



The Schwarz Alternating Method for Multiscale Coupling in Solid Mechanics

Alejandro Mota¹, Irina Tezaur¹, Coleman Alleman¹, Greg Phlipot²

¹Sandia National Laboratories, Livermore, CA, USA. ²California Institute of Technology, Pasadena, CA, USA.

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







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Motivation for Concurrent Multiscale Coupling

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

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



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



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.







 Ω_1

Schwarz Alternating Method for Domain Decomposition

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

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.

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

Iterate until convergence:

Initialize:

- 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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Basic Schwarz Algorithm

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

Iterate until convergence:

Initialize:

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

- 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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Basic Schwarz Algorithm

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

Iterate until convergence:

Initialize:

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

- 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 Ω₂) on Ω₁ w/ Dirichlet BCs on Γ₁ that are the values just obtained for Ω₂.
- Schwarz alternating method most commonly used as a *preconditioner* for Krylov iterative methods to solve linear algebraic equations.







Schwarz Alternating Method for Domain Decomposition

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

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

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

Iterate until convergence:

Initialize:

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

- 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 Ω₂) on Ω₁ w/ Dirichlet BCs on Γ₁ that are the values just obtained for Ω₂.
- 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 Sandia Coupling in Quasistatics



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*.

- <u>S. L. Sobolev (1936)</u>: posed Schwarz method for *linear elasticity* in variational form and *proved method's convergence* by proposing a convergent sequence of energy functionals.
- <u>S. G. Mikhlin (1951)</u>: 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 $\Phi[\varphi]$ 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

Four Variants* of Schwarz





Full Schwarz



$1: \boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)} \text{ in } \Omega_1, \boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)}) \text{ on } \partial_{\boldsymbol{\varphi}} \Omega_1, \boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)} \text{ on } \Gamma_1$	\triangleright initialize for Ω_1
2: $\boldsymbol{x}_B^{(2)} \leftarrow \boldsymbol{X}_B^{(2)}$ in $\Omega_2, \boldsymbol{x}_b^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_2, \boldsymbol{x}_{\beta}^{(2)} \leftarrow \boldsymbol{X}_{\beta}^{(2)}$ on Γ_2	\triangleright initialize for Ω_2
$\begin{array}{ccc} \text{3. repeat} \\ \text{4:} & \boldsymbol{x}_{\beta}^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_{\beta}^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_{b}^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_{\beta}^{(2)} \end{array}$	\triangleright project from Ω_2 to Γ_1
5: $\Delta \mathbf{x}_{B}^{(1)} \leftarrow -\mathbf{K}_{AB}^{(1)}(\mathbf{x}_{B}^{(1)}; \mathbf{x}_{b}^{(1)}; \mathbf{x}_{\beta}^{(1)}) \setminus \mathbf{R}_{A}^{(1)}(\mathbf{x}_{B}^{(1)}; \mathbf{x}_{b}^{(1)}; \mathbf{x}_{\beta}^{(1)})$	⊳ linear system
6: $oldsymbol{x}_B^{(1)} \leftarrow oldsymbol{x}_B^{(1)} + riangle oldsymbol{x}_B^{(1)}$	
7: $x_{eta}^{(2)} \leftarrow P_{21}x_{B}^{(1)} + Q_{21}x_{b}^{(1)} + G_{21}x_{eta}^{(1)}$	\triangleright project from Ω_1 to Γ_2
8: $\Delta \boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)}; \boldsymbol{x}_b^{(2)}; \boldsymbol{x}_\beta^{(2)}) \setminus \boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)}; \boldsymbol{x}_b^{(2)}; \boldsymbol{x}_\beta^{(2)})$	⊳ linear system
9: $oldsymbol{x}_B^{(2)} \leftarrow oldsymbol{x}_B^{(2)} + riangle oldsymbol{x}_B^{(2)}$	
$10: \text{ until } \left[\left(\triangle \boldsymbol{x}_B^{(1)} / \boldsymbol{x}_B^{(1)} \right)^2 + \left(\triangle \boldsymbol{x}_B^{(2)} / \boldsymbol{x}_B^{(2)} \right)^2 \right]^{1/2} \le \epsilon_{\text{machine}}$	⊳ tight tolerance

Modified Schwarz



Monolithic Schwarz

Inexact Schwarz

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

Four Variants* of Schwarz



Most performant method: monotonic convergence, theoretical convergence guarantee.



Full Schwarz



\triangleright initialize for Ω_1	1: $\boldsymbol{x}_{B}^{(1)} \leftarrow \boldsymbol{X}_{B}^{(1)}$ in $\Omega_{1}, \boldsymbol{x}_{b}^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_{b}^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_{1}, \boldsymbol{x}_{\beta}^{(1)} \leftarrow \boldsymbol{X}_{\beta}^{(1)}$ on Γ_{1}
\triangleright initialize for Ω_2	2: $\boldsymbol{x}_{B}^{(2)} \leftarrow \boldsymbol{X}_{B}^{(2)}$ in $\Omega_{2}, \boldsymbol{x}_{b}^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_{b}^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_{2}, \boldsymbol{x}_{\beta}^{(2)} \leftarrow \boldsymbol{X}_{\beta}^{(2)}$ on Γ_{2}
▷ Newton-Schwarz loop	3: repeat
\triangleright project from Ω_2 to Γ_1	$\begin{vmatrix} 4: & \bm{x}_{\beta}^{(1)} \leftarrow \bm{P}_{12}\bm{x}_{B}^{(2)} + \bm{Q}_{12}\bm{x}_{b}^{(2)} + \bm{G}_{12}\bm{x}_{\beta}^{(2)} \end{vmatrix}$
⊳ linear system	5: $\Delta \boldsymbol{x}_{B}^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_{B}^{(1)};\boldsymbol{x}_{b}^{(1)};\boldsymbol{x}_{\beta}^{(1)}) \setminus \boldsymbol{R}_{A}^{(1)}(\boldsymbol{x}_{B}^{(1)};\boldsymbol{x}_{b}^{(1)};\boldsymbol{x}_{\beta}^{(1)})$
	6: $\boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{x}_B^{(1)} + riangle \boldsymbol{x}_B^{(1)}$
\triangleright project from Ω_1 to Γ_2	$\left \begin{array}{cc} 7: & m{x}_{eta}^{(2)} \leftarrow m{P}_{21}m{x}_{B}^{(1)} + m{Q}_{21}m{x}_{b}^{(1)} + m{G}_{21}m{x}_{eta}^{(1)} \end{array} ight.$
⊳ linear system	8: $\Delta \boldsymbol{x}_B^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_B^{(2)}; \boldsymbol{x}_b^{(2)}; \boldsymbol{x}_\beta^{(2)}) \setminus \boldsymbol{R}_A^{(2)}(\boldsymbol{x}_B^{(2)}; \boldsymbol{x}_b^{(2)}; \boldsymbol{x}_\beta^{(2)})$
	9: $oldsymbol{x}_B^{(2)} \leftarrow oldsymbol{x}_B^{(2)} + riangle oldsymbol{x}_B^{(2)}$
⊳ tight tolerance	$ \left 10: \text{ 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}} $

Modified Schwarz



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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*.

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 - 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



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



Schwarz Iteration

with Sandia National Laboratories

Cuboid Problem: Convergence with Overlap & Refinement



Cuboid Problem: Schwarz Error





Subdomain	u_3 relative error	σ_{33} relative error	
$\Omega_1 \ \Omega_2$	1.24×10^{-14} 7.30×10^{-15}	$\begin{array}{c} 2.31 \times 10^{-13} \\ 3.06 \times 10^{-13} \end{array}$	





- *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





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



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.

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*.



Quasistatic Example #3: Laser Weld





- 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). •





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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 *spacetime 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 *spacetime discretizations*.

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

Con ②: *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



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

Controller time stepper = convenient checkpoint to facilitate implementation

Controller time stepper

Time integrator for Ω_1

Time integrator for Ω_2



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

<u>Step 1</u>: 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 $T_i + n\Delta t_1$.



Time integrator for Ω_2

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

Integrate using Δt_2

 Ω_2

<u>Step 1</u>: 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 $T_i + n\Delta t_1$.

from Ω_1 to Γ_2

<u>Step 2</u>: 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 $T_i + n\Delta t_2$.


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

<u>Step 1</u>: 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 $T_i + n\Delta t_1$.

<u>Step 2</u>: 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 $T_i + n\Delta t_2$.

<u>Step 3</u>: Check for convergence at time T_{i+1} .



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

<u>Step 1</u>: 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 $T_i + n\Delta t_1$.

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<u>Step 3</u>: Check for convergence at time T_{i+1} .

If unconverged, return to Step 1.



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

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<u>Step 3</u>: Check for convergence at time T_{i+1} .

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



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

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<u>Step 3</u>: Check for convergence at time T_{i+1} .

- ➢ 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) $\Phi[\tilde{\varphi}^{(0)}] \ge \Phi[\tilde{\varphi}^{(1)}] \ge \cdots \ge \Phi[\tilde{\varphi}^{(n-1)}] \ge \Phi[\tilde{\varphi}^{(n)}] \ge \cdots \ge \Phi[\varphi]$, where φ is the minimizer of $\Phi[\varphi]$ over S.
- (b) The sequence $\{\tilde{\varphi}^{(n)}\}\$ defined in (39) converges to the minimizer φ of $\Phi[\varphi]$ in S.
- (c) The Schwarz minimum values $\Phi[\tilde{\varphi}^{(n)}]$ converge monotonically to the minimum value $\Phi[\varphi]$ in 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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Albany

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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: $\Omega_0 = (0,0.001) \times (0.001) \times (0,0.75), \Omega_1 = (0,0.001) \times (0.001) \times (0.25,1).$



Elastic Wave Propagation



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

	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



- For clamped beam problem, total energy (TE = $0.5x^TKx + 0.5\dot{x}^TM\dot{x}$) 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 J₂ 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





*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.



- $\Omega_1 = \text{bolts}$ (composite tet 10), $\Omega_2 = \text{parts}$ (hex).
- Inelastic J₂ material model in both subdomains.
 - Ω_1 : steel
 - Ω_2 : steel component, aluminum (bottom) plate



- 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.







Bolted Joint Problem





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.

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
 - Implementation
 - Numerical Examples
- 4. Summary
- 5. Future Work







Summary



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).



- ③ *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!).
- ③ *"Plug-and-play" framework*: simplifies task of meshing complex geometries!
 - Oblight to couple regions with *different non-conformal meshes*, *different element types* and *different levels of refinement*.
 - ③ Ability to use *different solvers/time-integrators* in different regions.
- ⓒ Coupling does not introduce *nonphysical artifacts.*
- Theoretical convergence properties/guarantees (③ 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 © Springer-Verlag Berlin Heidelberg 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 meshdependent 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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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.

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

Appendix. Full Schwarz Method

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

1: $\boldsymbol{x}_{B}^{(1)} \leftarrow \boldsymbol{X}_{B}^{(1)}$ in $\Omega_{1}, \boldsymbol{x}_{b}^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_{b}^{(1)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_{1}, \boldsymbol{x}_{\beta}^{(1)} \leftarrow \boldsymbol{X}_{\beta}^{(1)}$ on Γ_{1} \triangleright initialize for Ω_1 2: $\boldsymbol{x}_{B}^{(2)} \leftarrow \boldsymbol{X}_{B}^{(2)}$ in $\Omega_{2}, \boldsymbol{x}_{b}^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_{b}^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_{2}, \boldsymbol{x}_{\beta}^{(2)} \leftarrow \boldsymbol{X}_{\beta}^{(2)}$ on Γ_{2} \triangleright initialize for Ω_2 3: repeat ▷ Schwarz loop $oldsymbol{u}^{(1)} \leftarrow oldsymbol{x}_{\mathrm{D}}^{(1)}$ 4: \triangleright for convergence check $m{x}_eta^{(1)} \leftarrow m{P}_{12} m{x}_B^{(2)} + m{Q}_{12} m{x}_b^{(2)} + m{G}_{12} m{x}_eta^{(2)}$ 5: \triangleright project from Ω_2 to Γ_1 \triangleright Newton loop for Ω_1 6: $\triangle \boldsymbol{x}_{B}^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_{B}^{(1)}; \boldsymbol{x}_{b}^{(1)}; \boldsymbol{x}_{\beta}^{(1)}) \backslash \boldsymbol{R}_{A}^{(1)}(\boldsymbol{x}_{B}^{(1)}; \boldsymbol{x}_{b}^{(1)}; \boldsymbol{x}_{\beta}^{(1)})$ 7: \triangleright linear system $oldsymbol{x}_B^{(1)} \leftarrow oldsymbol{x}_B^{(1)} + riangle oldsymbol{x}_B^{(1)}$ 8: until $|| \triangle \boldsymbol{x}_{B}^{(1)} || / || \boldsymbol{x}_{B}^{(1)} || \leq \epsilon_{\text{machine}}$ 9: \triangleright tight tolerance $oldsymbol{y}^{(2)} \leftarrow oldsymbol{x}^{(2)}_B$ 10: \triangleright for convergence check $oldsymbol{x}_eta^{(2)} \leftarrow oldsymbol{P}_{21}oldsymbol{x}_B^{(1)} + oldsymbol{Q}_{21}oldsymbol{x}_b^{(1)} + oldsymbol{G}_{21}oldsymbol{x}_eta^{(1)}$ 11: \triangleright project from Ω_1 to Γ_2 12: \triangleright Newton loop for Ω_2 repeat $\triangle \bm{x}_B^{(2)} \leftarrow -\bm{K}_{AB}^{(2)}(\bm{x}_B^{(2)};\bm{x}_b^{(2)};\bm{x}_\beta^{(2)}) \backslash \bm{R}_A^{(2)}(\bm{x}_B^{(2)};\bm{x}_b^{(2)};\bm{x}_\beta^{(2)})$ 13: \triangleright linear system $oldsymbol{x}_{\mathrm{D}}^{(2)} \leftarrow oldsymbol{x}_{\mathrm{D}}^{(2)} + riangle oldsymbol{x}_{\mathrm{D}}^{(2)}$ 14: until $|| \triangle \boldsymbol{x}_{B}^{(2)} || / || \boldsymbol{x}_{B}^{(2)} || \leq \epsilon_{\text{machine}}$ 15: \triangleright tight tolerance 16: until $\left[\left(||\boldsymbol{y}^{(1)} - \boldsymbol{x}_{B}^{(1)}||/||\boldsymbol{x}_{B}^{(1)}||\right)^{2} + \left(||\boldsymbol{y}^{(2)} - \boldsymbol{x}_{B}^{(2)}||/||\boldsymbol{x}_{B}^{(2)}||\right)^{2}\right]^{1/2} \leq \epsilon_{\text{machine}}$ \triangleright 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*.



Appendix. Monolithic Schwarz Method



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

$$\begin{array}{ll} 1: \ \boldsymbol{x}_{B}^{(1)} \leftarrow \boldsymbol{X}_{B}^{(1)} \text{ in } \Omega_{1}, \ \boldsymbol{x}_{b}^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_{b}^{(1)}) \text{ on } \partial_{\boldsymbol{\varphi}} \Omega_{1}, & \triangleright \text{ initialize for } \Omega_{1} \\ 2: \ \boldsymbol{x}_{B}^{(2)} \leftarrow \boldsymbol{X}_{B}^{(2)} \text{ in } \Omega_{2}, \ \boldsymbol{x}_{b}^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_{b}^{(2)}) \text{ on } \partial_{\boldsymbol{\varphi}} \Omega_{2}, & \triangleright \text{ initialize for } \Omega_{2} \\ 3: \ \mathbf{repeat} & \triangleright \text{ Newton-Schwarz loop} \\ 4: \quad \left\{ \begin{array}{c} \Delta \boldsymbol{x}_{B}^{(1)} \\ \Delta \boldsymbol{x}_{B}^{(2)} \end{array} \right\} \leftarrow \left(\begin{array}{c} \boldsymbol{K}_{AB}^{(1)} + \boldsymbol{K}_{A\beta}^{(1)} \boldsymbol{H}_{11} & \boldsymbol{K}_{A\beta}^{(1)} \boldsymbol{H}_{12} \\ \boldsymbol{K}_{A\beta}^{(2)} \boldsymbol{H}_{21} & \boldsymbol{K}_{AB}^{(2)} + \boldsymbol{K}_{A\beta}^{(2)} \boldsymbol{H}_{22} \end{array} \right) \setminus \left\{ \begin{array}{c} -\boldsymbol{R}_{A}^{(1)} \\ -\boldsymbol{R}_{A}^{(2)} \end{array} \right\} & \triangleright \text{ linear system} \\ 5: \quad \boldsymbol{x}_{B}^{(1)} \leftarrow \boldsymbol{x}_{B}^{(1)} + \Delta \boldsymbol{x}_{B}^{(1)} \\ 6: \quad \boldsymbol{x}_{B}^{(2)} \leftarrow \boldsymbol{x}_{B}^{(2)} + \Delta \boldsymbol{x}_{B}^{(2)} \\ 7: \ \text{ until } \left[\left(||\Delta \boldsymbol{x}_{B}^{(1)}||/||\boldsymbol{x}_{B}^{(1)}|| \right)^{2} + \left(||\Delta \boldsymbol{x}_{B}^{(2)}||/||\boldsymbol{x}_{B}^{(2)}|| \right)^{2} \right]^{1/2} \leq \epsilon_{\text{machine}} \qquad \triangleright \text{ tight tolerance} \end{array}$$

Advantages:

By-passes Schwarz loop.

Disadvantages:

• Off-diagonal coupling terms \rightarrow 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.

$1: \boldsymbol{x}_B^{(1)} \leftarrow \boldsymbol{X}_B^{(1)} \text{ in } \Omega_1, \boldsymbol{x}_b^{(1)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_b^{(1)}) \text{ on } \partial_{\boldsymbol{\varphi}}\Omega_1, \boldsymbol{x}_\beta^{(1)} \leftarrow \boldsymbol{X}_\beta^{(1)} \text{ on } \Gamma_1$	\triangleright initialize for Ω_1
2: $\boldsymbol{x}_{B}^{(2)} \leftarrow \boldsymbol{X}_{B}^{(2)}$ in $\Omega_{2}, \boldsymbol{x}_{b}^{(2)} \leftarrow \boldsymbol{\chi}(\boldsymbol{X}_{b}^{(2)})$ on $\partial_{\boldsymbol{\varphi}}\Omega_{2}, \boldsymbol{x}_{\beta}^{(2)} \leftarrow \boldsymbol{X}_{\beta}^{(2)}$ on Γ_{2} 3: repeat 4: $\boldsymbol{x}_{\beta}^{(1)} \leftarrow \boldsymbol{P}_{12}\boldsymbol{x}_{B}^{(2)} + \boldsymbol{Q}_{12}\boldsymbol{x}_{b}^{(2)} + \boldsymbol{G}_{12}\boldsymbol{x}_{\beta}^{(2)}$	\triangleright initialize for Ω_2 \triangleright Newton-Schwarz loop \triangleright project from Ω_2 to Γ_1
5: $\Delta \boldsymbol{x}_{B}^{(1)} \leftarrow -\boldsymbol{K}_{AB}^{(1)}(\boldsymbol{x}_{B}^{(1)};\boldsymbol{x}_{\beta}^{(1)}) \setminus \boldsymbol{R}_{A}^{(1)}(\boldsymbol{x}_{B}^{(1)};\boldsymbol{x}_{\beta}^{(1)};\boldsymbol{x}_{\beta}^{(1)})$ 6: $\boldsymbol{x}_{B}^{(1)} \leftarrow \boldsymbol{x}_{B}^{(1)} + \Delta \boldsymbol{x}_{B}^{(1)}$	⊳ linear system
7: $\boldsymbol{x}_{\beta}^{(2)} \leftarrow \boldsymbol{P}_{21} \boldsymbol{x}_{B}^{(1)} + \boldsymbol{Q}_{21} \boldsymbol{x}_{b}^{(1)} + \boldsymbol{G}_{21} \boldsymbol{x}_{\beta}^{(1)}$	\triangleright project from Ω_1 to Γ_2
8: $\Delta \boldsymbol{x}_{B}^{(2)} \leftarrow -\boldsymbol{K}_{AB}^{(2)}(\boldsymbol{x}_{B}^{(2)};\boldsymbol{x}_{\beta}^{(2)}) \setminus \boldsymbol{K}_{A}^{(2)}(\boldsymbol{x}_{B}^{(2)};\boldsymbol{x}_{\beta}^{(2)};\boldsymbol{x}_{\beta}^{(2)})$ 9: $\boldsymbol{x}_{B}^{(2)} \leftarrow \boldsymbol{x}_{B}^{(2)} + \Delta \boldsymbol{x}_{B}^{(2)}$	⊳ linear system
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

Considerin Proof of Proof of



A. Moto, I. Tezaut, C. Alleman Schwarz Alternating Method in Solid Mechanics

2 Formulation of the Schwarz Alternating Method

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

2.1 Variational Formulation on a Single Domain

2.1 Variations formations on a single to omain factor is a single to omain factor is a loss of a single to obtain the single to grant a single single

 $\Phi[\varphi] := \int_{\Omega} A(F, Z) dV - \int_{\Omega} RB \cdot \varphi dV - \int_{\Omega \cap \Omega} T \cdot \varphi dS,$ (1)

in which A(F, Z) is the Helmholtz free-mergy density and Z is a collection of internal variables. The weak form of the problem is obtained by minimizing the energy functional $\Phi(\mu)$ over the Sobolev space $W_1(0)$ that is comprised of all functions that are square integrable and have source integrable first derivatives. Define $S := \{\varphi \in W_2^1(\Omega) : \varphi = \chi \text{ on } \partial_{\varphi}\Omega\}$ (2)

and $\mathcal{V} := \{ \xi \in W_2^1(\Omega) : \xi = 0 \text{ on } \partial_{\varphi} \Omega \}$

(3) ν := γξ ∈ W₂(x), ζ = 0 on φ₂(y) = ζ = 0 on φ₂(y) = ζ = φ₁φ₂(y) = φ₁φ₂ + ζξ for all φ₂φ₂(x) = φ₂(x) = φ₂(x) = φ₂φ₂(x) = φ₂φ₂(x) = φ₂φ₂(x) = φ₂φ₂(x) = φ₂(x) = φ

 $D\Phi[\varphi](\xi) = \int_{\Omega} \mathbf{P} : \text{Grad} \, \xi \, dV - \int_{\Omega} R\mathbf{B} \cdot \xi \, dV - \int_{\partial \gamma \Omega} \mathbf{T} \cdot \xi \, dS = 0,$ (4) where $P = \partial A/\partial F$ denotes the first Piola Kirchhoff stress. The Euler-Lagrange equation corresponding to the variational statement (4) is

Div P + RB = 0, in Ω , PN = T, on $\partial_T \Omega$,

(5)

 $\varphi = \chi$, on $\partial_{\varphi} \Omega$. 2.2 Coupling Two or More Subdomains via the Schwarz Alternating Method

In this section, we describe the Solwarz adversaria gradeal test externation for the section of $n \in \mathbb{N}^{0} = \{0, 1, 2, ...\}, \quad i = 2 - n + 2 \left\lfloor \frac{n}{2} \right\rfloor \in \{1, 2\}, \quad j = n + 1 - 2 \left\lfloor \frac{n}{2} \right\rfloor \in \{1, 2\},$ (6)

5

A. Mota, I. Tezaur, C. Allema	n Schwar; Alternating Method	in Solid Mechanics
A Proof of Conve Finite-Deforma	rgence of the Schwarz Alternating Me ttion Inelastic Problem	thod for the
In this section we give a pro- remarks. Assume properties	of of Theorem 1. The proof relies on several properties, j -5 enumerated in Section 3 hold.	presented below as
Remark 1 By the coercivity his functional over S exists, i.e	of $\Phi[\varphi]$, it follows from the Lax-Milgram theorem that a u , the minimization of $\Phi[\varphi]$ is well-posed.	nique minimizer to
Remark 2 By the Stampace	in theorem, the minimization of $\Phi[\varphi]$ in $\mathcal S$ is equivalent to (finding $\varphi \in \mathcal{S}$ such
IMI	$(\Phi'[\varphi], \xi - \varphi) \ge 0$	(51)
or all $\xi \in S$.		
Remark 3 Recall that the st	ict convexity property of $\Phi[\varphi]$ can be written as	
	$\Phi[\psi_2] - \Phi[\psi_1] - (\Phi'[\psi_1], \psi_2 - \psi_1) \ge 0,$	(52)
$\psi_1, \psi_2 \in S$. From (36), rema $n \alpha_R > 0$ such that $\forall \psi_1, \psi_2 \in$	is that if $\Phi[\varphi]$ is strictly convex over $S \forall R \in \mathbb{R}$ such that $R \in K_R$ we have	$l < \infty$, we can find
$\Phi \psi_2$	$ -\Phi[\psi_1] - (\Phi'[\psi_1], \psi_2 - \psi_1) \ge a_R \psi_2 - \psi_1 ^2.$	(53)
Remark 4 By property 5, th	cuniform continuity of $\Phi'[\varphi]$, there exists a modulus of con-	tinuity $\omega > 0$, with
$: X_R \rightarrow X_R$, sten uar	$ \Phi'(\psi_1) - \Phi'(\psi_2) \le \omega(\psi_1 - \psi_2),$	(54)
$\psi_1, \psi_2 \in K_R$. By definition,	$v(\epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$.	
Remark 5 It was shown in	35] that in the case $\Omega_1 \cap \Omega_2 \neq \emptyset$, $\forall \varphi \in S$, there exist ζ_1	$\in S_1$ and $\zeta_2 \in S_2$
Den mar	$\varphi = \zeta_1 + \zeta_2$,	(55)
nd	$\max(\zeta_1 , \zeta_2) \le C_0 \varphi ,$	(56)
or some $C_0 > 0$ independent of	fφ.	
Remark 6 Note that (39) ca	be written as	
(8	$\forall [\hat{\varphi}^{(n)}], \xi^{(i)}) = 0$, for $\hat{\varphi}^{(n)} \in \hat{S}_n, \forall \xi^{(i)} \in S_i$,	(57)
or $i \in \{1, 2\}$ and $n \in \{0, 1, 2,$ of the solution to each minimiz \tilde{S}_n .) (recall from (6) the relation between i and n). This is dation problem over \hat{S}_n and the definition of $\hat{\varphi}^{(v)}$ as the mini-	te to the uniqueness inizer of $\Phi[\varphi]$ over
Benneds 2 (as \$(0) < \$	ad let \$ 6 \$ By Remark 5 there exist \$, 6 \$, and \$, 6 \$	2 march allows

 $(\Phi'[\hat{\omega}^{(n)}], \ell) = (\Phi'[\hat{\omega}^{(n)}], \ell_1 + \ell_2),$ (58)

34



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that is i = 1 and j = 2 if n is odd, and i = 2 and j = 1 if n is even. Introduce the following definitions for each subdomain i:			
 Closure: \$\overline{a}\$ > \$\overline{a}\$ / \$ 			
Dirichlet boundary: @ III) := @ III) III).			
 Neumann boundary: @ ID := @ ID1 ID. 			
 Schwarz boundary: Γ_i := @lo 1 IIQ. 			
Note that with these definitions we guarantee that $\otimes i \otimes i \otimes i \otimes j \otimes j = j$, $\otimes i \otimes i \cap j = j$ and $\otimes i \otimes i \cap j = j$. Now define the spaces			
$S_i := \{ ' \ 2 \ W_2^1(\mathbb{Z}) : ' = \chi \text{ on } \otimes \mathbb{Z}_{i}, ' = P_{\mathbb{Z}_i / \Gamma_i} ['(\mathbb{Z}_i)] \text{ on } \Gamma_i \}$ (7)			
and			
$V_i := \{ e^2 W_2^i(20) : e = 0 \text{ on } @ 20 [\Gamma_i],$ (8)			
where the symbol P_{α_1} , r_1 () downloar the projection (from the acbidomian its) onto the Schwarz boundary (r_1 . This projection operating plays a contrain of the Schwarz about significant the advector and implementation are discussed in subsequent sections. For the moment it is sufficient to assume that the operator is able to project a lefed '' from one subsequent sections is the Schwarz boundary of the other subsequent sections ('') The Schwarz attracting method schwarz boundary of the other subsequent ('). The solution '' (o) for the			
8 S			
rid for n = 0			
$(\alpha) = \frac{\langle id_{\chi}, for n = 0;}{: \arg \min_{2 \leq \alpha} \Phi_i(')}, for n > 0;$ (9)			
$(a) = \frac{\langle id_X, for n = 0, \\ r_{2E} = \frac{\langle id_X, for n > 0, \\ r_{2E} = $			
(ii) ≤ 0 = 0 (ii) (iii)			
$\begin{array}{c} \cdot (u_{i}^{-1} & \mathrm{ch}^{-1}, & \mathrm{ch}^{$			

A. Mota, I. Tezaur, C. Alleman	Schwarz Alternating Method in Solid Mech	unic)
By (57), $(\Phi'[\hat{\varphi}^{(w-1)}], \zeta_2) = 0$. Hence,		
$(\Phi'[\phi^{(\alpha)}],\zeta_1+\zeta_2)=(\Phi'[\phi^{(\alpha)}],\zeta_1+\zeta_2)-(\Phi'[\phi^{(\alpha-1)}],\zeta_1+\zeta_2)-(\Phi'[\phi^{($	$[0], \zeta_2) = (\Phi'[\phi^{(\alpha)}], \zeta_2) - (\Phi'[\phi^{(\alpha-1)}], \zeta_2),$	(59)
since $(\Phi^{i}[\hat{\varphi}^{(n)}], \zeta_{1}) = 0$, also by (57). By the Cauchy-Sch	warz inequality,	
$(\Phi'[\phi^{(n)}],\zeta_2)-(\Phi'[\phi^{(n-1)}],\zeta_2)=(\Phi'[\phi^{(n)}]-\Phi'[\phi^{(n)}]$	$ -1 $, $\zeta_2) \le \Phi'[\phi^{(n)}] - \Phi'[\phi^{(n-1)}] \cdot \zeta_2 .$	(60)
Again using (57) and also (58) in (60) leads to		
$(\Phi'[\phi^{(u)}] - \Phi'[\phi^{(u-1)}], \xi_2) = (\Phi'[\phi^{(u)}], \xi)$	$ \le \Phi'[\tilde{\varphi}^{(n)}] - \Phi'[\tilde{\varphi}^{(n-1)}] \cdot \zeta_2 .$	(61)
and substituting (56) into (61) we finally obtain that		
$(\Phi'[\hat{\varphi}^{(n)}], \xi) \le C_0[\Phi'[\hat{\varphi}^{(n)}]]$	$-\Phi'[\hat{\varphi}^{(n-1)}] \cdot \xi ,$	(62)
$\forall \xi \in S.$		
Remark 8 For part (d) of Theorem 1, recall the definition	on of geometric convergence:	
$E_{n+1} \le C$	E_n ,	(63)
$\forall n \in \{0, 1, 2,\}$ for some $C > 0$, where		
$E_n := \phi^{(n+1)} $	$-\phi^{(n)} .$	(64)
Remark 9 Recall from the definition of continuity that there exists a constant $K \ge 0$ such that	if $\Phi^{i}[\varphi]$ is Lipshitz continuous at $\tilde{\varphi}^{(a)}$ near φ	, then
$\frac{ \Phi'[\phi^{(u)}] - \Phi'[}{ \phi^{(u)} - \phi }$	$\frac{\rho }{ } \le K.$	(65)
Considering that $\Phi'[\varphi] = 0$ since φ is the minimizer of Φ	$[\varphi]$, (65) is equivalent to	
$ \Phi'[\varphi^{(n)}] \le K $	$\phi^{(u)} = \phi .$	(65)
Proof of Theorem 1		
$\begin{split} & Preof of (a). \mbox{ Let } \hat{\varphi}^{(1)} = \arg\min_{\psi \in \hat{\mathcal{S}}_1} \Phi[\varphi]. \mbox{ By } (40), \\ & \text{ and suppose } \Phi[\hat{\varphi}^{*}] > \Phi[\hat{\varphi}^{(1)}]. \mbox{ But this is a contradiction } \\ & \text{ that } \Phi[\hat{\varphi}^{(1)}] < \Phi[\hat{\varphi}^{(2)}] \mbox{ where } \hat{\varphi}^{(2)} = \arg\min_{\psi \in \hat{\mathcal{S}}_1} \Phi[\varphi] \end{split}$	$\hat{S}^{(1)} \in \hat{S}_2$. Let $\hat{\varphi}^*$ be the minimizer of $\Phi(\varphi)$ ov 1, since we can take $\hat{\varphi}^* = \hat{\varphi}^{(1)}$. Hence, it can be follows by induction that	er Ŝ ₂ 101 be
$\Phi(\hat{\varphi}^{(n)}) \leq \Phi$	$[\hat{\varphi}^{(n-1)}]$	(67
for $n \in \{1, 2, 3,\}$. Now let φ be the minimizer of i unique. Hence $\Phi[\varphi] \leq \Phi[\hat{\varphi}^{(n)}]$ for all $n \in \{1, 2, 3,\}$	$\mathbb{P}[\varphi]$ over S . Since the problem is well-posed.	iφi □

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▷ initialize for Ω ₂ ▷ Newton-Schwarz loop
P ADVOD-SCINIZZ (reg
to linear system
> tight tolerance

[35, 34, 4]. Although we do not provide here formal convergence proofs for the remaining variants of the Schwarz method, we offer some numerical results illustrating their convergence in Section 4. Consider the energy functional $\Phi[\phi]$ defined in (1). We will denote by $\langle \cdot, \cdot \rangle$ the usual L^2 inner product m = 0 when it. over Ω , that is, $(\psi_1, \psi_2) := \int_{-}^{-} \psi_1 \cdot \psi_2 \, dV,$ (35) for $\psi_1, \psi_2 \in W_2^1(\Omega)$, with corresponding nerm $\|\cdot\|_{\infty}^{-1}$ proof of the convergence of the Schwarz alternating method requires that the functional $\Phi[\varphi]$ satisfy the following properties over the space S defined in (2): 1. $\Phi[\varphi]$ is coercive. 2. $\Phi[\varphi]$ is Fréchet differentiable, with $\Phi'[\varphi]$ denoting its Fréchet derivative. Φ[φ] is strictly convex. 4. $\Phi[\varphi]$ is lower semi-contin 5. $\Phi'[\phi]$ is uniformly continuous on $\mathcal{K}_{\mathrm{R}},$ where $\mathcal{K}_R := \{ \varphi \in S : \Phi[\varphi] < R, R \in \mathbb{R}, R < \infty \}$. (36) It can be shown that the energy functional $\vartheta(\varphi)$ defined in (1) is strictly convex in S (property 3) provided that the Helmholtz free-energy density $\mathcal{A}(F, Z)$ is a quasi-convex function of F [26]. Properties 1, 2, 4 and 5 follow from the strict convexity of $\vartheta(\varphi)$. Next, then we conditional sets of spaces $\hat{S}_{n} := \left\{ \varphi \in S : \varphi = P_{\Omega_{i} \to \Gamma_{1}} | \varphi^{(n-1)}(\Omega_{j}) \right\} \text{ on } \Gamma_{i}, \varphi = \varphi^{(n-1)} \text{ on } \Omega \setminus \Omega_{i} \right\},$ (37) and $\tilde{V}_i := \{ \xi \in S : \xi = 0 \text{ in } \Omega \setminus \Omega_i \},\$ (38)

where i = 1 and j = 2 if n is odd, and i = 2 and j = 1 if n is even for $n \in \{1, 2, ...\}$ as given by (6) and with the function $q^{(0)} \in S$ an initial gauss. Note that the spaces S_n in (37) are extensions of the spaces S_n in (7) to the entities domain 10. With this notation in place, the solution to be -nd problem $(9) \leftarrow (13)$ and be recarded as (12) + (12 $\bar{\varphi}^{(n)} = \begin{cases} \mathrm{id}_{\boldsymbol{X}}, & \text{for } n = 0; \\ \arg\min_{\boldsymbol{w} \in \mathcal{N}} \Phi[\varphi], & \text{for } n > 0. \end{cases}$ (39)

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Proof of (b) By (a) $\Phi(3(2)) \rightarrow 1$ as $n \rightarrow \infty$ for m	ma $l \in \mathbb{R}$. Now, combining (51) and (53), we have the
bound	the first restriction of the second states of the second
$\Phi[\hat{\varphi}^{(n)}] - \Phi[\hat{\varphi}^{(n+1)}] \ge \Phi[\hat{\varphi}^{(n)}] - \Phi[\hat{\varphi}^{(n+1)}] - \left(e^{i\theta_n - 1} - e^{i\theta_n - 1} \right) = 0$	$\Psi[\tilde{\varphi}^{(n+1)}], \tilde{\varphi}^{(n)} - \tilde{\varphi}^{(n+1)}) \ge \alpha_B \tilde{\varphi}^{(n)} - \tilde{\varphi}^{(n+1)} ^2,$ (68)
for all $n \in \{1, 2, 3,\}$. Since $\Phi[\tilde{\varphi}^{(n)}] \rightarrow l$ as $n \rightarrow$	∞ , it follows that $\Phi[\hat{\varphi}^{(n)}] - \Phi[\hat{\varphi}^{(n+1)}] \rightarrow 0$ as $n \rightarrow \infty$.
From (68), we have that $\lim_{n\to\infty} \hat{\varphi}^{(n)} -$	$-\tilde{\varphi}^{(n+1)} ^2 = 0,$ (69)
from which we can conclude that $\hat{\varphi}^{(n)} - \hat{\varphi}^{(n+1)} \rightarrow$ We must now show that $\hat{\varphi}^{(n)}$ converges to φ , if $\psi_2 = \hat{\varphi}^{(n)}$, we have	0 as $n\to\infty.$ he minimizer of $\Phi[\phi]$ on ${\cal S}.$ By (53) with $\psi_1=\phi$ and
$ \varphi - \tilde{\varphi}^{(n)} ^2 \le \frac{1}{\alpha_R} \left\{ \Phi[\varphi] - \Phi[\varphi] - \Phi[\varphi] - \Phi[\varphi] \right\}$	$\theta[\hat{\varphi}^{(n)}] = \left(\Phi'[\hat{\varphi}^{(n)}], \varphi - \hat{\varphi}^{(n)} \right) \right\}.$ (70)
Since φ is the minimum of $\Phi[\varphi]$, by (a) we have th	at $\Phi[\varphi] \le \Phi[\tilde{\varphi}^{(n)}]$. It follows that
$-\Phi[\varphi]-\Phi[\bar{\varphi}^{(n)}]-\left(\Phi'[\bar{\varphi}^{(n)}],\varphi-\bar{\varphi}^{(n)}\right)\leq -\left($	$\Phi'[\hat{\varphi}^{(n)}], \varphi - \hat{\varphi}^{(n)} = (\Phi'[\hat{\varphi}^{(n)}], \hat{\varphi}^{(n)} - \varphi).$ (71)
Substituting (71) into (70) we have	
$ \varphi - \overline{\varphi}^{(n)} ^2 \le \frac{1}{\alpha_R}$	$(\Phi' \bar{\varphi}^{(n)} , \bar{\varphi}^{(n)} - \varphi).$ (72)
Now by (62) (Remark 7),	
$\left(\Phi'[\tilde{\varphi}^{(n)}], \tilde{\varphi}^{(n)} - \varphi\right) \le C_0 \Phi' $	$[\tilde{\varphi}^{(n)}] = \Phi'[\tilde{\varphi}^{(n-1)}] \cdot \tilde{\varphi}^{(n)} - \varphi .$ (73)
Substituting (73) into (72) leads to	
$ \tilde{\varphi}^{(\alpha)} - \varphi \le \frac{C_0}{\alpha_R} $	$\Phi'[\hat{\varphi}^{(n)}] - \Phi'[\hat{\varphi}^{(n-1)}] .$ (74)
Applying the uniform continuity assumption (54), w	e obtain
$ \hat{\varphi}^{(n)} - \varphi \le \frac{C_0}{\alpha_H}$	$\omega \left(\tilde{\varphi}^{(n)} - \tilde{\varphi}^{(n-1)} \right).$ (75)
By (69), $ \tilde{\varphi}^{(n)} - \tilde{\varphi}^{(n-1)} \rightarrow 0$ as $n \rightarrow \infty$. From $n \rightarrow \infty$.	n this we obtain the result, namely that $\hat{\varphi}^{(v)} ightarrow \varphi$ as
Proof of (c). This follows immediately from (a) and	i (b).
Proof of (d). By (b), for large enough n, there exist	s some $C_1 > 0$ independent of n such that
$ \phi^{(n)} - \phi ^2 \le 0$	$C_1 \hat{\varphi}^{(n+1)} - \hat{\varphi}^{(n)} ^2.$ (76)
Let us choose C_1 such that $C_1 > \alpha_R/K$, where K (68) with (76) leads to	is the Lipshitz continuity constant in (66). Combining
$\frac{1}{\alpha_N} \left(\Phi[\hat{\varphi}^{(n)}] - \Phi[\hat{\varphi}^{(n+1)}] \right) \ge _{\hat{\theta}}$	$\hat{\varphi}^{(n+1)} - \hat{\varphi}^{(n)} ^2 \ge \frac{1}{C_1} \hat{\varphi}^{(n)} - \varphi ^2.$ (77)

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Remark that [50] $\hat{\mathcal{S}}_n = \hat{\varphi}^{(n-1)} + \hat{\mathcal{V}}_i \quad \text{for} \quad \hat{\varphi}^{(n-1)} \in \hat{\mathcal{S}}_{n-1} \Rightarrow \hat{\varphi}^{(n-1)} \in \hat{\mathcal{S}}_n.$ (40) **Theorem 1.** Assume that the energy functional $\Phi(\varphi)$ ratisfies properties $l \rightarrow 3$ above. Consider the Schwarz alternating method of Section 2 defined by (9)–(13) and its equivalent form (39). Then $(a) \ \Phi[\hat{\varphi}^{(0)}] \geq \Phi[\hat{\varphi}^{(1)}] \geq \cdots \geq \Phi[\hat{\varphi}^{(n-1)}] \geq \Phi[\hat{\varphi}^{(n)}] \geq \cdots \geq \Phi[\varphi], \text{ where } \varphi \text{ is the minimizer of } \Phi[\varphi]$ (b) the sequence $\{\tilde{\varphi}^{(n)}\}$ defined in (39) converges to the minimizer φ of $\Phi[\varphi]$ in S.

(c) the Schwarz minimum values $\Phi[\vec{\varphi}^{(n)}]$ converge monotonically to the minimum value $\Phi[\varphi]$ in S starting from any initial guess $\vec{\varphi}^{(0)}$.

(d) if Φ[†](φ) is Lipschit; continuous in a neighborhood of φ, then the sequence {φ^(ψ)} converges geometrically to the minimizer φ². Proof. See Appendix A. п

Finally, while most of works cited above present their analysis for the specific case of two subdomains extension to multiple subdomains is in general straightforward. The case of multiple subdomains is considered specifically in Liesen [35], Baler [4], and Li Shan and Faran [34].

4 Numerical Examples

Interactive Learning to the second second

4.1 Implementation

The four variants of the Schwarz alternating method described in Section 2.4 have been implemented in a non-dimensional MATLAN code. The objective is to determine the convergence behavior, efficiency, and performance of each variant. This code has been optimized both in terms of memory usage and essecution record.

eeed. In addition, the Modified variant of the Schwarz alternating method described in Section 2.4 has been generated in ALBANY, an oppressure multiphysics research platform developed mainly at Sandia National ³See Remark 3 in the Appendix for a definition of generatic consequence. 15

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Using the identity $\Phi[\hat{\varphi}^{(n)}] - \Phi[\hat{\varphi}^{(n+1)}] = (\Phi[\hat{\varphi}^{(n)}] - \Phi[\varphi]) - that$	$\left(\Phi[\hat{\varphi}^{(\alpha+1)}] - \Phi[\varphi]\right)$, it follows from (77)
$\left(\Phi[\phi^{(n)}] - \Phi[\phi]\right) - \left(\Phi[\phi^{(n+1)}] - \Phi[\phi]\right)$	$\geq \frac{\alpha_R}{C_1} \hat{\varphi}^{(n)} - \varphi ^2.$ (78)
Substituting $\psi_1 = \phi^{(\alpha)}$ and $\psi_2 = \phi$ into (53) and rearranging, w	e obtain
$\left(\Phi'[\phi^{(n)}], \varphi - \phi^{(n)}\right) \le \left(\Phi'[\phi^{(n)}], \varphi - \phi^{(n)}\right) + \alpha_R$	$ \varphi - \hat{\varphi}^{(n)} \le \Phi \varphi - \Phi [\hat{\varphi}^{(n)}]$ (79)
since $\alpha_R \geq 0.$ Now, by the Cauchy-Schwarz inequality followed b of $\Phi'[\varphi]$ (66) we can write	y the application of the Lipshitz continuity
$\left(\Phi' \hat{\varphi}^{(n)}), \varphi - \hat{\varphi}^{(n)}\right) \le \Phi' \hat{\varphi}^{(n)} \cdot \varphi - \hat{\varphi} $	$ m \le K \varphi - \hat{\varphi}^{(u)} ^3$. (80)
Hence, from (79), $\Phi[\partial^{(n)}] - \Phi[\omega] \leq K \partial^{(n)} $	- all ² (81)
Moreover, by (53) since $\Phi'[\varphi] = 0$,	
$\Phi[\hat{\varphi}^{(n)}] - \Phi[\varphi] \ge \alpha_B[\hat{\varphi}^{(n)}]$	$-\varphi ^2$. (82)
Using (81) and (82) we obtain	
$\left(\Phi[\hat{\varphi}^{(n)}] - \Phi[\varphi]\right) - \left(\Phi[\hat{\varphi}^{(n+1)}] - \Phi[\varphi]\right) \le K \hat{\varphi}^{(n+1)} $	$ \dot{\varphi} ^{2} - \varphi ^{2} - \alpha_{R} \dot{\varphi}^{(n+1)} - \varphi ^{2}$. (83)
Combining (83) and (78) leads to	
$\frac{\alpha_R}{C_1} \vec{\varphi}^{(u)} - \varphi ^2 \leq \left(\Phi[\vec{\varphi}^{(u)}] - \Phi[\varphi] \right) - \left(\Phi[\vec{\varphi}^{(u+1)}] - \Phi[\varphi] \right)$	$\leq K \phi^{(n)} - \phi ^2 - \alpha_R \phi^{(n+1)} - \phi ^2$. (84)
or $ \dot{\varphi}^{(n+1)} - \varphi \leq B \dot{\varphi}^{(n)} $	- $\varphi $ (85)
with $B := \sqrt{\frac{K}{\alpha_F} - \frac{1}{C_1}},$	(86)
and $B \in \mathbb{R}$ as we chose $C_1 > \alpha_R/K$. Furthermore, since the seq the minimizer φ of $\Phi[\varphi]$ by (b) and (c), it follows that $B \in (0, 1)$	uence $\{\phi^{(n)}\}$ converges monotonically to 1). Define $C := 1 - B \in (0, 1)$, then (85)
can be recast as $ \hat{\varphi}^{(n+1)} - \hat{\varphi}^{(n)} \le C \hat{\varphi}^{(n)} -$	$\hat{\varphi}^{(n-1)}$ (87)
whereupon the claim is proven.	0
B Analytic Solution for Linear-Elastic Sit	ngular Bar
As reference, herein we provide the solution of the singular ba equilibrium equation is	r of Section 4.3 for linear elasticity. The
$P=\sigma(X)A(X)={\rm const.}, \sigma(X)=E\epsilon(X), e(X):=$	$u'(X)$, $A(X) = A_3 \left(\frac{X}{L}\right)^{\frac{3}{2}}$, (88)
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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.



- 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 Varia



Appendix. Notched Cylinder: HEX-HEX Coupling



Appendix. Notched Cylinder: Nonconform



Appendix. Notched Cylinder: Nonconform



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



Appendix. Parallelization via DTK: Strong Scaling on Cubes Problem



Appendix. Rubiks Cube Problem





Appendix. Tensile Bar





ASTM tensile geometry

Appendix. Tensile Bar: Meso-Macroscale

Mesoscale

SPARKS-generated microstructure (F. Abdeljawad)

cubic elastic constant : $C_{11} = 204.6$ GPa cubic elastic constant : $C_{12} = 137.7$ GPa cubic elastic constant : $C_{44} = 126.2$ GPa

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

rate sensitivity factor : m = 20

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

initial hardness : $g_0 = 90$ MPa

saturation hardness : $g_s = 202 \text{ MPa}$

saturation exponent : $\omega = 0.01$

Fix microstructure, investigate ensembles





Load microstructural ensembles in uniaxial stress
 Fit flow curves with a macroscale J₂ plasticity model



Appendix. Tensile Bar: Results





Appendix. Schwarz Alternating Method for Dynamics



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 Distance

- 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).





- 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

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 $\Delta t = 1e-6$.
- Results compared to single-domain solution on mesh conformal with Schwarz domain meshes.



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

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 Ω_{ref}

 Ω_0

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}



 Ω_1

 Ω_0

 $\Omega_{\rm ref}$



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

Time: 0.000000

disp Y

-5.131++03 -0.002 0.00014 0.003 5.989+03









Schwarz

Appendix. Bolted Joint Problem

z-displacement

Time: 0.000000







Schwarz

disp /

1.211+-02