The Schwarz Alternating Method for Multiscale Coupling in Solid Mechanics

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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

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NEW!

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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.
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.

**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 $\Omega_1$ w/ initial guess for Dirichlet BCs on $\Gamma_1$.

**Iterate until convergence:**
- Solve PDE by any method (can be different than for $\Omega_1$) on $\Omega_2$ w/ Dirichlet BCs on $\Gamma_2$ that are the values just obtained for $\Omega_1$.
- Solve PDE by any method (can be different than for $\Omega_2$) on $\Omega_1$ w/ Dirichlet BCs on $\Gamma_1$ that are the values just obtained for $\Omega_2$. 
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**Requirement for convergence:** $\Omega_1 \cap \Omega_2 \neq \emptyset
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- Schwarz alternating method most commonly used as a *preconditioner* for Krylov iterative methods to solve linear algebraic equations.

H. Schwarz (1843 – 1921)
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**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

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 $\Phi[\varphi]$ defined below), and determined a *geometric convergence rate* for the finite deformation quasi-static problem.

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

\[
\nabla \cdot P + B = 0
\]

*S. L. Sobolev (1908 – 1989)*

*S. G. Mikhlin (1908 – 1990)*

*A. Mota, I. Tezaur, C. Alleman*
Four Variants* of Schwarz

Full Schwarz

1. $x_1^{(1)} \leftarrow X_1^{(1)}$ in $\Omega_1$, $x_1^{(1)} \leftarrow \chi(X_1^{(1)})$ on $\partial \Omega_1$, $x_1^{(1)} \leftarrow X_1^{(1)}$ on $\Gamma_1$
2. $x_2^{(1)} \leftarrow X_2^{(1)}$ in $\Omega_2$, $x_2^{(1)} \leftarrow \chi(X_2^{(1)})$ on $\partial \Omega_2$, $x_2^{(1)} \leftarrow X_2^{(1)}$ on $\Gamma_2$
3. repeat
4. $y^{(1)} \leftarrow x_1^{(1)}$
5. $x_1^{(n+1)} \leftarrow P_2 y^{(1)} + Q_{12} x_2^{(1)} + G_{12} x_2^{(1)}$
6. repeat
7. $\Delta x_1^{(1)} \leftarrow -K_{12}^{A1}(x_1^{(1)}; x_2^{(1)}; x_2^{(1)})R_{A1}^{2}(x_2^{(1)}; x_2^{(1)}; x_2^{(1)})$
8. $x_1^{(n+1)} \leftarrow x_1^{(n+1)} + \Delta x_1^{(1)}$
9. until $||\Delta x_1^{(1)}||/||x_1^{(1)}|| \leq \varepsilon_{\text{machine}}$
10. $y^{(1)} \leftarrow x_1^{(1)}$
11. $x_2^{(1)} \leftarrow P_2 y^{(1)} + Q_{12} x_2^{(1)} + G_{12} x_2^{(1)}$
12. repeat
13. $\Delta x_2^{(1)} \leftarrow -K_{21}^{A2}(x_2^{(1)}; x_2^{(1)}; x_2^{(1)})R_{A2}^{2}(x_2^{(1)}; x_2^{(1)}; x_2^{(1)})$
14. $x_2^{(n+1)} \leftarrow x_2^{(n+1)} + \Delta x_2^{(1)}$
15. until $||\Delta x_2^{(1)}||/||x_2^{(1)}|| \leq \varepsilon_{\text{machine}}$
16. until $\left[\left(||y^{(1)} - x_1^{(1)}||/||x_1^{(1)}||\right)^2 + \left(||y^{(2)} - x_2^{(2)}||/||x_2^{(2)}||\right)^2\right]^{1/2} \leq \varepsilon_{\text{machine}}$

Modified Schwarz

1. $x_1^{(1)} \leftarrow X_1^{(1)}$ in $\Omega_1$, $x_1^{(1)} \leftarrow \chi(X_1^{(1)})$ on $\partial \Omega_1$, $x_1^{(1)} \leftarrow X_1^{(1)}$ on $\Gamma_1$
2. $x_2^{(1)} \leftarrow X_2^{(1)}$ in $\Omega_2$, $x_2^{(1)} \leftarrow \chi(X_2^{(1)})$ on $\partial \Omega_2$, $x_2^{(1)} \leftarrow X_2^{(1)}$ on $\Gamma_2$
3. repeat
4. $x_2^{(1)} \leftarrow P_2 x_2^{(2)} + Q_{12} x_2^{(1)} + G_{12} x_2^{(1)}$
5. $\Delta x_2^{(1)} \leftarrow -K_{21}^{A2}(x_2^{(1)}; x_2^{(2)}; x_2^{(2)})R_{A2}^{2}(x_2^{(2)}; x_2^{(2)}; x_2^{(2)})$
6. $x_2^{(1)} \leftarrow x_2^{(1)} + \Delta x_2^{(1)}$
7. $x_2^{(2)} \leftarrow P_2 x_2^{(2)} + Q_{12} x_2^{(1)} + G_{12} x_2^{(1)}$
8. $\Delta x_2^{(2)} \leftarrow -K_{21}^{A2}(x_2^{(2)}; x_2^{(2)}; x_2^{(2)})R_{A2}^{2}(x_2^{(2)}; x_2^{(2)}; x_2^{(2)})$
9. $x_2^{(2)} \leftarrow x_2^{(2)} + \Delta x_2^{(2)}$
10. until $\left[\left(||y^{(1)} - x_1^{(1)}||/||x_1^{(1)}||\right)^2 + \left(||y^{(2)} - x_2^{(2)}||/||x_2^{(2)}||\right)^2\right]^{1/2} \leq \varepsilon_{\text{machine}}$

Inexact Schwarz

1. $x_1^{(1)} \leftarrow X_1^{(1)}$ in $\Omega_1$, $x_1^{(1)} \leftarrow \chi(X_1^{(1)})$ on $\partial \Omega_1$, $x_1^{(1)} \leftarrow X_1^{(1)}$ on $\Gamma_1$
2. $x_2^{(1)} \leftarrow X_2^{(1)}$ in $\Omega_2$, $x_2^{(1)} \leftarrow \chi(X_2^{(1)})$ on $\partial \Omega_2$, $x_2^{(1)} \leftarrow X_2^{(1)}$ on $\Gamma_2$
3. repeat
4. $x_2^{(1)} \leftarrow P_2 x_2^{(2)} + Q_{12} x_2^{(1)} + G_{12} x_2^{(1)}$
5. $\Delta x_2^{(1)} \leftarrow -K_{21}^{A2}(x_2^{(1)}; x_2^{(2)}; x_2^{(2)})R_{A2}^{2}(x_2^{(2)}; x_2^{(2)}; x_2^{(2)})$
6. $x_2^{(1)} \leftarrow x_2^{(1)} + \Delta x_2^{(1)}$
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9. $x_2^{(2)} \leftarrow x_2^{(2)} + \Delta x_2^{(2)}$
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Monolithic Schwarz

1. $x_1^{(1)} \leftarrow X_1^{(1)}$ in $\Omega_1$, $x_1^{(1)} \leftarrow \chi(X_1^{(1)})$ on $\partial \Omega_1$, $x_1^{(1)} \leftarrow X_1^{(1)}$ on $\Gamma_1$
2. $x_2^{(1)} \leftarrow X_2^{(1)}$ in $\Omega_2$, $x_2^{(1)} \leftarrow \chi(X_2^{(1)})$ on $\partial \Omega_2$, $x_2^{(1)} \leftarrow X_2^{(1)}$ on $\Gamma_2$
3. repeat
4. $x_2^{(1)} \leftarrow P_2 x_2^{(2)} + Q_{12} x_2^{(1)} + G_{12} x_2^{(1)}$
5. $\Delta x_2^{(1)} \leftarrow -K_{21}^{A2}(x_2^{(1)}; x_2^{(2)}; x_2^{(2)})R_{A2}^{2}(x_2^{(2)}; x_2^{(2)}; x_2^{(2)})$
6. $x_2^{(1)} \leftarrow x_2^{(1)} + \Delta x_2^{(1)}$
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9. $x_2^{(2)} \leftarrow x_2^{(2)} + \Delta x_2^{(2)}$
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Four Variants* of Schwarz

**Most performant method:** monotonic convergence, theoretical convergence guarantee.

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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*. 

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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.
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 \( \mu \) 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

<table>
<thead>
<tr>
<th>Subdomain</th>
<th>$u_3$ relative error</th>
<th>$\sigma_{33}$ relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Omega_1$</td>
<td>$1.24 \times 10^{-14}$</td>
<td>$2.31 \times 10^{-13}$</td>
</tr>
<tr>
<td>$\Omega_2$</td>
<td>$7.30 \times 10^{-15}$</td>
<td>$3.06 \times 10^{-13}$</td>
</tr>
</tbody>
</table>
Quasistatic Example #2: Notched Cylinder

- Notched cylinder that is stretched along its axial direction.
- Domain decomposed into two subdomains.
- Neohookean-type material model.
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) $\Omega_1$

(b) $\Omega_2$

<table>
<thead>
<tr>
<th>Absolute residual tolerance</th>
<th>$u_3$ relative error $\Omega_1$</th>
<th>$u_3$ relative error $\Omega_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.0 \times 10^{-14}$</td>
<td>$9.27 \times 10^{-3}$</td>
<td>$3.70 \times 10^{-3}$</td>
</tr>
</tbody>
</table>
Notched Cylinder: Coupling Different Materials

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

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

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

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

Coupled Schwarz discretization (50% reduction in model size)
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**

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

---

**Controller time stepper** = convenient checkpoint to facilitate implementation

Controller time stepper

Time integrator for $\Omega_1$

Time integrator for $\Omega_2$
Step 0: Initialize $i = 0$ (controller time index).

Step 1: Advance $\Omega_1$ solution from time $T_i$ to time $T_{i+1}$ using time-stepper in $\Omega_1$ with time-step $\Delta t_1$, using solution in $\Omega_2$ interpolated to $\Gamma_1$ at times $T_i + n\Delta t_1$. 

Controller time stepper = convenient checkpoint to facilitate implementation

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Schwarz Alternating Method for Dynamic Multiscale Coupling

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

  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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- 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*.

*Current dynamic Schwarz implementation in Albany requires same $\Delta t$ in different subdomains.*
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
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**: $\Omega_0 = (0,0.001) \times (0.001) \times (0,0.75)$, $\Omega_1 = (0,0.001) \times (0.001) \times (0.25,1)$.

![Clamped Beam Gaussian Z Problem]

*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 $\Delta t$.

*Meshes:* hexes, tets
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

<table>
<thead>
<tr>
<th></th>
<th>Implicit-Implicit</th>
<th>Explicit(CM)-Implicit</th>
<th>Explicit(LM)-Implicit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conformal hex-hex</td>
<td>2.79e-3</td>
<td>7.32e-3</td>
<td>3.53e-3</td>
</tr>
<tr>
<td>Nonconformal hex-hex</td>
<td>2.90e-3</td>
<td>7.10e-3</td>
<td>2.82e-3</td>
</tr>
<tr>
<td>Tet-hex</td>
<td>2.79e-3</td>
<td>7.58e-3</td>
<td>3.52e-3</td>
</tr>
</tbody>
</table>

LM = Lumped Mass, CM = Consistent Mass
For clamped beam problem, total energy (\(TE = 0.5x^T Kx + 0.5\dot{x}^T M\dot{x}\)) should be conserved.

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

- Total energy is calculated in 2 ways: with most of contribution from \(\Omega_0\) and from \(\Omega_1\).
Example #2: Tension Specimen

- Uniaxial aluminum cylindrical tensile specimen with \textit{inelastic J}_2 \textit{material model}.

- Domain decomposition into \textbf{two subdomains} (right): \(\Omega_0 = \text{ends, } \Omega_1 = \text{gauge.}\)

- \textit{Nonconformal hex + composite tet 10} coupling via Schwarz.

- \textit{Implicit} Newmark time-integration with \textit{adaptive time-stepping} algorithm employed in both subdomains.

- Slight \textit{imperfection} introduced at center of gauge to force \textit{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.

- \( \Omega_1 \) = bolts (composite tet 10), \( \Omega_2 \) = parts (hex).

- *Inelastic J*₂ *material model* in both subdomains.
  - \( \Omega_1 \): steel
  - \( \Omega_2 \): steel component, aluminum (bottom) plate

- BC: x-disp = 0.02 at \( T = 1.0 \times 10^{-3} \) on top of parts.
- Run until \( T = 5.0 \times 10^{-4} \) w/ \( dt = 1 \times 10^{-5} \) + implicit Newmark with analytic mass matrix for composite tet 10s.
Bolted Joint Problem

\[ \text{Single } \Omega \]

\[ \text{Schwarz} \]

\[ \text{x-displacement} \]
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.
Outline

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   • 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).

😊 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).
Outline

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   • Numerical Examples

4. Summary

5. Future Work
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.
References


Appendix. Previous Work

A multiscale overlapped coupling formulation for large-deformation strain localization

WaiChing Sun · Alejandro Mota

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

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

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

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

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

DOI 10.1007/s00466-014-1034-0

**ORIGINAL PAPER**

**A multiscale overlapped coupling formulation for large-deformation strain localization**

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Nevertheless, modeling strain localization with the conventional finite element method may lead to spurious mesh-dependent results due to the loss of ellipticity at the onset of strain localization [31]. To circumvent the loss of mate-
Method works well, but is difficult to implement into existing codes.
Appendix. Full Schwarz Method

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

1: $\mathbf{x}_B^{(1)} \leftarrow X_B^{(1)}$ in $\Omega_1$, $\mathbf{x}_b^{(1)} \leftarrow \chi(X_b^{(1)})$ on $\partial \varphi \Omega_1$, $\mathbf{x}_\beta^{(1)} \leftarrow X_\beta^{(1)}$ on $\Gamma_1$
2: $\mathbf{x}_B^{(2)} \leftarrow X_B^{(2)}$ in $\Omega_2$, $\mathbf{x}_b^{(2)} \leftarrow \chi(X_b^{(2)})$ on $\partial \varphi \Omega_2$, $\mathbf{x}_\beta^{(2)} \leftarrow X_\beta^{(2)}$ on $\Gamma_2$
3: **repeat**
   4: $\mathbf{y}^{(1)} \leftarrow \mathbf{x}_B^{(1)}$
   5: $\mathbf{x}_\beta^{(1)} \leftarrow P_{12}\mathbf{x}_B^{(2)} + Q_{12}\mathbf{x}_b^{(2)} + G_{12}\mathbf{x}_\beta^{(2)}$
   6: **repeat**
      7: $\Delta \mathbf{x}_B^{(1)} \leftarrow -K_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)}) \backslash R_A^{(1)}(\mathbf{x}_B^{(1)}; \mathbf{x}_b^{(1)}; \mathbf{x}_\beta^{(1)})$
      8: $\mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \Delta \mathbf{x}_B^{(1)}$
      9: until $\|\Delta \mathbf{x}_B^{(1)}\| / \|\mathbf{x}_B^{(1)}\| \leq \epsilon_{\text{machine}}$
   10: $\mathbf{y}^{(2)} \leftarrow \mathbf{x}_B^{(2)}$
   11: $\mathbf{x}_\beta^{(2)} \leftarrow P_{21}\mathbf{x}_B^{(1)} + Q_{21}\mathbf{x}_b^{(1)} + G_{21}\mathbf{x}_\beta^{(1)}$
   12: **repeat**
      13: $\Delta \mathbf{x}_B^{(2)} \leftarrow -K_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)}) \backslash R_A^{(2)}(\mathbf{x}_B^{(2)}; \mathbf{x}_b^{(2)}; \mathbf{x}_\beta^{(2)})$
      14: $\mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \Delta \mathbf{x}_B^{(2)}$
      15: until $\|\Delta \mathbf{x}_B^{(2)}\| / \|\mathbf{x}_B^{(2)}\| \leq \epsilon_{\text{machine}}$
16: until $\left[ \left( \|\mathbf{y}^{(1)} - \mathbf{x}_B^{(1)}\| / \|\mathbf{x}_B^{(1)}\| \right)^2 + \left( \|\mathbf{y}^{(2)} - \mathbf{x}_B^{(2)}\| / \|\mathbf{x}_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}$

- initialize for $\Omega_1$
- initialize for $\Omega_2$
- Schwarz loop
- for convergence check
- project from $\Omega_2$ to $\Gamma_1$
- Newton loop for $\Omega_1$
- linear system
- tight tolerance
- for convergence check
- project from $\Omega_1$ to $\Gamma_2$
- Newton loop for $\Omega_2$
- linear system
- tight tolerance
- tight tolerance
Appendix. Inexact Schwarz Method

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

```
1: \( x_B^{(1)} \leftarrow X_B^{(1)} \) in \( \Omega_1 \), \( x_b^{(1)} \leftarrow \chi(X_b^{(1)}) \) on \( \partial \Omega_1 \), \( x_\beta^{(1)} \leftarrow X_\beta^{(1)} \) on \( \Gamma_1 \)
2: \( x_B^{(2)} \leftarrow X_B^{(2)} \) in \( \Omega_2 \), \( x_b^{(2)} \leftarrow \chi(X_b^{(2)}) \) on \( \partial \Omega_2 \), \( x_\beta^{(2)} \leftarrow X_\beta^{(2)} \) on \( \Gamma_2 \)
3: repeat
   4: \( y^{(1)} \leftarrow x_B^{(1)} \)
   5: \( x_\beta^{(1)} \leftarrow P_{12} x_B^{(2)} + Q_{12} x_b^{(2)} + G_{12} x_\beta^{(2)} \)
   6: repeat
      7: \( \Delta x_B^{(1)} \leftarrow -K_{AB}^{(1)}(x_B^{(1)}; x_b^{(1)}; x_\beta^{(1)}) \backslash R_A^{(1)}(x_B^{(1)}; x_b^{(1)}; x_\beta^{(1)}) \)
      8: \( x_B^{(1)} \leftarrow x_B^{(1)} + \Delta x_B^{(1)} \)
   9: until \( \|\Delta x_B^{(1)}\|/\|x_B^{(1)}\| \leq \epsilon \)
   10: \( y^{(2)} \leftarrow x_B^{(2)} \)
   11: \( x_\beta^{(2)} \leftarrow P_{21} x_B^{(1)} + Q_{21} x_b^{(1)} + G_{21} x_\beta^{(1)} \)
   12: repeat
      13: \( \Delta x_B^{(2)} \leftarrow -K_{AB}^{(2)}(x_B^{(2)}; x_b^{(2)}; x_\beta^{(2)}) \backslash R_A^{(2)}(x_B^{(2)}; x_b^{(2)}; x_\beta^{(2)}) \)
      14: \( x_B^{(2)} \leftarrow x_B^{(2)} + \Delta x_B^{(2)} \)
   15: until \( \|\Delta x_B^{(2)}\|/\|x_B^{(2)}\| \leq \epsilon \)
16: until \( \left[ (\|y^{(1)} - x_B^{(1)}\|/\|x_B^{(1)}\|)^2 + (\|y^{(2)} - x_B^{(2)}\|/\|x_B^{(2)}\|)^2 \right]^{1/2} \leq \epsilon_{\text{machine}} \)
```

\( \triangleright \) initialize for \( \Omega_1 \)
\( \triangleright \) initialize for \( \Omega_2 \)
\( \triangleright \) Schwarz loop
\( \triangleright \) for convergence check
\( \triangleright \) project from \( \Omega_2 \) to \( \Gamma_1 \)
\( \triangleright \) Newton loop for \( \Omega_1 \)
\( \triangleright \) linear system
\( \triangleright \) loose tolerance, e.g. \( \epsilon \in [10^{-4}, 10^{-1}] \)
\( \triangleright \) for convergence check
\( \triangleright \) project from \( \Omega_1 \) to \( \Gamma_2 \)
\( \triangleright \) Newton loop for \( \Omega_2 \)
\( \triangleright \) solve linear system
\( \triangleright \) loose tolerance, e.g. \( \epsilon \in [10^{-4}, 10^{-1}] \)
\( \triangleright \) tight tolerance
Appendix. Monolithic Schwarz Method

Combines Schwarz and Newton loop into \textit{since Newton-Schwarz loop}, with \textit{elimination of Schwarz boundary DOFs}, and tight convergence tolerance.

\begin{align*}
1: & \quad x_B^{(1)} \leftarrow X_B^{(1)} \text{ in } \Omega_1, \quad x_b^{(1)} \leftarrow \chi(X_b^{(1)}) \text{ on } \partial \varphi \Omega_1, \\
2: & \quad x_B^{(2)} \leftarrow X_b^{(2)} \text{ in } \Omega_2, \quad x_b^{(2)} \leftarrow \chi(X_b^{(2)}) \text{ on } \partial \varphi \Omega_2, \\
3: & \quad \text{repeat} \\
4: & \quad \begin{cases}
\Delta x_B^{(1)} \\
\Delta x_B^{(2)}
\end{cases} \leftarrow \begin{pmatrix}
K_{AB}^{(1)} + K_{A\beta}^{(1)} H_{11} & K_{A\beta}^{(1)} H_{12} \\
K_{A\beta}^{(2)} H_{21} & K_{AB}^{(2)} + K_{A\beta}^{(2)} H_{22}
\end{pmatrix} \begin{pmatrix}
-R_A^{(1)} \\
-R_A^{(2)}
\end{pmatrix} \\
5: & \quad x_B^{(1)} \leftarrow x_B^{(1)} + \Delta x_B^{(1)} \\
6: & \quad x_B^{(2)} \leftarrow x_B^{(2)} + \Delta x_B^{(2)} \\
7: & \quad \text{until } \left[ \left( \frac{||\Delta x_B^{(1)}||}{||x_B^{(1)}||} \right)^2 + \left( \frac{||\Delta x_B^{(2)}||}{||x_B^{(2)}||} \right)^2 \right] \leq \epsilon_{\text{machine}}
\end{align*}

\textbf{Advantages:}

- By-passes Schwarz loop.

\textbf{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: \( x_B^{(1)} \leftarrow X_B^{(1)} \) in \( \Omega_1 \), \( x_b^{(1)} \leftarrow \chi(X_b^{(1)}) \) on \( \partial \varphi \Omega_1 \), \( x_{\beta}^{(1)} \leftarrow X_{\beta}^{(1)} \) on \( \Gamma_1 \)
2: \( x_B^{(2)} \leftarrow X_B^{(2)} \) in \( \Omega_2 \), \( x_b^{(2)} \leftarrow \chi(X_b^{(2)}) \) on \( \partial \varphi \Omega_2 \), \( x_{\beta}^{(2)} \leftarrow X_{\beta}^{(2)} \) on \( \Gamma_2 \)
3: repeat
   4: \( x_{\beta}^{(1)} \leftarrow P_{12}x_B^{(2)} + Q_{12}x_b^{(2)} + G_{12}x_{\beta}^{(2)} \)
   5: \( \triangle x_B^{(1)} \leftarrow -K_{AB}^{(1)}(x_B^{(1)}; x_b^{(1)}; x_{\beta}^{(1)})\backslash R_{A}^{(1)}(x_B^{(1)}; x_b^{(1)}; x_{\beta}^{(1)}) \)
   6: \( x_B^{(1)} \leftarrow x_B^{(1)} + \triangle x_B^{(1)} \)
   7: \( x_{\beta}^{(2)} \leftarrow P_{21}x_B^{(1)} + Q_{21}x_b^{(1)} + G_{21}x_{\beta}^{(1)} \)
   8: \( \triangle x_B^{(2)} \leftarrow -K_{AB}^{(2)}(x_B^{(2)}; x_b^{(2)}; x_{\beta}^{(2)})\backslash R_{A}^{(2)}(x_B^{(2)}; x_b^{(2)}; x_{\beta}^{(2)}) \)
   9: \( x_B^{(2)} \leftarrow x_B^{(2)} + \triangle x_B^{(2)} \)
10: until \[ \left( \frac{\|\triangle x_B^{(1)}\|}{\|x_B^{(1)}\|} \right)^2 + \left( \frac{\|\triangle x_B^{(2)}\|}{\|x_B^{(2)}\|} \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}
```

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
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 **hypereleastic** material model with no damage.
  - **MATLAB** implementation.

\[
\begin{align*}
  u(0) &= 0 \\
  A(X) &= A_0 \sqrt{X/L} \\
  u(L) &= \Delta
\end{align*}
\]

- **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

<table>
<thead>
<tr>
<th>Absolute residual tolerance</th>
<th>( u_3 ) relative error</th>
<th>( \Omega_1 )</th>
<th>( \Omega_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 1.0 \times 10^{-4} )</td>
<td>7.60 \times 10^{-3}</td>
<td>3.20 \times 10^{-3}</td>
<td></td>
</tr>
<tr>
<td>( 1.0 \times 10^{-8} )</td>
<td>3.10 \times 10^{-5}</td>
<td>1.71 \times 10^{-5}</td>
<td></td>
</tr>
<tr>
<td>( 1.0 \times 10^{-12} )</td>
<td>1.34 \times 10^{-9}</td>
<td>5.10 \times 10^{-10}</td>
<td></td>
</tr>
<tr>
<td>( 1.0 \times 10^{-14} )</td>
<td>1.23 \times 10^{-11}</td>
<td>4.69 \times 10^{-12}</td>
<td></td>
</tr>
<tr>
<td>( 2.5 \times 10^{-16} )</td>
<td>1.14 \times 10^{-13}</td>
<td>8.37 \times 10^{-14}</td>
<td></td>
</tr>
</tbody>
</table>
Appendix. Notched Cylinder: Nonconformal HEX-HEX Coupling

(a) $\Omega_1$ and $\Omega_2$
(b) $\Omega_{\text{ref}}$ mesh
(c) $\Omega_{\text{ref}}$ solution
Appendix. Notched Cylinder: Nonconformal HEX-HEX Coupling

<table>
<thead>
<tr>
<th>Absolute residual tolerance</th>
<th>$u_3$ relative error</th>
<th>$\Omega_1$</th>
<th>$\Omega_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.0 \times 10^{-8}$</td>
<td>$1.31 \times 10^{-3}$</td>
<td>$4.45 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>$1.0 \times 10^{-12}$</td>
<td>$1.30 \times 10^{-3}$</td>
<td>$4.43 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>$1.0 \times 10^{-14}$</td>
<td>$1.30 \times 10^{-3}$</td>
<td>$4.43 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>$2.5 \times 10^{-16}$</td>
<td>$1.30 \times 10^{-3}$</td>
<td>$4.43 \times 10^{-4}$</td>
<td></td>
</tr>
</tbody>
</table>
Appendix. Multiscale Modeling of Localization

Goals:

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

Strain localization can cause *localized necking* (left) and ultimately *fracture* (above).
Appendix. Parallelization via DTK: Weak Scaling on Cubes Problem

<table>
<thead>
<tr>
<th>Number of Processors</th>
<th>Total Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Processor</td>
<td>2.5*10³ DOF / proc</td>
</tr>
<tr>
<td>8 Processors</td>
<td>2.1*10³ DOF / proc</td>
</tr>
<tr>
<td>64 Processors</td>
<td>1.9*10³ DOF / proc</td>
</tr>
</tbody>
</table>

Graph showing the relationship between the number of processors and total time.
Appendix. Parallelization via DTK: Strong Scaling on Cubes Problem

Small problem (2.5*10^3 DOFs)

Medium problem (1.7*10^4 DOFs)

Large problem (1.6*10^5 DOFs)
Appendix. Rubik's Cube Problem

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
Appendix. Tensile Bar

Embed microstructure in ASTM tensile geometry
Appendix. Tensile Bar: Meso-Macroscale Coupling

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: $g_0 = 2.0 \times 10^4$ 1/s
- initial hardness: $g_0 = 90$ MPa
- saturation hardness: $g_s = 202$ MPa
- saturation exponent: $\omega = 0.01$

Fix microstructure, investigate ensembles

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

Macroscale

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

- Young’s modulus: $E = 195.0$ GPa
- Poisson’s ratio: $\nu = 0.3$
- yield stress: $\sigma_0 = 144$ MPa
- hardening modulus: $H = 300$ MPa
- saturation modulus: $S = 170$ MPa
- saturation exponent: $\alpha = 190$

$$\sigma_y = \sigma_0 + H\varepsilon_p + S(1 - e^{-\alpha\varepsilon_p})$$
Appendix. Tensile Bar: Results

Reduction in cross-sectional area over time

![Graph showing reduction in cross-sectional area over time.](image)
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.

![Diagram of overlapping non-matching meshes and time steps in dynamics.](image-url)
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.

![Diagram of coupled domains and time integrators]

- Controller time stepper
- Time integrator for $\Omega_1$
- Time integrator for $\Omega_2$
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 \( \Delta t \).

- 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*!

Displacement relative errors at final time ($T=0.002$)

Velocit comparable to single-domain solution on mesh conformal with Schwarz domain meshes.

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 $\Omega_0$ with hexes + implicit Newmark in $\Omega_1$.
- Reference solution is computed on fine hex mesh + implicit Newmark $\Omega_{\text{ref}}$

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

No dynamic artifacts!

Movie of $|\text{displacement}|$

*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

Time: 0.000000

Single \( \Omega \)

Schwarz
Appendix. Bolted Joint Problem

z-displacement

Single $\Omega$

Schwarz