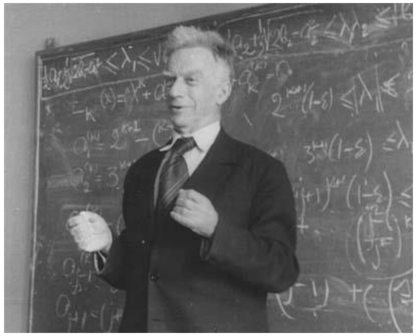
- **S. L. Sobolev (1936)**: posed Schwarz method for ***linear elasticity*** in variational form and ***proved method's convergence*** by proposing a convergent sequence of energy functionals.



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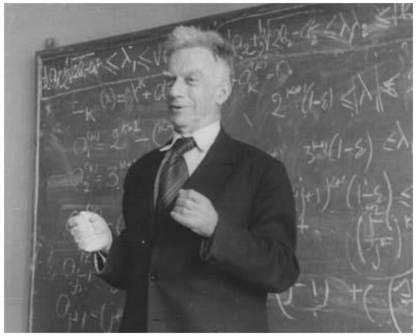

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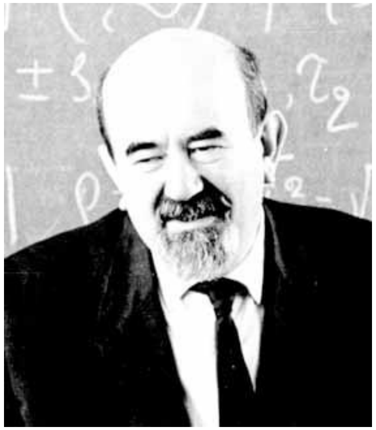

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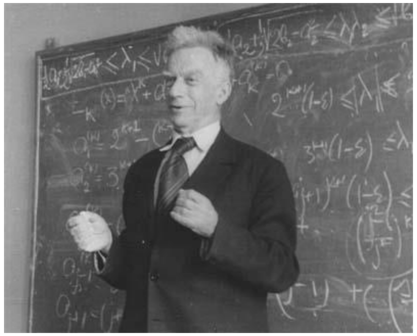
- **A. Mota, I. Tezaur, C. Alleman (2017)*:** derived a ***proof of convergence*** of the alternating Schwarz method for the ***finite deformation quasi-static nonlinear PDEs*** (with energy functional $\boldsymbol{\Phi}[\boldsymbol{\varphi}]$ defined below), and determined a ***geometric convergence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

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



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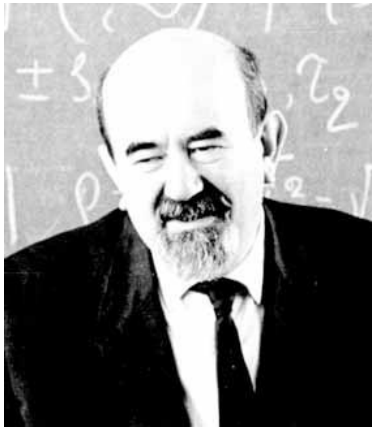

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*A. Mota, **I. Tezaur**, C. Alleman. "The Schwarz Alternating Method in Solid Mechanics", *CMAME* 319 (2017), 19-51.

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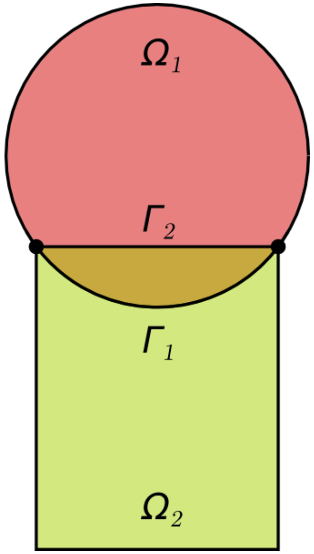

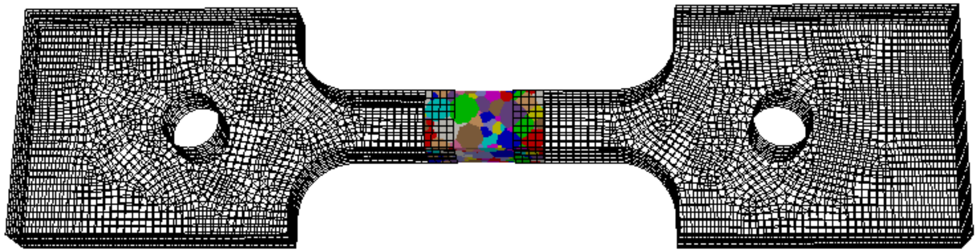

Schwarz Alternating Method for Multiscale Coupling in Quasistatics

$\boldsymbol{\varphi}^{(0)} \leftarrow \mathrm{id}_{\boldsymbol{X}}$ in Ω_2 ▷ initialize to zero displacement or a better guess in Ω_2

$n \leftarrow 1$

repeat ▷ Schwarz loop

$\quad \boldsymbol{\varphi}^{(n)} \leftarrow \boldsymbol{\chi}$ on $\partial_{\boldsymbol{\varphi}}\Omega_i$ ▷ Dirichlet BC for Ω_i

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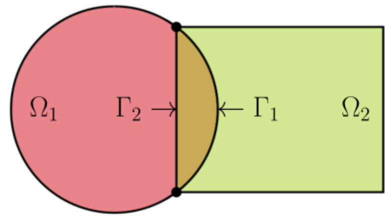
$\quad n \leftarrow n + 1$

until converged



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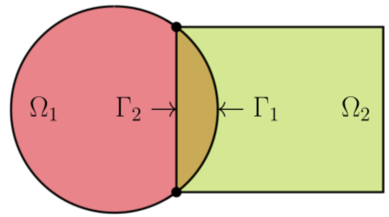

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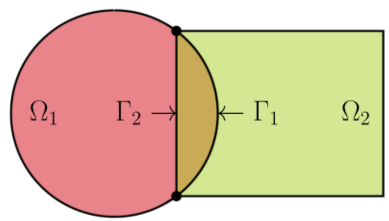

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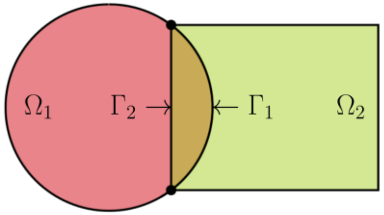

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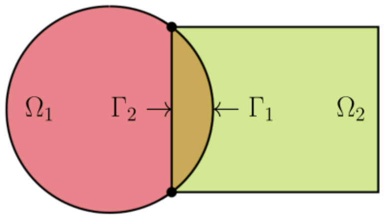

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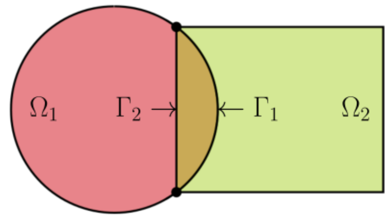

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- ***Different solvers*** can be used for the different regions.
- ***Different material models*** can be coupled provided that they are compatible in the overlap region.
- Simplifies the task of ***meshing complex geometries*** for the different scales.

Four Variants* of the Schwarz Alternating Method

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
  $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  repeat ▷ Newton loop for Ω_1
    $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  until $\|\triangle\boldsymbol{x}_B^{(1)}\|/\|\boldsymbol{x}_B^{(1)}\| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance
  $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  repeat ▷ Newton loop for Ω_2
    $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
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  until $\|\triangle\boldsymbol{x}_B^{(2)}\|/\|\boldsymbol{x}_B^{(2)}\| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance
until $\left[\left(\|\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}\|/\|\boldsymbol{x}_B^{(1)}\|\right)^2 + \left(\|\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}\|/\|\boldsymbol{x}_B^{(2)}\|\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Full Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Newton-Schwarz loop
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
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  $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
  $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
until $\left[\left(\|\triangle\boldsymbol{x}_B^{(1)}\|/\|\boldsymbol{x}_B^{(1)}\|\right)^2 + \left(\|\triangle\boldsymbol{x}_B^{(2)}\|/\|\boldsymbol{x}_B^{(2)}\|\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Modified Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
  $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  repeat ▷ Newton loop for Ω_1
    $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  until $\|\triangle\boldsymbol{x}_B^{(1)}\|/\|\boldsymbol{x}_B^{(1)}\| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
  $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  repeat ▷ Newton loop for Ω_2
    $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ solve linear system
    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
  until $\|\triangle\boldsymbol{x}_B^{(2)}\|/\|\boldsymbol{x}_B^{(2)}\| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
until $\left[\left(\|\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}\|/\|\boldsymbol{x}_B^{(1)}\|\right)^2 + \left(\|\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}\|/\|\boldsymbol{x}_B^{(2)}\|\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Inexact Schwarz

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

Monolithic Schwarz

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

Four Variants* of the Schwarz Alternating Method

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

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \chi(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \chi(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2

repeat ▷ Schwarz loop

$\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check

$\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1

repeat ▷ Newton loop for Ω_1

$\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$

until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

$\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check

$\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2

repeat ▷ Newton loop for Ω_2

$\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$

until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Full Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \chi(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \chi(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2

repeat ▷ Newton-Schwarz loop

$\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1

$\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$

$\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2

$\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$

until $\left[\left(||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Modified Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \chi(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \chi(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2

repeat ▷ Schwarz loop

$\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check

$\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1

repeat ▷ Newton loop for Ω_1

$\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$

until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$

$\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check

$\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2

repeat ▷ Newton loop for Ω_2

$\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ solve linear system

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$

until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$

until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Inexact Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \chi(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, ▷ initialize for Ω_1

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \chi(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, ▷ initialize for Ω_2

repeat ▷ Newton-Schwarz loop

$\begin{Bmatrix} \triangle\boldsymbol{x}_B^{(1)} \\ \triangle\boldsymbol{x}_B^{(2)} \end{Bmatrix} \leftarrow \begin{pmatrix} \boldsymbol{K}_{AB}^{(1)} + \boldsymbol{K}_{A\beta}^{(1)}\boldsymbol{H}_{11} & \boldsymbol{K}_{A\beta}^{(1)}\boldsymbol{H}_{12} \\ \boldsymbol{K}_{A\beta}^{(2)}\boldsymbol{H}_{21} & \boldsymbol{K}_{AB}^{(2)} + \boldsymbol{K}_{A\beta}^{(2)}\boldsymbol{H}_{22} \end{pmatrix} \backslash \begin{Bmatrix} -\boldsymbol{R}_A^{(1)} \\ -\boldsymbol{R}_A^{(2)} \end{Bmatrix}$ ▷ linear system

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$

until $\left[\left(||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Monolithic Schwarz

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

Implementations*

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

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
  $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  repeat ▷ Newton loop for Ω_1
    $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \le \epsilon_{\text{machine}}$ ▷ tight tolerance
  $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  repeat ▷ Newton loop for Ω_2
    $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
  until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \le \epsilon_{\text{machine}}$ ▷ tight tolerance
until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \le \epsilon_{\text{machine}}$ ▷ tight tolerance

Full Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Newton-Schwarz loop
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
  $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
  $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
until $\left[\left(||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \le \epsilon_{\text{machine}}$ ▷ tight tolerance

Modified Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
  $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  repeat ▷ Newton loop for Ω_1
    $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \le \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
  $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  repeat ▷ Newton loop for Ω_2
    $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ solve linear system
    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
  until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \le \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \le \epsilon_{\text{machine}}$ ▷ tight tolerance

Inexact Schwarz

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

Monolithic Schwarz

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

Implementations*

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

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_\varphi\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_\varphi\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
  $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  repeat ▷ Newton loop for Ω_1
    $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \le \epsilon_{\text{machine}}$ ▷ tight tolerance
  $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  repeat ▷ Newton loop for Ω_2
    $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
  until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \le \epsilon_{\text{machine}}$ ▷ tight tolerance
until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \le \epsilon_{\text{machine}}$ ▷ tight tolerance

Full Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_\varphi\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_\varphi\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Newton-Schwarz loop
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
  $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
  $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
until $\left[\left(||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \le \epsilon_{\text{machine}}$ ▷ tight tolerance

Modified Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_\varphi\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_\varphi\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
  $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  repeat ▷ Newton loop for Ω_1
    $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \le \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
  $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  repeat ▷ Newton loop for Ω_2
    $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ solve linear system
    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
  until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \le \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \le \epsilon_{\text{machine}}$ ▷ tight tolerance

Inexact Schwarz

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

Monolithic Schwarz

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

Implementations*

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

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
  $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  repeat ▷ Newton loop for Ω_1
    $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance
  $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  repeat ▷ Newton loop for Ω_2
    $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
  until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance
until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Full Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Newton-Schwarz loop
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
  $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system
  $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
until $\left[\left(||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Modified Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2
repeat ▷ Schwarz loop
  $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1
  repeat ▷ Newton loop for Ω_1
    $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system
    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
  $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check
  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2
  repeat ▷ Newton loop for Ω_2
    $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ solve linear system
    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
  until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$
until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Inexact Schwarz

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, ▷ initialize for Ω_1
$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, ▷ initialize for Ω_2
repeat ▷ Newton-Schwarz loop

$$\begin{Bmatrix}\triangle\boldsymbol{x}_B^{(1)}\\ \triangle\boldsymbol{x}_B^{(2)}\end{Bmatrix} \leftarrow \begin{pmatrix}\boldsymbol{K}_{AB}^{(1)} + \boldsymbol{K}_{A\beta}^{(1)}\boldsymbol{H}_{11} & \boldsymbol{K}_{A\beta}^{(1)}\boldsymbol{H}_{12}\\ \boldsymbol{K}_{A\beta}^{(2)}\boldsymbol{H}_{21} & \boldsymbol{K}_{AB}^{(2)} + \boldsymbol{K}_{A\beta}^{(2)}\boldsymbol{H}_{22}\end{pmatrix}\backslash\begin{Bmatrix}-\boldsymbol{R}_A^{(1)}\\ -\boldsymbol{R}_A^{(2)}\end{Bmatrix}$$ ▷ linear system

  $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$
  $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$
until $\left[\left(||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

Monolithic Schwarz

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

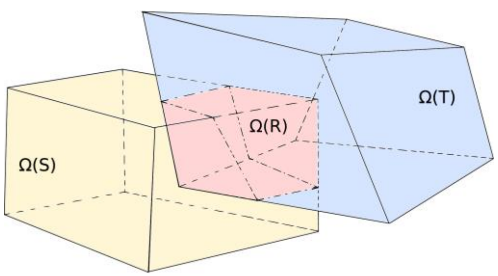
Schwarz Alternating Method in *Albany* Code

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***.

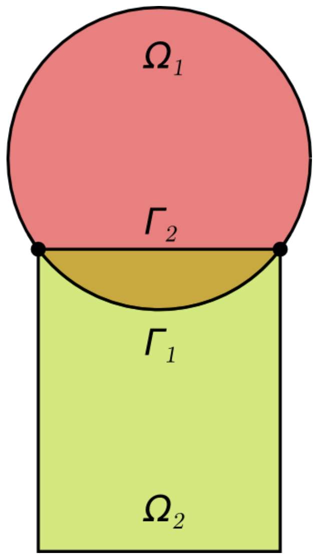
https://github.com/trilinos/trilinos

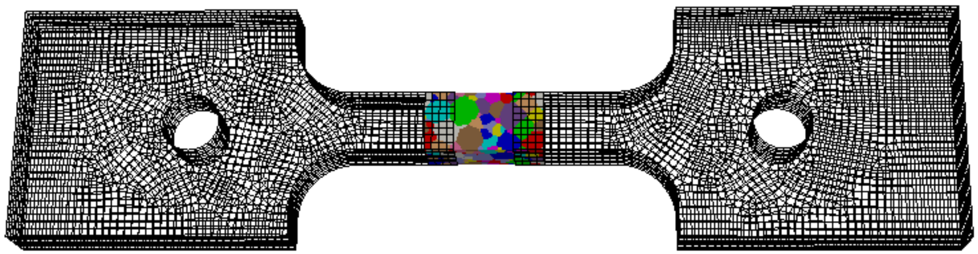


https://github.com/ORNL-CEES/DataTransferKit

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

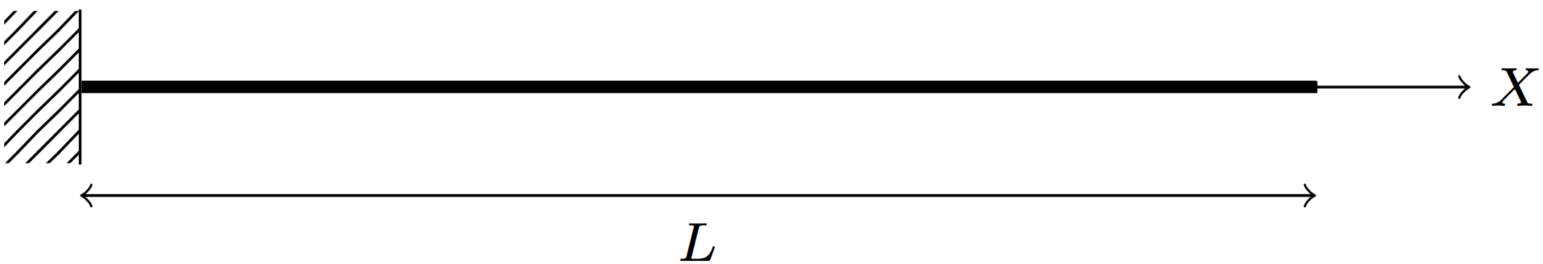




Example #1: Foulk's Singular Bar

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

$u(0) = 0$ $\qquad A(X) = A_0\sqrt{X/L}$ $\qquad u(L) = \Delta$



- ***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

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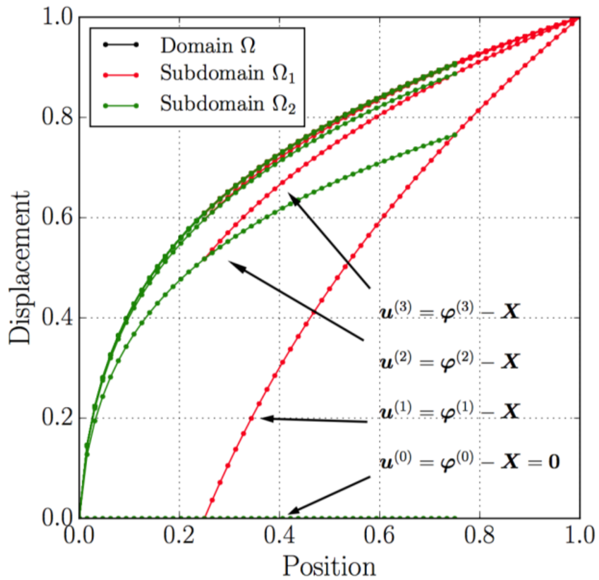
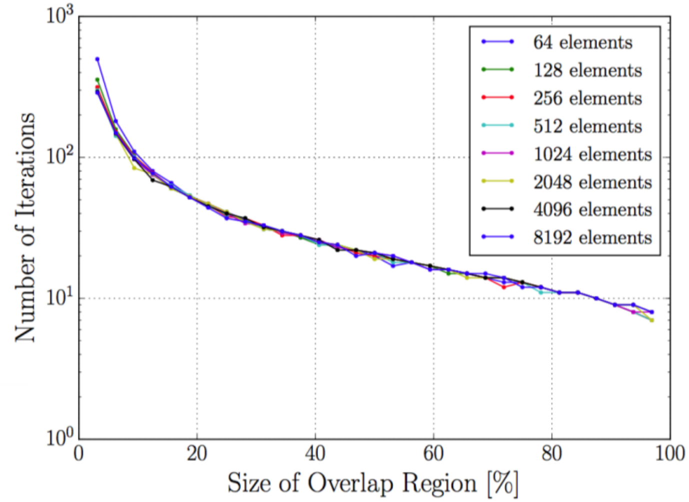
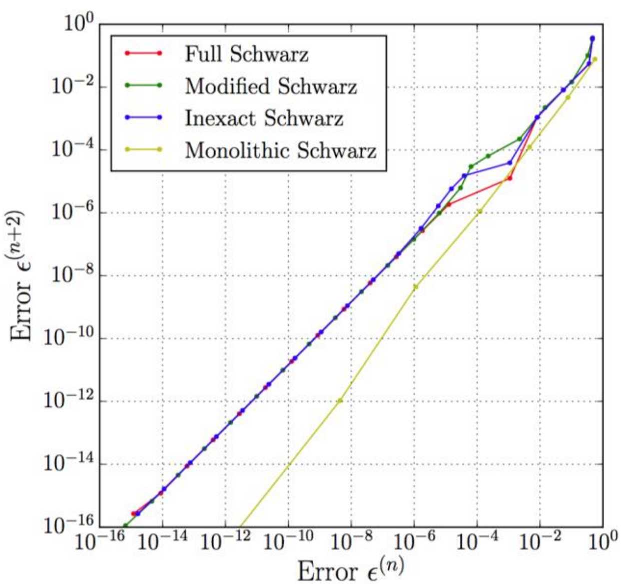
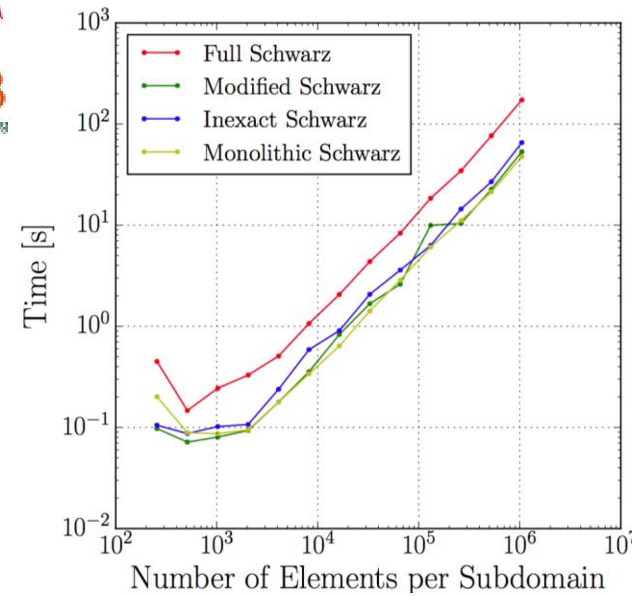
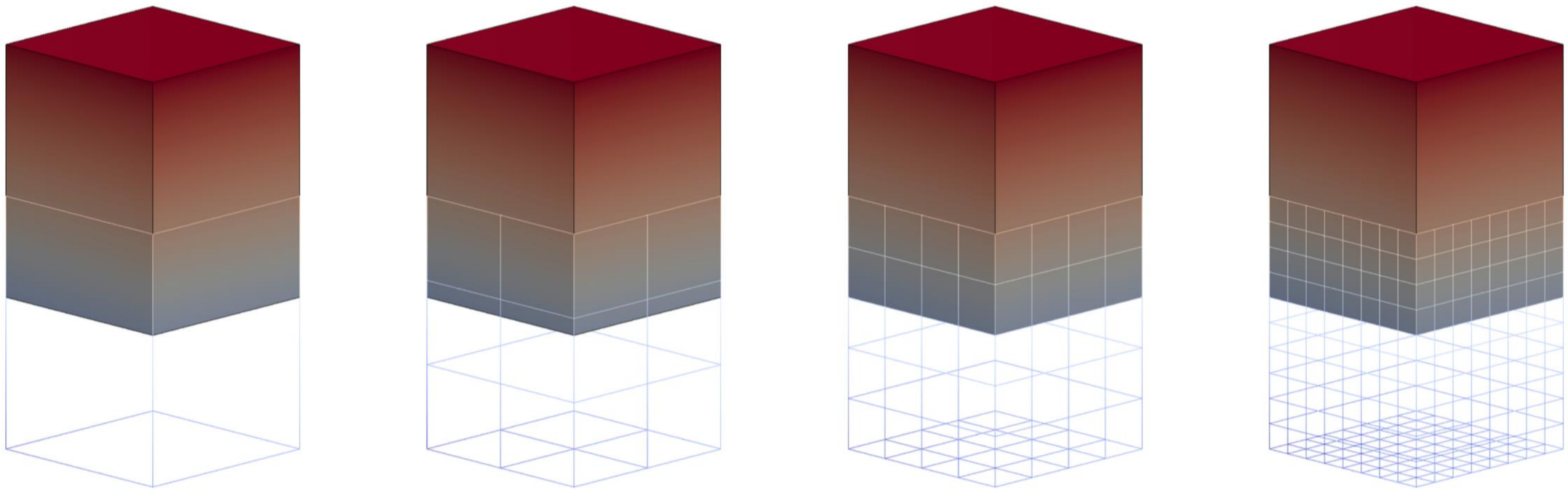




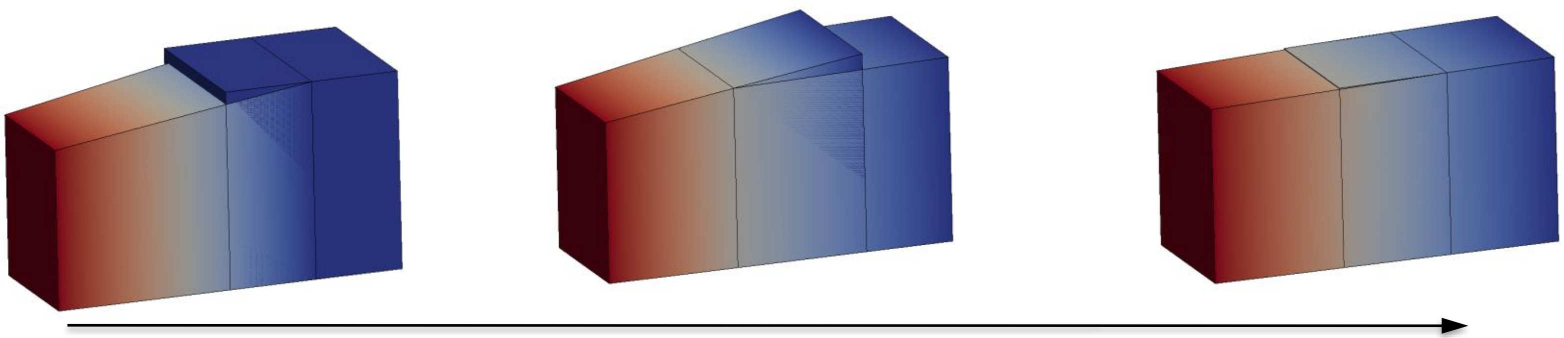




Example #2: Cuboid Problem



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



Combined Newton-Schwarz Iteration

Cuboid Problem: Convergence with Overlap & Refinement

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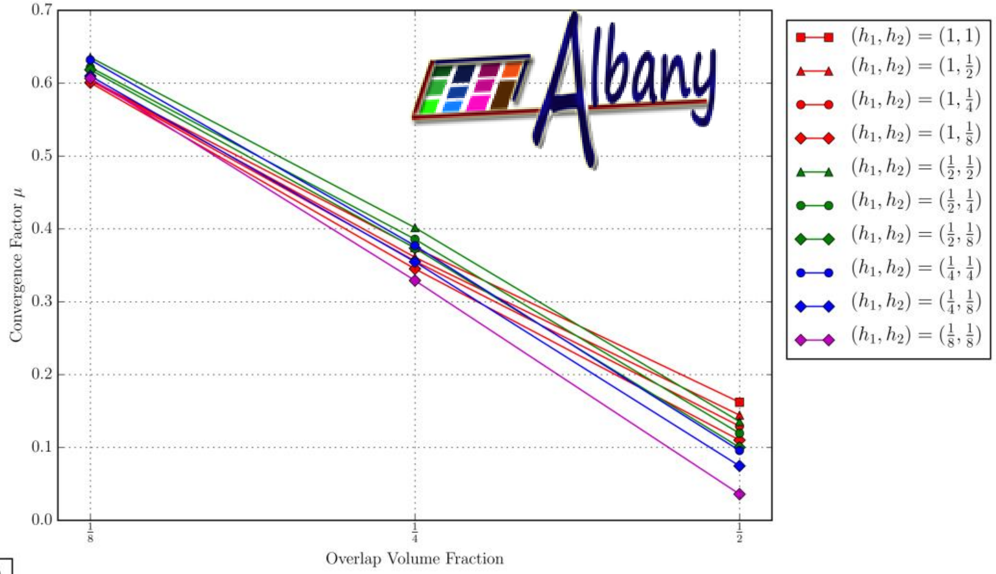
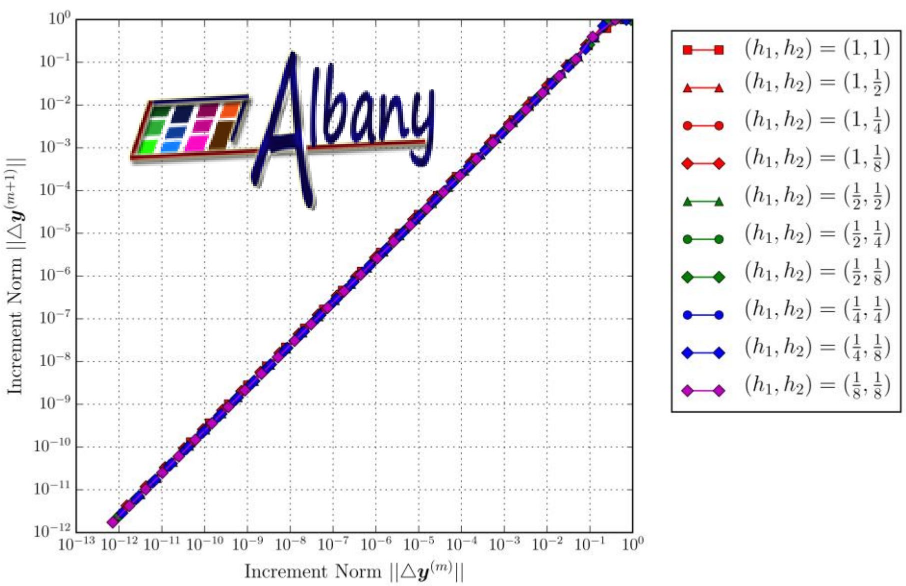


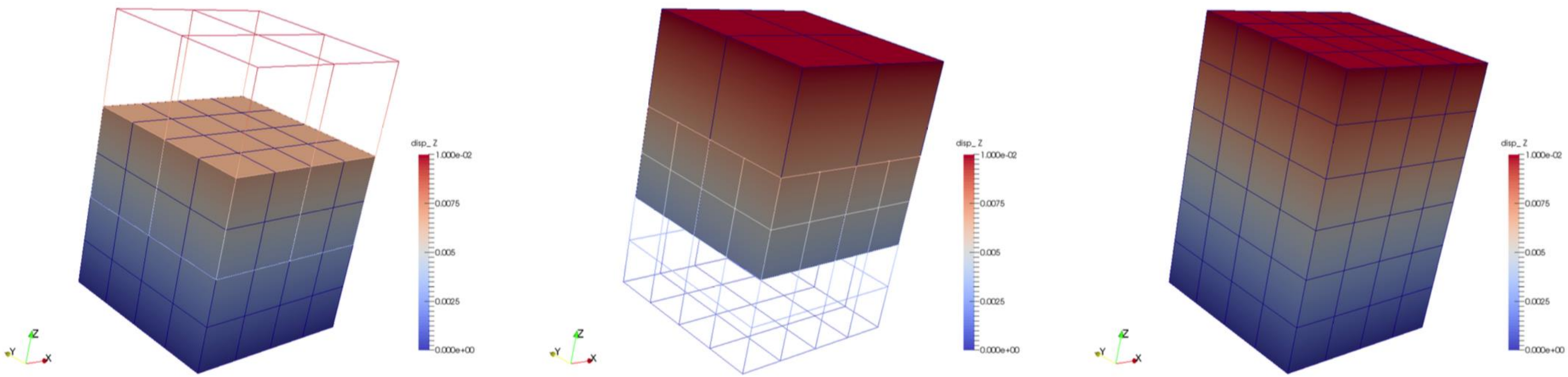
Below: Convergence of the cuboid problem for different mesh sizes and fixed overlap volume fraction. The Schwarz alternating method converges ***linearly***.



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

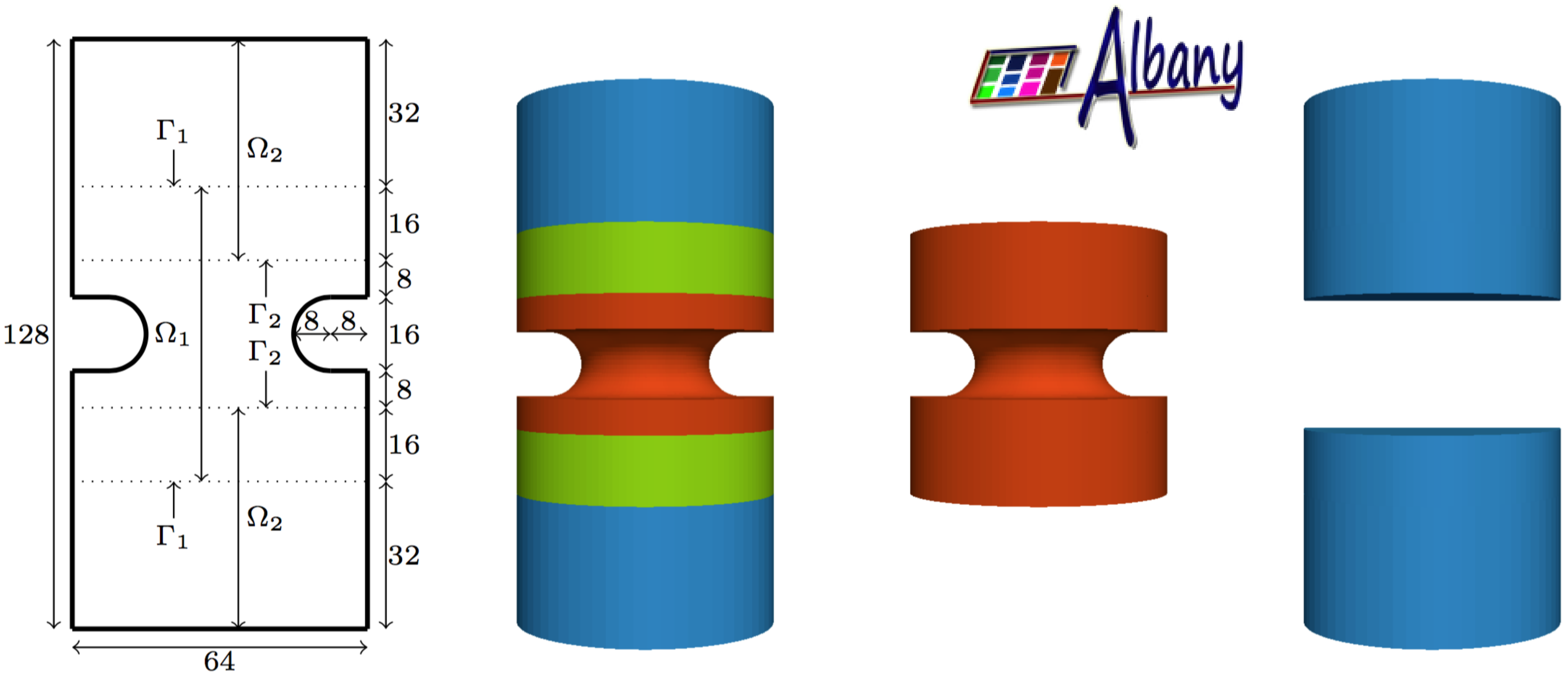
$$\Delta y^{(m+1)} \leq \mu \Delta y^{(m)}$$

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}

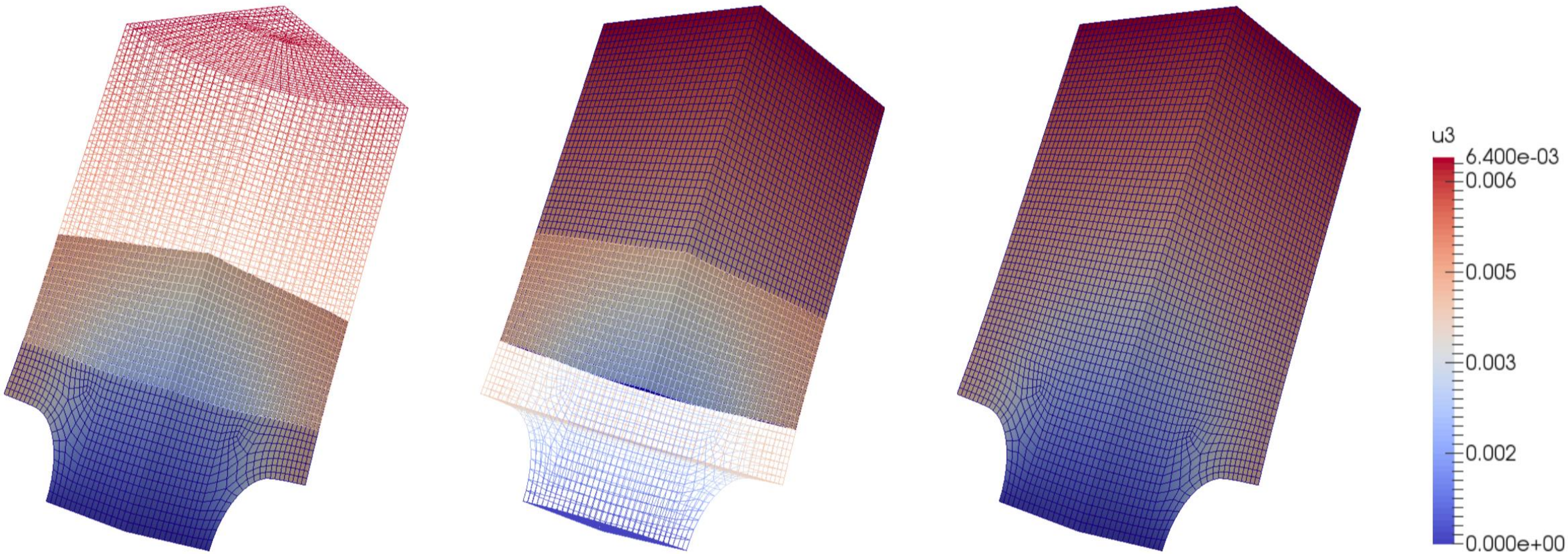
Example #3: Notched Cylinder



(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

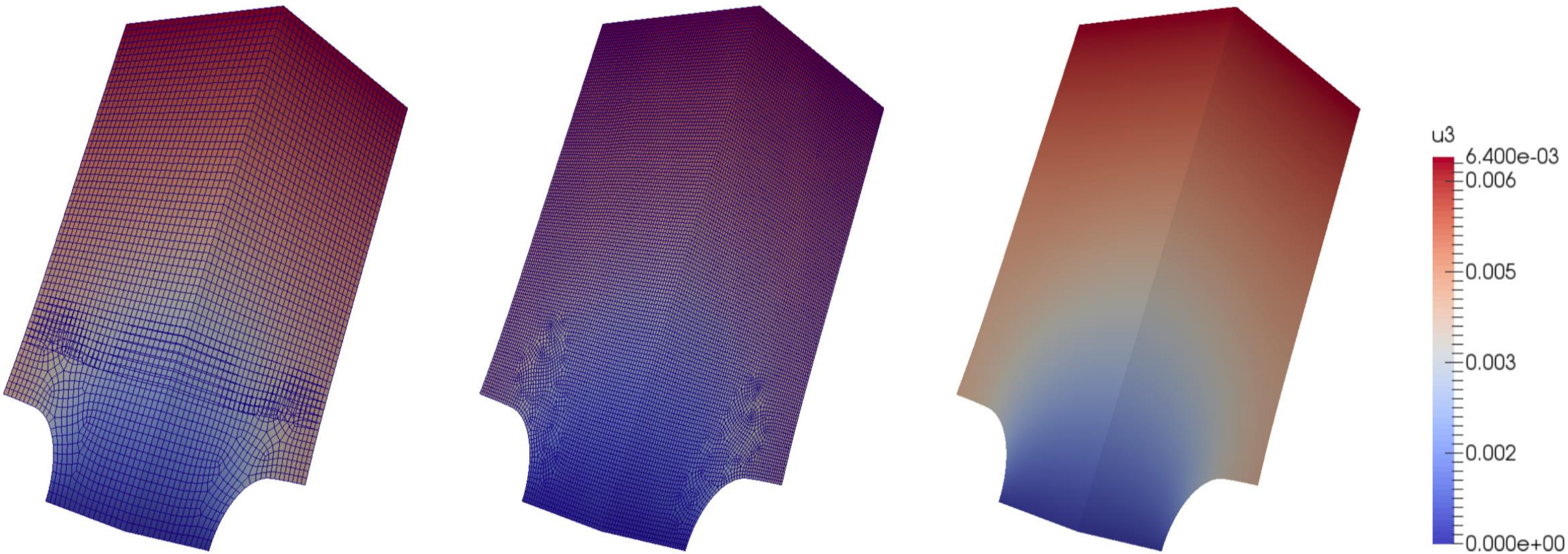


(a) Ω_1 **(b)** Ω_2 **(c)** Ω_{ref}

	u_3 relative error	
Absolute residual tolerance	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}

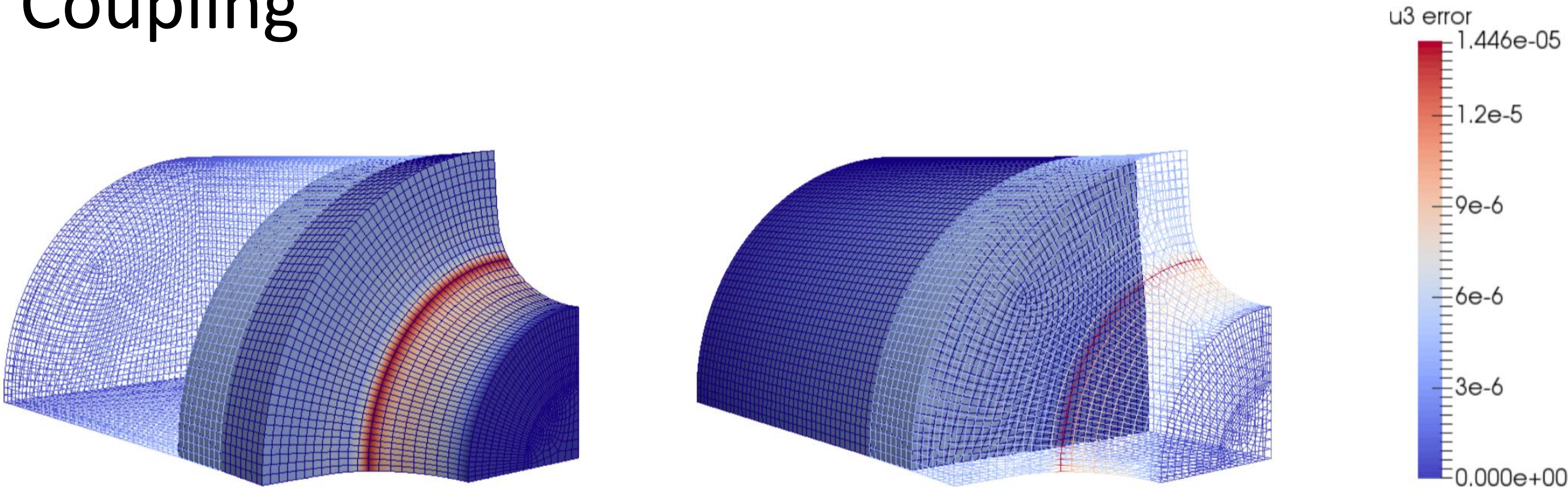
Albany

Notched Cylinder: Nonconformal HEX-HEX Coupling



(a) Ω_1 and Ω_2 **(b)** Ω_{ref} mesh **(c)** Ω_{ref} solution

Notched Cylinder: Nonconformal HEX-HEX Coupling

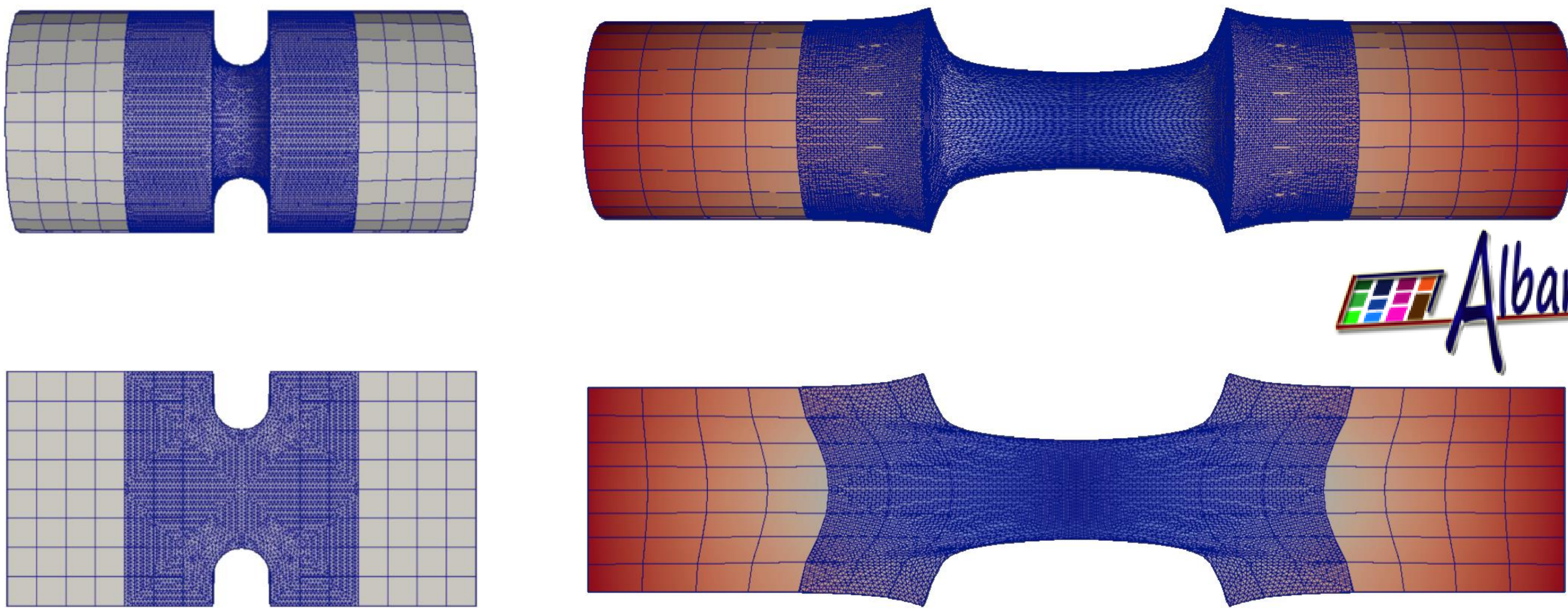


(a) Ω_1 **(b)** Ω_2

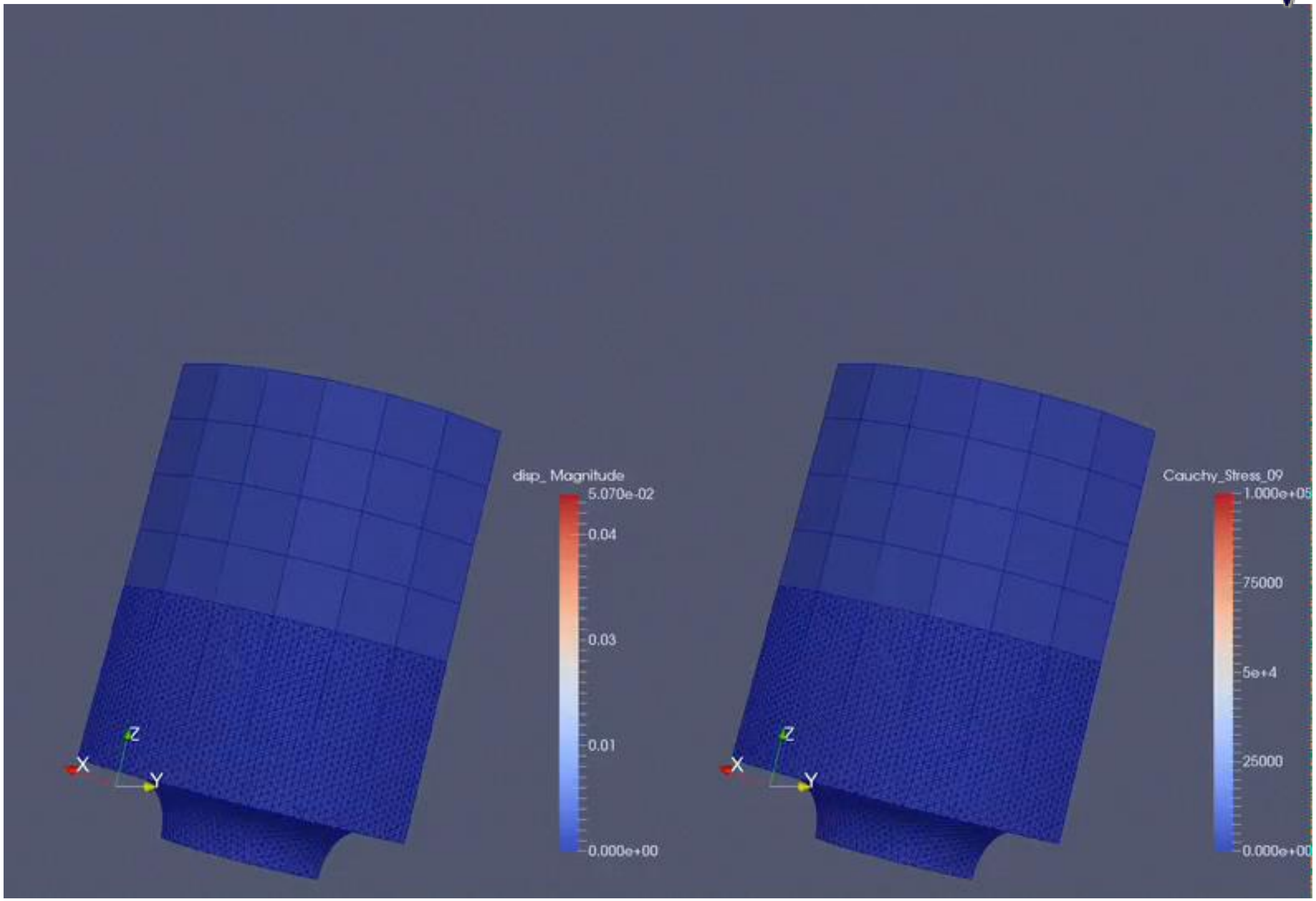
Absolute residual tolerance	u_3 relative error Ω_1	Ω_2
1.0×10^{-8}	1.31×10^{-3}	4.45×10^{-4}
1.0×10^{-12}	1.30×10^{-3}	4.43×10^{-4}
1.0×10^{-14}	1.30×10^{-3}	4.43×10^{-4}
2.5×10^{-16}	1.30×10^{-3}	4.43×10^{-4}

Notched Cylinder: TET-HEX Coupling

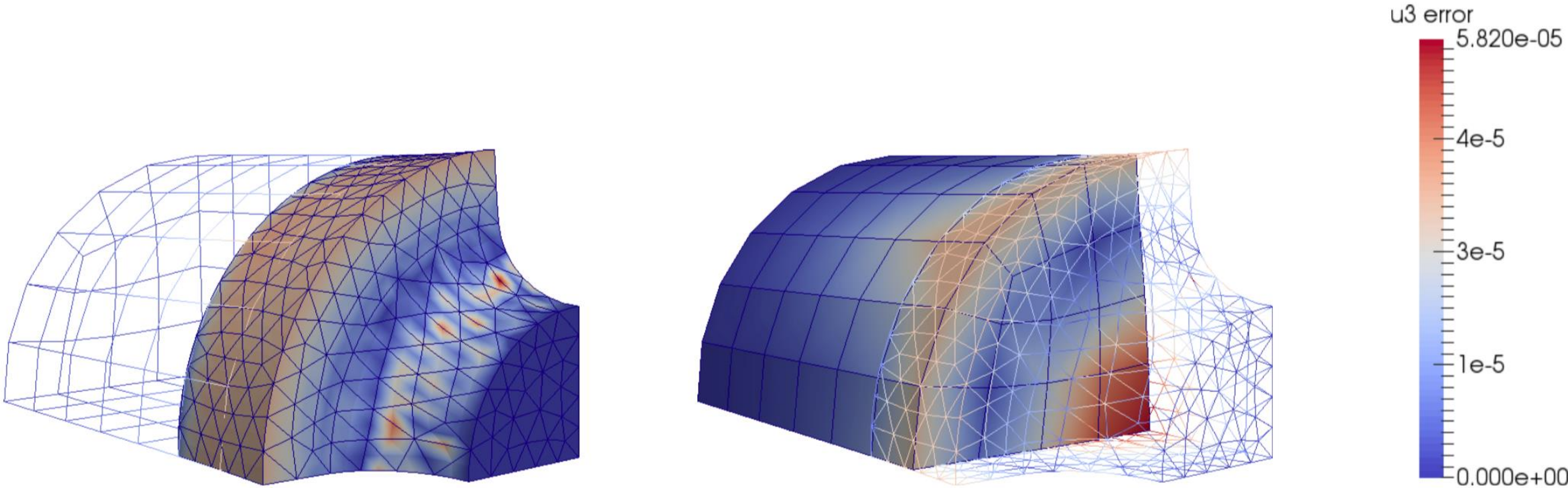
- The Schwarz alternating method is capable of coupling ***different mesh topologies***.
- The notched region, where stress concentrations are expected, is ***finely*** meshed with ***tetrahedral*** elements.
- The top and bottom regions, presumably of less interest, are meshed with ***coarser hexahedral***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



Notched Cylinder: TET-HEX Coupling



Notched Cylinder: Conformal TET-HEX Coupling



(a) Ω_1 **(b)** Ω_2

Absolute residual tolerance	u_3 relative error Ω_1	u_3 relative error 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***.

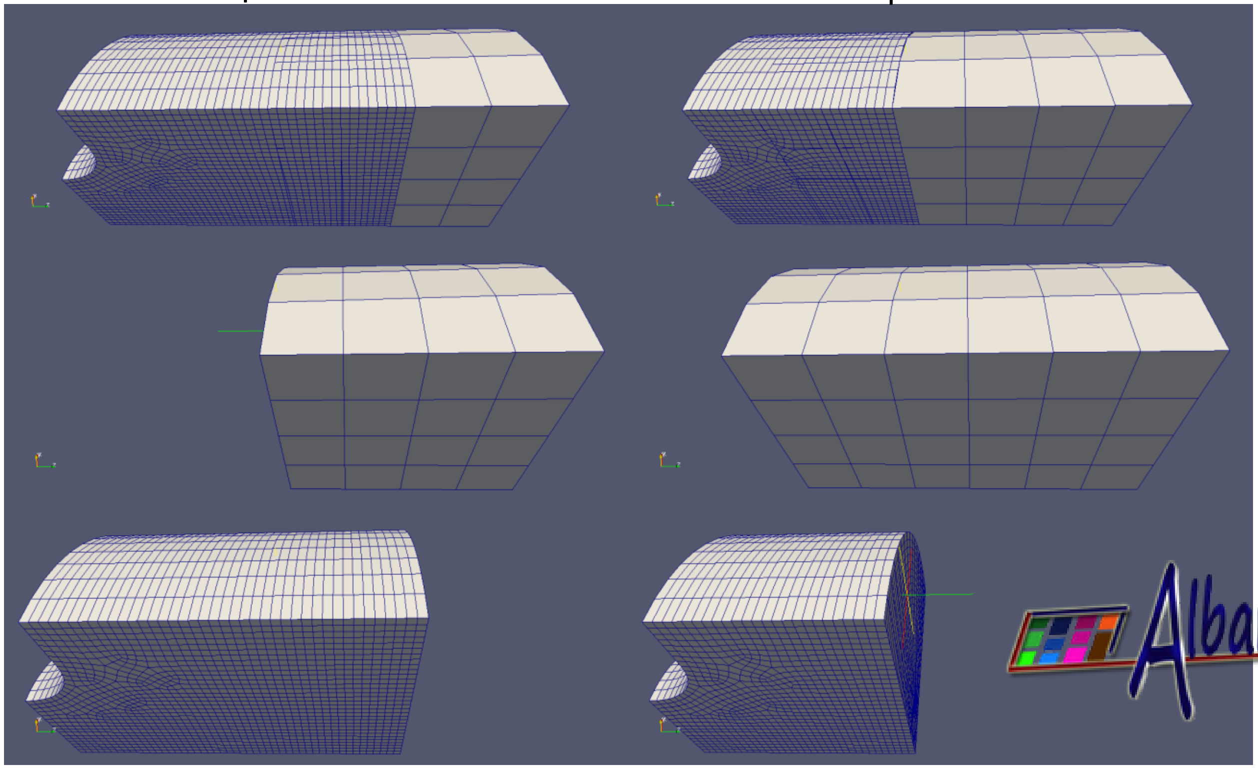
- Notched cylinder subjected to tensile load with an ***elastic*** and ***J2 elasto-plastic*** regions.
- ***Coarse*** region is ***elastic*** and ***fine*** region is ***elasto-plastic***.
- The ***overlap region*** in the first mesh is nearer the notch, where plastic behavior is expected.

Overlap far from notch. | Overlap near notch.

Coupled regions

Coarse, elastic region

Fine, elasto-plastic region

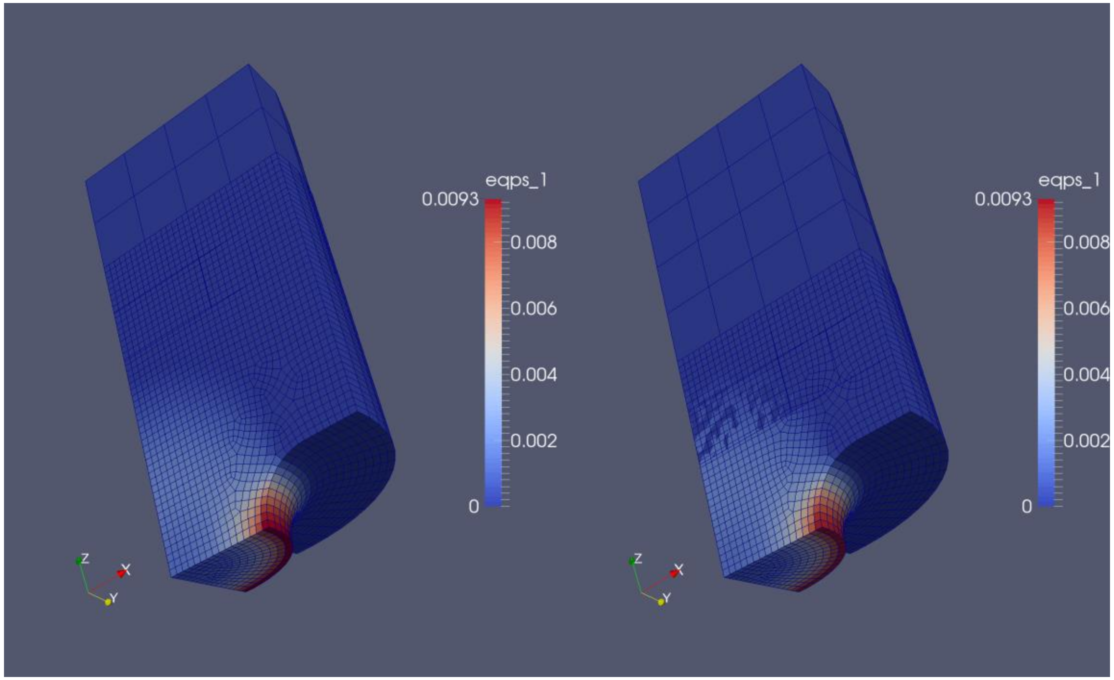


Notched Cylinder: Coupling Different Materials

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***.

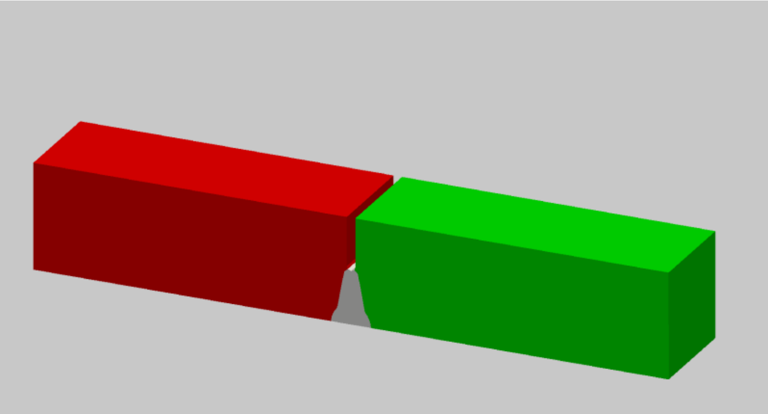
Albany



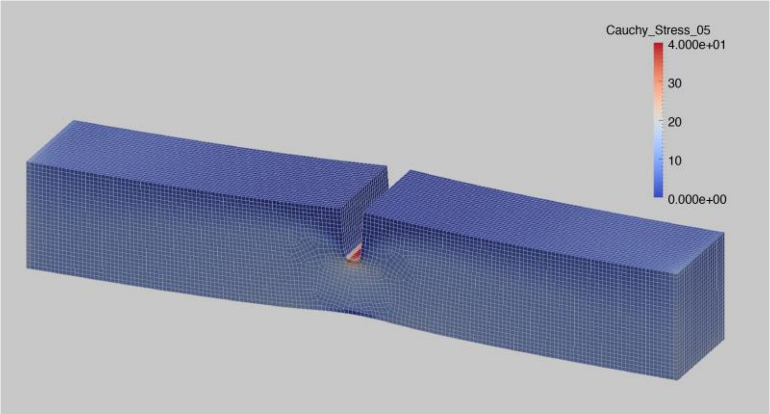
Overlap far from notch. Overlap near notch.

Example #4: Laser Weld with 3 Subdomains

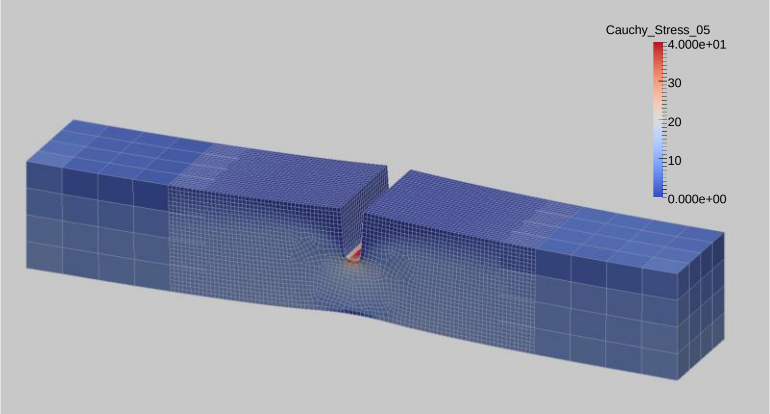
Laser weld specimen



Single domain discretization

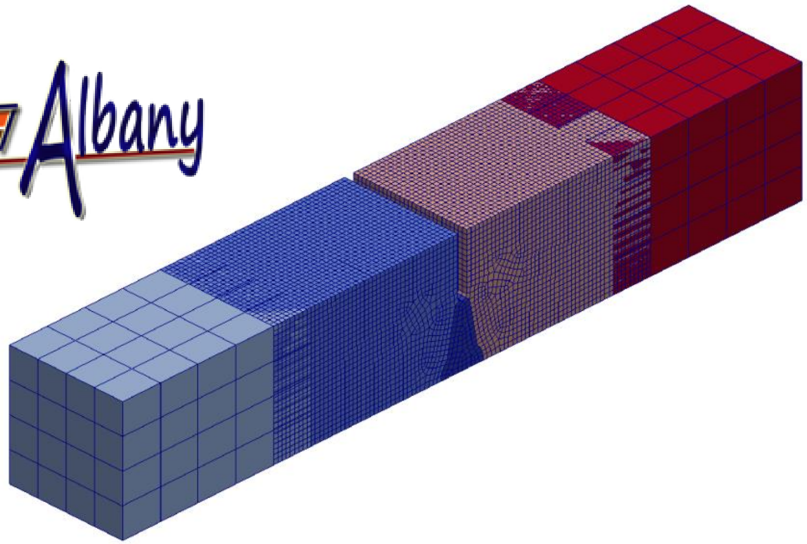


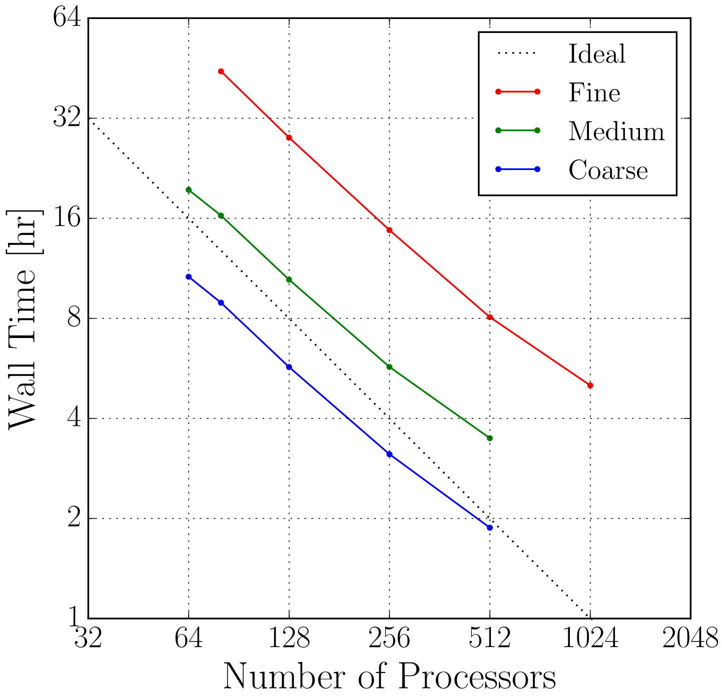
Coupled Schwarz discretization
(50% reduction in model size)



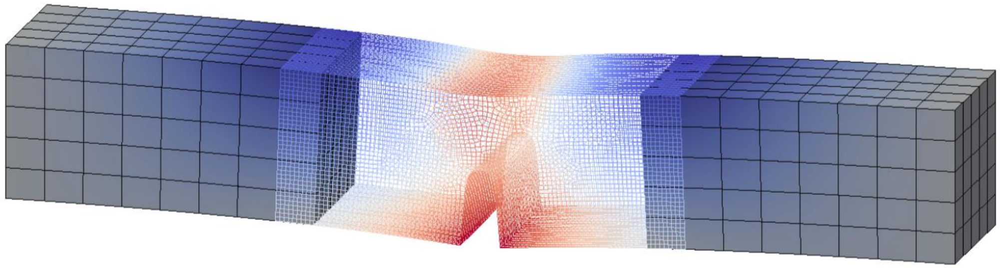
- Problem of ***practical scale (~200K dofs).***
- ***Isotropic elasticity*** and ***J2 plasticity*** with linear isotropic hardening.
- ***Identical parameters*** for weld and base materials for proof of concept, to become independent models.

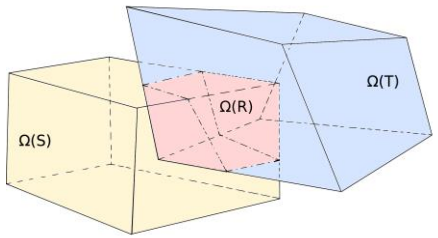
Laser Weld: Strong Scalability of Parallel Schwarz with DTK





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

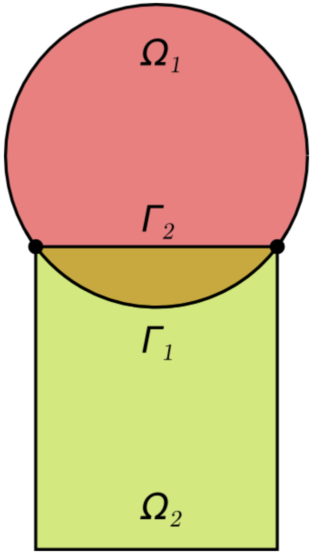


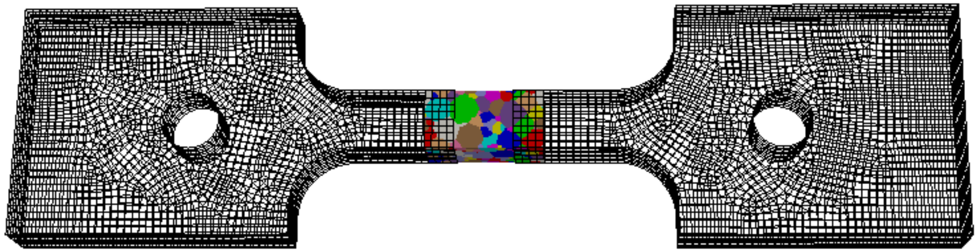


Data Transfer Kit (DTK)

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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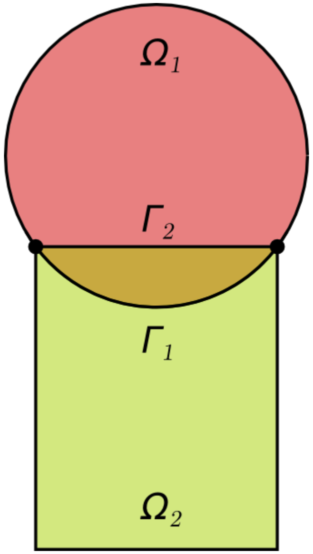

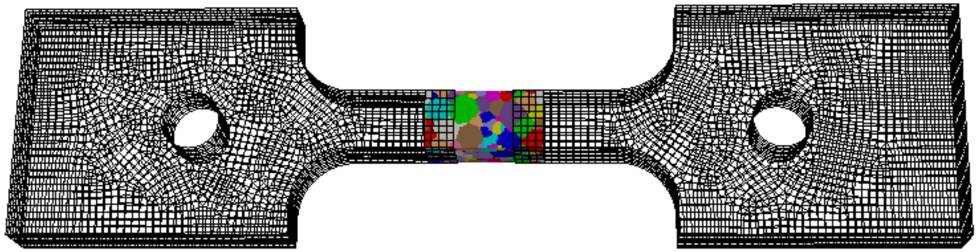

Future Work

- 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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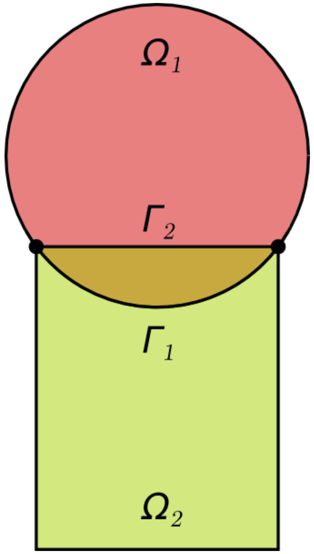

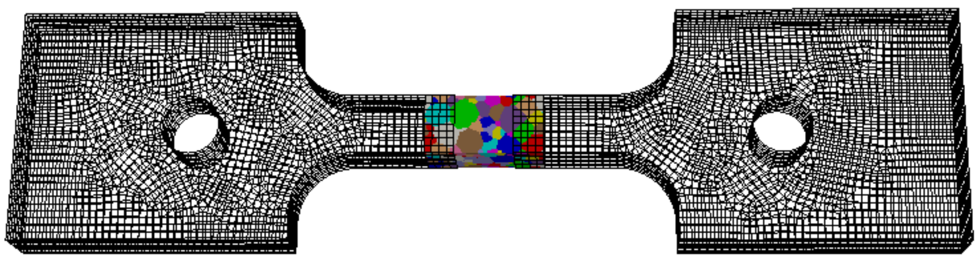

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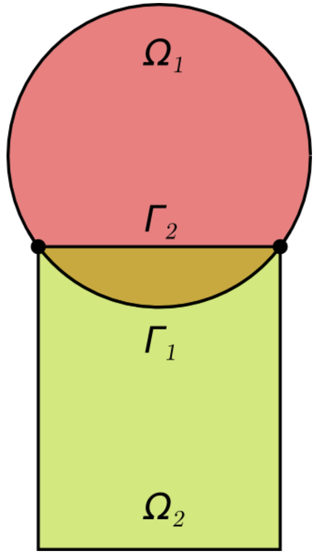

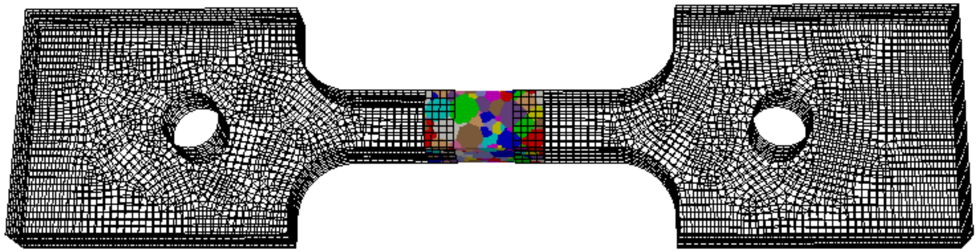

Appendix. Previous Work

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

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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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-

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*** ($\epsilon_{machine}$).

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2

repeat ▷ Schwarz loop

  $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check

  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1

  repeat ▷ Newton loop for Ω_1

    $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system

    $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$

  until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

  $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check

  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2

  repeat ▷ Newton loop for Ω_2

    $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system

    $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$

  until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ 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***.

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2

repeat ▷ Schwarz loop

    $\boldsymbol{y}^{(1)} \leftarrow \boldsymbol{x}_B^{(1)}$ ▷ for convergence check

    $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1

    repeat ▷ Newton loop for Ω_1

        $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system

        $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$

    until $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$

    $\boldsymbol{y}^{(2)} \leftarrow \boldsymbol{x}_B^{(2)}$ ▷ for convergence check

    $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2

    repeat ▷ Newton loop for Ω_2

        $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ solve linear system

        $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$

    until $||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}|| \leq \epsilon$ ▷ loose tolerance, e.g. $\epsilon \in [10^{-4}, 10^{-1}]$

until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ 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: $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, ▷ initialize for Ω_1

2: $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, ▷ initialize for Ω_2

3: **repeat** ▷ Newton-Schwarz loop

4: $\begin{Bmatrix} \triangle\boldsymbol{x}_B^{(1)} \\ \triangle\boldsymbol{x}_B^{(2)} \end{Bmatrix} \leftarrow \begin{pmatrix} \boldsymbol{K}_{AB}^{(1)} + \boldsymbol{K}_{A\beta}^{(1)}\boldsymbol{H}_{11} & \boldsymbol{K}_{A\beta}^{(1)}\boldsymbol{H}_{12} \\ \boldsymbol{K}_{A\beta}^{(2)}\boldsymbol{H}_{21} & \boldsymbol{K}_{AB}^{(2)} + \boldsymbol{K}_{A\beta}^{(2)}\boldsymbol{H}_{22} \end{pmatrix} \backslash \begin{Bmatrix} -\boldsymbol{R}_A^{(1)} \\ -\boldsymbol{R}_A^{(2)} \end{Bmatrix}$ ▷ linear system

5: $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$

6: $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$

7: **until** $\left[\left(||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ 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.

$\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)}$ in Ω_1, $\boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_1 ▷ initialize for Ω_1

$\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in Ω_2, $\boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2

repeat ▷ Newton-Schwarz loop

  $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_B^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_b^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_\beta^{(2)}$ ▷ project from Ω_2 to Γ_1

  $\triangle\boldsymbol{x}_B^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})\backslash\boldsymbol{R}_A^{(1)}(\boldsymbol{x}_B^{(1)};\boldsymbol{x}_b^{(1)};\boldsymbol{x}_\beta^{(1)})$ ▷ linear system

  $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + \triangle\boldsymbol{x}_B^{(1)}$

  $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{P}_{21}\boldsymbol{x}_B^{(1)} + \boldsymbol{Q}_{21}\boldsymbol{x}_b^{(1)} + \boldsymbol{G}_{21}\boldsymbol{x}_\beta^{(1)}$ ▷ project from Ω_1 to Γ_2

  $\triangle\boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})\backslash\boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)};\boldsymbol{x}_b^{(2)};\boldsymbol{x}_\beta^{(2)})$ ▷ linear system

  $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{x}_B^{(2)} + \triangle\boldsymbol{x}_B^{(2)}$

until $\left[\left(||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

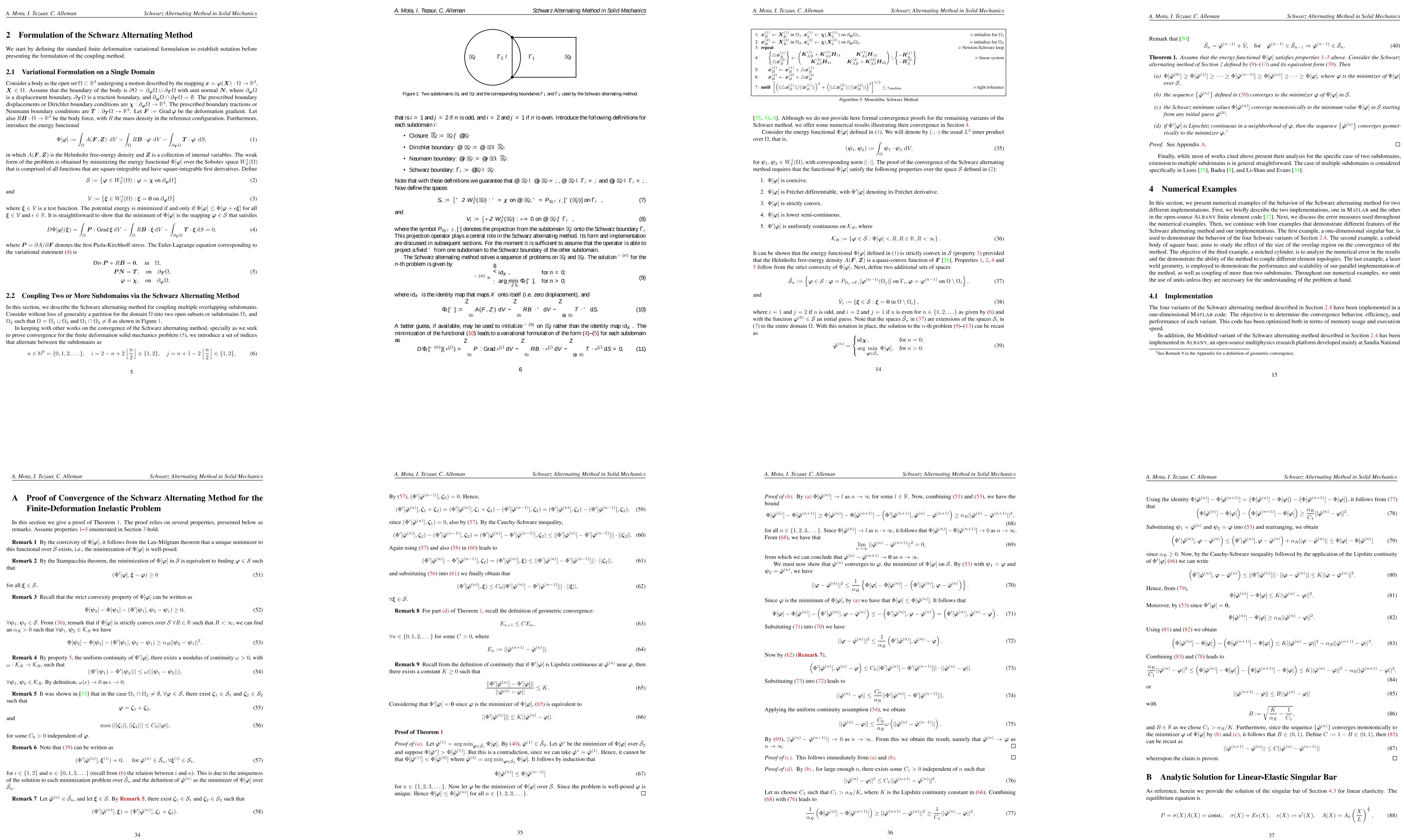
Advantages:

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

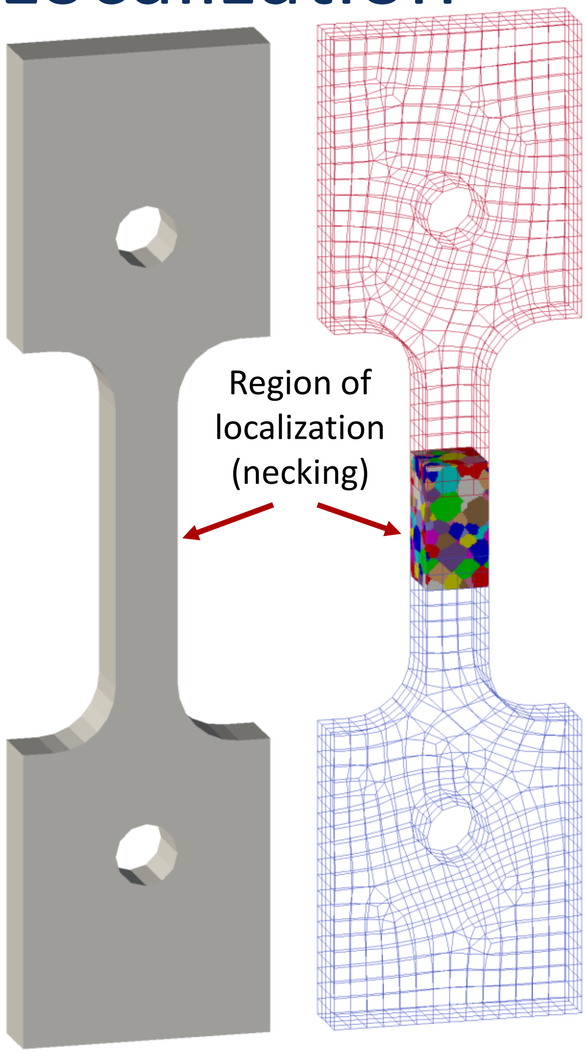
Least-intrusive variant: by-passes Schwarz iteration, no need for block solver.

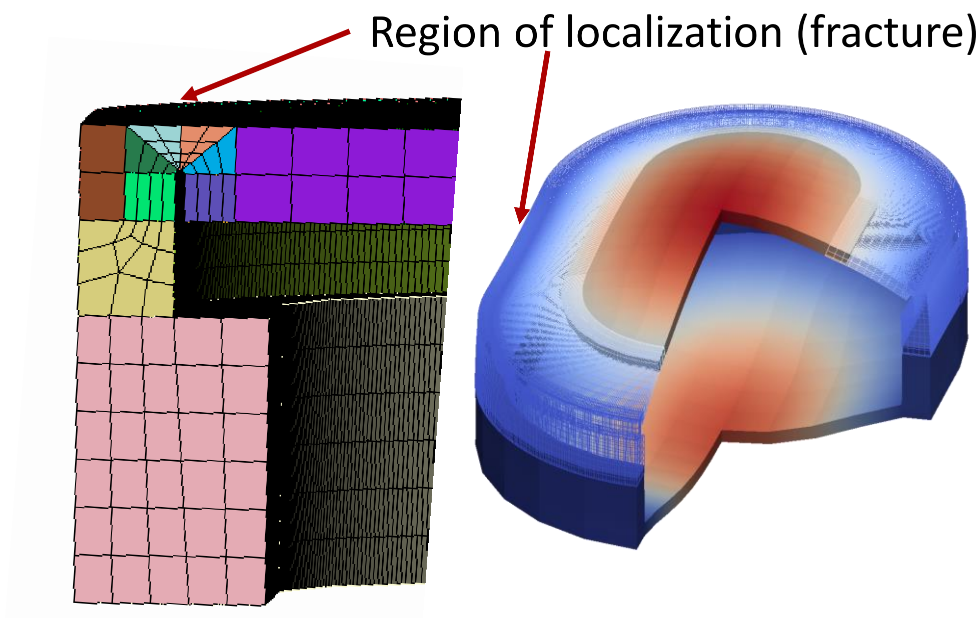
Appendix. Convergence Proof

Sandia National Laboratories



Appendix. Multiscale Modeling of Localization



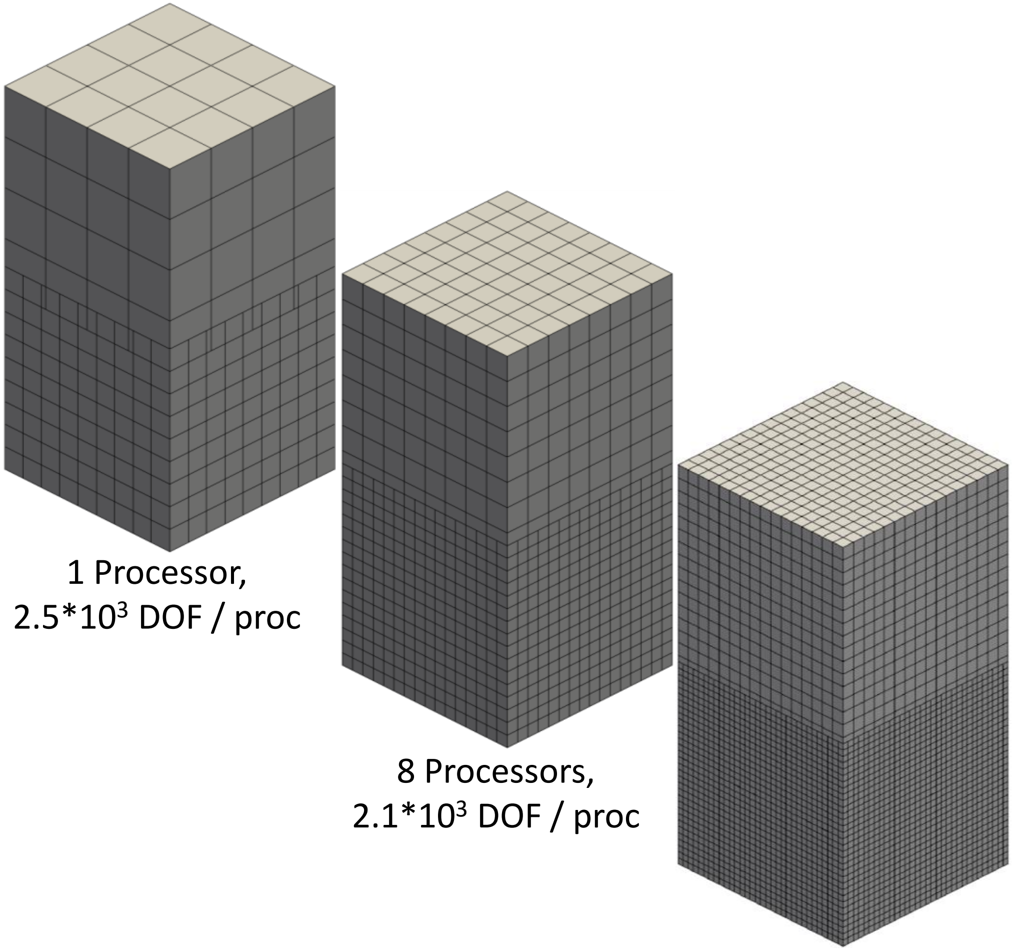


Strain localization can cause ***localized necking*** (left) and ultimately ***fracture*** (above).

Goals:

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

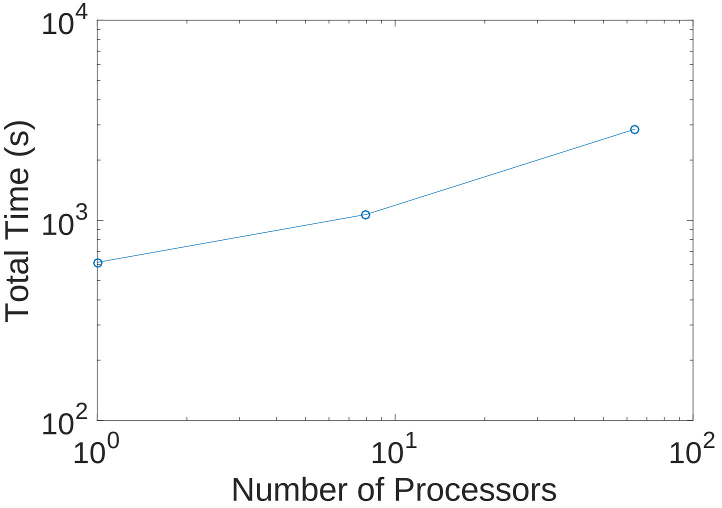
Appendix. Parallelization via DTK: Weak Scaling on Cubes Problem



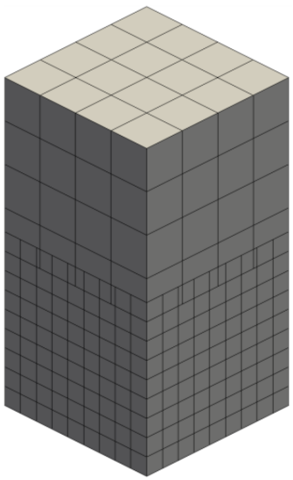
1 Processor,
2.5*10^3 DOF / proc

8 Processors,
2.1*10^3 DOF / proc

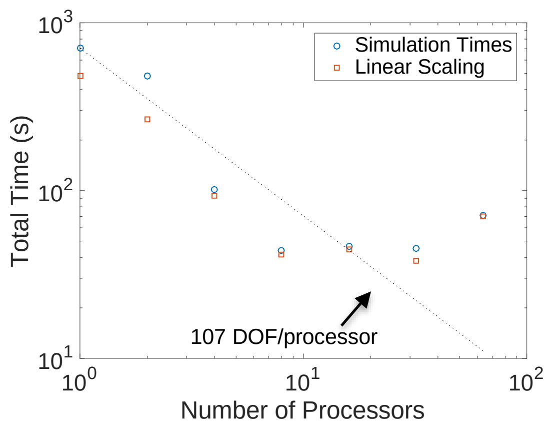
64 Processors,
1.9*10^3 DOF / proc



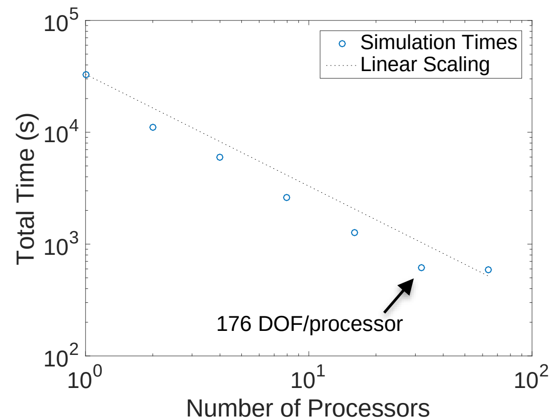
Appendix. Parallelization via DTK: Strong Scaling on Cubes Problem

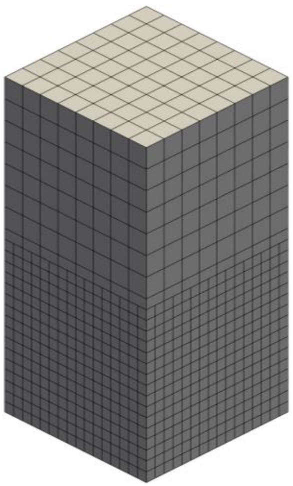


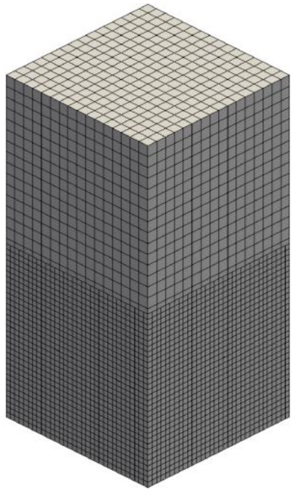
Small problem ($2.5*10^3$ DOFs)



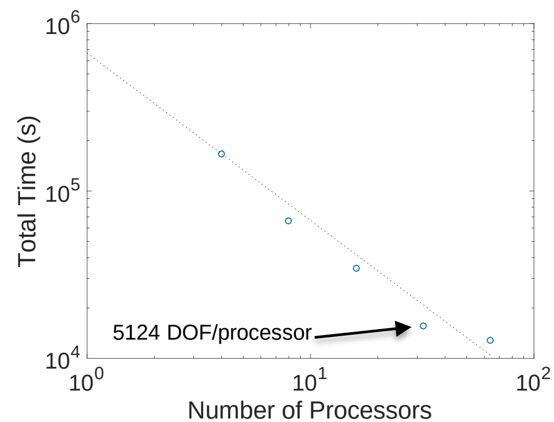
Medium problem ($1.7*10^4$ DOFs)





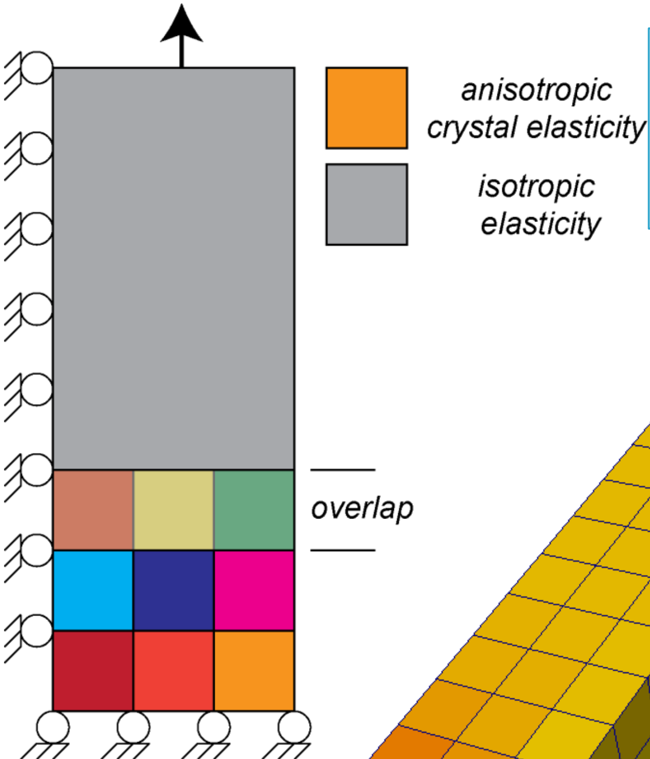


Large problem ($1.6*10^5$ DOFs)

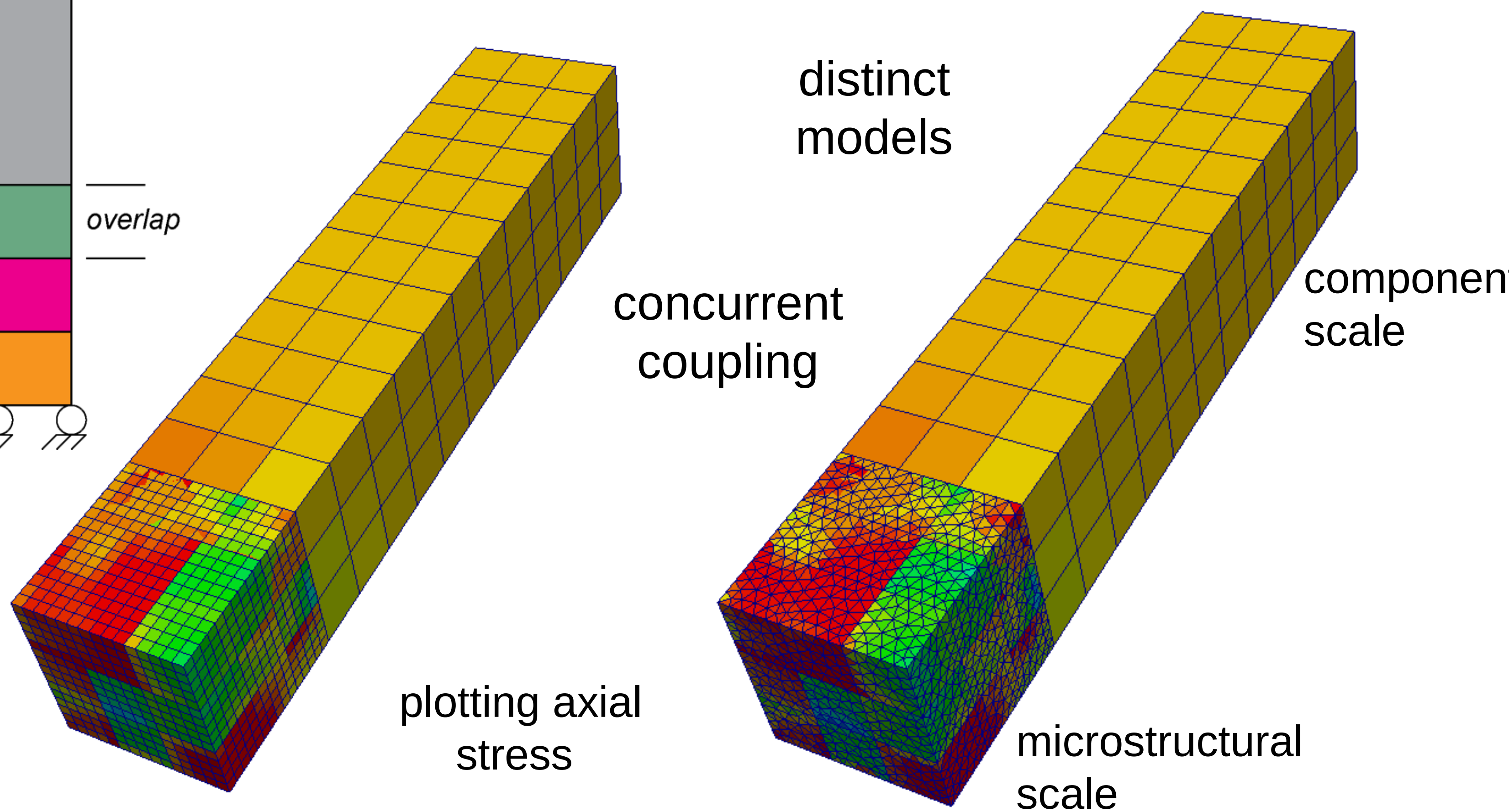


Appendix. Rubiks Cube Problem

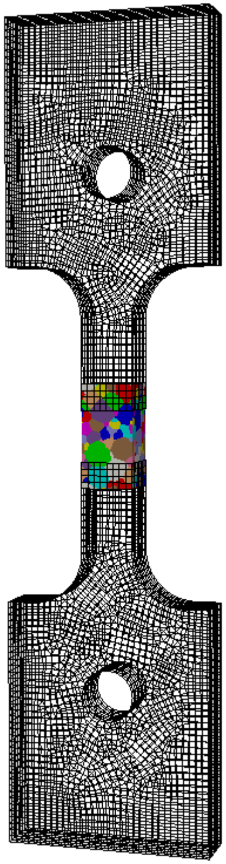
Work by J. Foulk, D. Littlewood, C. Battaile, H. Lim



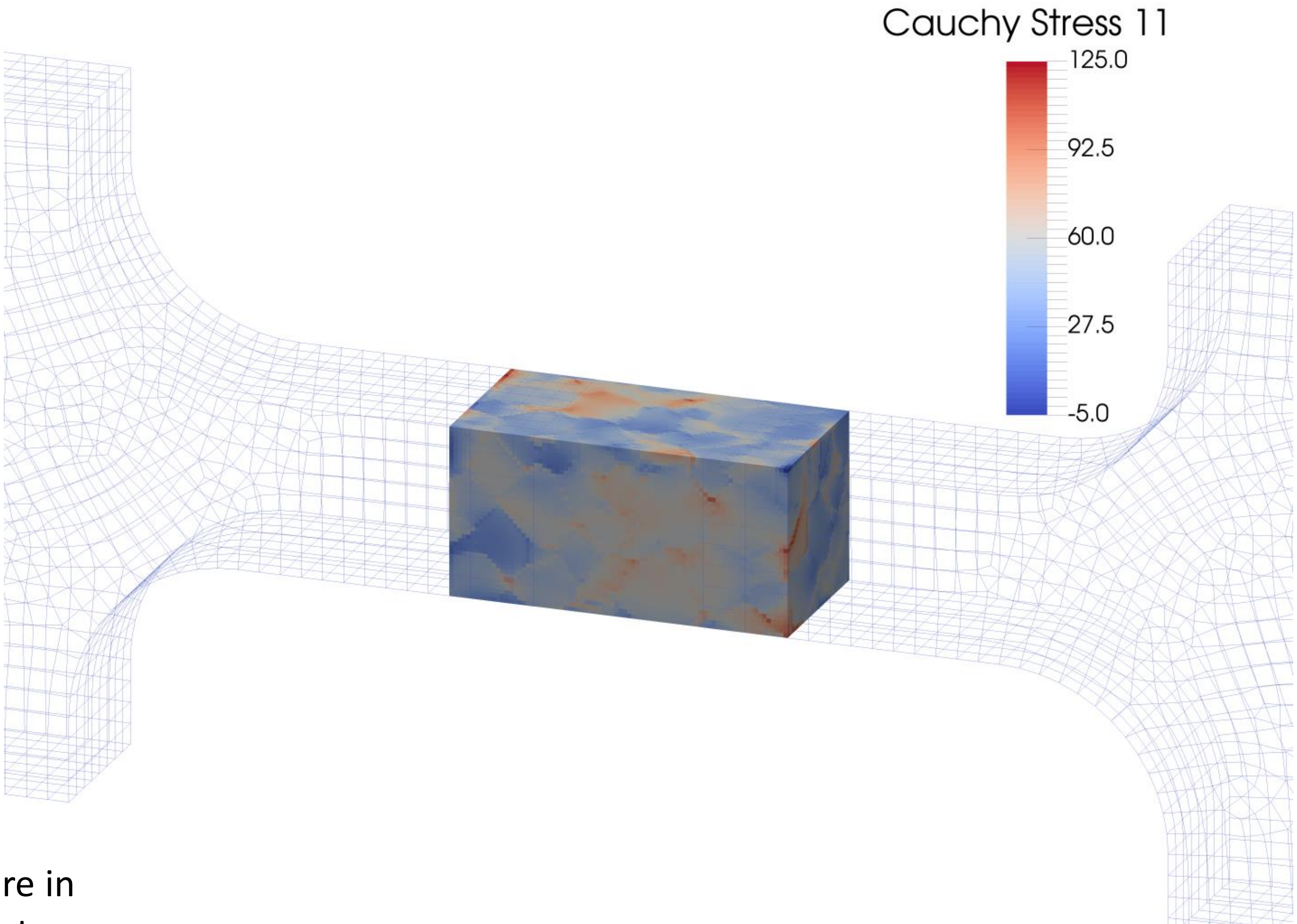
Two distinct bodies, the component scale and the microstructural scale, are coupled iteratively with alternating Schwarz



Appendix. Tensile Bar



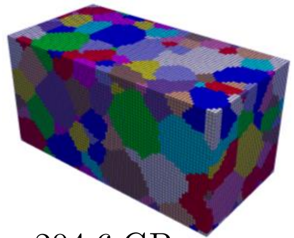
Embed microstructure in
ASTM tensile geometry



Appendix. Tensile Bar: Meso-Macroscale Coupling

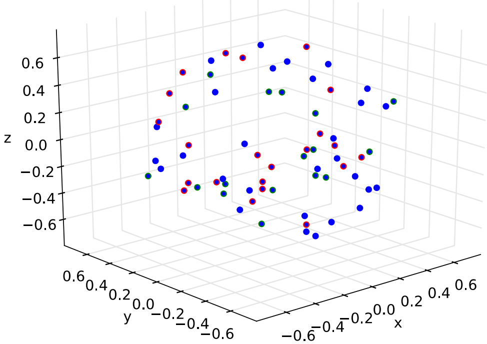
Mesoscale

SPARKS-generated microstructure (F. Abdeljawad)



$$\text{cubic elastic constant} : C_{11} = 204.6 \text{ GPa}$$
$$\text{cubic elastic constant} : C_{12} = 137.7 \text{ GPa}$$
$$\text{cubic elastic constant} : C_{44} = 126.2 \text{ GPa}$$
$$\text{reference shear rate} : \dot{\gamma}_0 = 1.0 \text{ 1/s}$$
$$\text{rate sensitivity factor} : m = 20$$
$$\text{hardening rate parameter} : \dot{g}_0 = 2.0 \times 10^4 \text{ 1/s}$$
$$\text{initial hardness} : g_0 = 90 \text{ MPa}$$
$$\text{saturation hardness} : g_s = 202 \text{ MPa}$$
$$\text{saturation exponent} : \omega = 0.01$$

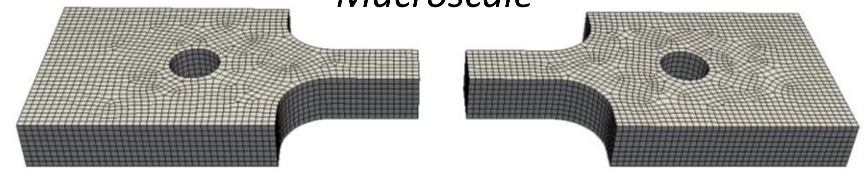
Fix microstructure, investigate ensembles



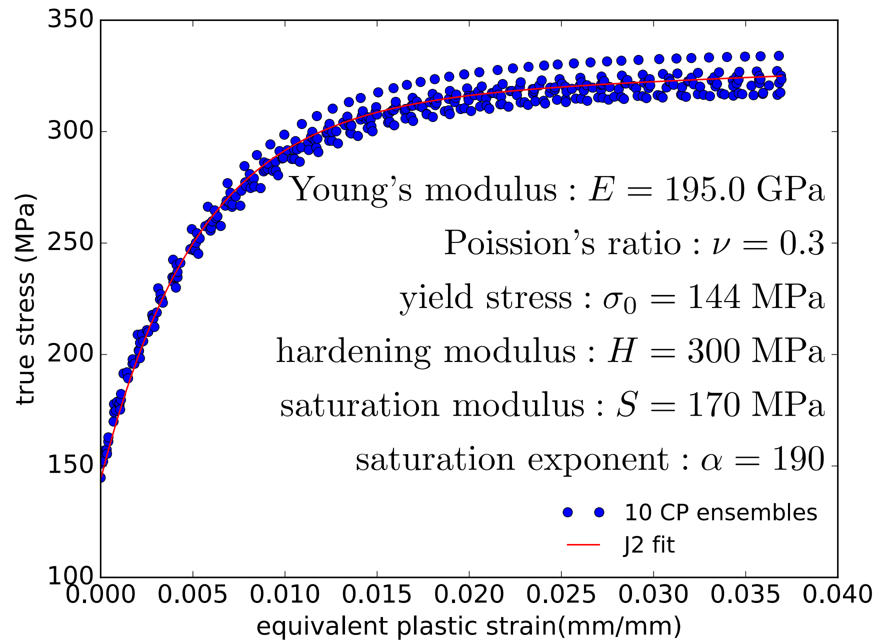
151 axial vectors from 3 of the 10 ensembles of random rotations (blue, green, red)

+

Macroscale



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

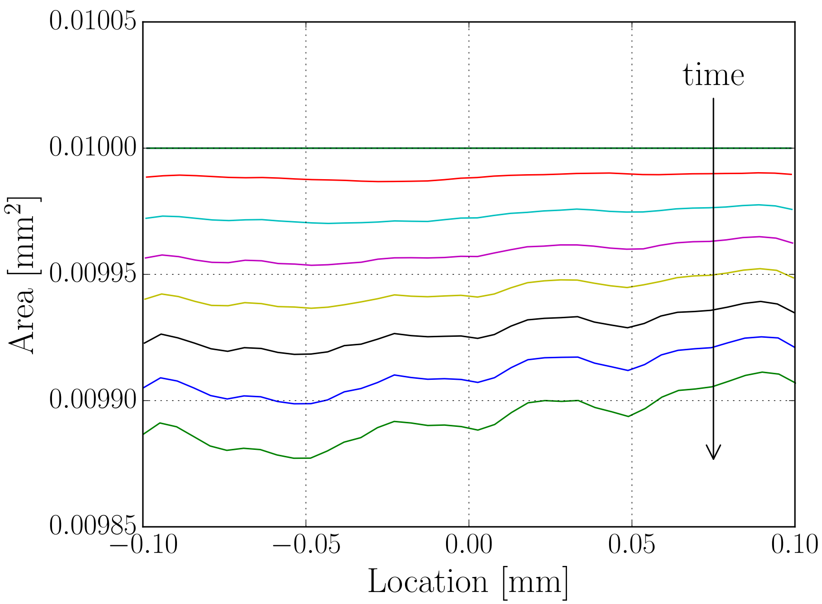


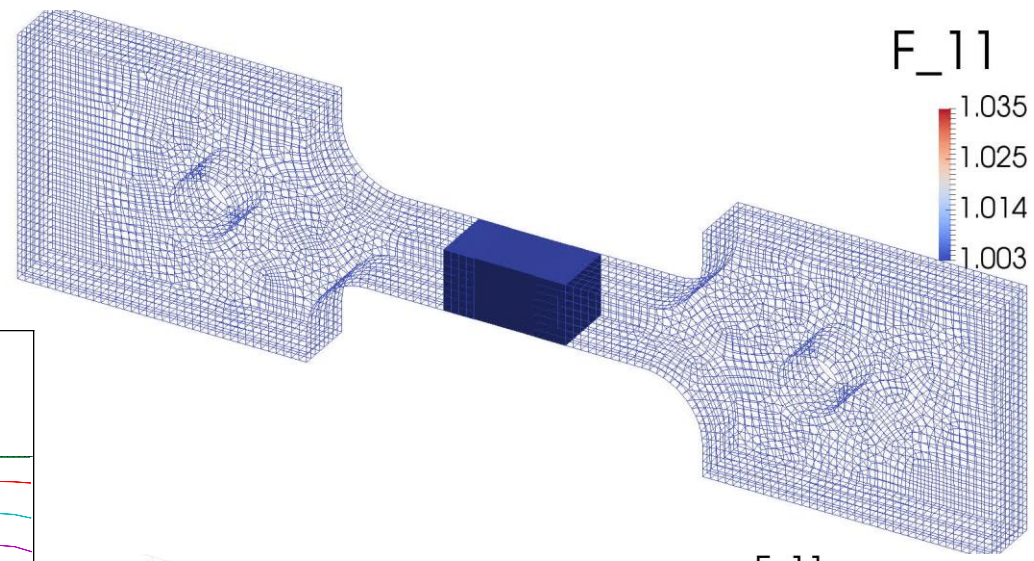
$$\text{Young's modulus} : E = 195.0 \text{ GPa}$$
$$\text{Poission's ratio} : \nu = 0.3$$
$$\text{yield stress} : \sigma_0 = 144 \text{ MPa}$$
$$\text{hardening modulus} : H = 300 \text{ MPa}$$
$$\text{saturation modulus} : S = 170 \text{ MPa}$$
$$\text{saturation exponent} : \alpha = 190$$

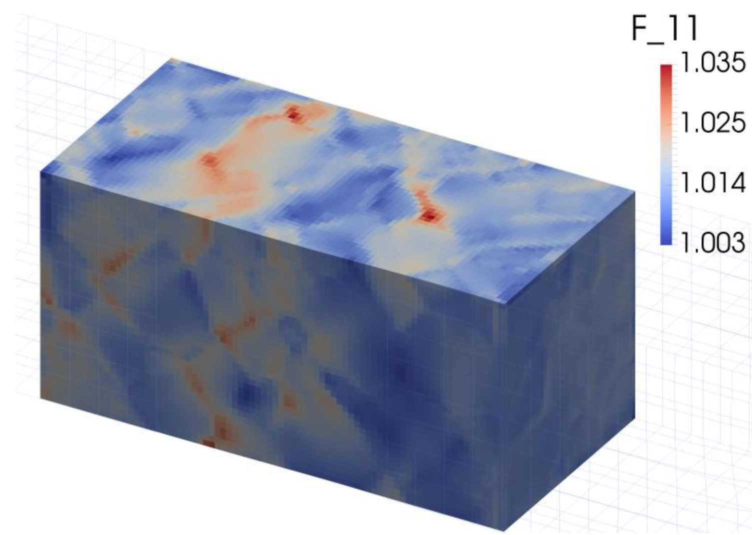
$$\sigma_y = \sigma_0 + H\epsilon_p + S(1 - e^{-\alpha\epsilon_p})$$

Appendix. Tensile Bar: Results

Reduction in cross-sectional area over time

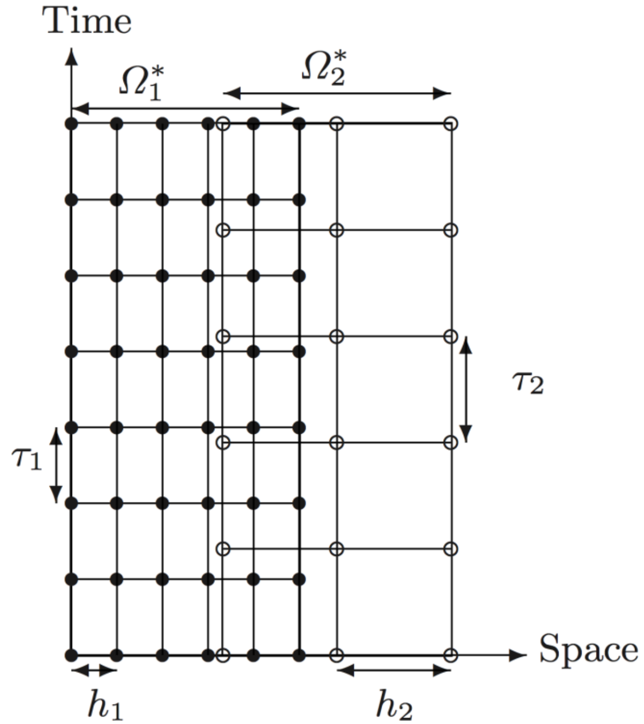






Appendix. Schwarz Alternating Method for Dynamics

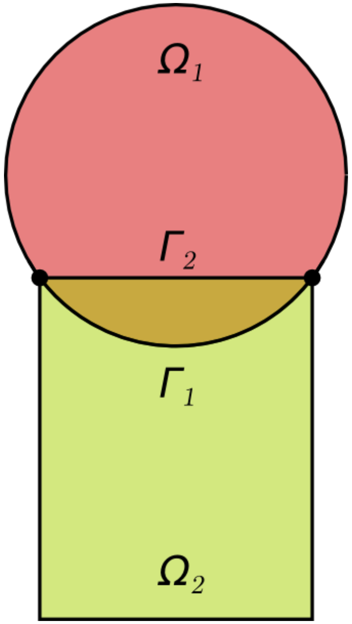
- In the literature the Schwarz method is applied to dynamics by using ***space-time discretizations***.
- This was deemed ***unfeasible*** given the design of our current codes and size of simulations.

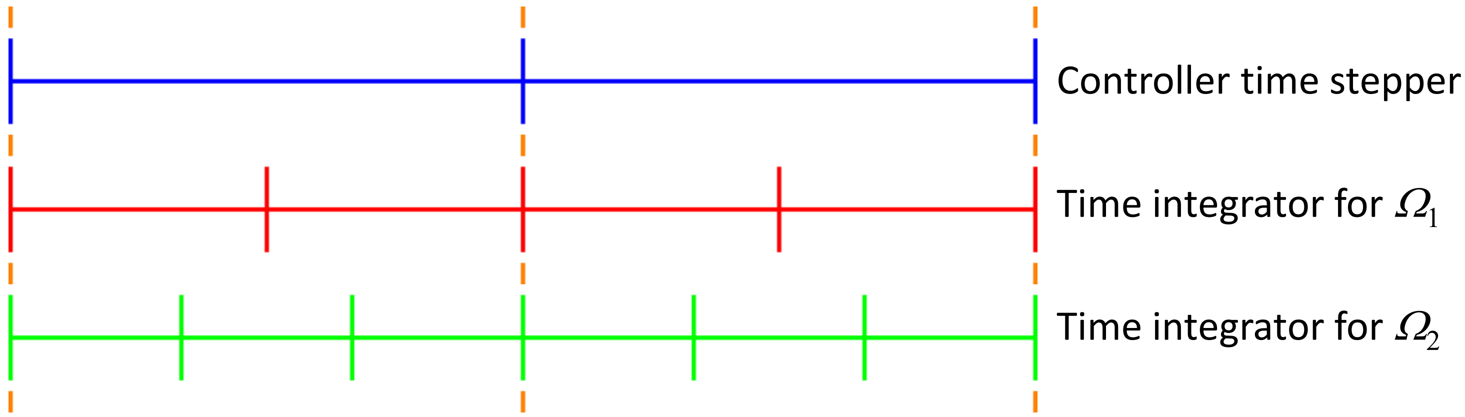


Overlapping non-matching meshes and time steps in dynamics.

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).