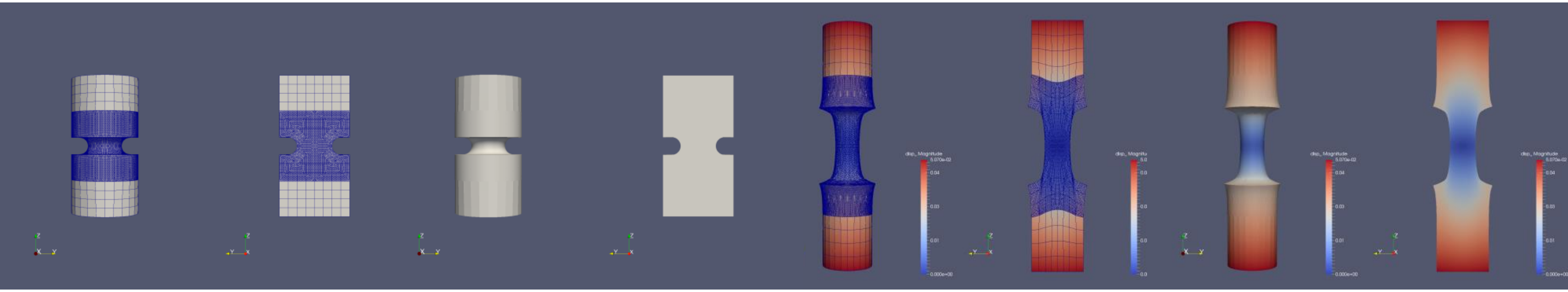

The Schwarz Alternating Method for Multiscale Coupling in Solid Mechanics

Alejandro Mota[1], Irina Tezaur[1], Coleman Alleman[1], Greg Phlipot[2]

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Outline

1. Motivation
2. Schwarz Alternating Method for Concurrent Multiscale Coupling for Quasistatics
   - Formulation
   - Implementation
   - Numerical Examples
3. Schwarz Alternating Method for Concurrent Multiscale Coupling for Dynamics
   - Formulation
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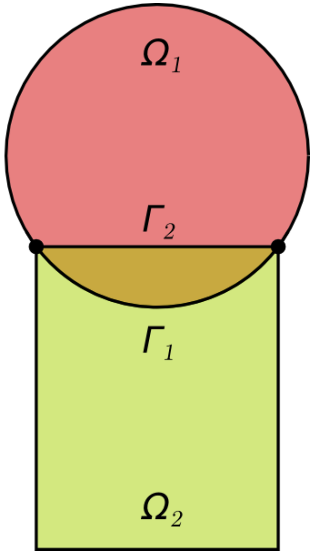
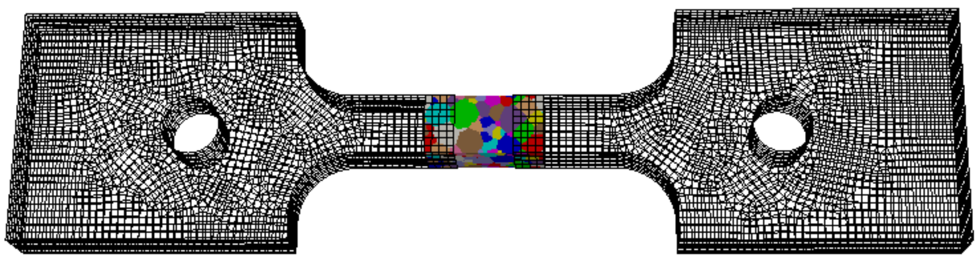
   - Numerical Examples
4. Summary
5. Future Work





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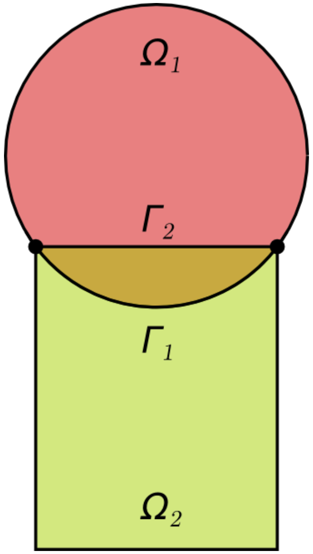
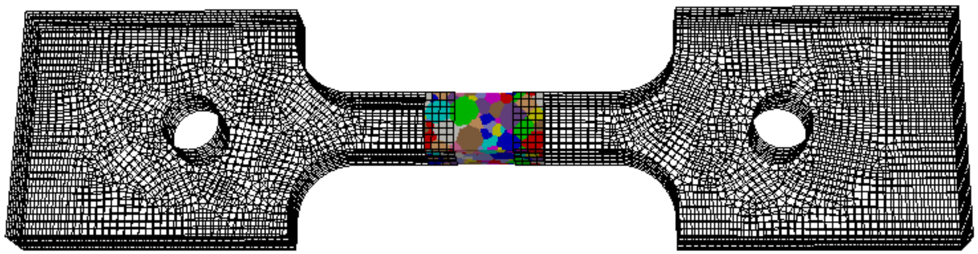




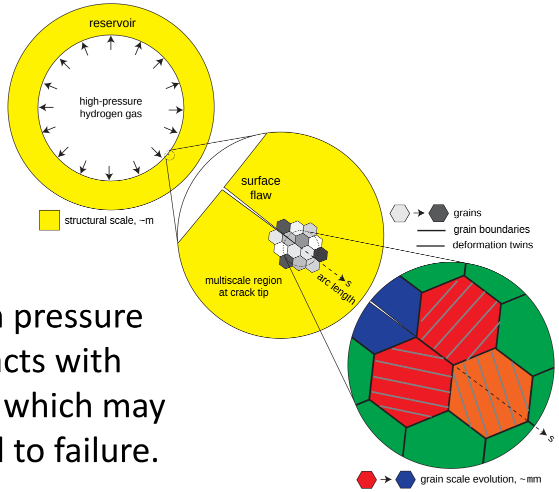
Motivation for Concurrent Multiscale Coupling

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).

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

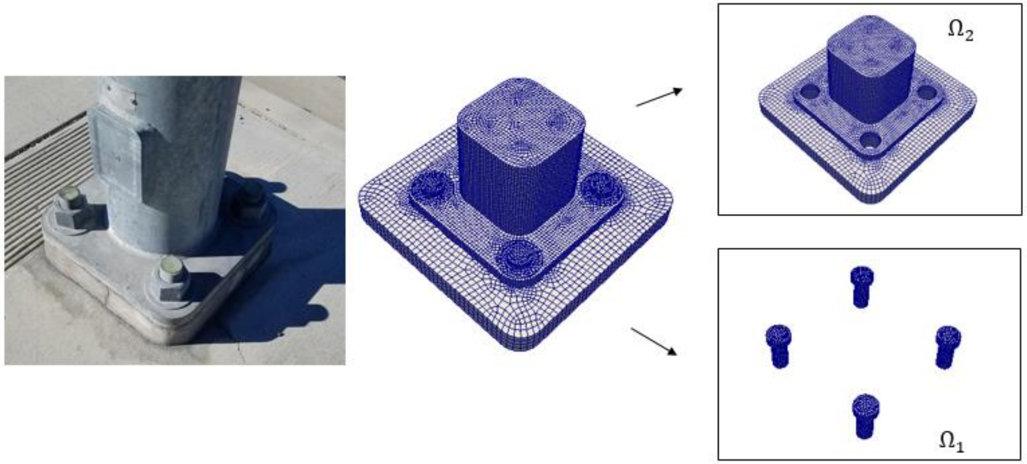
Concurrent multiscale methods are ***essential*** for understanding and prediction of behavior of engineering systems when a ***small scale failure*** determines the performance of the entire system.



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

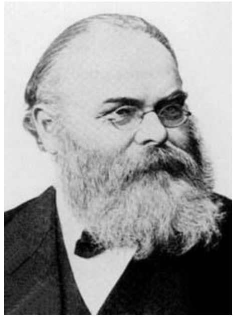
Requirements for Multiscale Coupling Method

- Coupling is ***concurrent*** (two-way).
- ***Ease of implementation*** into existing massively-parallel HPC codes.
- ***Scalable, fast, robust*** (we target ***real*** engineering problems, e.g., analyses involving failure of bolted components!).
- ***"Plug-and-play" framework***: simplifies task of meshing complex geometries!
  - Ability to couple regions with ***different non-conformal meshes***, ***different element types*** and ***different levels of refinement.***
  - Ability to use ***different solvers/time-integrators*** in different regions.
- Coupling does not introduce ***nonphysical artifacts.***
- ***Theoretical*** convergence properties/guarantees.



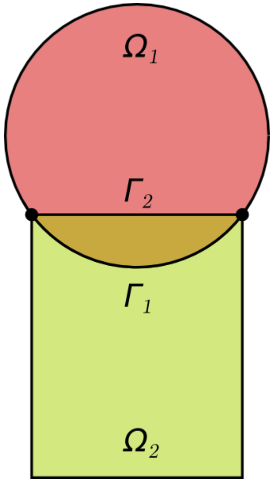
Schwarz Alternating Method for Domain Decomposition

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



H. Schwarz (1843 – 1921)

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



Basic Schwarz Algorithm

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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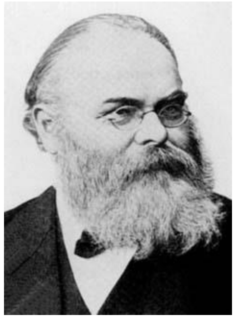

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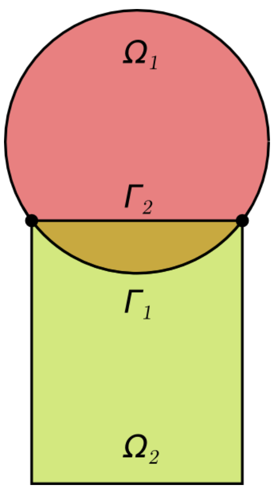

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<u>Requirement for convergence</u>: $\Omega_1 \cap \Omega_2 \neq \emptyset$

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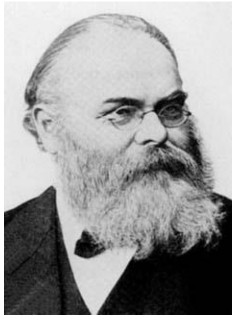

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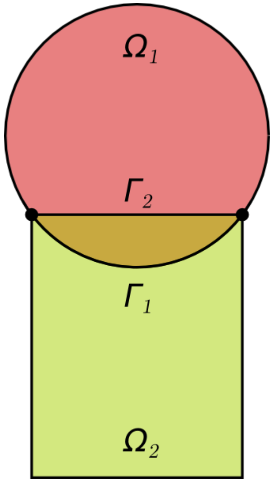

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- Schwarz alternating method most commonly used as a ***preconditioner*** for Krylov iterative methods to solve linear algebraic equations.

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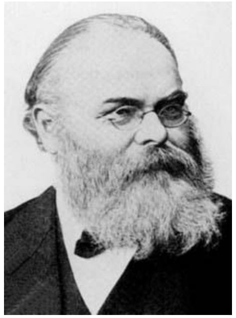

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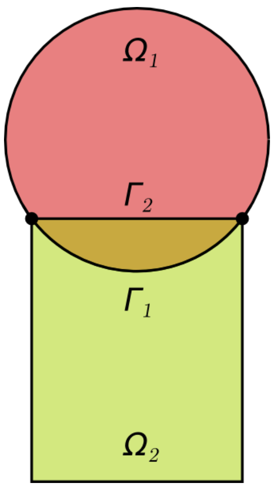

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- Schwarz alternating method most commonly used as a ***preconditioner*** for Krylov iterative methods to solve linear algebraic equations.

Novel idea: using the Schwarz alternating as a ***discretization method*** for solving multiscale partial differential equations (PDEs).

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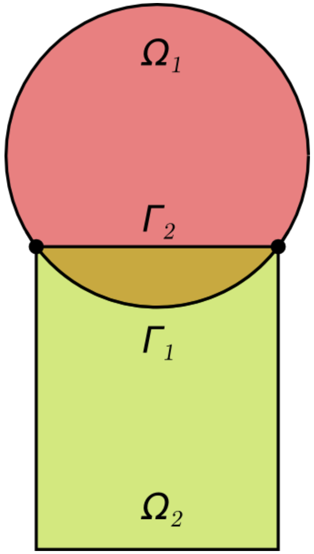
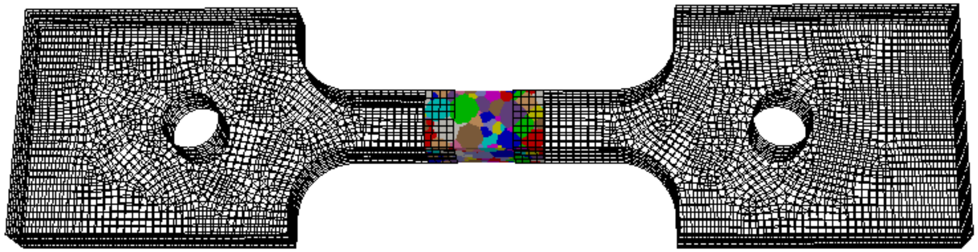




Schwarz Alternating Method for Multiscale Coupling in Quasistatics

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

$n \leftarrow 1$

repeat $\triangleright$ Schwarz loop

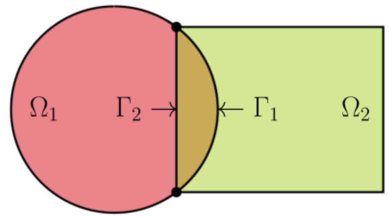
$\quad \boldsymbol{\varphi}^{(n)} \leftarrow \boldsymbol{\chi}$ on $\partial_{\boldsymbol{\varphi}}\Omega_i$ $\triangleright$ Dirichlet BC for Ω_i

$\quad \boldsymbol{\varphi}^{(n)} \leftarrow P_{\Omega_j \rightarrow \Gamma_i}[\boldsymbol{\varphi}^{(n-1)}]$ on Γ_i $\triangleright$ Schwarz BC for Ω_i

$\quad \boldsymbol{\varphi}^{(n)} \leftarrow \arg\min_{\boldsymbol{\varphi} \in \mathcal{S}_i} \Phi_i[\boldsymbol{\varphi}]$ in Ω_i $\triangleright$ solve in Ω_i

$\quad n \leftarrow n + 1$

until converged



Advantages:

- Conceptually very ***simple***.
- Allows the coupling of regions with ***different non-conforming meshes***, ***different element types***, and ***different levels of refinement***.
- Information is exchanged among two or more regions, making coupling ***concurrent***.
- ***Different solvers*** can be used for the different regions.
- ***Different material models*** can be coupled if they are compatible in the overlap region.
- Simplifies the task of ***meshing complex geometries*** for the different scales.

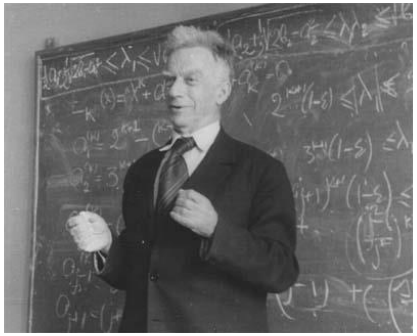
Theoretical Foundation

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

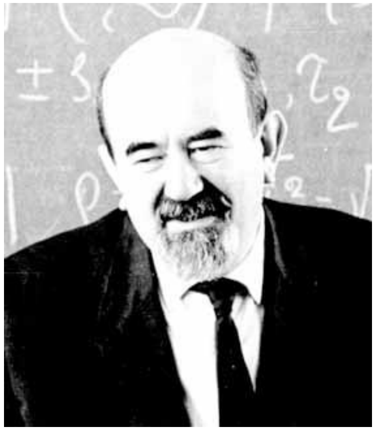
- S. L. Sobolev (1936): posed Schwarz method for ***linear elasticity*** in variational form and ***proved method's convergence*** by proposing a convergent sequence of energy functionals.
- S. G. Mikhlin (1951): ***proved convergence*** of Schwarz method for general linear elliptic PDEs.
- A. Mota, 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.

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

$$\nabla \cdot \boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



S. L. Sobolev (1908 – 1989)



S. G. Mikhlin (1908 – 1990)

A. Mota, I. Tezaur, C. Alleman

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

Four Variants* of 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 $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \leq \epsilon_{\text{machine}}$ ▷ 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

Four Variants* of Schwarz

Most performant method: monotonic convergence, theoretical convergence guarantee.

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

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1. Motivation
2. **Schwarz Alternating Method for Concurrent Multiscale Coupling for Quasistatics**
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   - **Implementation**
   - Numerical Examples
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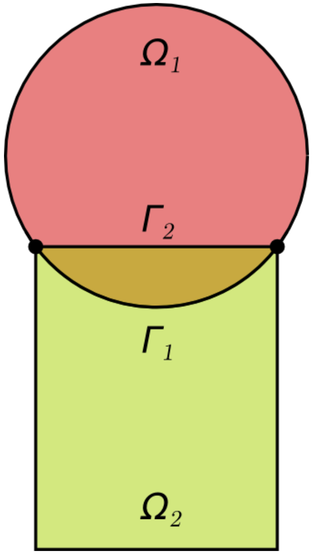
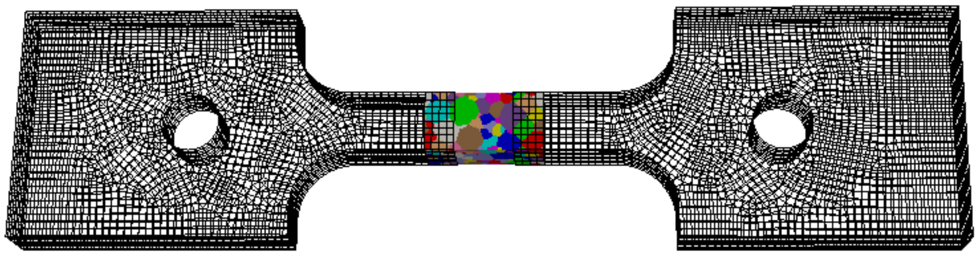




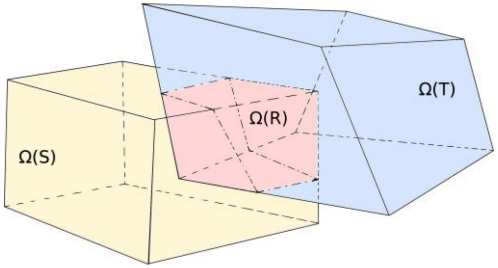
Implementation within *Albany* Code

The proposed ***quasistatic alternating Schwarz method*** is implemented within the ***LCM project*** in Sandia's open-source parallel, C++, multi-physics, finite element code, ***Albany***.

- ***Component-based*** design for rapid development of capabilities.
- Contains a wide variety of ***constitutive models***.
- 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/gahansen/Albany

https://github.com/trilinos/trilinos



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

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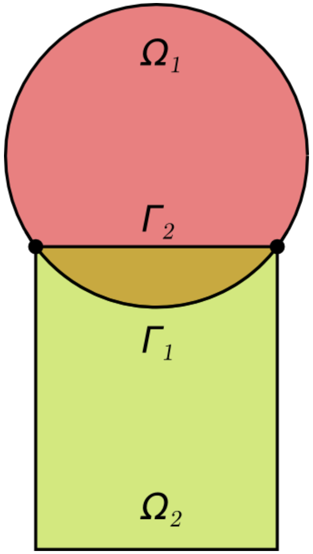
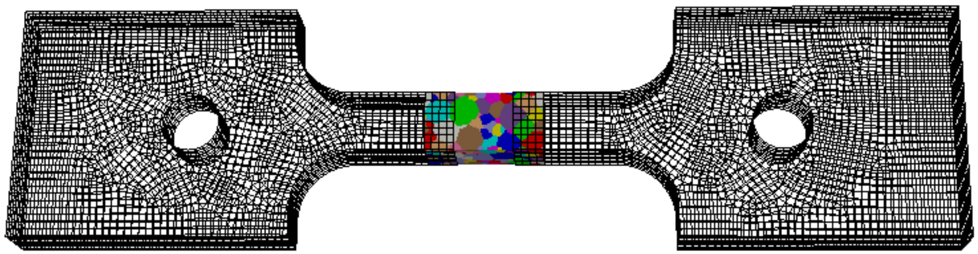
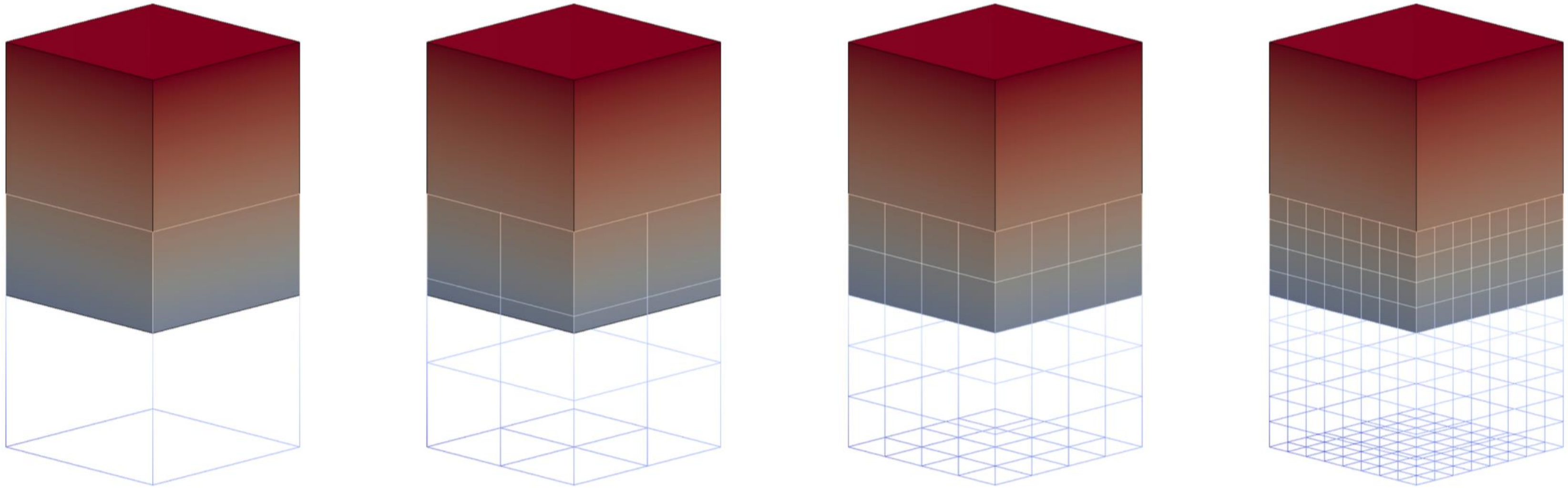
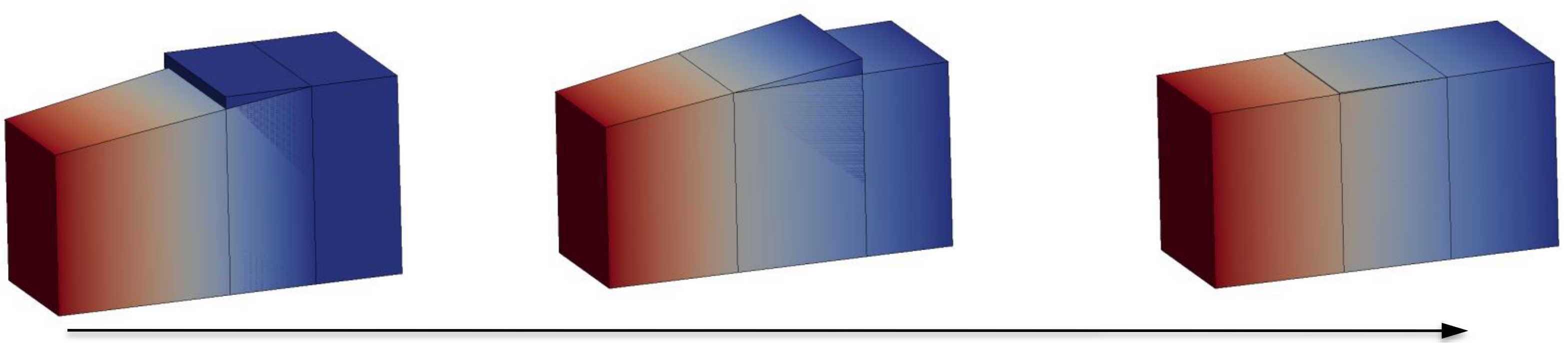




Quasistatic Example #1: Cuboid Problem



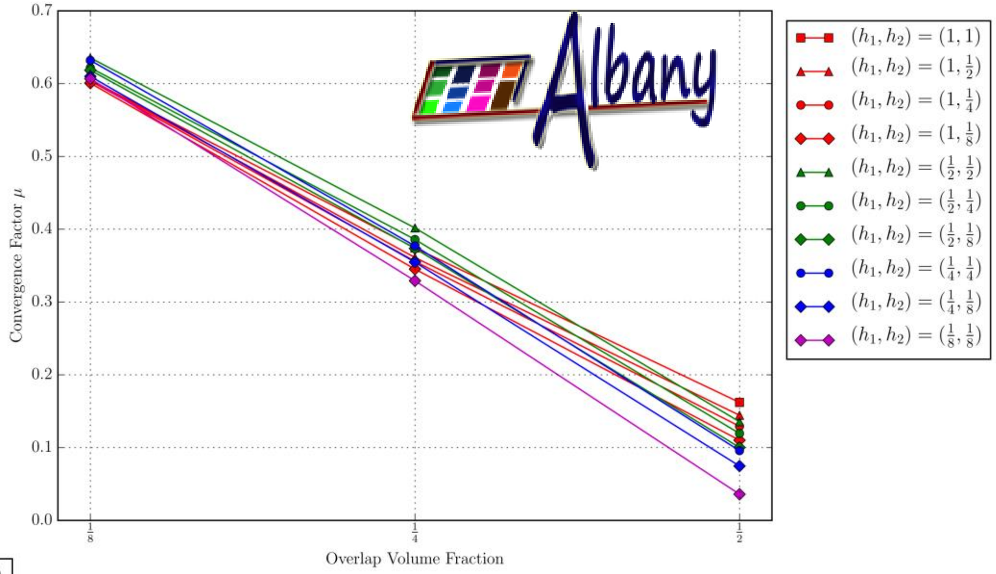
- Coupling of ***two cuboids*** with square base (above).
- ***Neohookean***-type material model.

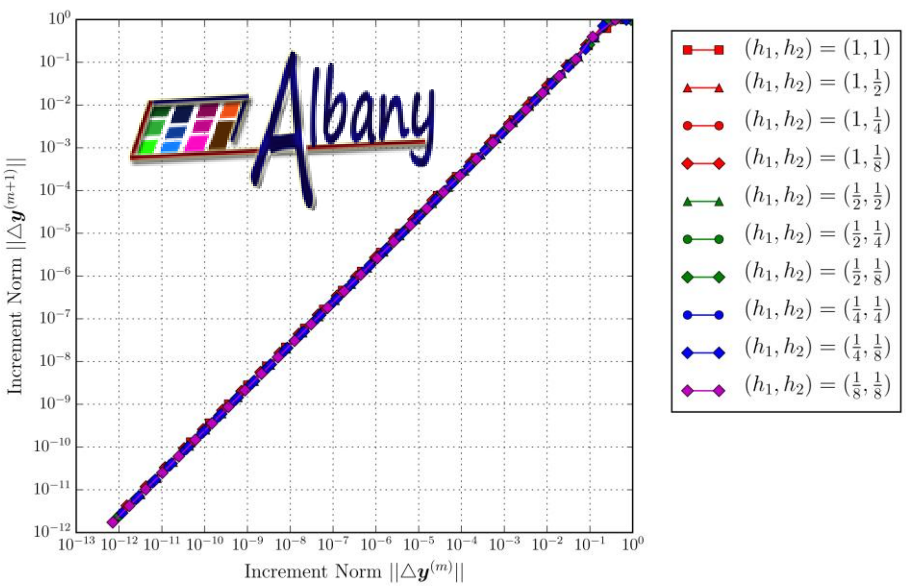


Schwarz Iteration

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***.

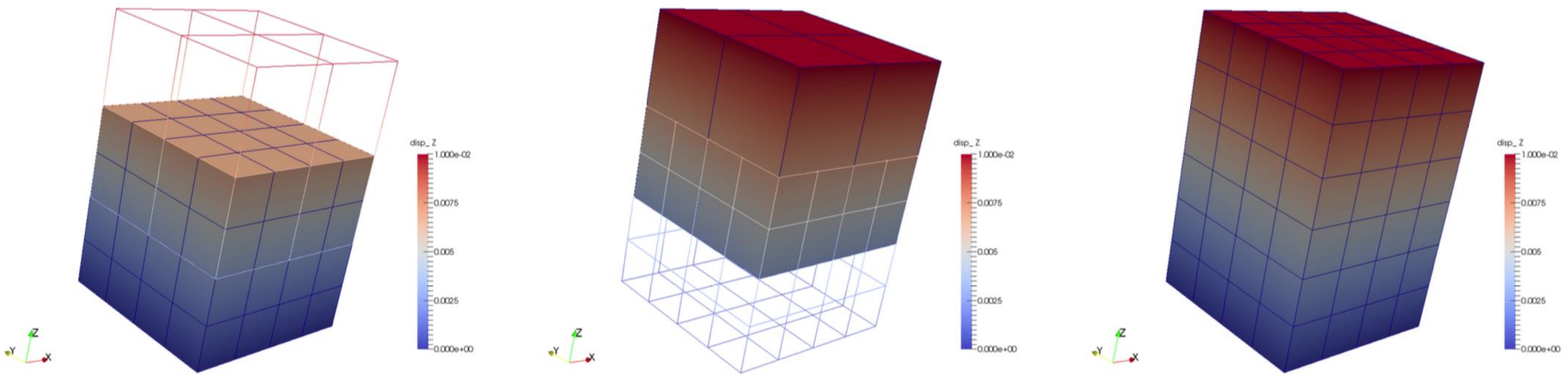




Above: Convergence factor μ as a function of overlap volume and different mesh. There is ***faster linear convergence*** with increasing ***overlap volume fraction***.

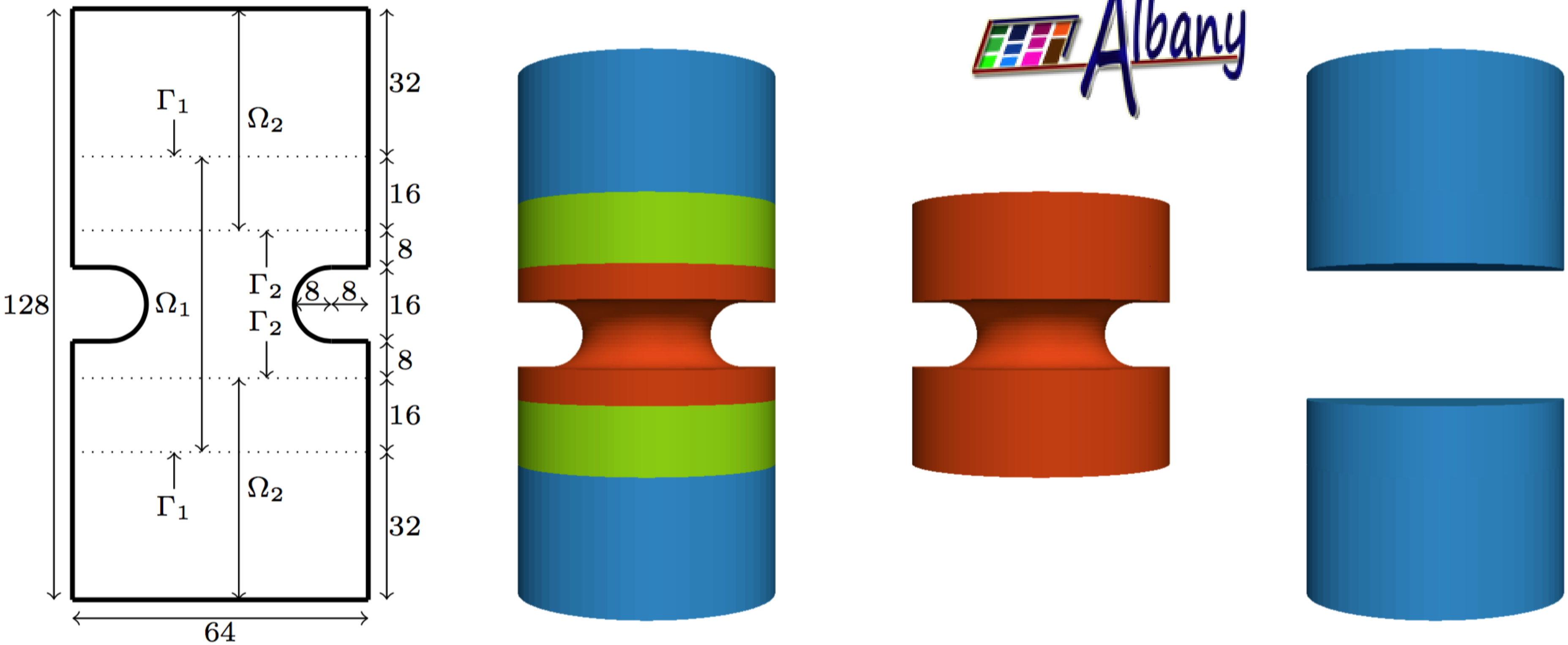
$$\Delta y^{(m+1)} \leq \mu \Delta y^{(m)}$$

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}

Quasistatic Example #2: Notched Cylinder

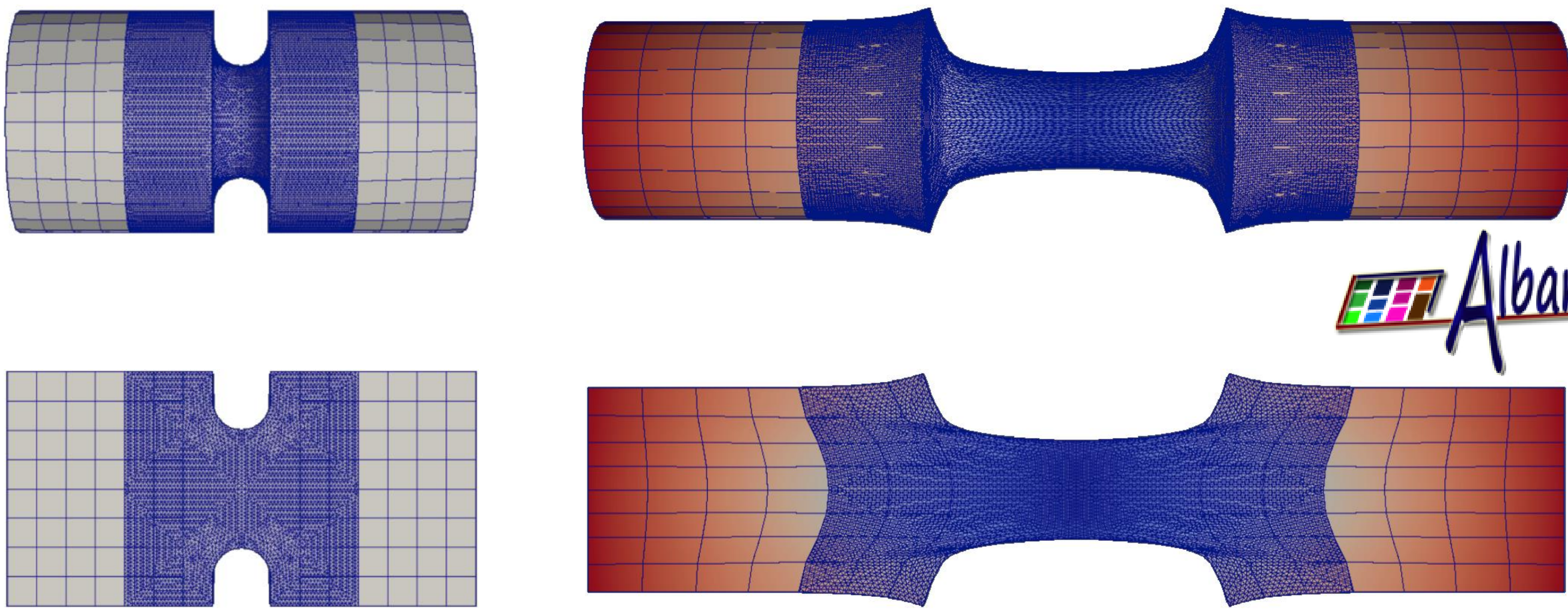


(a) Schematic **(b)** Entire Domain Ω **(c)** Fine Region Ω_1 **(d)** Coarse Region Ω_2

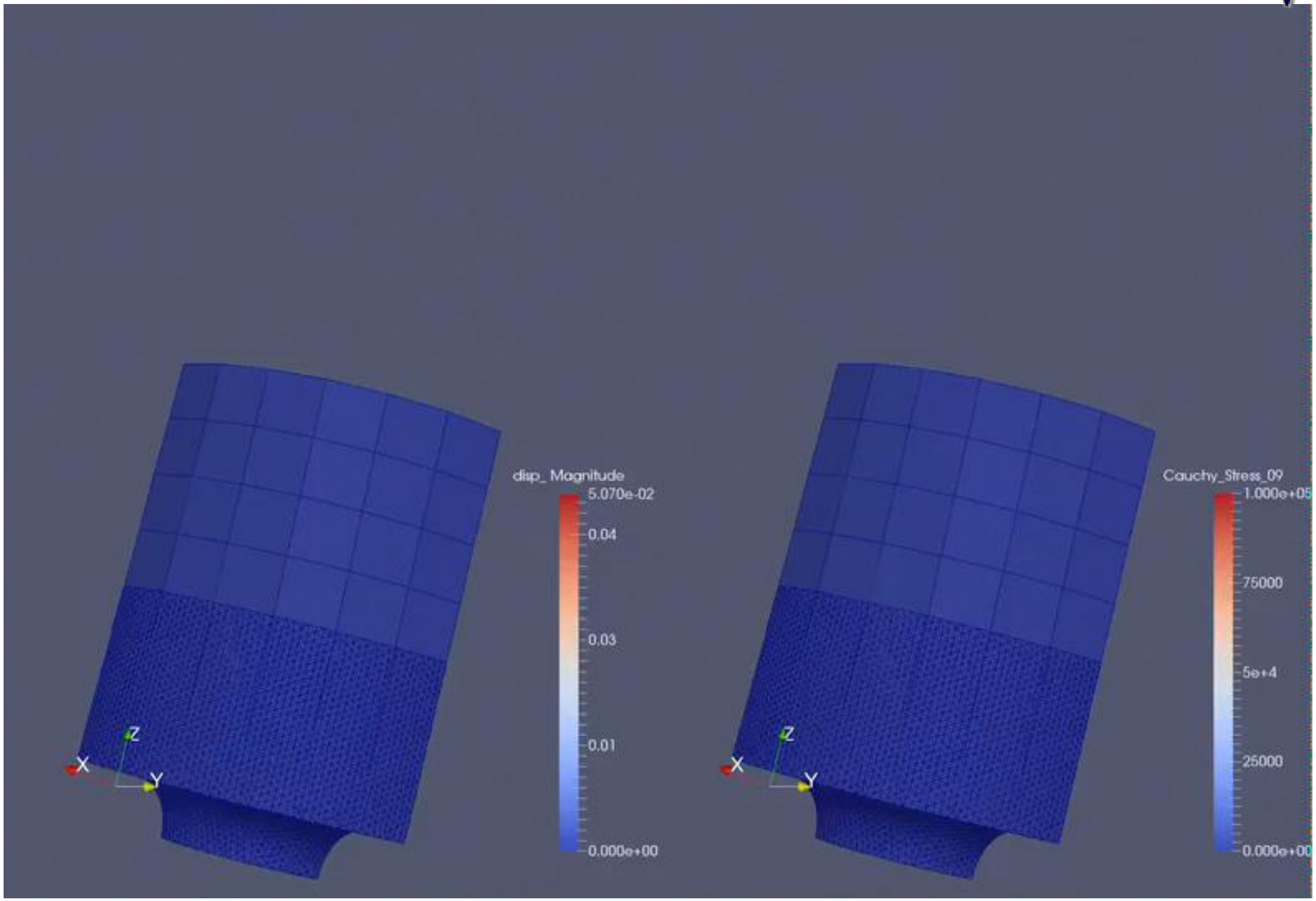
- ***Notched cylinder*** that is stretched along its axial direction.
- Domain decomposed into ***two subdomains***.
- ***Neohookean***-type material model.

Notched Cylinder: TET-HEX Coupling

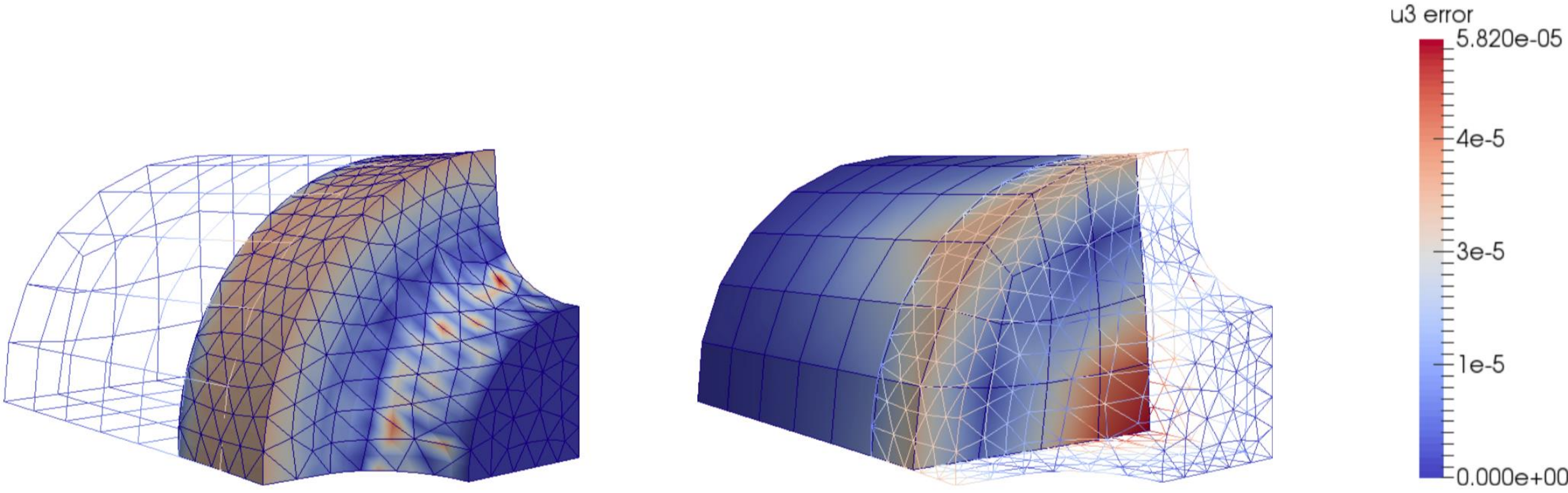
- The Schwarz alternating method is capable of coupling ***different mesh topologies***.
- The notched region, where stress concentrations are expected, is ***finely*** meshed with ***tetrahedral*** elements.
- The top and bottom regions, presumably of less interest, are meshed with ***coarser hexahedral***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



Notched Cylinder: TET-HEX Coupling



Notched Cylinder: Conformal TET-HEX Coupling



(a) Ω_1 **(b)** Ω_2

	u_3 relative error	
Absolute residual tolerance	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.

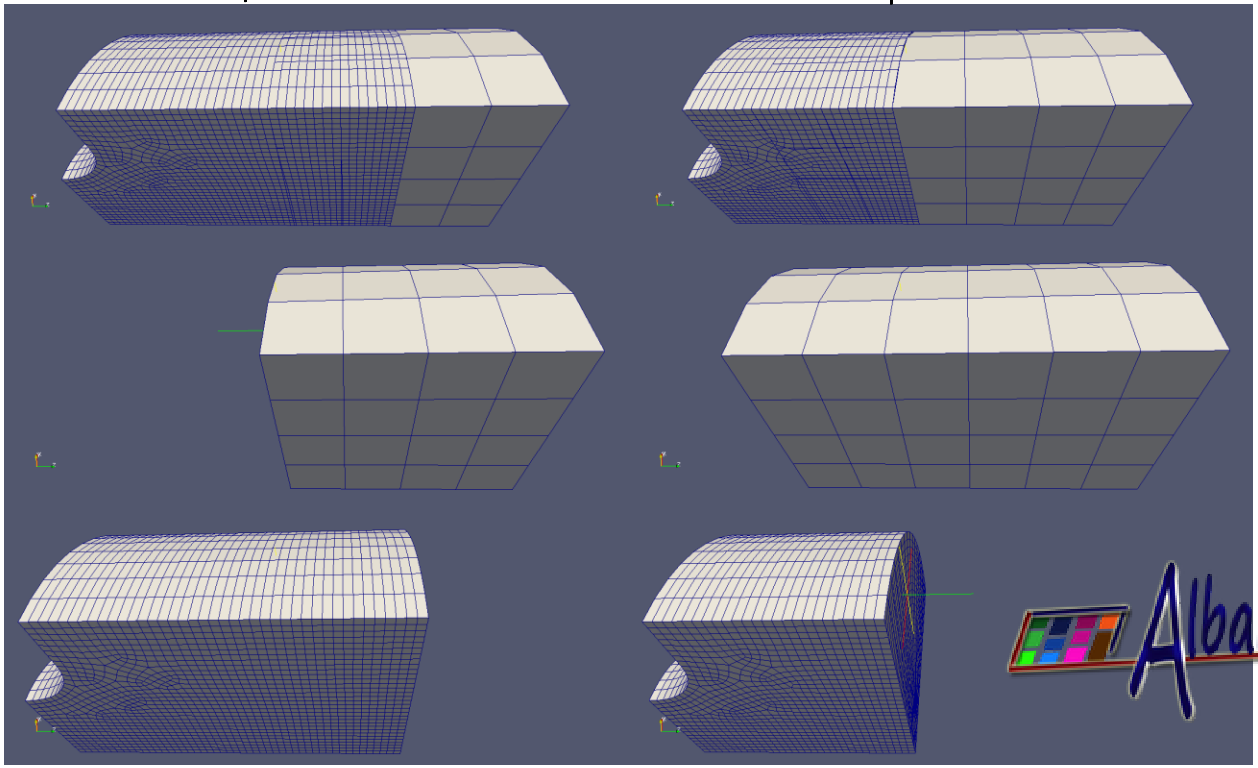
Overlap far from notch.

Overlap near notch.

Coupled regions

Coarse, elastic region

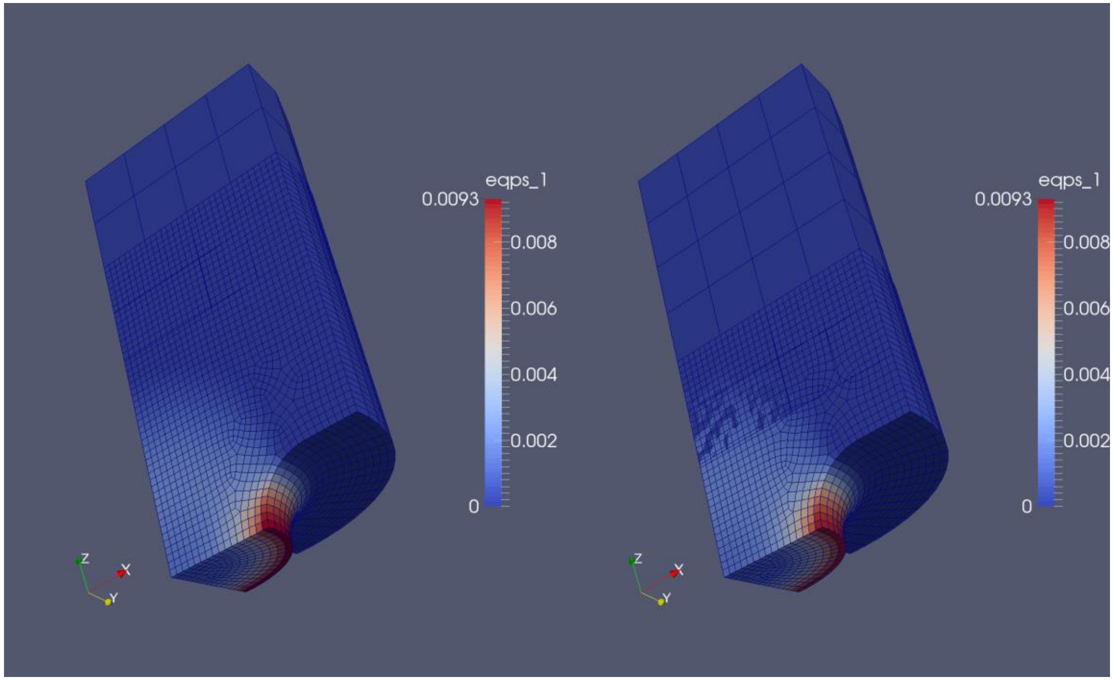
Fine, elasto-plastic region



Notched Cylinder: Coupling Different Materials

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

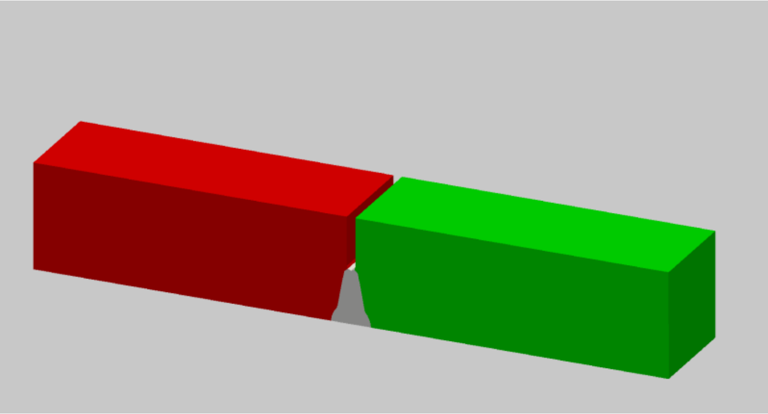
- When the ***overlap*** region is ***far from the notch***, no plastic deformation exists in it: the coarse and fine regions predict the ***same behavior***.
- When the ***overlap*** region is ***near the notch***, plastic deformation spills onto it and the two models predict different behavior, affecting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



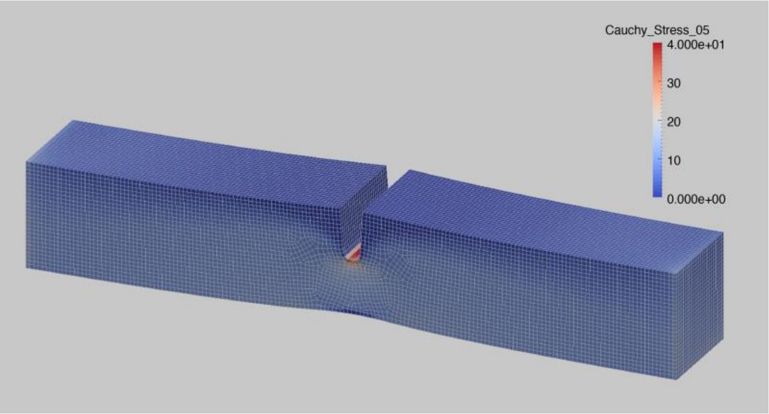
Overlap far from notch. Overlap near notch.

Quasistatic Example #3: Laser Weld

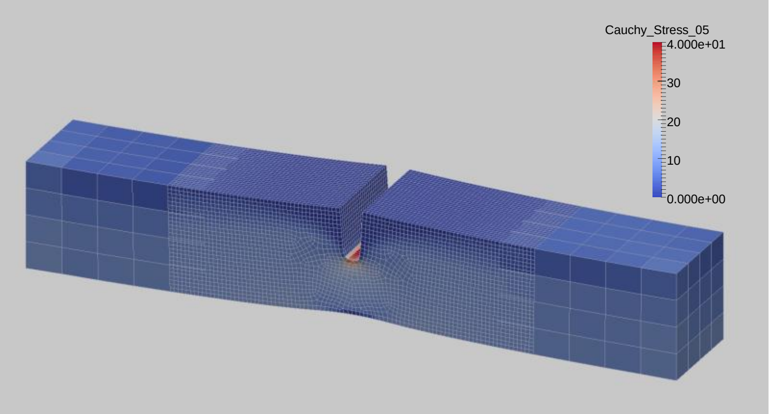
Laser weld specimen



Single domain discretization

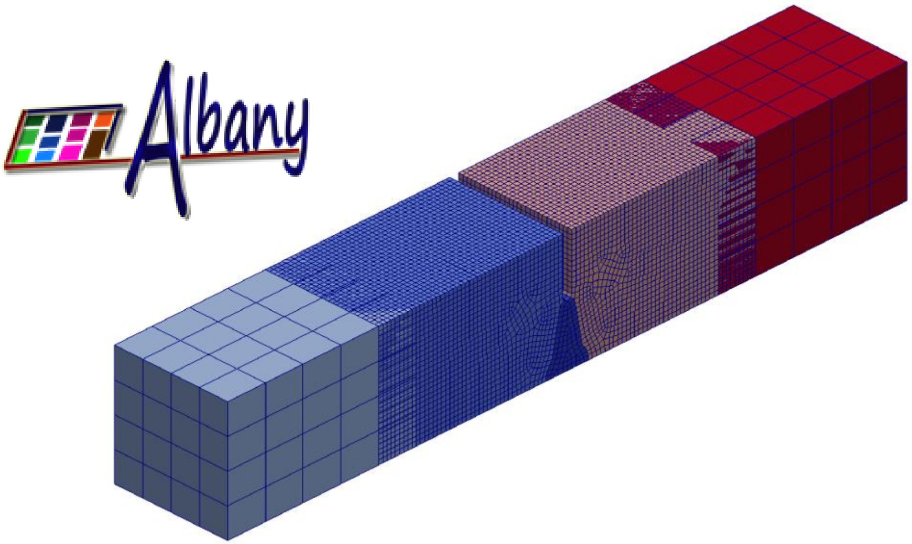


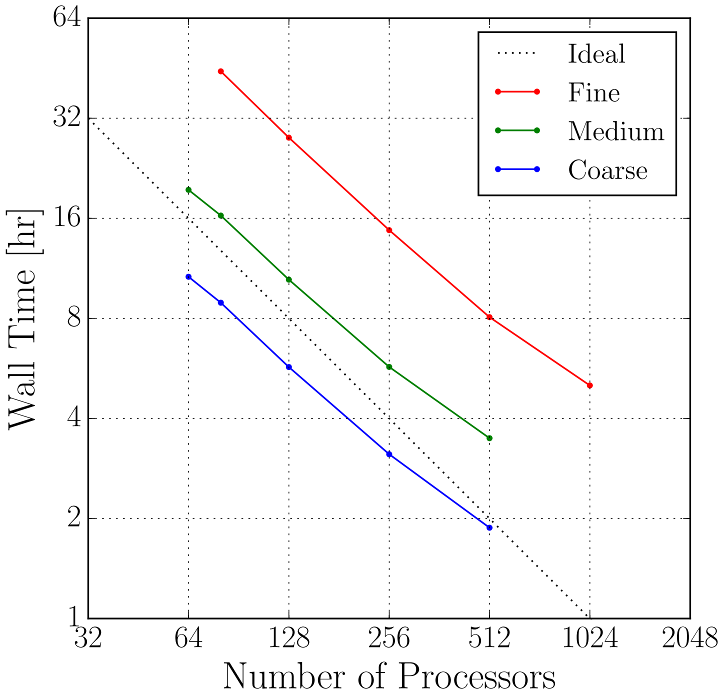
Coupled Schwarz discretization
(50% reduction in model size)



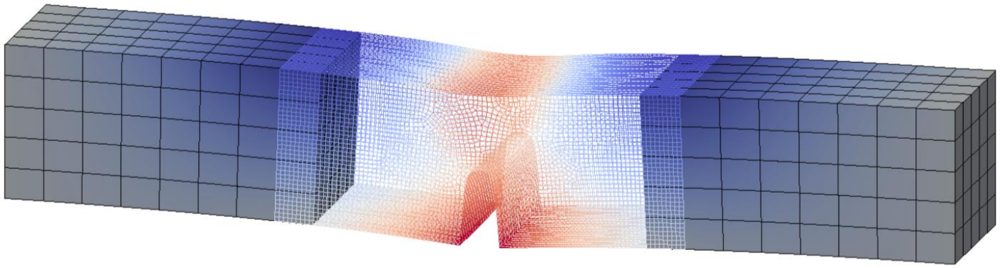
- Problem of ***practical scale (~200K dofs).***
- ***Isotropic elasticity*** and ***J2 plasticity*** with linear isotropic hardening.
- ***Identical parameters*** for weld and base materials for proof of concept, to become independent models.

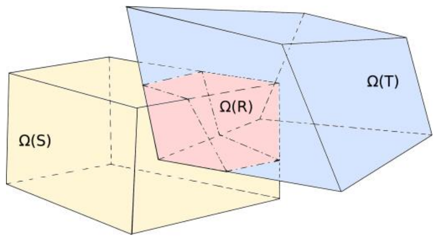
Laser Weld: Strong Scalability of Parallel Schwarz with DTK





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





Data Transfer Kit (DTK)

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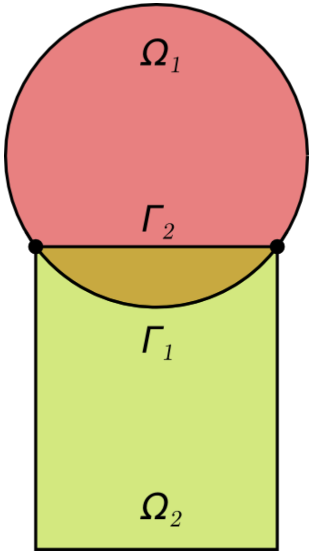
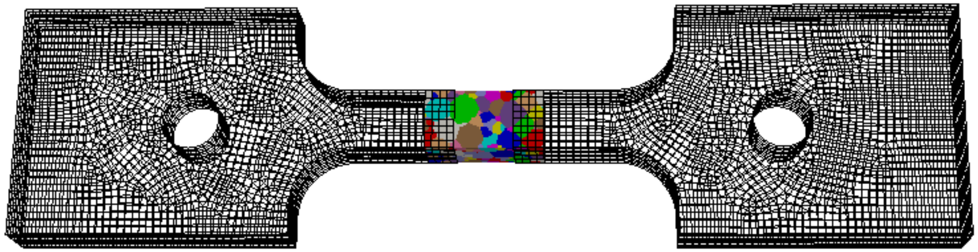
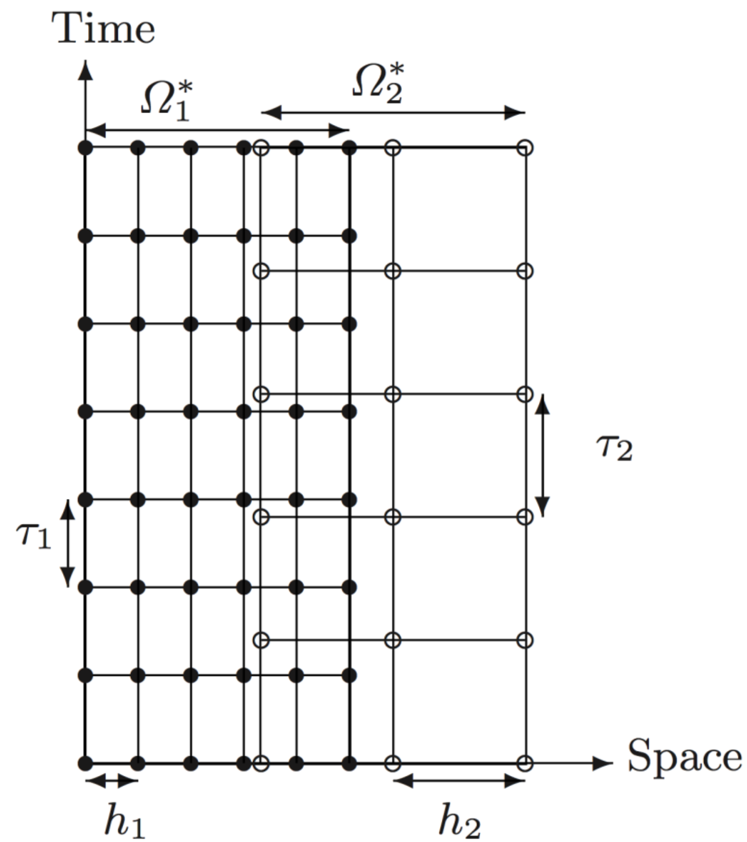




Schwarz Alternating Method for Dynamics

- In the literature the Schwarz method is applied to dynamics by using ***space-time discretizations***.



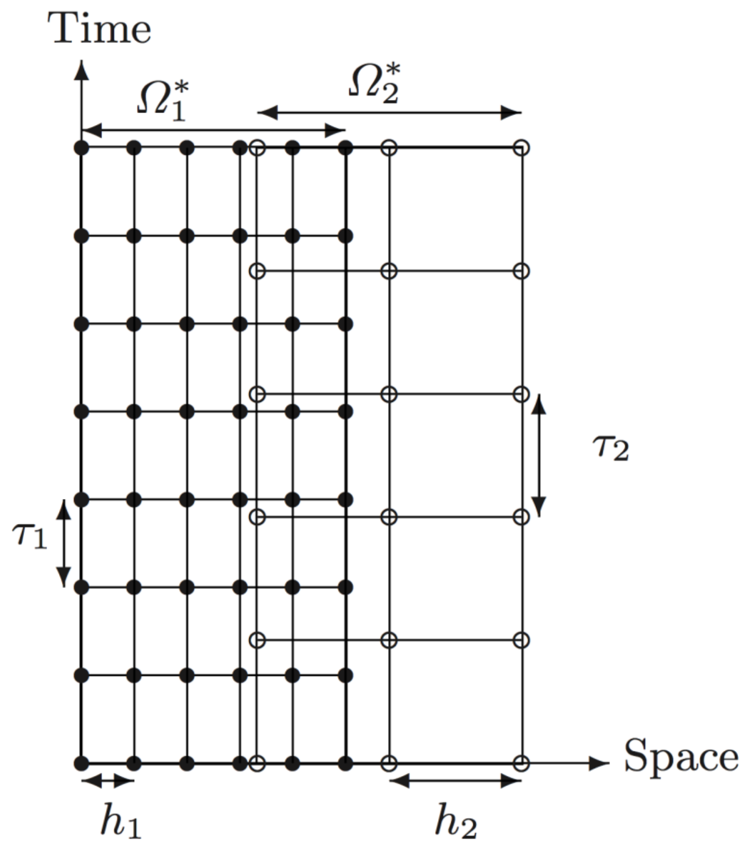
Overlapping non-matching meshes and time steps in dynamics.

Schwarz Alternating Method for Dynamics

- In the literature the Schwarz method is applied to dynamics by using ***space-time discretizations***.

Pro ☺: Can use ***non-matching*** meshes and time-steps (see right figure).

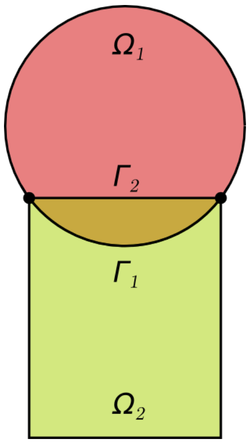
Con ☹: ***Unfeasible*** given the design of our current codes and size of simulations.

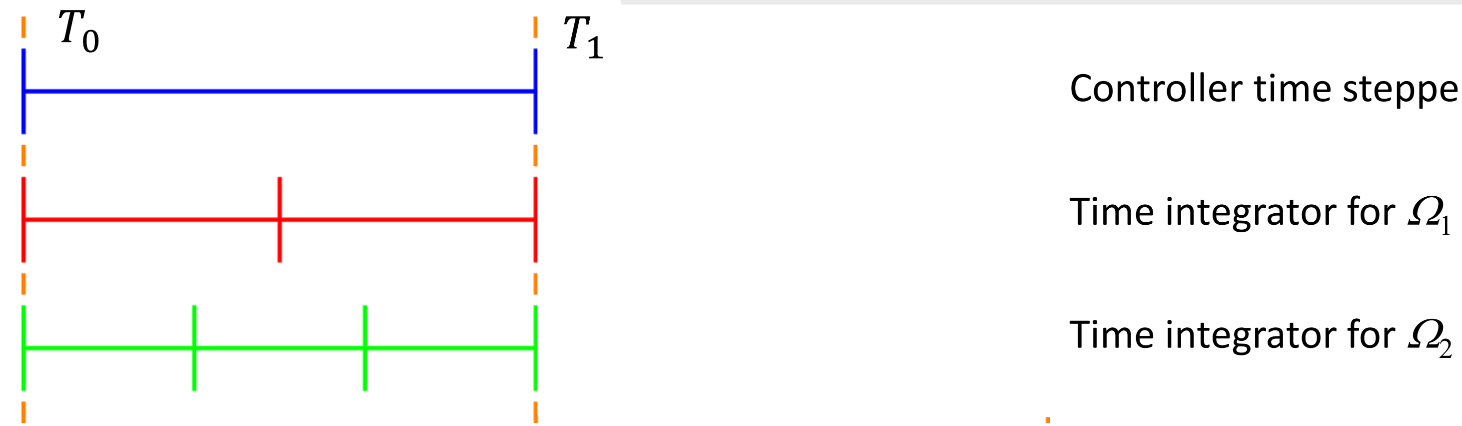


Overlapping non-matching meshes and time steps in dynamics.

Schwarz Alternating Method for Dynamic Multiscale Coupling

Controller time stepper = convenient checkpoint to facilitate implementation

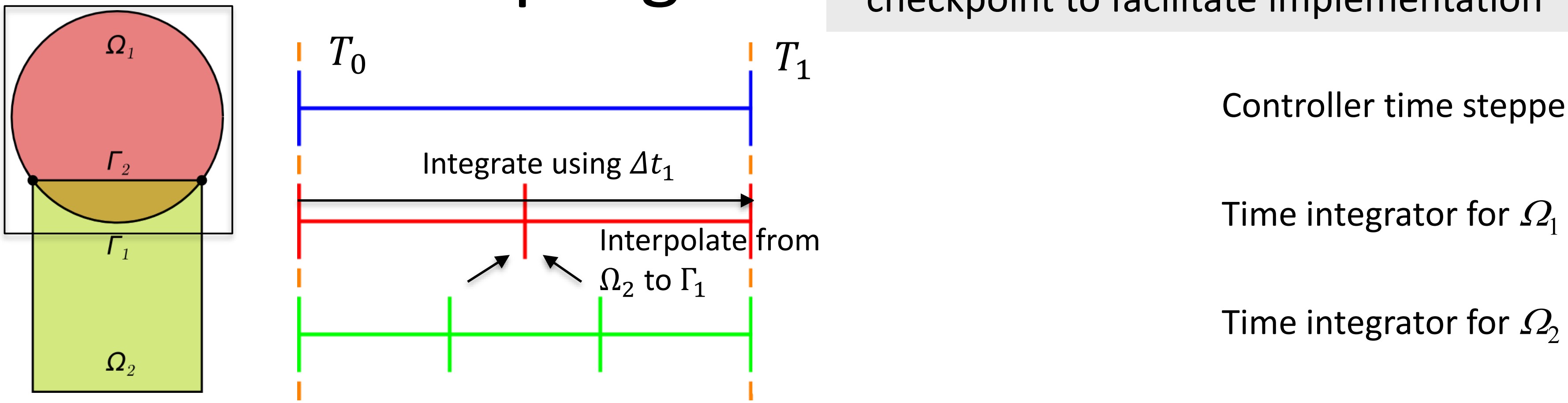




<u>Step 0</u>: Initialize $i = 0$ (controller time index).

Schwarz Alternating Method for Dynamic Multiscale Coupling

Controller time stepper = convenient checkpoint to facilitate implementation

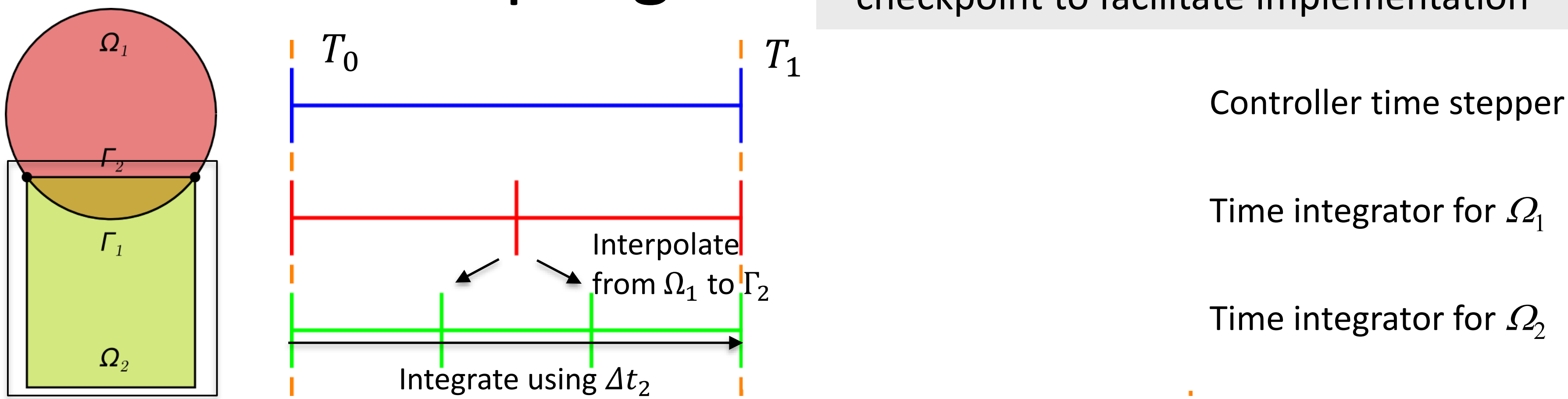


Step 0: Initialize $i = 0$ (controller time index).

Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ_1 at times $T_i + n\Delta t_1$.

Schwarz Alternating Method for Dynamic Multiscale Coupling

Controller time stepper = convenient checkpoint to facilitate implementation



Step 0: Initialize $i = 0$ (controller time index).

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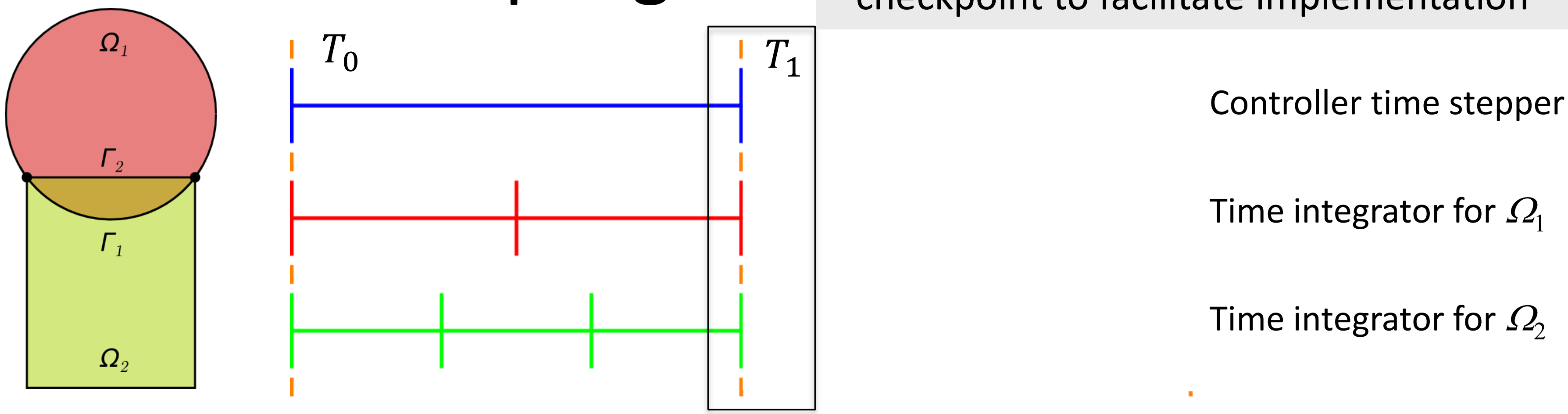
Step 2: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ_2 at times $T_i + n\Delta t_2$.

Schwarz Alternating Method for Dynamic Multiscale Coupling

Controller time stepper = convenient checkpoint to facilitate implementation



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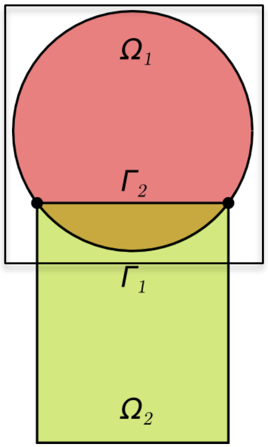
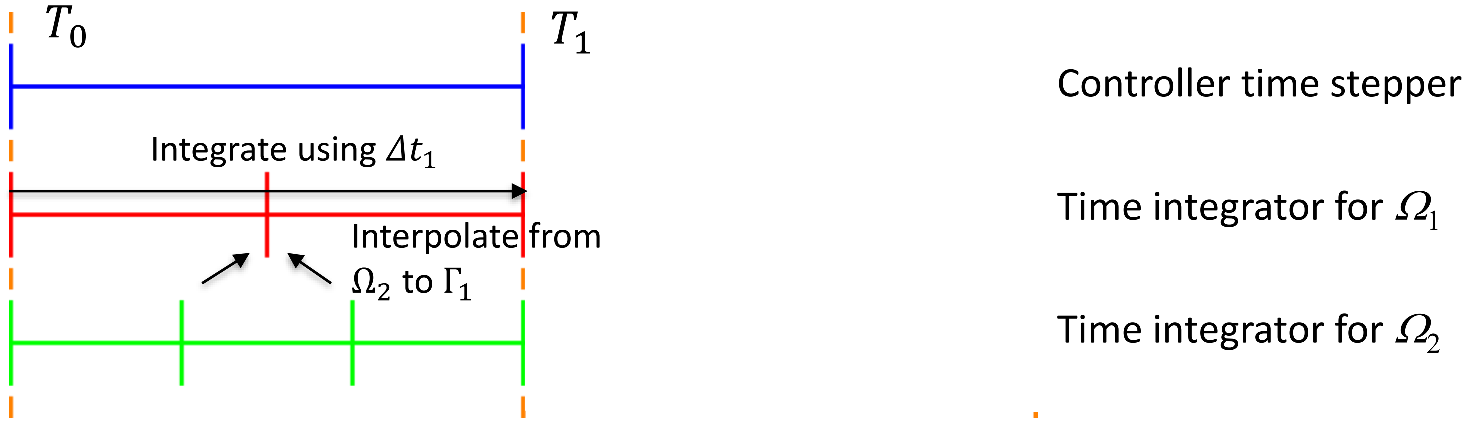
Step 2: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ_2 at times $T_i + n\Delta t_2$.

Step 3: Check for convergence at time T_{i+1}.

Schwarz Alternating Method for Dynamic Multiscale Coupling

Controller time stepper = convenient checkpoint to facilitate implementation





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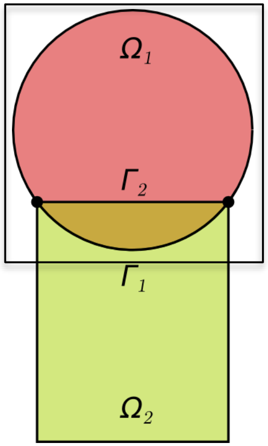
Step 2: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ_2 at times $T_i + n\Delta t_2$.

Step 3: Check for convergence at time T_{i+1}.

- If unconverged, return to Step 1.

Schwarz Alternating Method for Dynamic Multiscale Coupling



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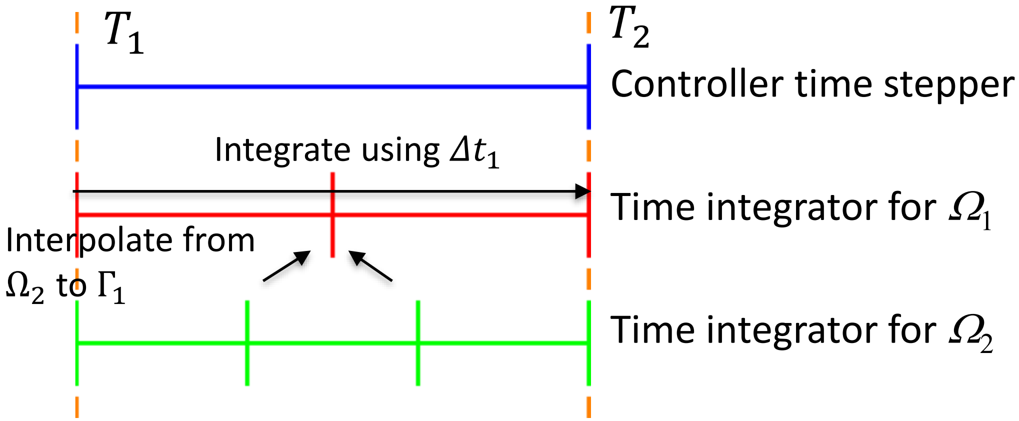

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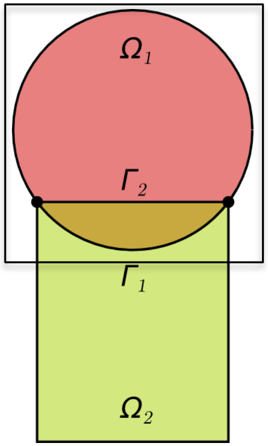
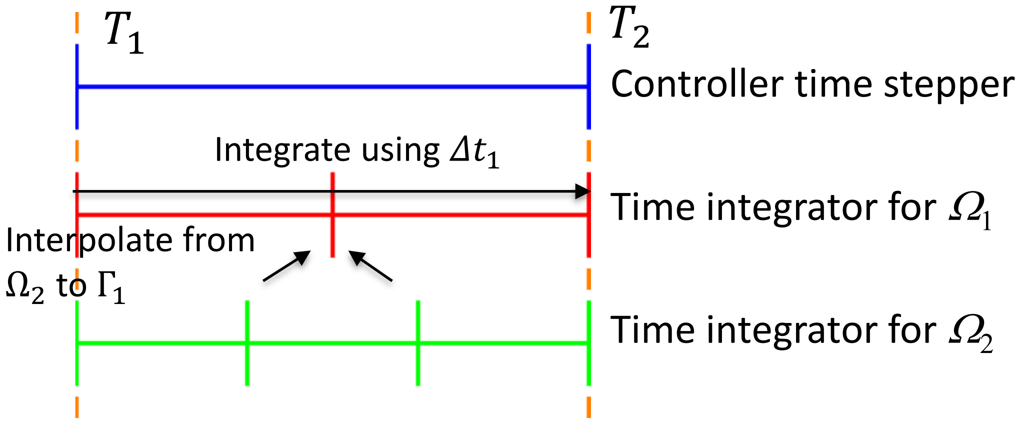
Schwarz Alternating Method for Dynamic Multiscale Coupling

Controller time stepper = convenient checkpoint to facilitate implementation





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- If unconverged, return to Step 1.
- If converged, set $i = i + 1$ and return to Step 1.

Can use ***different integrators*** with ***different time steps*** within each domain!

Schwarz Alternating Method for Dynamic Multiscale Coupling: Theory

- For quasistatics, we derived a ***proof of convergence*** of the alternating Schwarz method for the ***finite deformation*** problem, and determined a ***geometric convergence rate*** [(Mota, Tezaur, Alleman, *CMAME,* 2017) and previous talk].

Theorem 1. *Assume that the energy functional $\Phi[\varphi]$ satisfies properties 1–5 above. Consider the Schwarz alternating method of Section 2 defined by (9)–(13) and its equivalent form (39). Then*

(a) $\Phi[\tilde{\varphi}^{(0)}] \geq \Phi[\tilde{\varphi}^{(1)}] \geq \cdots \geq \Phi[\tilde{\varphi}^{(n-1)}] \geq \Phi[\tilde{\varphi}^{(n)}] \geq \cdots \geq \Phi[\varphi]$, *where φ is the minimizer of $\Phi[\varphi]$ over $\mathcal{S}$.*
(b) *The sequence $\{\tilde{\varphi}^{(n)}\}$ defined in (39) converges to the minimizer φ of $\Phi[\varphi]$ in $\mathcal{S}$.*
(c) *The Schwarz minimum values $\Phi[\tilde{\varphi}^{(n)}]$ converge monotonically to the minimum value $\Phi[\varphi]$ in $\mathcal{S}$ starting from any initial guess $\tilde{\varphi}^{(0)}$.*

Extending these results to ***dynamics*** is ***work in progress***.

- Quasistatic proof ***extends naturally*** assuming conformal meshes and the same time step is used in each Schwarz subdomain.
- Some analysis of Schwarz for evolution problems was performed in (Lions, 1988) and may be possible to ***leverage***.
- Our numerical results suggest theoretical analysis is ***possible***.

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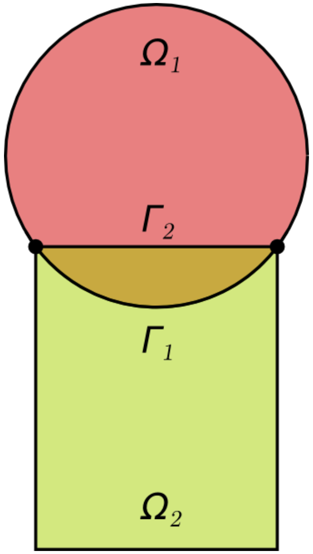
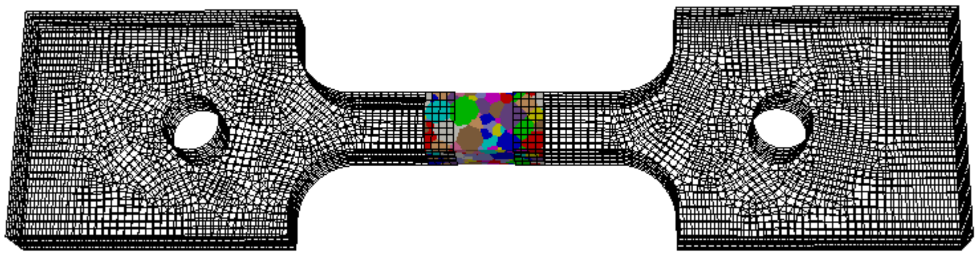




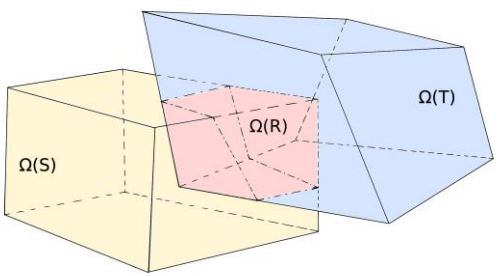
Implementation within *Albany* Code

The proposed ***dynamic alternating Schwarz method*** is 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.
- Contains a wide variety of ***constitutive models***.
- 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 ***Tempus*** package for ***time-integration****.
- ***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

* Current dynamic Schwarz implementation in Albany requires same Δt in different subdomains.

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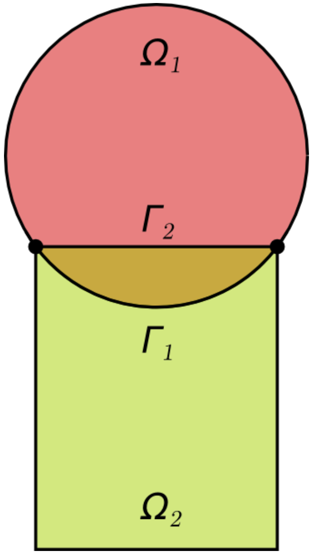
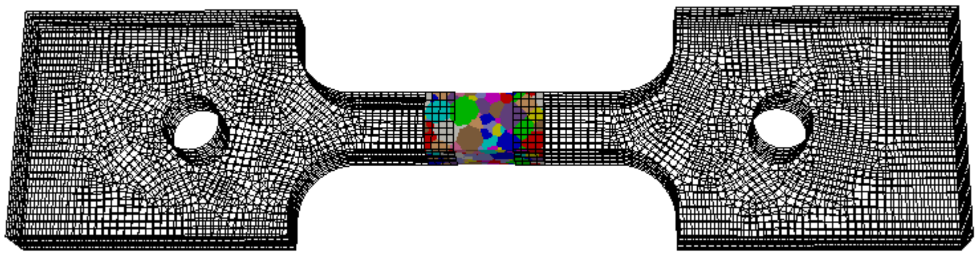
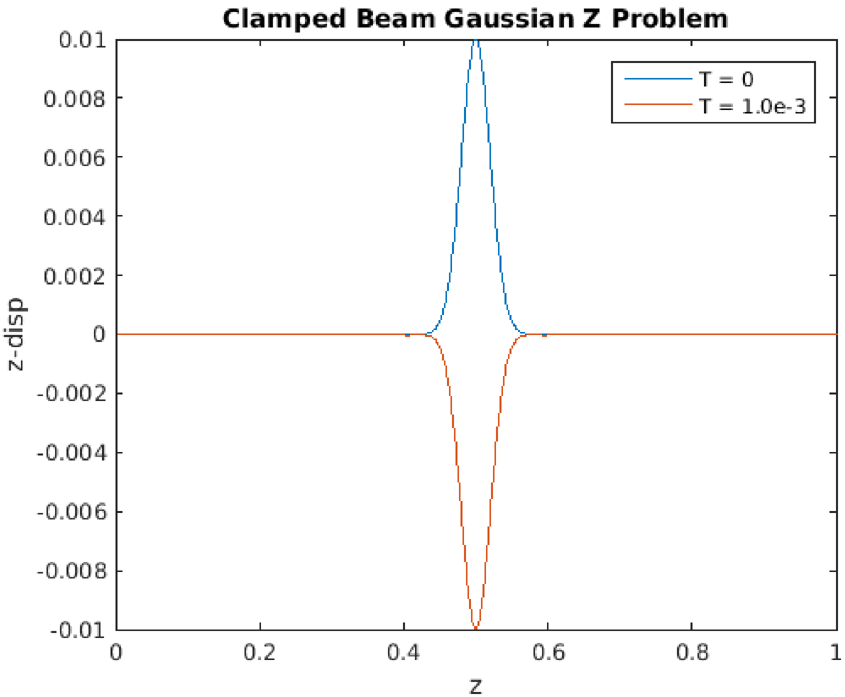




Dynamic Example #1: Elastic Wave Propagation

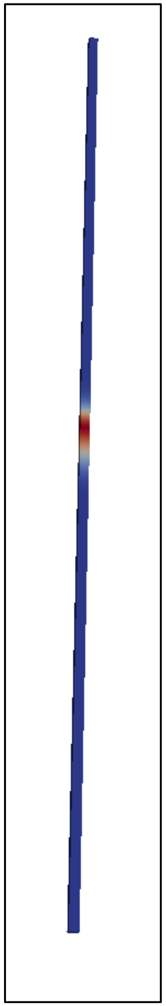
- Linear elastic ***clamped beam*** with Gaussian initial condition for the z-displacement (see figures to the right and below).
- Simple problem with analytical exact solution but very ***stringent test*** for discretization methods.
- Test Schwarz with ***2 subdomains***: $\Omega_0 = (0{,}0.001) \times (0.001) \times (0{,}0.75), \Omega_1 = (0{,}0.001) \times (0.001) \times (0.25{,}1)$.



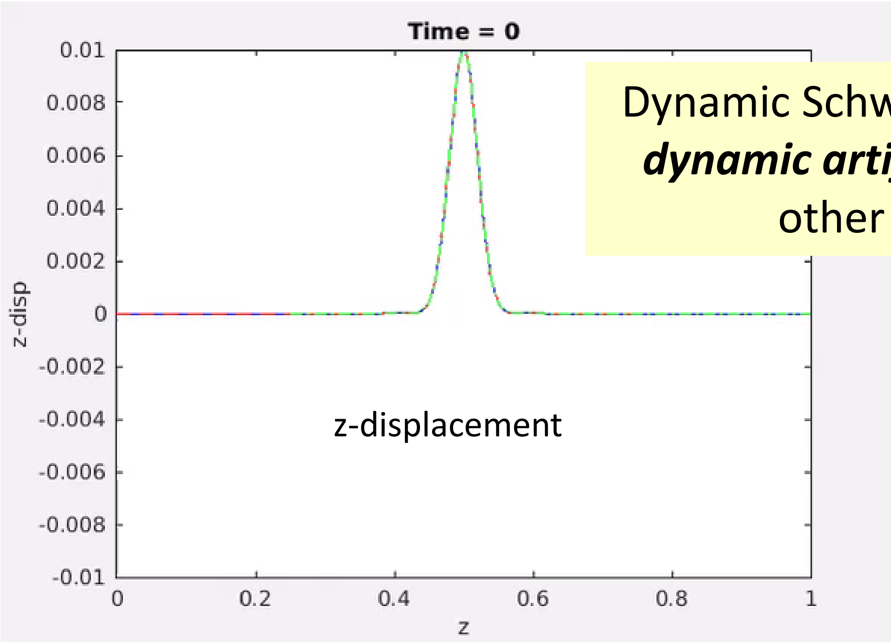
Left: Initial condition (blue) and final solution (red). Wave profile is negative of initial profile at time T = 1.0e-3.

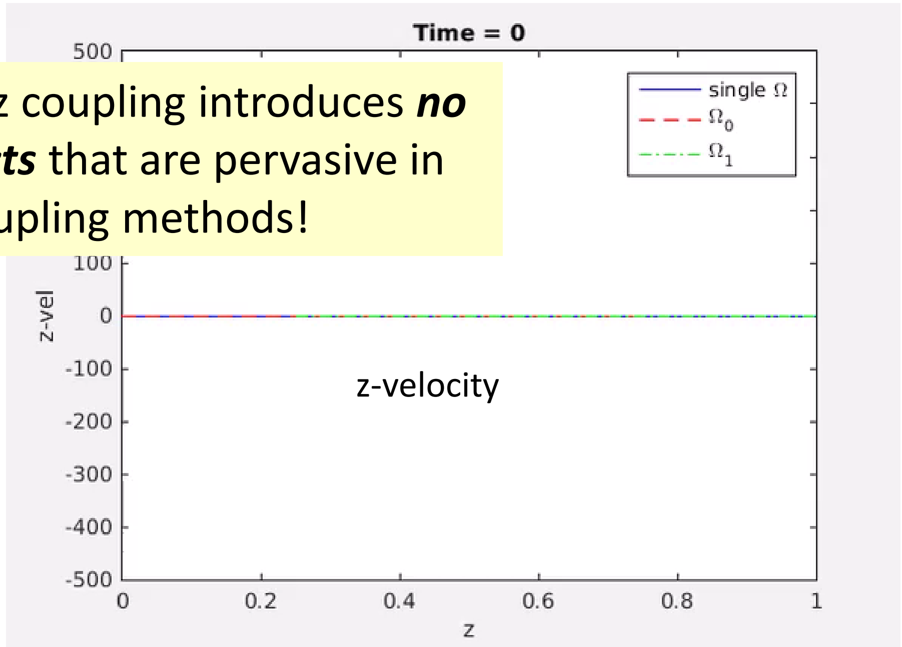
Time-discretizations: Newmark-Beta (implicit, explicit) with same Δt.

Meshes: hexes, tets



Elastic Wave Propagation





Dynamic Schwarz coupling introduces ***no dynamic artifacts*** that are pervasive in other coupling methods!

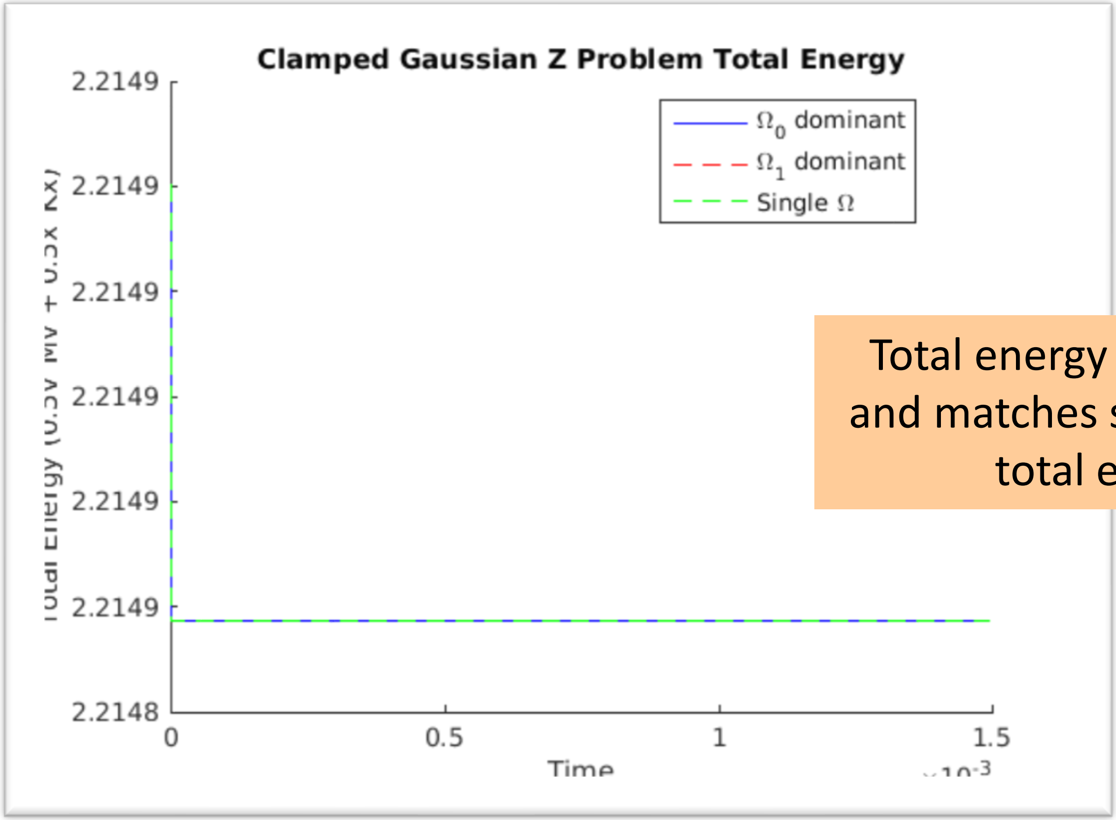
Table 1: Averaged (over times + domains) relative errors in **z–displacement** (blue) and **z-velocity** (green) for several different Schwarz couplings, 50% overlap volume fraction

	Implicit-Implicit		**Explicit(CM)-Implicit**		**Explicit(LM)-Implicit**	
Conformal hex-hex	2.79e-3	7.32e-3	3.53e-3	8.70e-3	4.72e-3	1.19e-2
Nonconformal hex-hex	2.90e-3	7.10e-3	2.82e-3	7.29e-3	2.84e-3	7.33e-3
Tet-hex	2.79e-3	7.58e-3	3.52e-3	8.92e-3	4.72e-3	1.19e-2

LM = Lumped Mass, CM = Consistent Mass

Elastic Wave Propagation

Energy Conservation

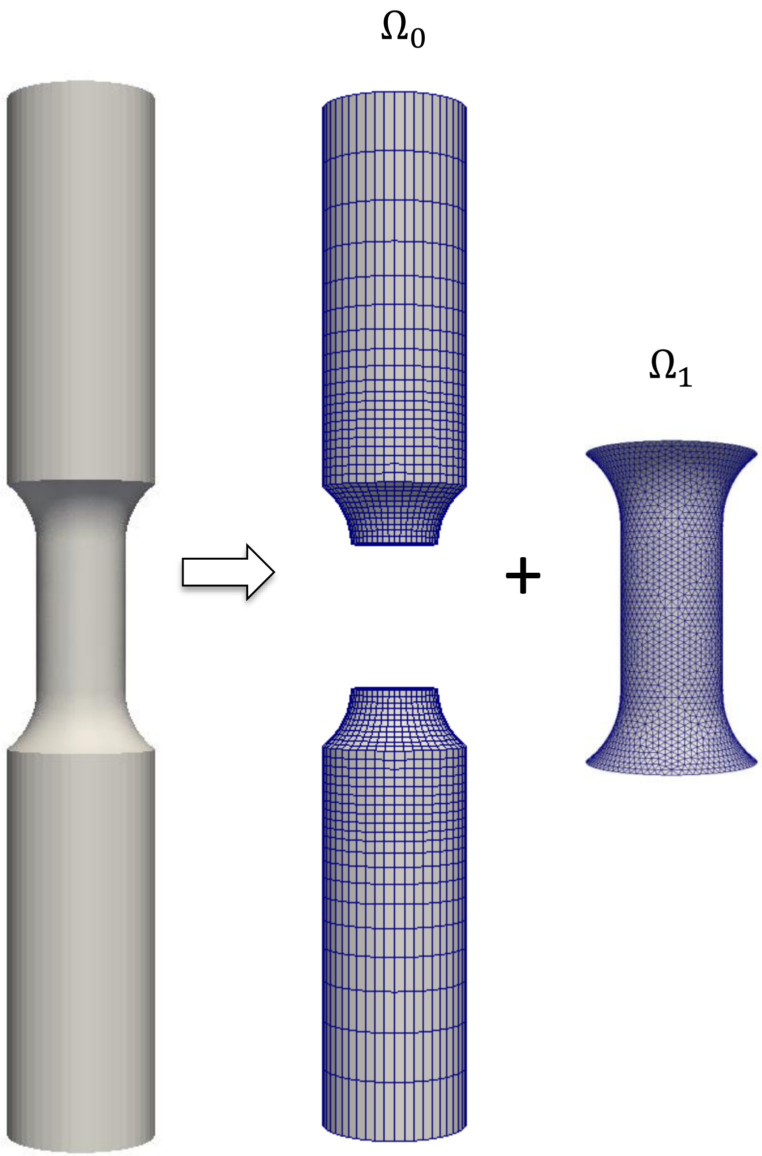


Total energy is **conserved** and matches single-domain total energy.

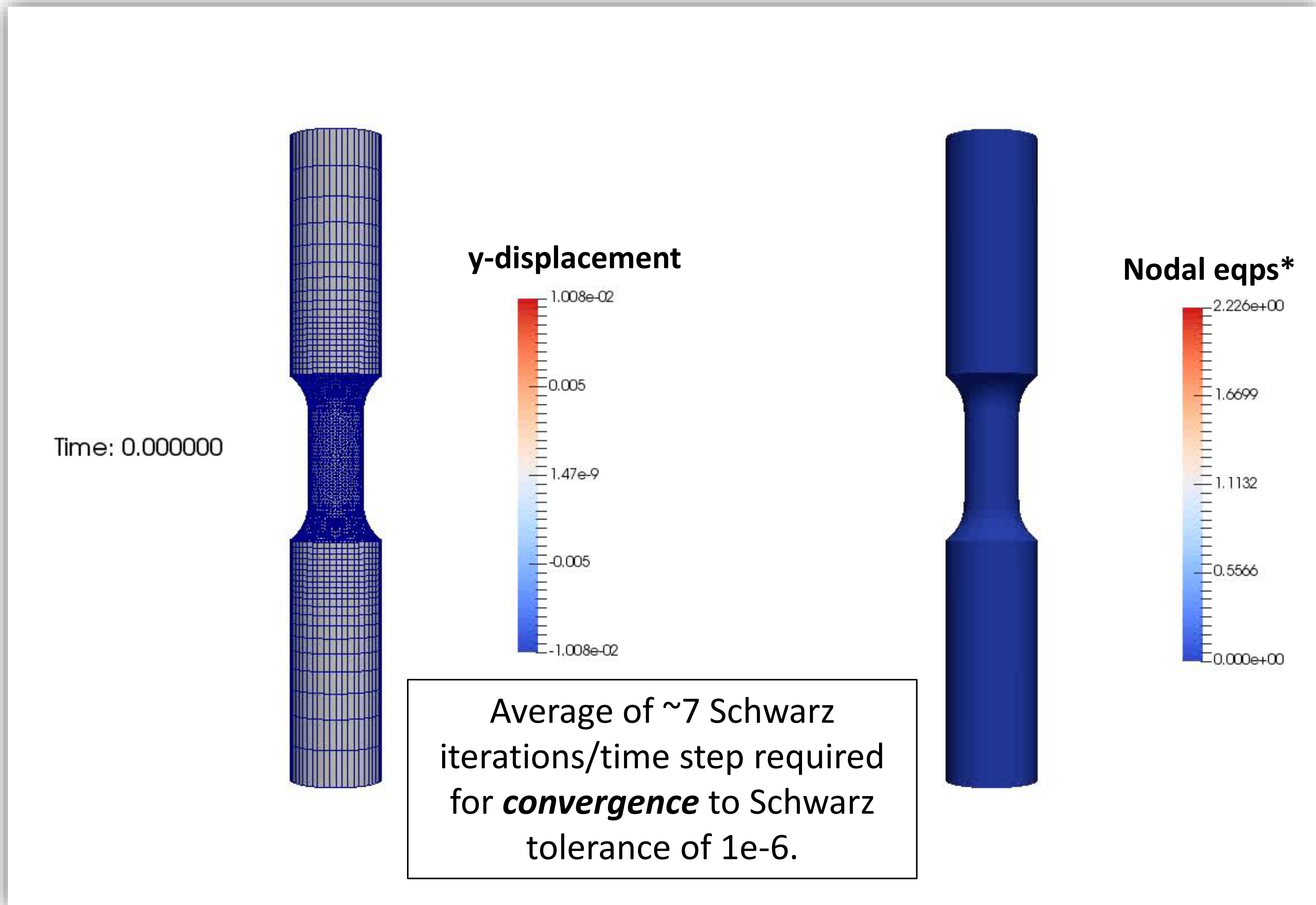
- For clamped beam problem, total energy (TE = $0.5\boldsymbol{x}^T\boldsymbol{K}\boldsymbol{x} + 0.5\dot{\boldsymbol{x}}^T\boldsymbol{M}\dot{\boldsymbol{x}}$) should be conserved.
- Total energy is calculated in 2 ways: with most of contribution from Ω_0 and from Ω_1.

Example #2: Tension Specimen

- Uniaxial aluminum cylindrical tensile specimen with ***inelastic J_2 material model***.
- Domain decomposition into ***two subdomains*** (right): Ω_0 = ends, Ω_1 = gauge.
- ***Nonconformal hex + composite tet 10*** coupling via Schwarz.
- ***Implicit*** Newmark time-integration with ***adaptive time-stepping*** algorithm employed in both subdomains.
- Slight ***imperfection*** introduced at center of gauge to force ***necking*** upon pulling in vertical direction.



Tension Specimen



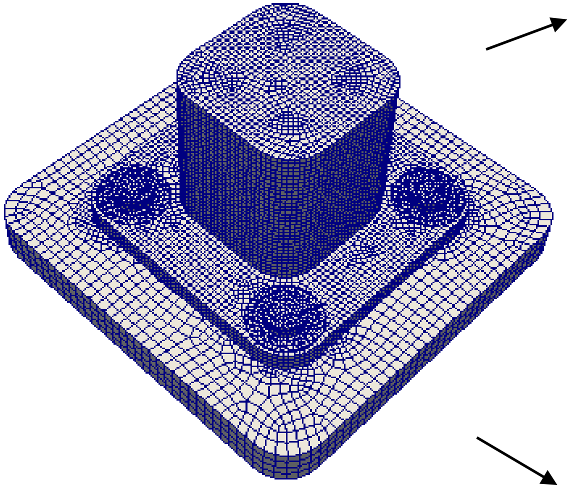
Average of ~7 Schwarz iterations/time step required for ***convergence*** to Schwarz tolerance of 1e-6.

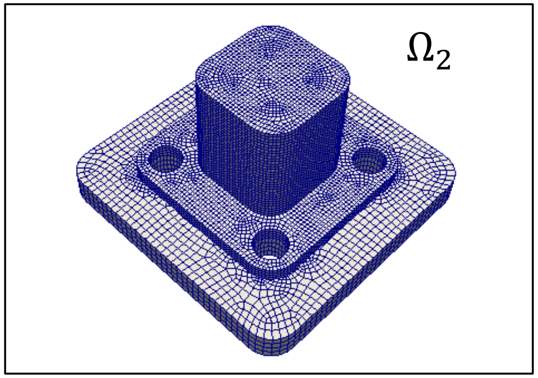
*Nodal eqps = equivalent plastic strain computed via weighted volume average.

Example #3: Bolted Joint Problem

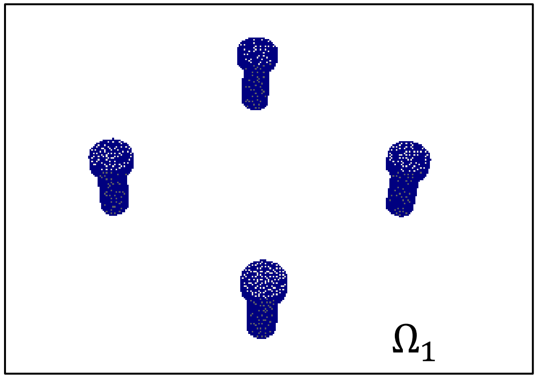
Problem of ***practical scale***.

- Schwarz solution compared to single-domain solution on composite tet 10 mesh.



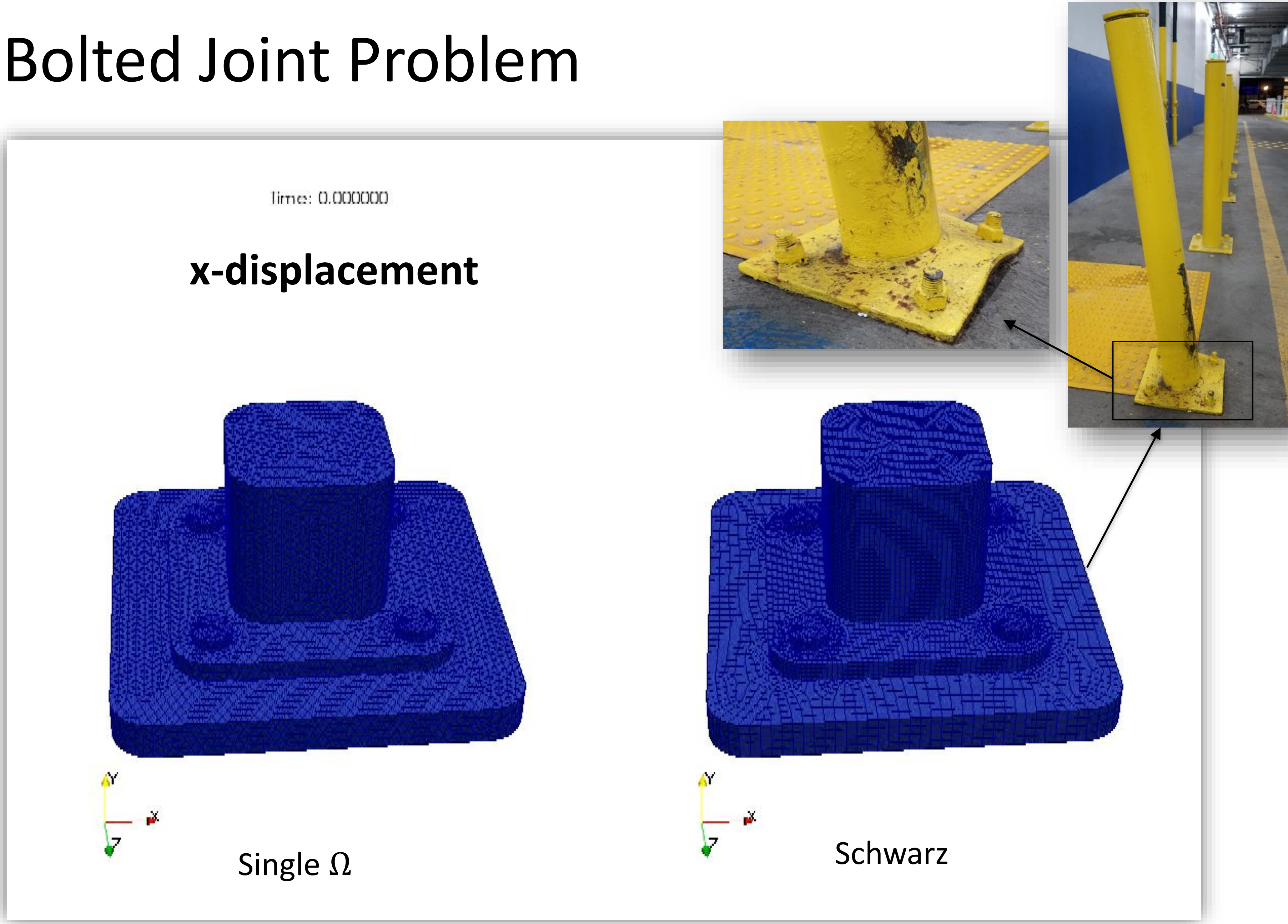


- BC: x-disp = 0.02 at T = 1.0e-3 on top of parts.
- Run until T = 5.0e-4 w/ dt = 1e-5 + implicit Newmark with analytic mass matrix for composite tet 10s.



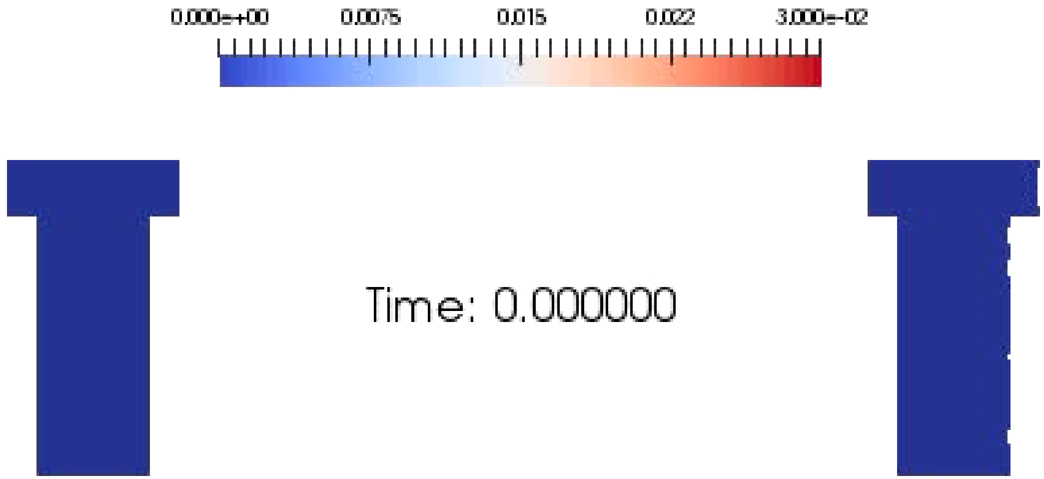
- Ω_1 = bolts (composite tet 10), Ω_2 = parts (hex).
- ***Inelastic J_2 material model*** in both subdomains.
  - Ω_1: steel
  - Ω_2: steel component, aluminum (bottom) plate

Bolted Joint Problem

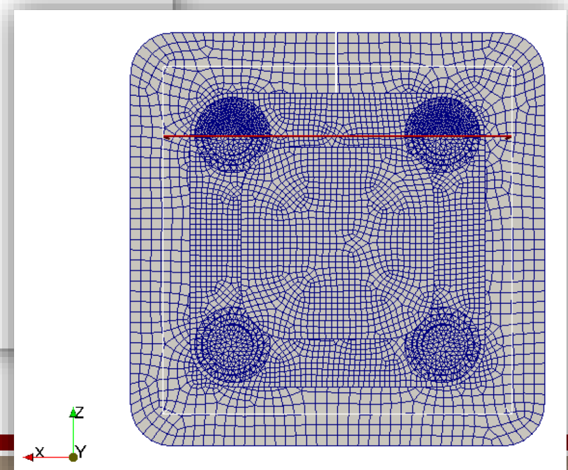


Bolted Joint Problem

Nodal Equivalent Plastic Strain (eqps)



Cross-section of bolts obtained via clip (right)

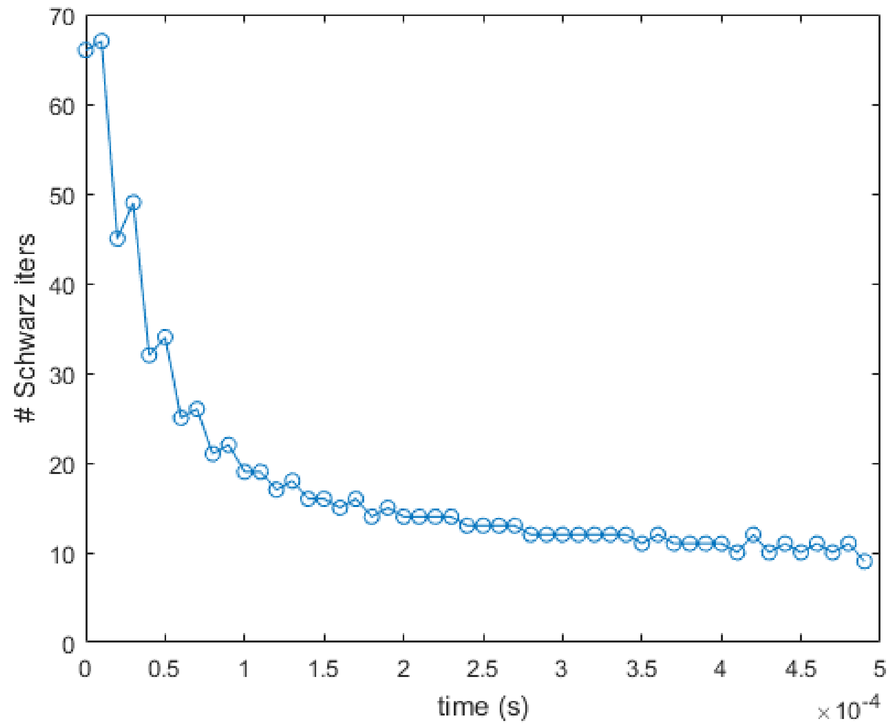


Bolted Joint Problem

Some Performance Results

Schwarz / solver settings

- Relatively loose Schwarz tolerances were used:
  - Relative Tolerance: 1.0e-3.
  - Absolute Tolerance: 1.0e-4.
- Newton tolerance on NormF: 1e-8
- Linear solver tolerance: 1e-5
- MueLu preconditioner



- ***Top right plot:*** # Schwarz iterations for each time step.
  - After start-up, # Schwarz iterations / time step is ~9-10. This is not bad given how small is the size of the overlap region for this problem.

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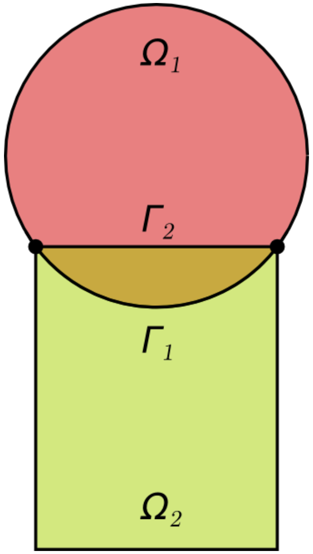

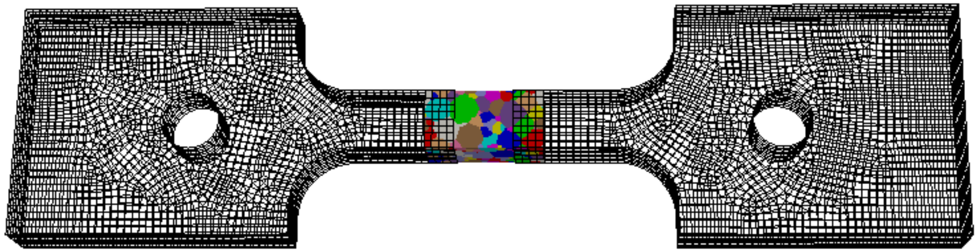

Summary

Sandia National Laboratories

The **alternating Schwarz** coupling method has been developed/implemented for **concurrent multiscale quasistatic & dynamic modeling** in Sandia's Albany/LCM code.

- ☺ Coupling is ***concurrent*** (two-way).
- ☺ ***Ease of implementation*** into existing massively-parallel HPC codes.
- ☺ ***Scalable, fast, robust*** (we target ***real*** engineering problems, e.g., analyses involving failure of bolted components!).
- ☺ ***"Plug-and-play" framework***: simplifies task of meshing complex geometries!
  - ☺ Ability to couple regions with ***different non-conformal meshes***, ***different element types*** and ***different levels of refinement.***
  - ☺ Ability to use ***different solvers/time-integrators*** in different regions.
- ☺ Coupling does not introduce ***nonphysical artifacts.***
- 😐 ***Theoretical*** convergence properties/guarantees (☺ for quasistatics).

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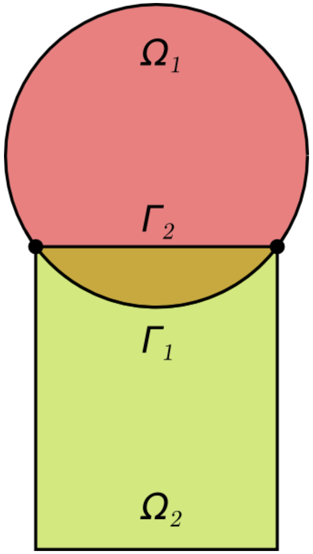
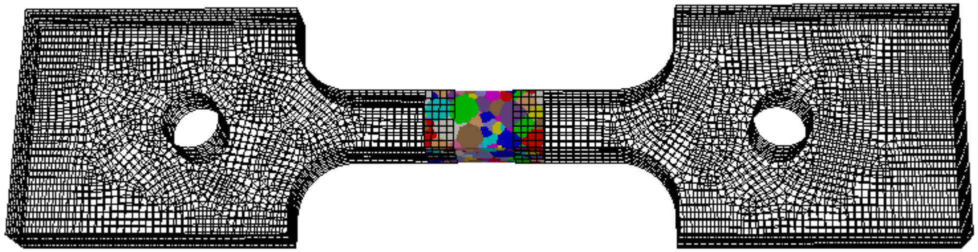
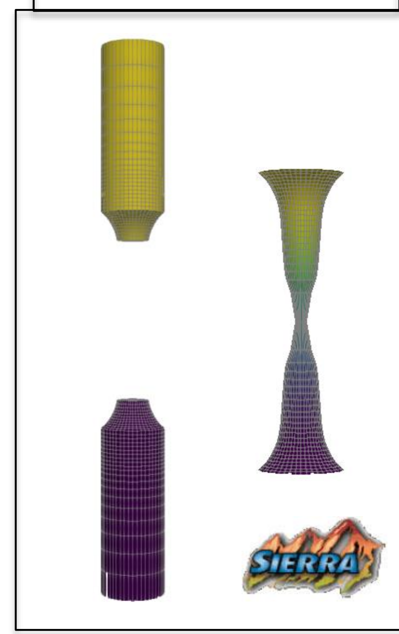




Ongoing/Future Work

- Develop ***theory*** for dynamic alternating Schwarz formulation.
- ***Journal article*** on dynamic Schwarz formulation.
- Extension of Albany/LCM dynamic Schwarz implementation to allow for ***different time steps*** in different subdomains.
- Apply dynamic Schwarz to problem of interest to ***production***.
- Implement alternating Schwarz method in Sandia ***production codes*** (Sierra Solid Mechanics).
- Development of a ***multi-physics coupling framework*** based on variational formulations and the Schwarz alternating method.



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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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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-

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, $\boldsymbol{x}_b^{(1)} \leftarrow \chi(\boldsymbol{X}_b^{(1)})$ 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 $||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}|| \le \epsilon$ ▷ 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

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.

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 $\partial_{\boldsymbol{\varphi}}\Omega_1$, $\boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)}$ on Γ_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 $\partial_{\boldsymbol{\varphi}}\Omega_2$, $\boldsymbol{x}_\beta^{(2)} \leftarrow \boldsymbol{X}_\beta^{(2)}$ on Γ_2 ▷ initialize for Ω_2

3: **repeat** ▷ Newton-Schwarz loop

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

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

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

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

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

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

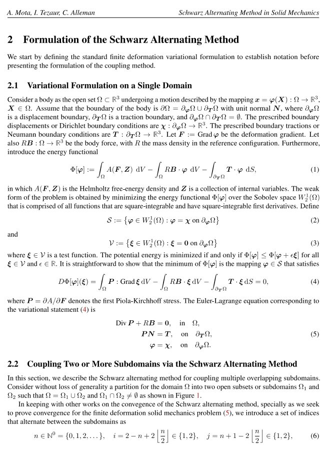
10: **until** $\left[\left(||\triangle\boldsymbol{x}_B^{(1)}||/||\boldsymbol{x}_B^{(1)}||\right)^2 + \left(||\triangle\boldsymbol{x}_B^{(2)}||/||\boldsymbol{x}_B^{(2)}||\right)^2\right]^{1/2} \leq \epsilon_{\text{machine}}$ ▷ tight tolerance

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


A. Mota, I. Tezaur, C. Alleman — Schwarz Alternating Method in Solid Mechanics

2 Formulation of the Schwarz Alternating Method

2.1 Variational Formulation on a Single Domain

2.2 Coupling Two or More Subdomains via the Schwarz Alternating Method

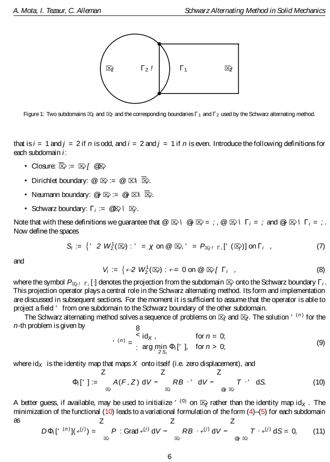
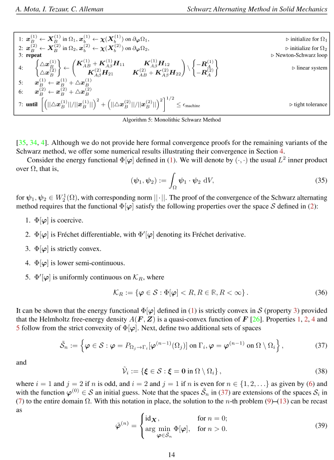
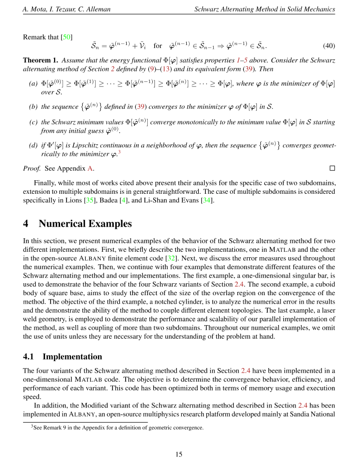
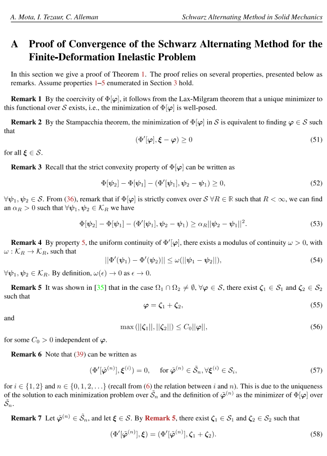


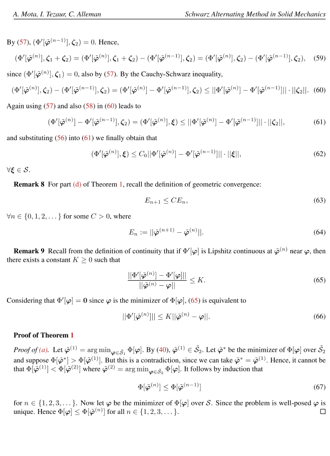
Figure 1: Two subdomains Ω_1 and Ω_2 and the corresponding boundaries Γ_1 and Γ_2 used by the Schwarz alternating method.

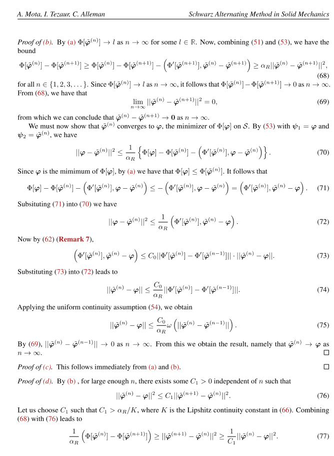

Algorithm 5: Monolithic Schwarz Method

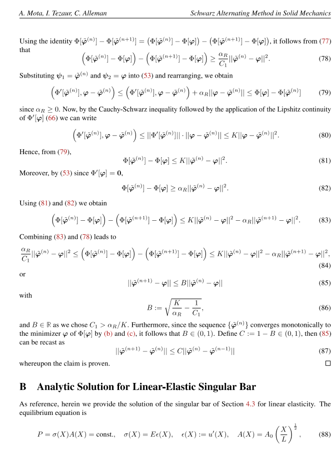

4 Numerical Examples

4.1 Implementation


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


Proof of Theorem 1

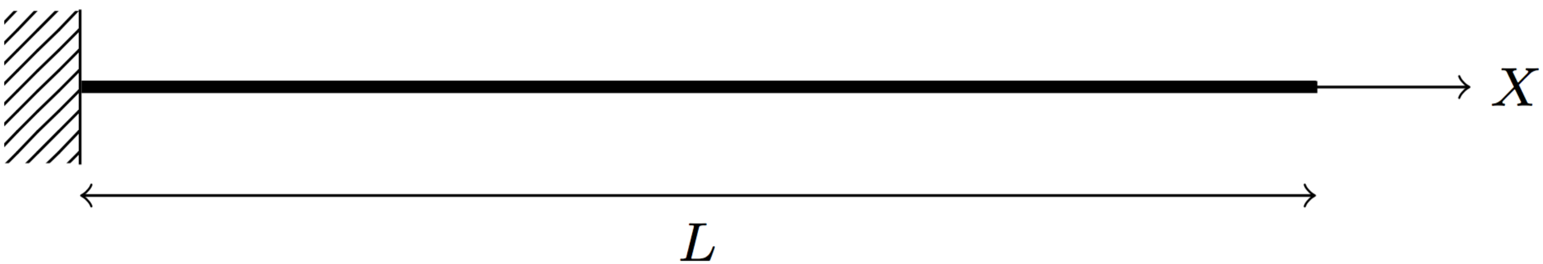



B Analytic Solution for Linear-Elastic Singular Bar

Appendix. Foulk's Singular Bar

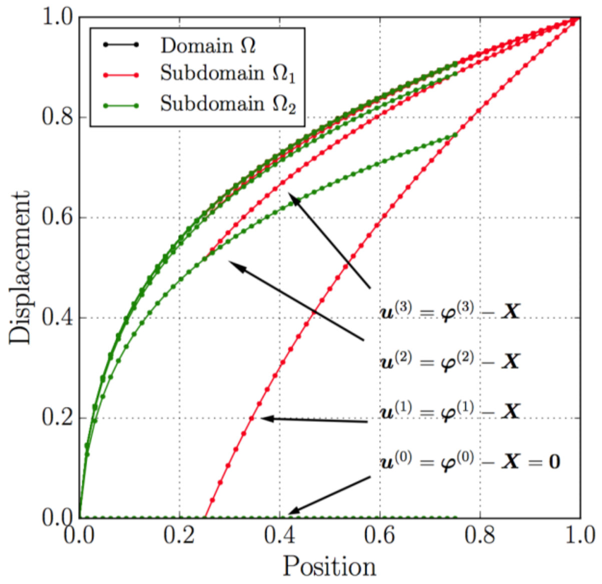
- ***1D proof of concept*** problem:
  - ***1D bar*** with area proportional to square root of length.
  - Strong ***singularity*** on left end of bar.
  - Simple ***hyperelestic*** material model with no damage.
  - ***MATLAB*** implementation.

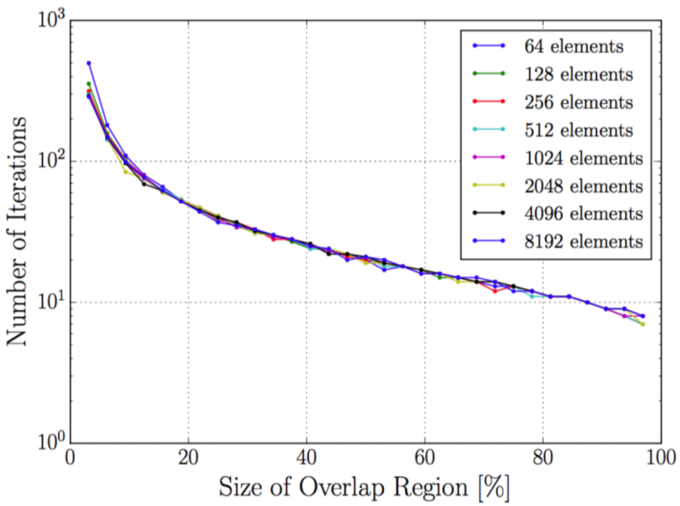
$$u(0) = 0 \qquad A(X) = A_0\sqrt{X/L} \qquad u(L) = \Delta$$

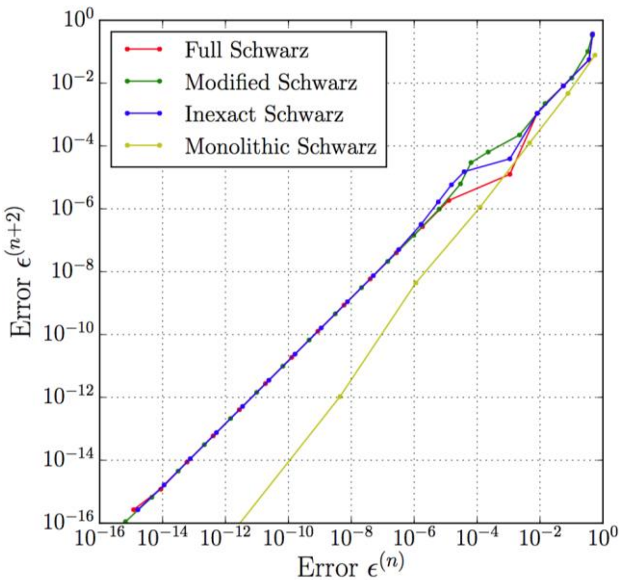


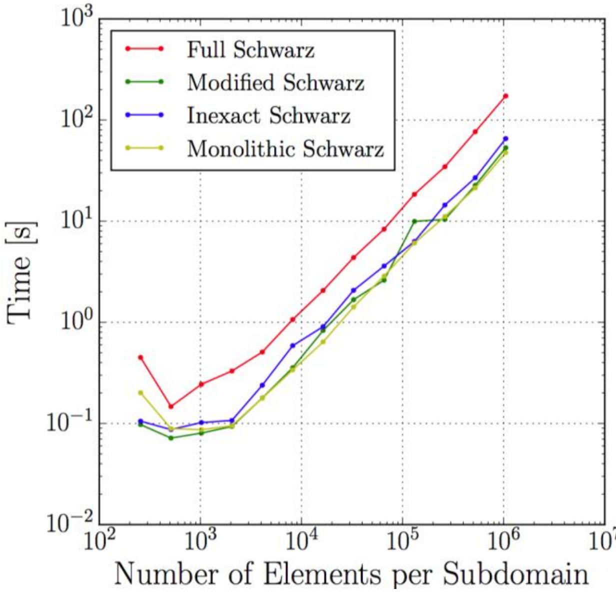
- ***Problem goals***:
  - Explore ***viability*** of ***4 variants*** of the Schwarz alternating method.
  - Test ***convergence*** and compare with literature (Evans, 1986).
    - Expect ***faster convergence*** in ***fewer iterations*** with ***increased overlap***.

Appendix. Singular Bar and Schwarz Variants

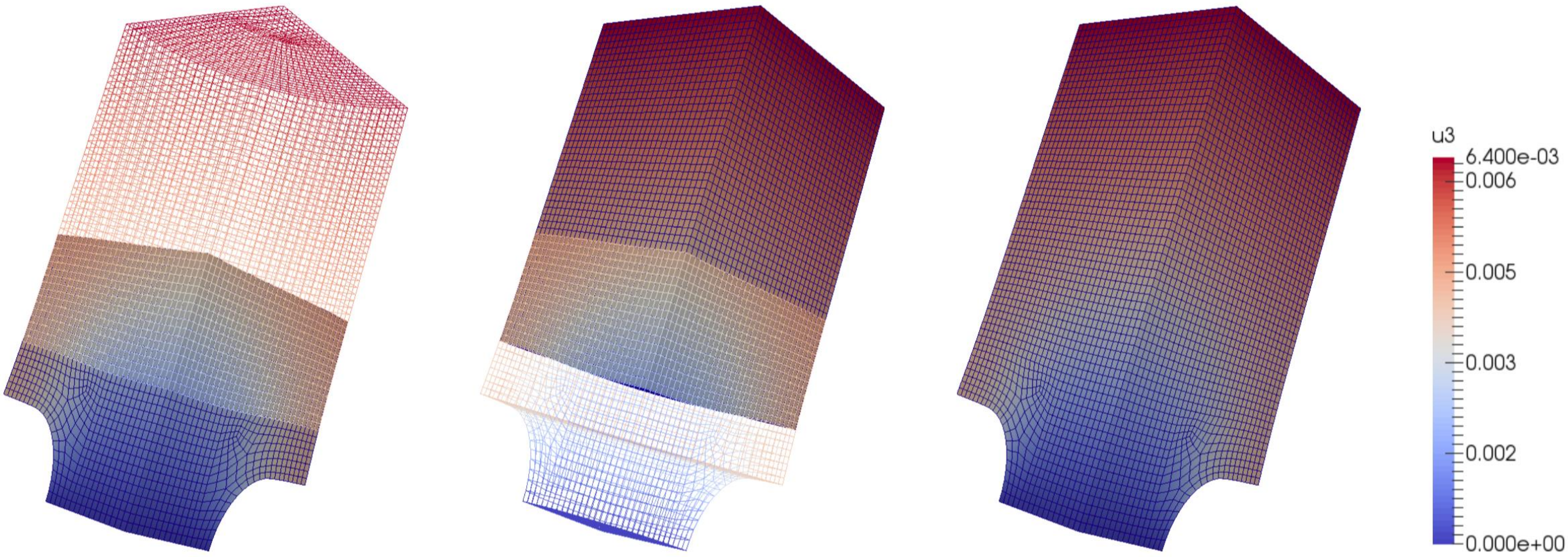








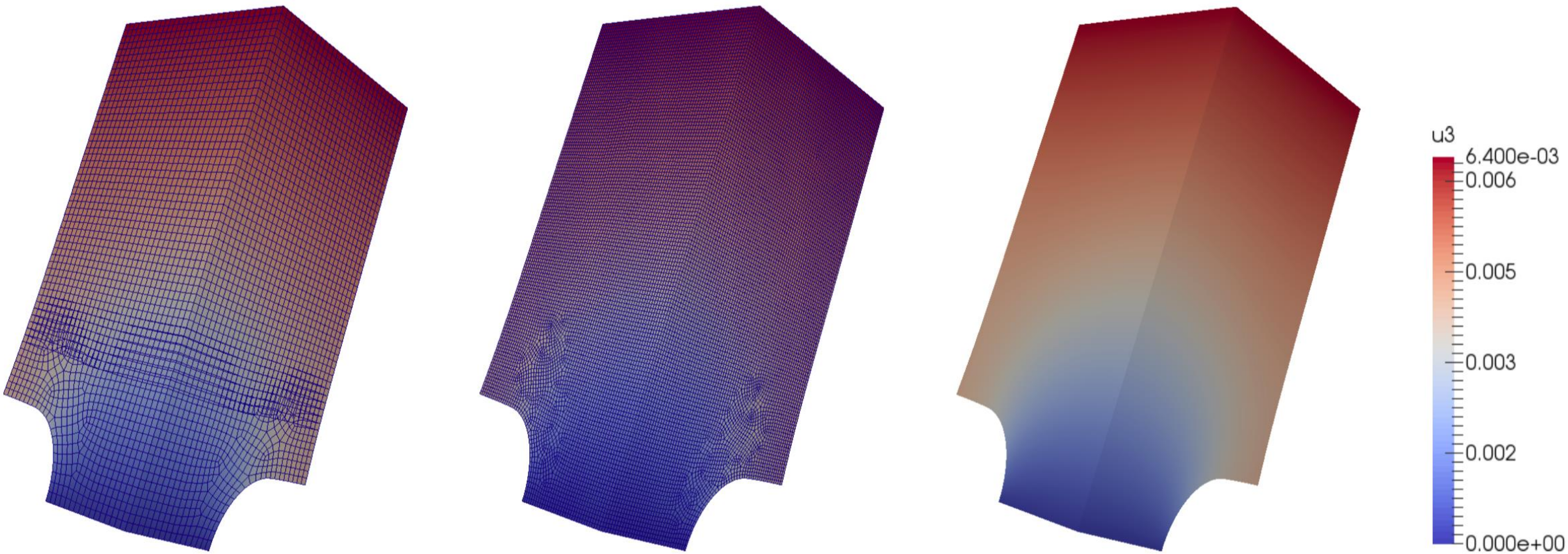
Appendix. Notched Cylinder: HEX-HEX Coupling



(a) Ω_1 **(b)** Ω_2 **(c)** Ω_{ref}

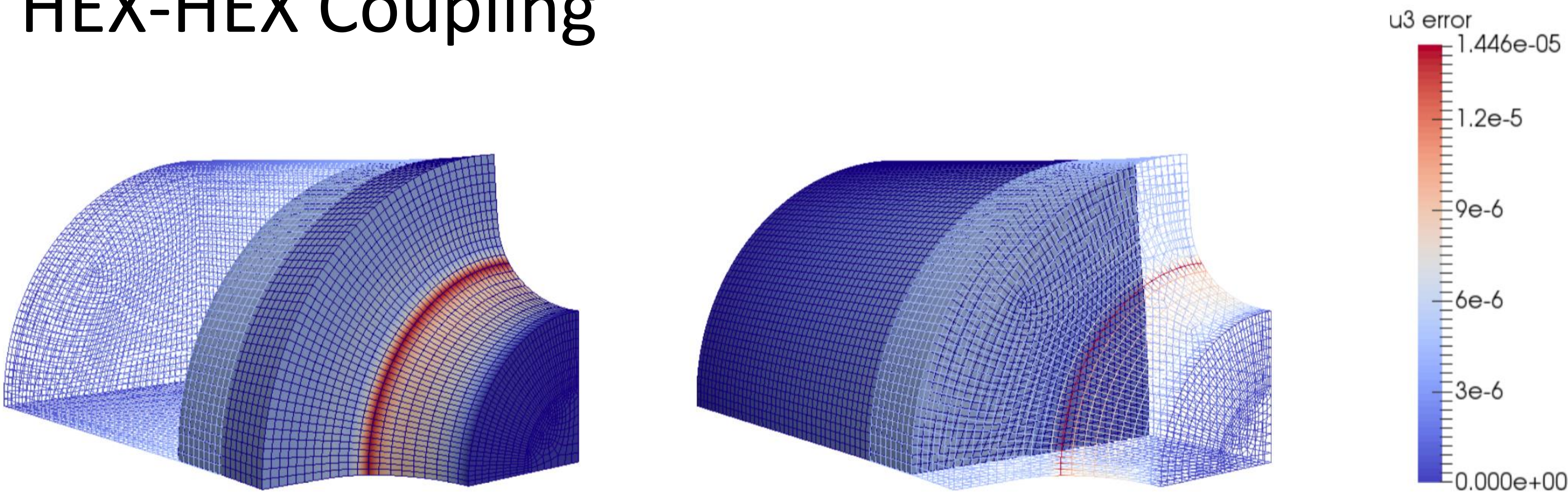
Absolute residual tolerance	u_3 relative error Ω_1	Ω_2
1.0×10^{-4}	7.60×10^{-3}	3.20×10^{-3}
1.0×10^{-8}	3.10×10^{-5}	1.71×10^{-5}
1.0×10^{-12}	1.34×10^{-9}	5.10×10^{-10}
1.0×10^{-14}	1.23×10^{-11}	4.69×10^{-12}
2.5×10^{-16}	1.14×10^{-13}	8.37×10^{-14}

Appendix. Notched Cylinder: Nonconformal HEX-HEX Coupling



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

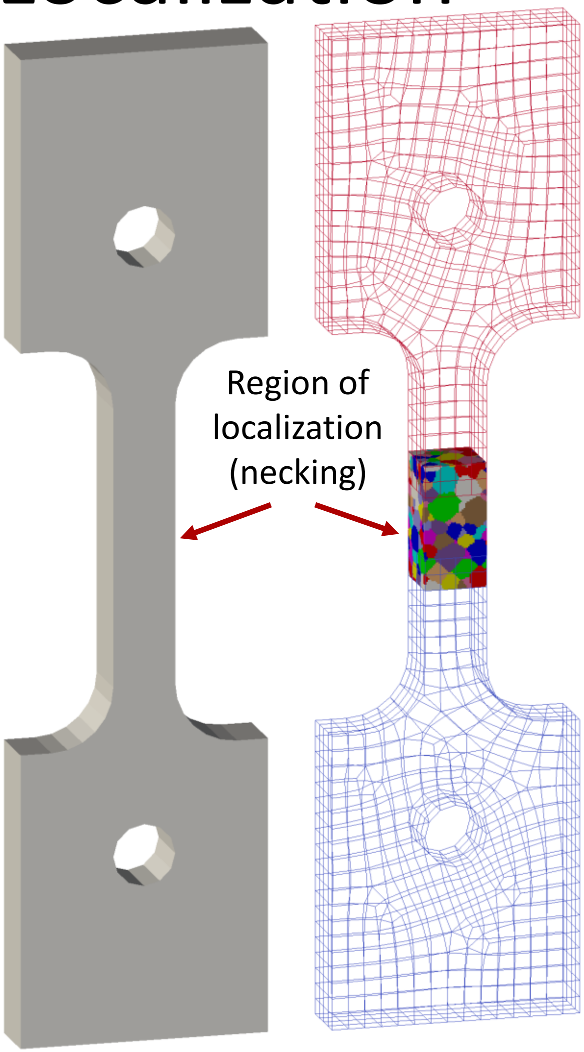
Appendix. Notched Cylinder: Nonconformal HEX-HEX Coupling

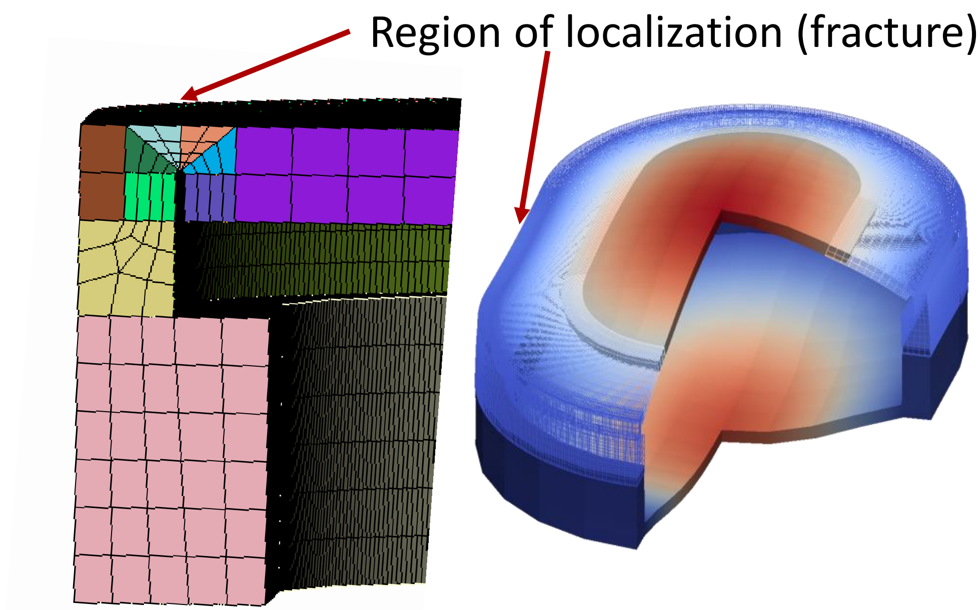


(a) Ω_1 **(b)** Ω_2

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}

Appendix. Multiscale Modeling of Localization



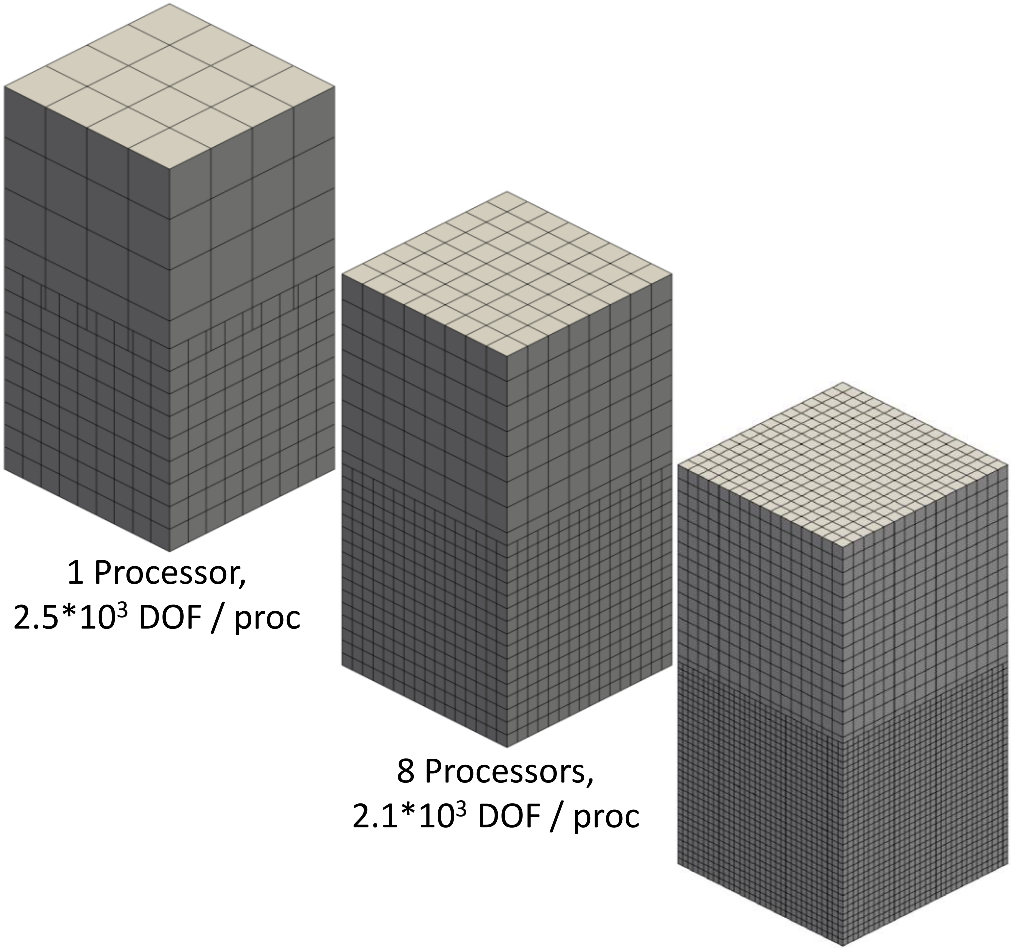


Strain localization can cause ***localized necking*** (left) and ultimately ***fracture*** (above).

Goals:

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

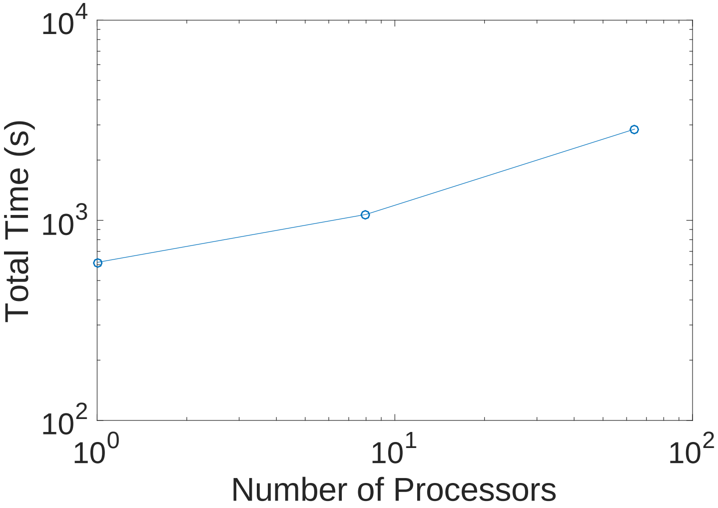
Appendix. Parallelization via DTK: Weak Scaling on Cubes Problem



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

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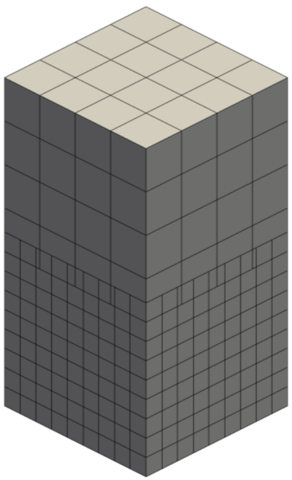
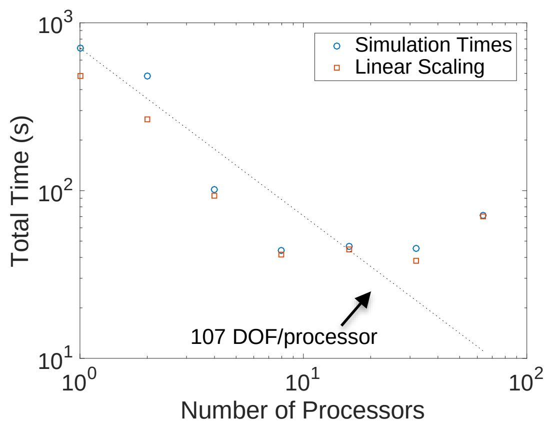
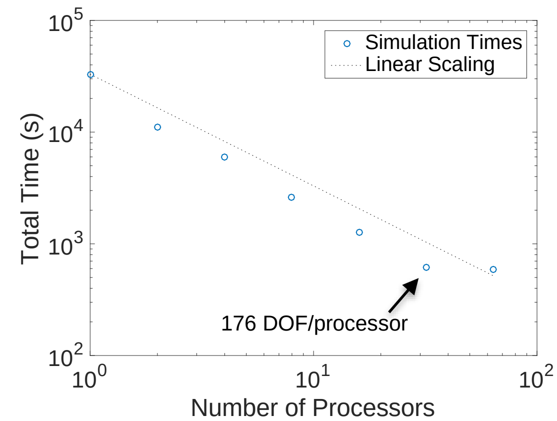
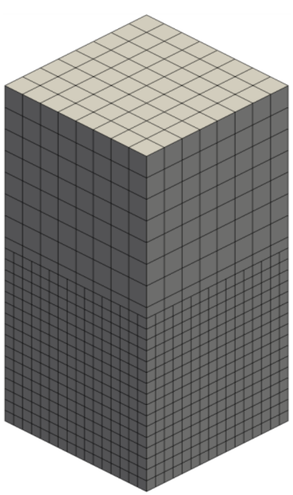


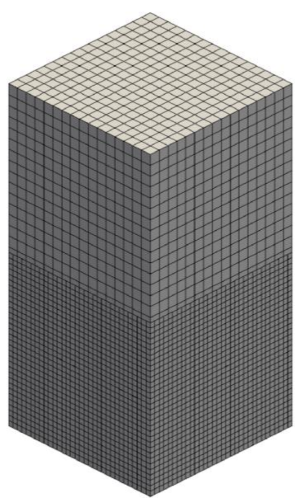
Small problem ($2.5*10^3$ DOFs)



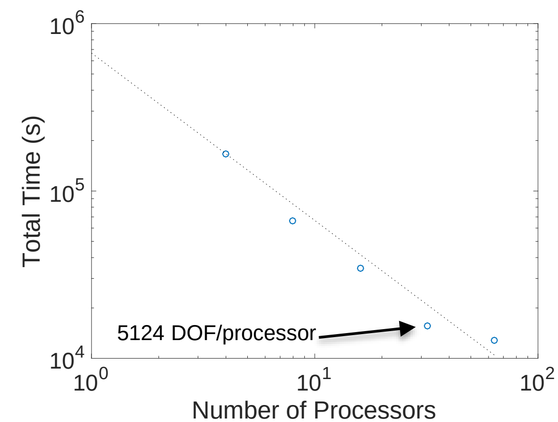
Medium problem ($1.7*10^4$ DOFs)







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



Appendix. Rubiks Cube Problem

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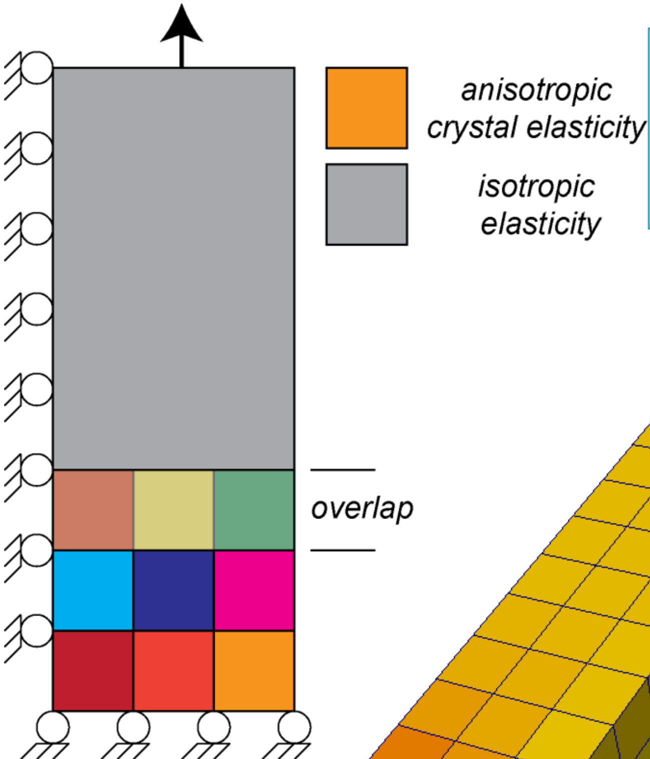
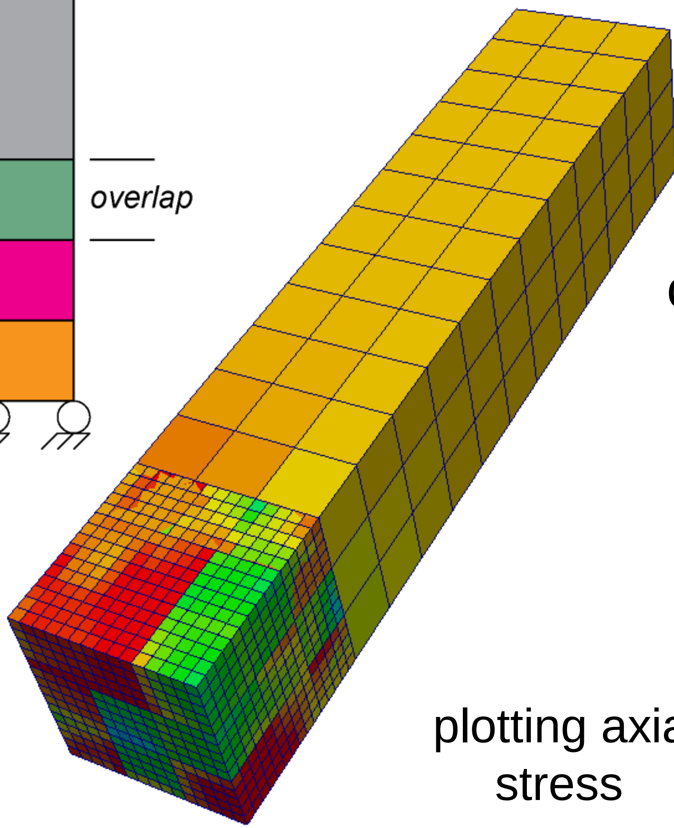


Two distinct bodies, the component scale and the microstructural scale, are coupled iteratively with alternating Schwarz

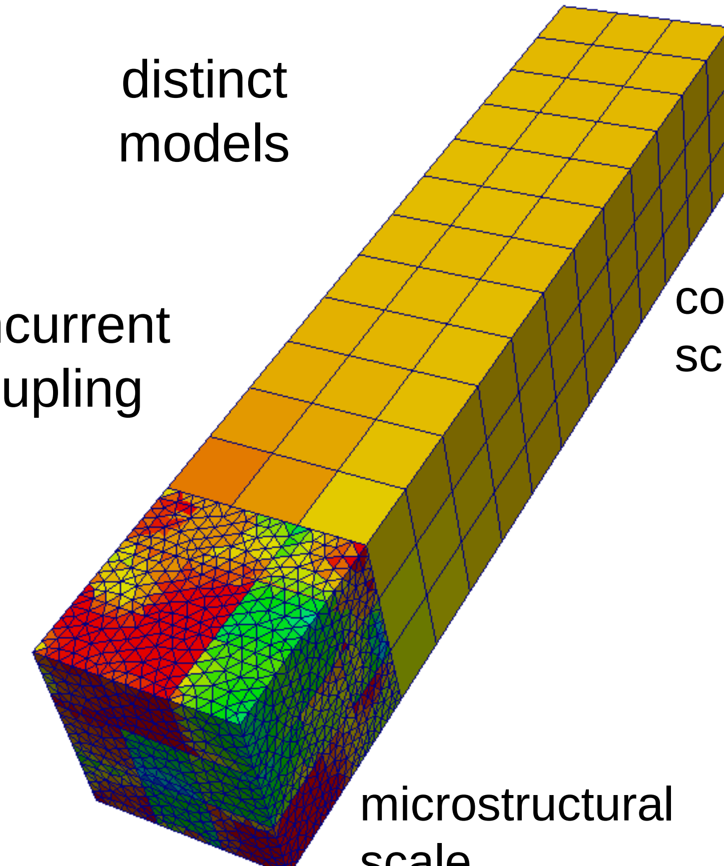
Work by J. Foulk, D. Littlewood, C. Battaile, H. Lim



distinct models

concurrent coupling

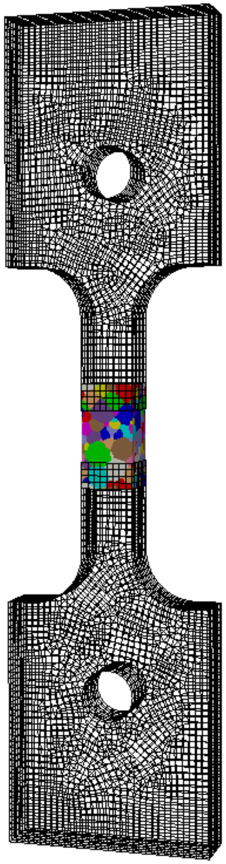
plotting axial stress



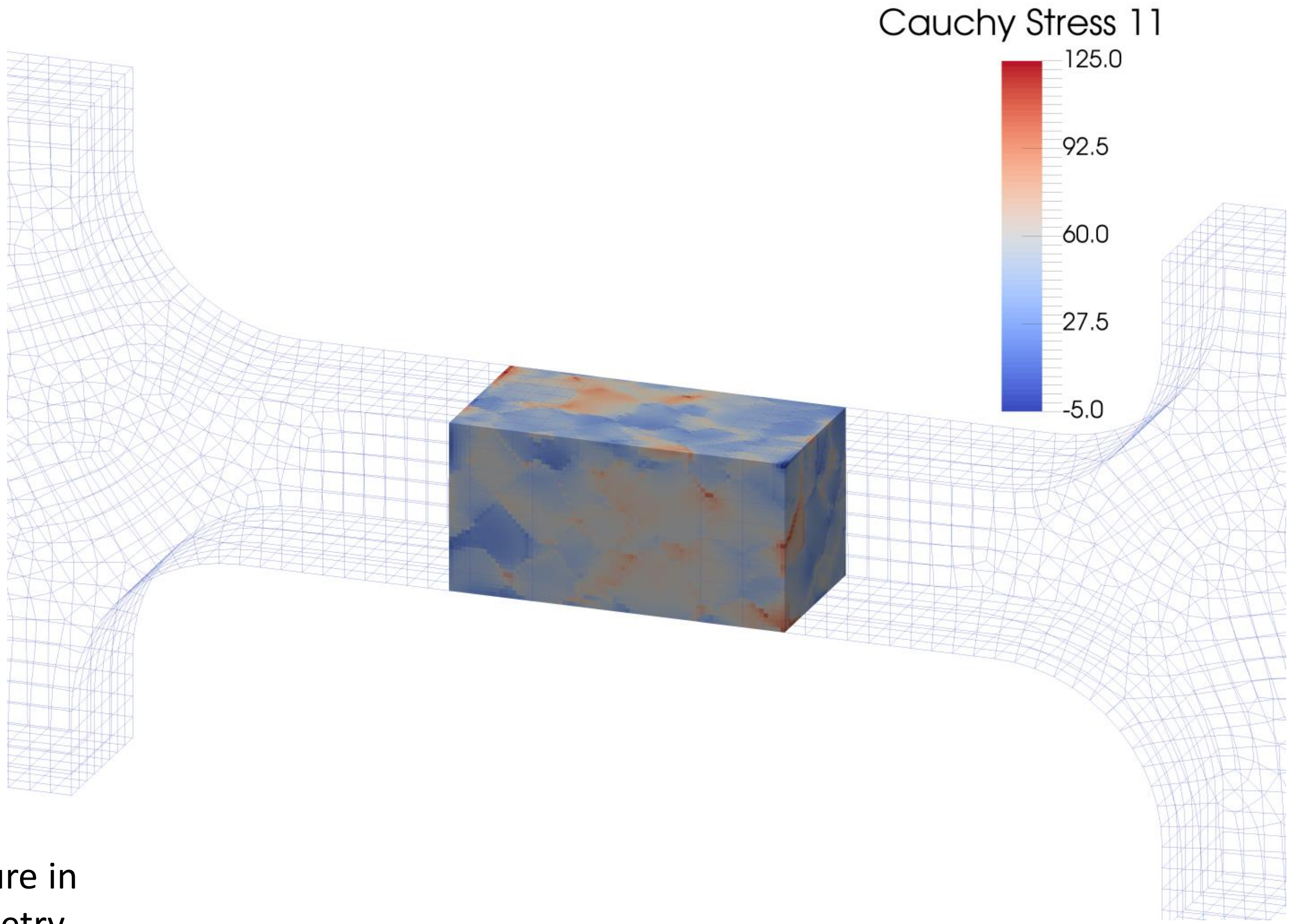
component scale

microstructural scale

Appendix. Tensile Bar



Embed microstructure in ASTM tensile geometry



Appendix. Tensile Bar: Meso-Macroscale Coupling

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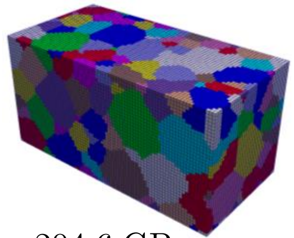
Mesoscale

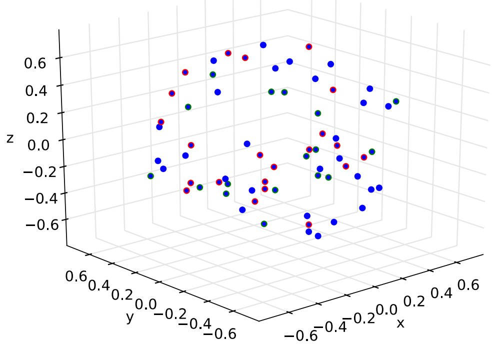
SPARKS-generated microstructure (F. Abdeljawad)



+

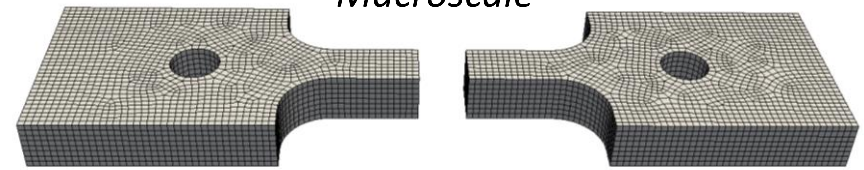
$$\text{cubic elastic constant}: C_{11} = 204.6 \text{ GPa}$$
$$\text{cubic elastic constant}: C_{12} = 137.7 \text{ GPa}$$
$$\text{cubic elastic constant}: C_{44} = 126.2 \text{ GPa}$$
$$\text{reference shear rate}: \dot{\gamma}_0 = 1.0 \text{ 1/s}$$
$$\text{rate sensitivity factor}: m = 20$$
$$\text{hardening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

Fix microstructure, investigate ensembles

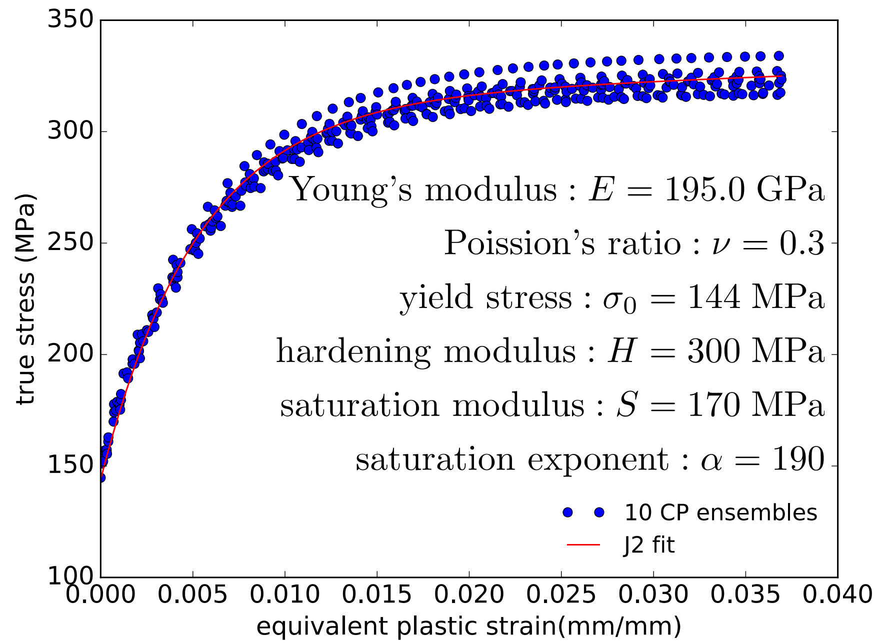


151 axial vectors from 3 of the 10 ensembles of random rotations (blue, green, red)

Macroscale



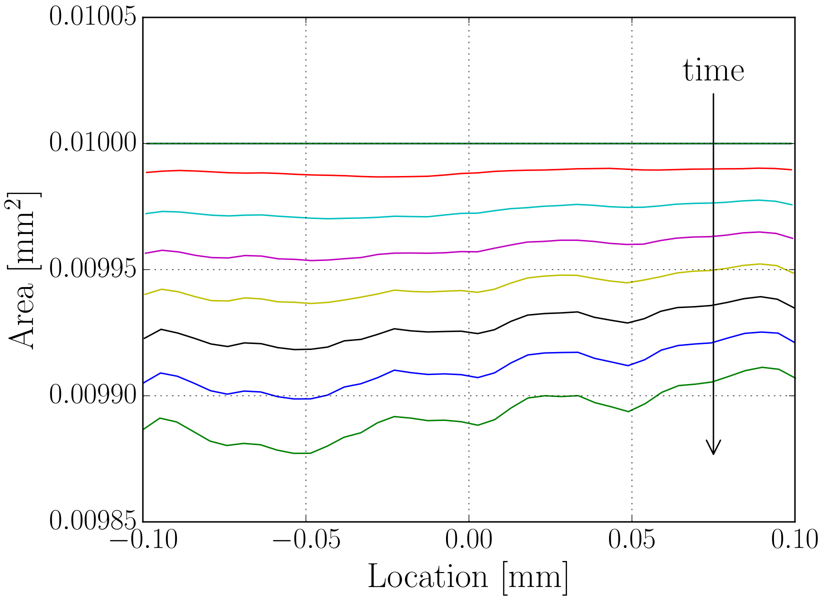
- Load microstructural ensembles in uniaxial stress
- Fit flow curves with a macroscale J_2 plasticity model

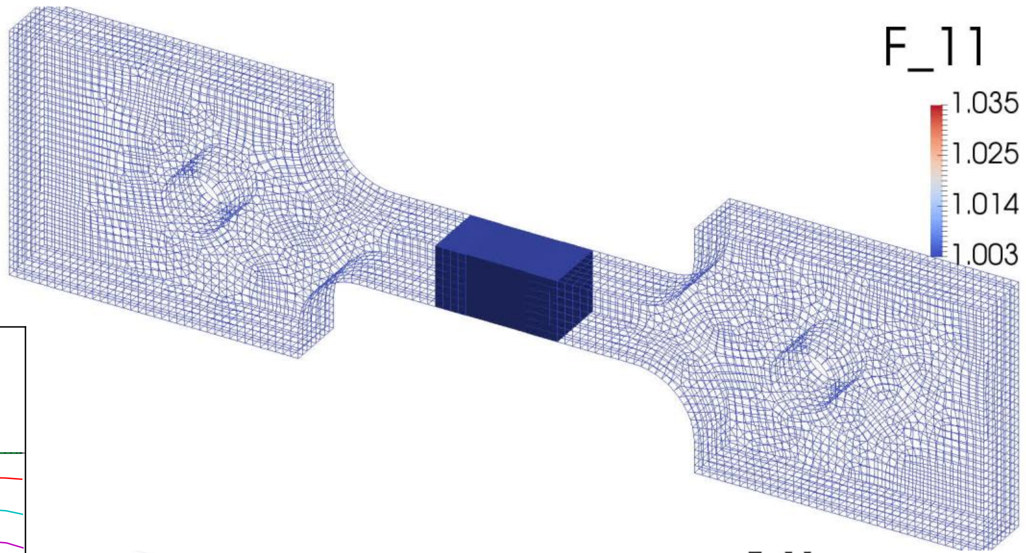


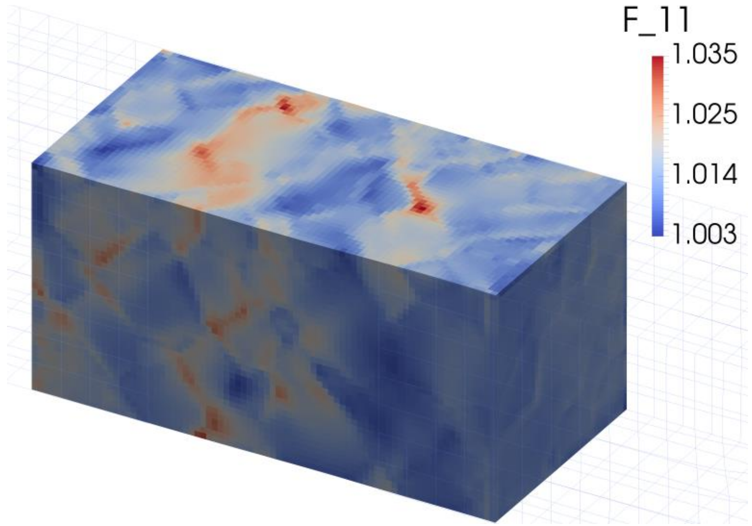
$$\sigma_y = \sigma_0 + H\epsilon_p + S(1 - e^{-\alpha\epsilon_p})$$

Appendix. Tensile Bar: Results

Reduction in cross-sectional area over time

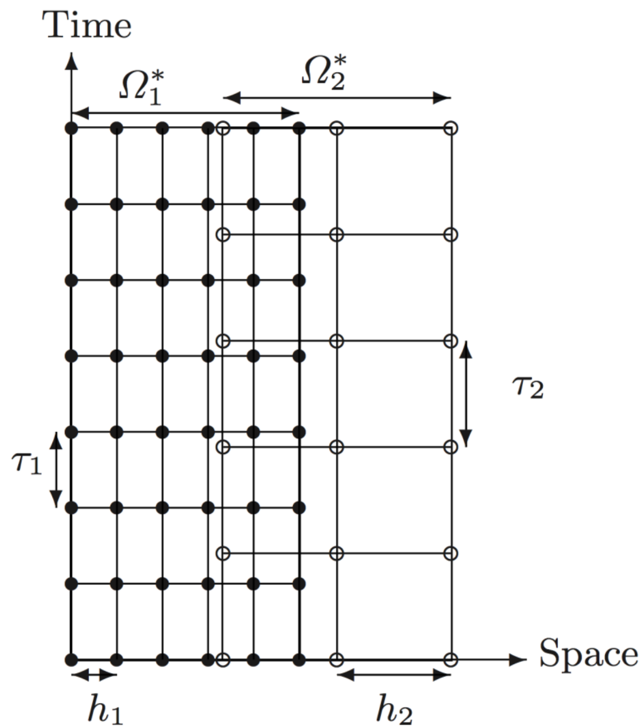






Appendix. Schwarz Alternating Method for Dynamics

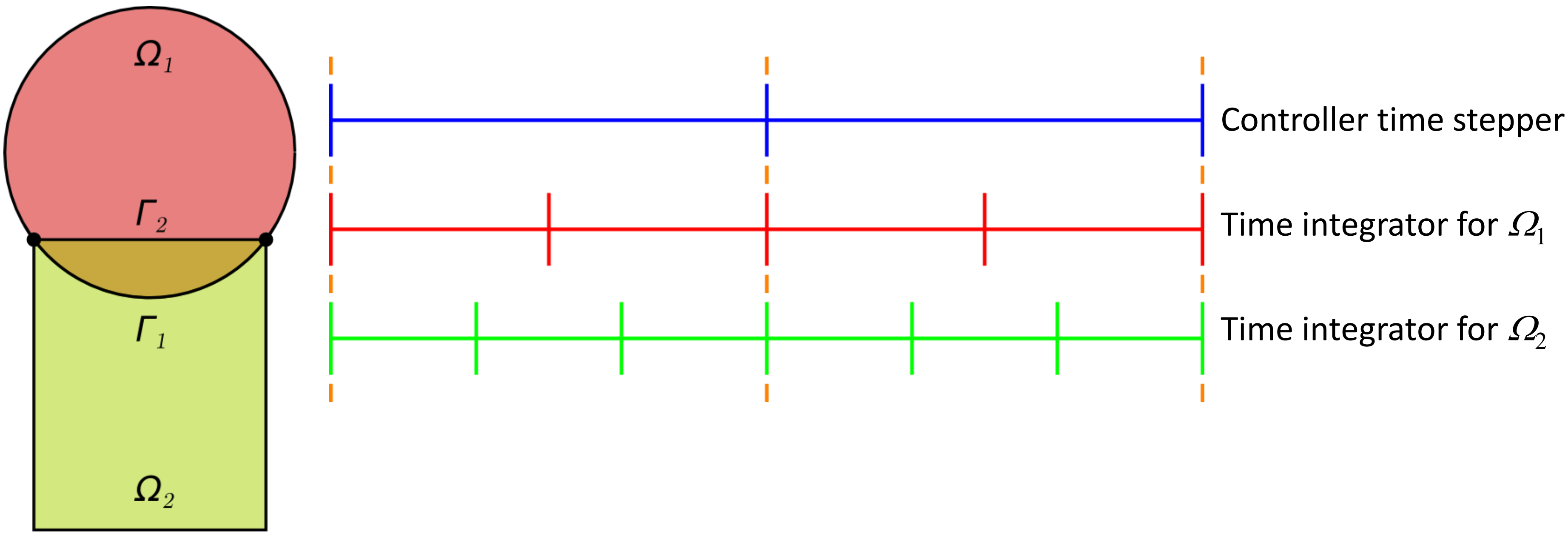
- In the literature the Schwarz method is applied to dynamics by using ***space-time discretizations***.
- This was deemed ***unfeasible*** given the design of our current codes and size of simulations.



Overlapping non-matching meshes and time steps in dynamics.

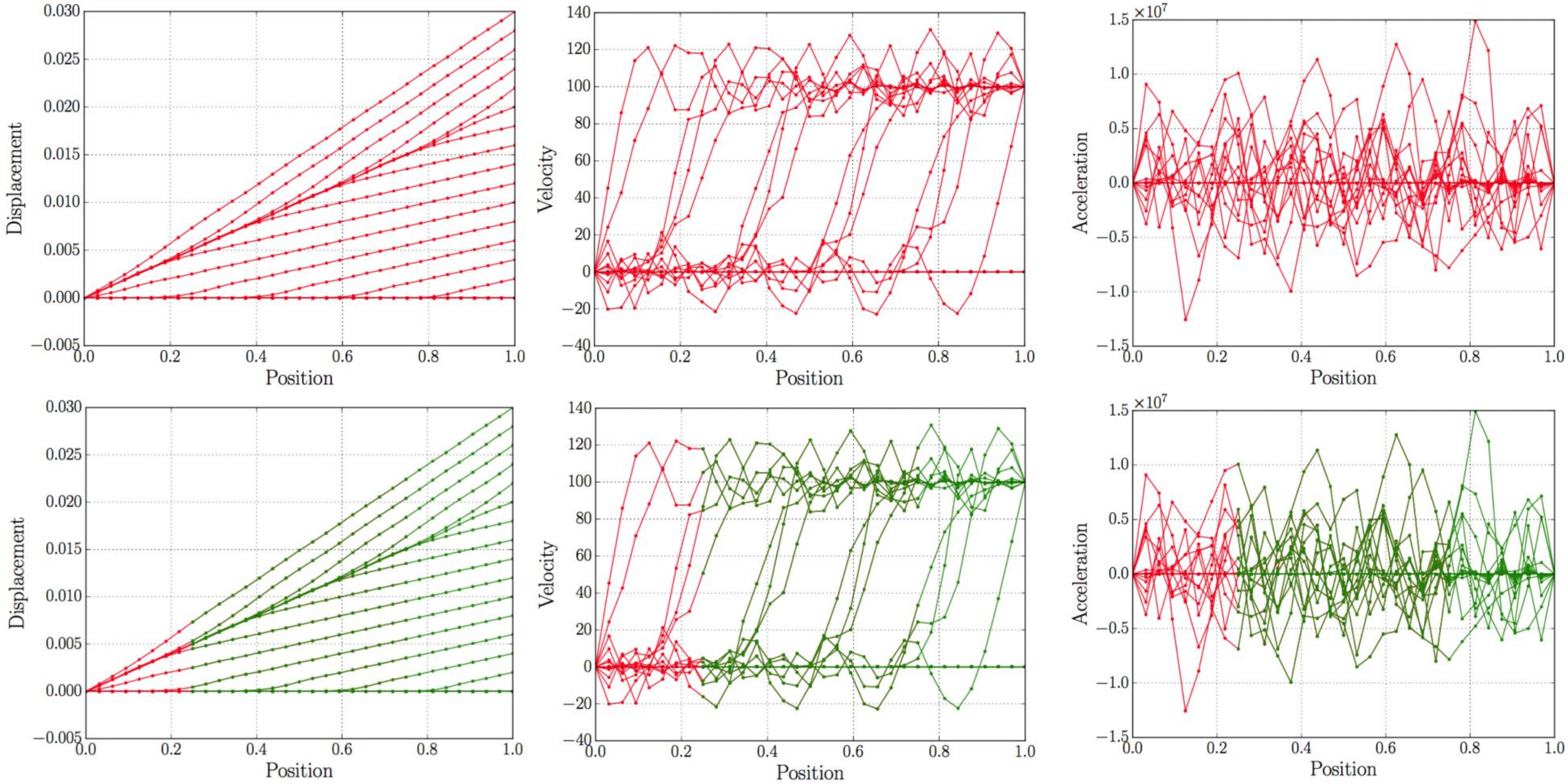
Appendix. A Schwarz-like Time Integrator

- 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.



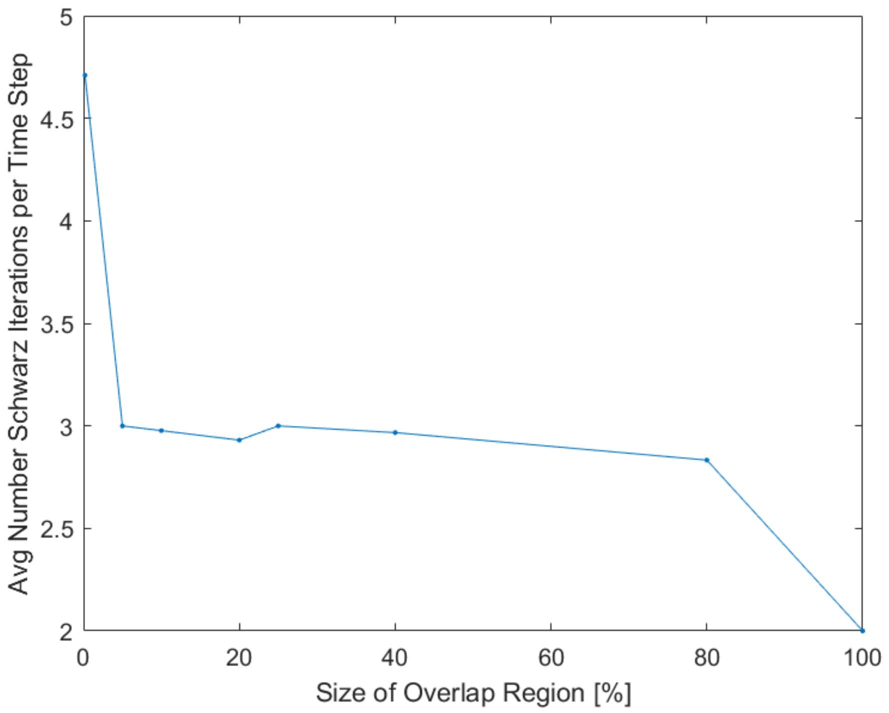
Appendix. Dynamic Singular Bar

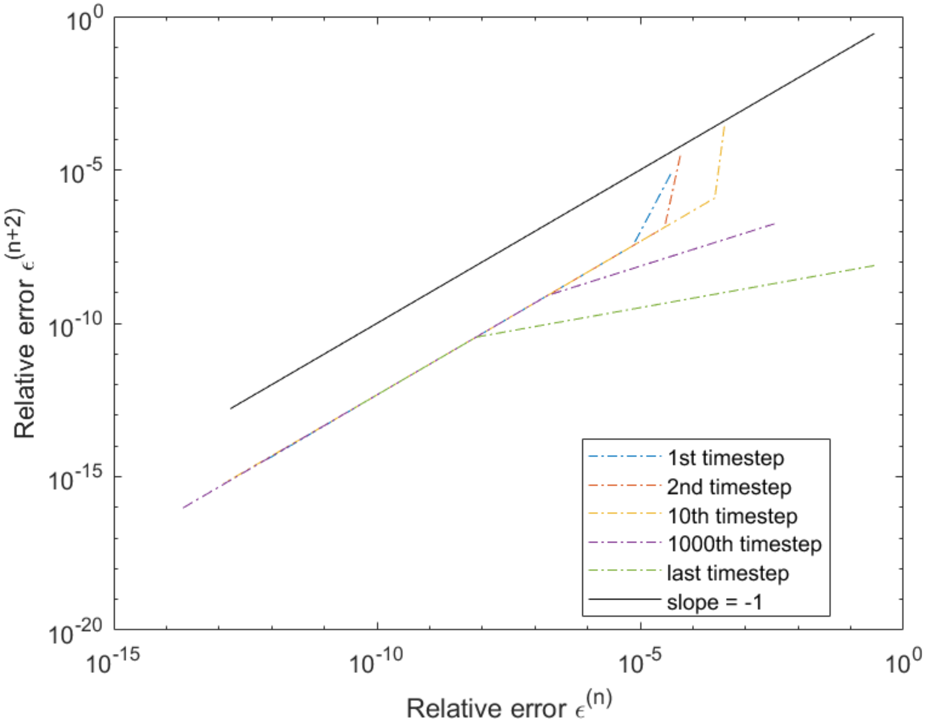
- Inelasticity masks problems by introducing ***energy dissipation***.
- Schwarz does ***not*** introduce ***numerical artifacts***.
- Can couple domains with ***different time integration schemes*** (***Explicit-Implicit*** below).



Appendix. Elastic Wave Propagation

Some Performance Results

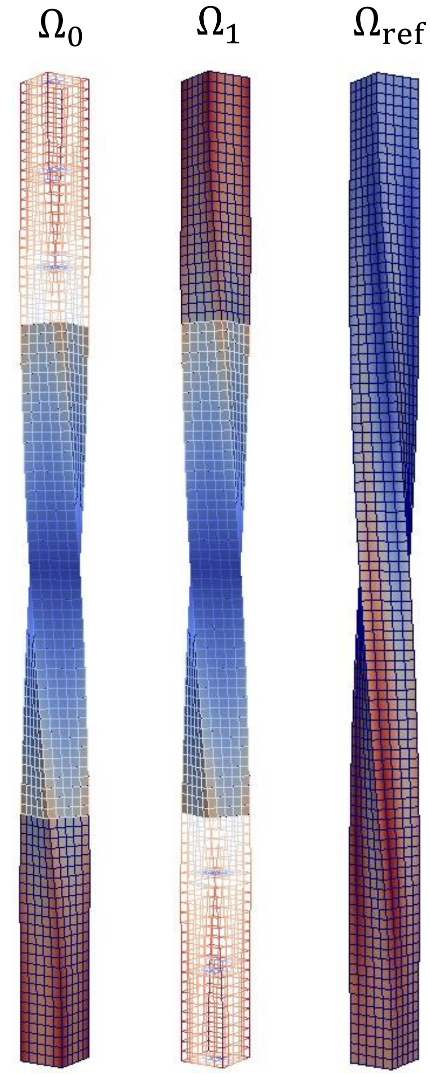




- Left figure shows ***# of iterations*** as a function of ***overlap region size*** for 2 subdomains. The method does not converge for 0% overlap. If the overlap is 100% then the single-domain solution is recovered for each of the subdomains.
- Right figure shows ***linear convergence rate*** of dynamic Schwarz implementation (for small overlap fraction of 0.2%).

Appendix. Torsion

- Nonlinear elastic bar (Neohookean material model) subjected to a high degree of ***torsion***.
- The ***domain*** is $\Omega = (-0.025, 0.025) \times (-0.025, 0.025) \times (-0.5, 0.5)$.
- We evaluate ***dynamic Schwarz*** with 2 subdomains: $\Omega_0 = (-0.025, 0.025) \times (-0.025, 0.025) \times (-0.5, 0.25)$, $\Omega_1 = (-0.025, 0.025) \times (-0.025, 0.025) \times (-0.25, 0.5)$.
- ***Time-discretizations***: Newmark-Beta (implicit, explicit) with same Δt.
- ***Meshes:*** hexes, composite tet 10s.



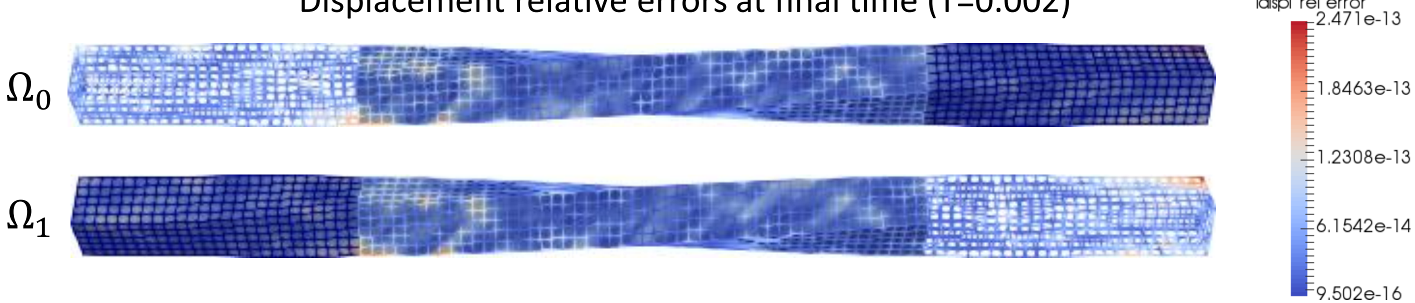
Appendix. Torsion

Schwarz and single-domain results agree to almost ***machine-precision***!

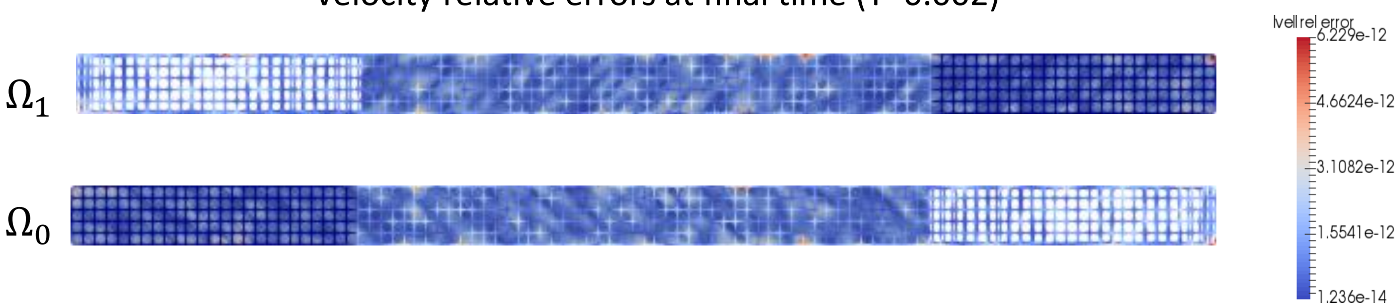
Conformal Hex + Hex Coupling

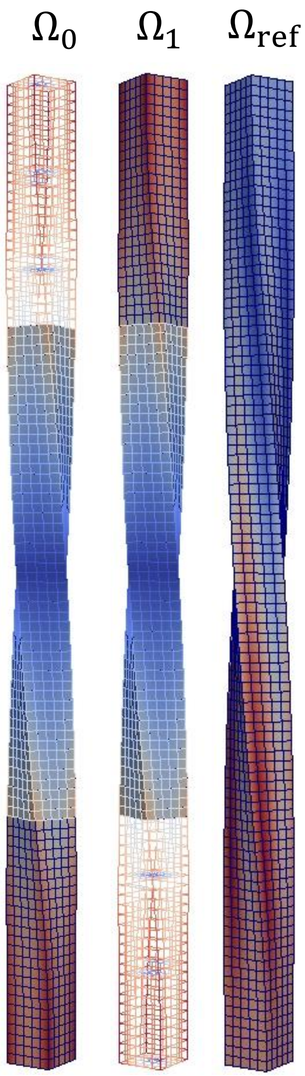
- Each subdomain discretized using **uniform hex mesh** with $\Delta x_i = 0.01$, and advanced in time using implicit Newmark-Beta scheme with Δt =1e-6.
- Results compared to single-domain solution on mesh **conformal** with Schwarz domain meshes.

Displacement relative errors at final time (T=0.002)



Velocity relative errors at final time (T=0.002)





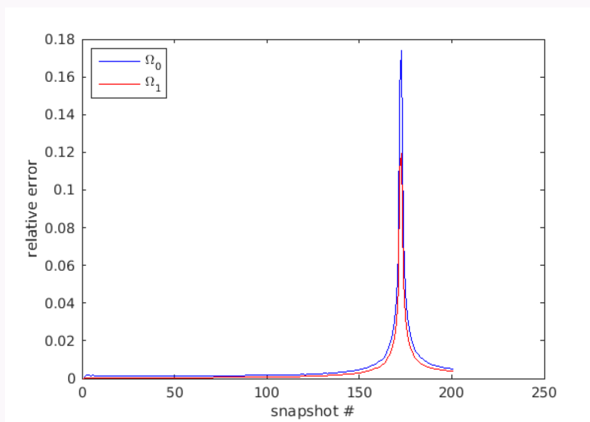
Appendix. Torsion

Hex + Composite Tet 10 Coupling

- Coupling of composite tet 10s + explicit Newmark with consistent mass in Ω_0 with hexes + implicit Newmark in Ω_1.
- Reference solution is computed on fine hex mesh + implicit Newmark Ω_{ref}

Relative error <1% and does not grow in time!

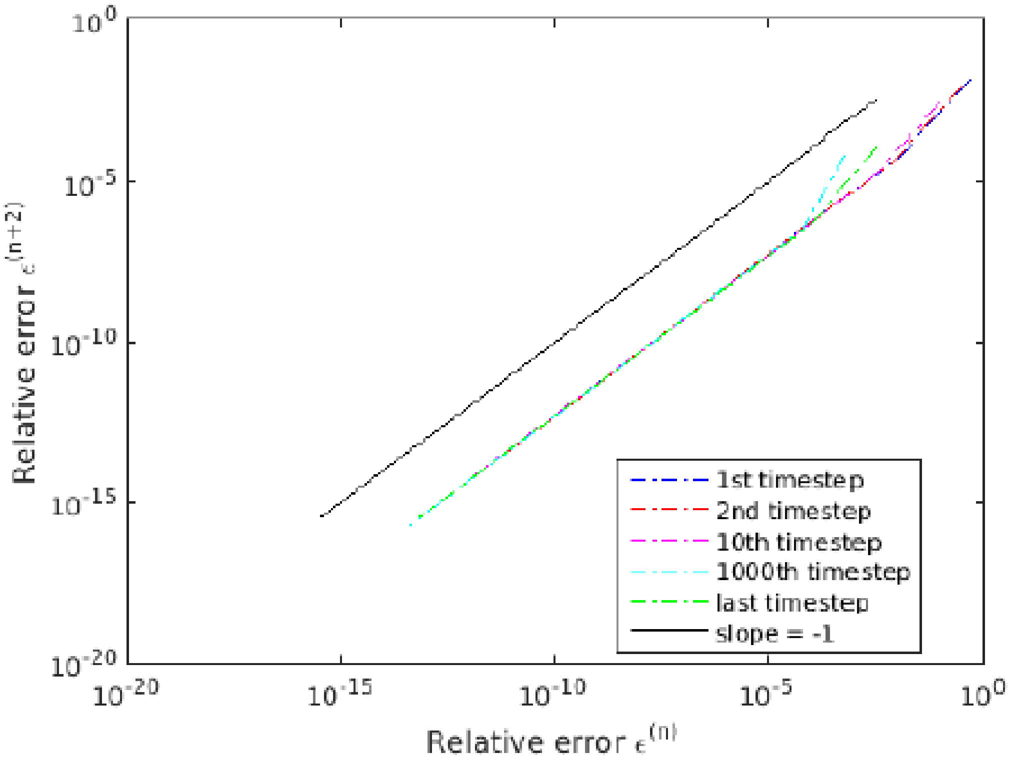
No dynamic artifacts!



Movie of |displacement|
Left: Single-domain,
Right: Schwarz

Appendix. Torsion

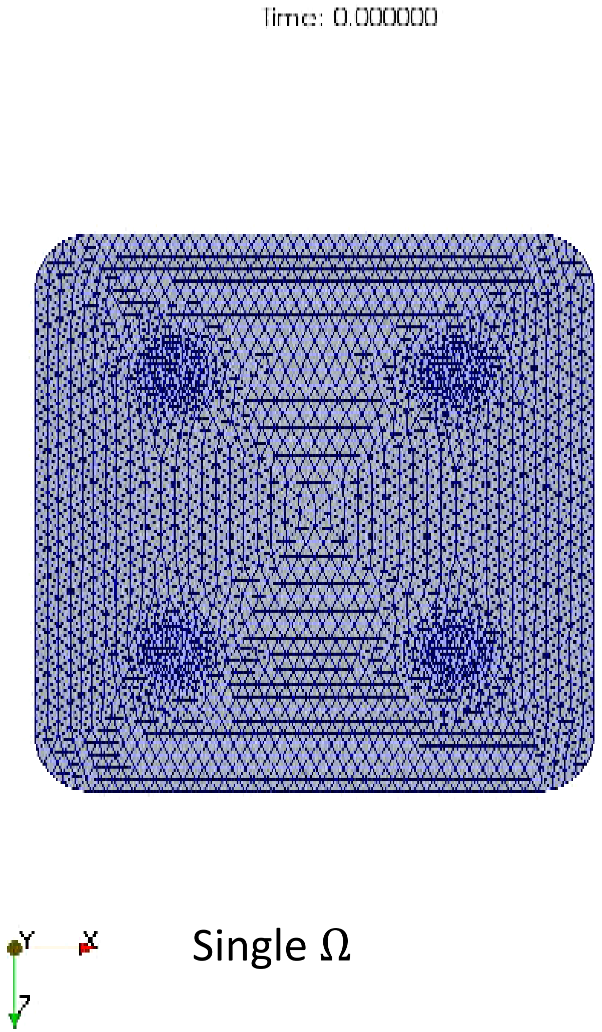
Some Performance Results



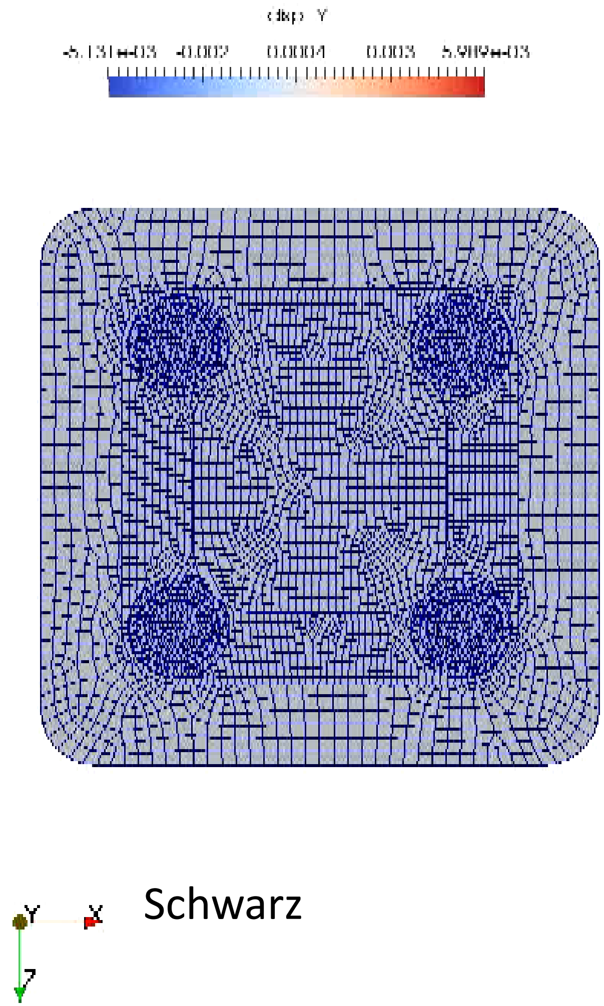
- Convergence behavior of the dynamic Schwarz algorithm for the torsion problem for small overlap volume fraction (2%) in which each subdomain is discretized using a hexahedral mesh. The plot shows that a ***linear convergence rate*** is achieved.

Appendix. Bolted Joint Problem

y-displacement



Single Ω

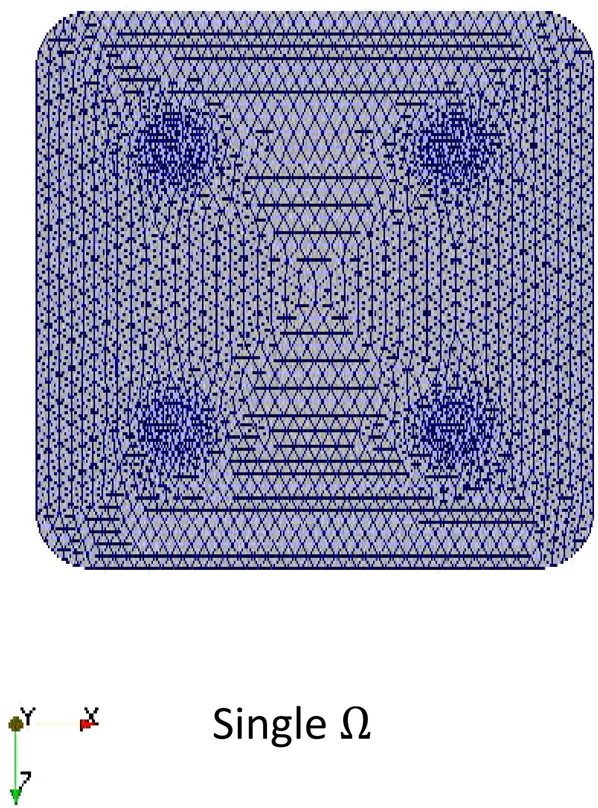


Schwarz

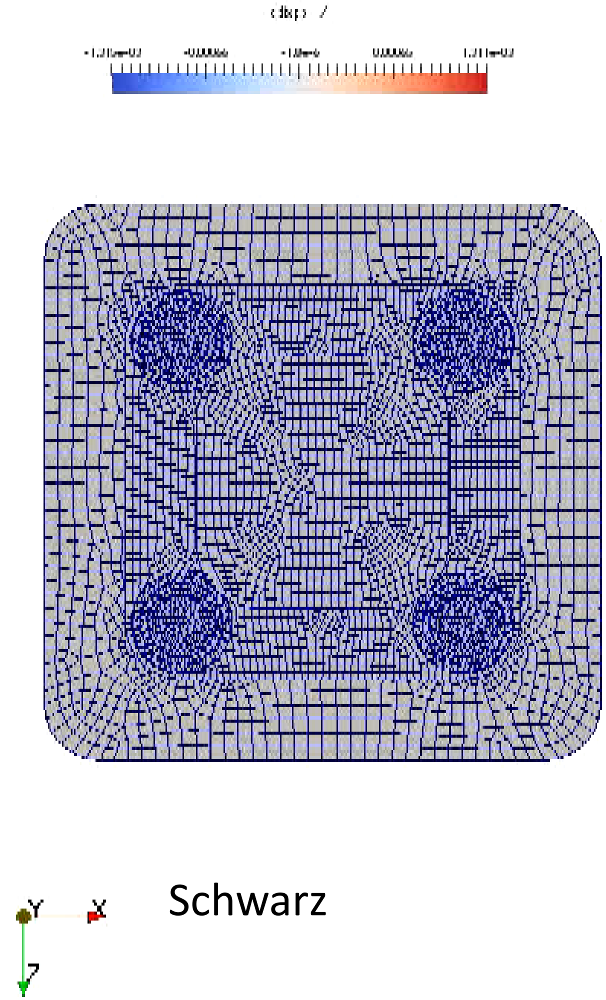
Appendix. Bolted Joint Problem

z-displacement

Time: 0.000000



Single Ω



Schwarz