The Schwarz alternating method for concurrent multiscale coupling in solid mechanics

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Outline

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

- **Large scale** structural ***failure*** frequently originates from **small scale** phenomena such as defects, microcracks, inhomogeneities and more, which grow quickly in an unstable manner.

- Failure occurs due to **tightly coupled interaction** between small scale (stress concentrations, material instabilities, cracks, etc.) and large scale (vibration, impact, high loads and other perturbations).

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

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

Surface flaw in pressure vessel: interacts with microstructure, which may or may not lead to failure.
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Schwarz Alternating Method for Domain Decomposition

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

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

---

**Schwarz Alternating Method**

**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.

**Requirement for convergence:** $\Omega_1 \cap \Omega_2 \neq \emptyset$
Using the Schwarz alternating as a \textit{discretization method} for PDEs is natural idea with a sound \textit{theoretical foundation}.
Schwarz Alternating Method after Schwarz

Using the Schwarz alternating as a discretization method for PDEs is a 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. L. Sobolev (1908 – 1989)
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Using the Schwarz alternating as a **discretization method** for PDEs is a 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.

$$\Phi[\varphi] = \int_B W(F,Z,T) \, dV - \int_B B \cdot \varphi \, dV - \int_{\partial T_B} \bar{T} \cdot \varphi \, dS$$

$$\nabla \cdot P + B = 0$$

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Schwarz Alternating Method for Multiscale Coupling in Quasistatics

**Advantages:**

- Conceptually very simple.
Schwarz Alternating Method for Multiscale Coupling in Quasistatics

1. \( \varphi^{(0)} \leftarrow \text{id}_X \) in \( \Omega_2 \)
2. \( n \leftarrow 1 \)
3. \textbf{repeat}
4. \( \varphi^{(n)} \leftarrow \chi \) on \( \partial \varphi \Omega_i \)
5. \( \varphi^{(n)} \leftarrow P_{\Omega_j \rightarrow \Gamma_i}[\varphi^{(n-1)}] \) on \( \Gamma_i \)
6. \( \varphi^{(n)} \leftarrow \arg \min_{\varphi \in \mathcal{S}_i} \Phi_i[\varphi] \) in \( \Omega_i \)
7. \( n \leftarrow n + 1 \)
8. \textbf{until} converged

\( \Omega_1 \rightarrow \Gamma_2 \rightarrow \Gamma_1 \rightarrow \Omega_2 \)

\( \triangleright \) initialize to zero displacement or a better guess in \( \Omega_2 \)

\( \triangleright \) Schwarz loop

\( \triangleright \) Dirichlet BC for \( \Omega_i \)

\( \triangleright \) Schwarz BC for \( \Omega_i \)

\( \triangleright \) solve in \( \Omega_i \)

Advantages:

- Conceptually very \textit{simple}.
- Allows the coupling of regions with \textit{different non-conforming meshes, different element types}, and \textit{different levels of refinement}. 
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- Conceptually very \textit{simple}.
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- Conceptually very simple.
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- Different solvers can be used for the different regions.

```
1: \varphi^{(0)} \leftarrow \text{id}_{\mathcal{X}} \text{ in } \Omega_2
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4: \varphi^{(n)} \leftarrow \chi \text{ on } \partial \varphi \Omega_i
5: \varphi^{(n)} \leftarrow P_{\Omega_i \rightarrow \Gamma_i}[\varphi^{(n-1)}] \text{ on } \Gamma_i
6: \varphi^{(n)} \leftarrow \arg \min_{\varphi \in \mathcal{S}_i} \Phi_i[\varphi] \text{ in } \Omega_i
7: n \leftarrow n + 1
8: \text{until converged}
```

\( \varphi^{(n)} \) is initialized to zero displacement or a better guess in \( \Omega_2 \).

\( \varphi^{(n)} \) is updated using the Schwarz loop.

\( \varphi^{(n)} \) is solved in \( \Omega_i \).

\( \varphi^{(n)} \) is updated with Dirichlet BC for \( \Omega_i \).

\( \varphi^{(n)} \) is updated with Schwarz BC for \( \Omega_i \).

\( \varphi^{(n)} \) is updated with solve in \( \Omega_i \).
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8: \textbf{until} converged

Advantages:

- Conceptually very \textit{simple}.
- Allows the coupling of regions with \textit{different non-conforming meshes, different element types}, and \textit{different levels of refinement}.
- Information is exchanged among two or more regions, making coupling \textit{concurrent}.
- \textit{Different solvers} can be used for the different regions.
- \textit{Different material models} can be coupled provided that they are compatible in the overlap region.
Schwarz Alternating Method for Multiscale Coupling in Quasistatics

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- 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 provided that they are compatible in the overlap region.
- Simplifies the task of meshing complex geometries for the different scales.

Algorithm:

1. \( \varphi^{(0)} \leftarrow \text{id}_X \) in \( \Omega_2 \)
2. \( n \leftarrow 1 \)
3. repeat
4. \( \varphi^{(n)} \leftarrow \chi \) on \( \partial\varphi_{\Omega_i} \)
5. \( \varphi^{(n)} \leftarrow P_{\Omega_j \rightarrow \Gamma_i} [\varphi^{(n-1)}] \) on \( \Gamma_i \)
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7. \( n \leftarrow n + 1 \)
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Four Variants* of the Schwarz Alternating Method

Full Schwarz

Modified Schwarz

Inexact Schwarz

Monolithic Schwarz

Four Variants* of the Schwarz Alternating Method

Full Schwarz

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Monolithic Schwarz

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

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Implementations*

- All four variants implemented in 3D MATLAB code.

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Implementations*

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

---

<table>
<thead>
<tr>
<th>Variant</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full Schwarz</td>
<td>MATLAB code</td>
</tr>
<tr>
<td>Modified Schwarz</td>
<td>Parallel C++ Albany code</td>
</tr>
<tr>
<td>Inexact Schwarz</td>
<td></td>
</tr>
<tr>
<td>Monolithic Schwarz</td>
<td></td>
</tr>
</tbody>
</table>

---

Implementations*

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

Schwarz Alternating Method in *Albany* Code

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

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

https://github.com/gahansen/Albany

https://github.com/trilinos/trilinos

https://github.com/ORNL-CEES/DataTransferKit
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Example #1: Foulk’s Singular Bar

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

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

- **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**.
Singular Bar and Schwarz Variants

[Graphs and diagrams showing the performance of different Schwarz variants for various parameters and error metrics.]
Example #2: Cuboid Problem

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

Combined Newton-Schwarz Iteration
Cuboid Problem: Convergence with Overlap & Refinement

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

![Graph showing convergence](image)

**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>
Example #3: Notched Cylinder

- **Notched cylinder** that is stretched along its axial direction.
- Domain decomposed into **two subdomains**.
- **Neohookean**-type material model.
Notched Cylinder: Conformal 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>
Notched Cylinder: Nonconformal HEX-HEX Coupling

(a) $\Omega_1$ and $\Omega_2$
(b) $\Omega_{\text{ref}}$ mesh
(c) $\Omega_{\text{ref}}$ solution
Notched Cylinder: Nonconformal HEX-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>$1.0 \times 10^{-8}$</td>
<td>$1.31 \times 10^{-3}$</td>
<td>$4.45 \times 10^{-4}$</td>
</tr>
<tr>
<td>$1.0 \times 10^{-12}$</td>
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<td>$4.43 \times 10^{-4}$</td>
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</tr>
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</table>
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

\( \Omega_1 \)  
\( \Omega_2 \)

<table>
<thead>
<tr>
<th>Absolute residual tolerance</th>
<th>( u_3 ) relative error</th>
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</thead>
<tbody>
<tr>
<td>( 1.0 \times 10^{-14} )</td>
<td>( 9.27 \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.

Overlap far from notch.

Overlap near notch.

Coupled regions

Coarse, elastic region

Fine, elasto-plastic region
Notched Cylinder: Coupling Different Materials

- 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.

Need to be careful to do domain decomposition so that material models are consistent in overlap region.
Example #4: Laser Weld with 3 Subdomains

- 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).
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Summary

- We have proposed the **Schwarz alternating method** as a means of **concurrent multiscale coupling** in finite deformation quasistatic solid mechanics.

- We have developed **four variants** of the Schwarz alternating method (**Full Schwarz**, **Modified Schwarz**, **Inexact Schwarz**, **Monolithic Schwarz**).

- We have **proven** that the Full Schwarz variant converges geometrically for the solid mechanics problem.

- We have **demonstrated numerically** that the **convergence** of the Schwarz method in its four variants is **linear**.

- We have demonstrated coupling of **conformal** and **non-conformal meshes**, meshes with **different levels of refinement**, meshes with different **element topologies**, and **> two subdomains** via the proposed method.

- We have demonstrated that the **error** in the coupling can be decreased up to **numerical precision** provided that no other sources of error exist.

- We have developed a **parallel** implementation of the **Modified Schwarz** method in the **Albany code** and demonstrated that the **strong scalability** of our implementation is close to **ideal**.
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Future Work

- Extension of the methods presented herein to transient dynamics (hyperbolic) problems with the ability to use different time steps and time integrators for each subdomain.

- Development of a multi-physics coupling framework based on variational formulations and the Schwarz alternating method.

- **Analysis** of the convergence for the other Schwarz variants introduced herein, namely Modified Schwarz, Inexact Schwarz, and Monolithic Schwarz.

- Using the Schwarz alternating method with different solvers in different domains.

- Develop a hybrid FOM-ROM (full-order-model – reduced-order-model) framework using the Schwarz alternating method.

- Introduction of pervasive multi-threading into our Albany implementation of the Schwarz alternating method using the Kokkos framework.

- Multiscale coupling using the proposed Schwarz alternating method in other applications.
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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 mater-
Appendix. Previous Work

Three-field multiscale coupling formulation with compatibility enforced weakly using Lagrange multipliers.
Appendix. Previous Work

Method works well, but is difficult to implement into existing codes.
Classical algorithm originally proposed by Schwarz with outer Schwarz loop and inner Newton loop, each converged to a tight tolerance ($\epsilon_{\text{machine}}$).

\begin{align*}
1: & \quad x_B^{(1)} \leftarrow X_B^{(1)} \text{ in } \Omega_1, \, x_b^{(1)} \leftarrow \chi(X_b^{(1)}) \text{ on } \partial \Omega_1, \, x_\beta^{(1)} \leftarrow X_\beta^{(1)} \text{ on } \Gamma_1 \\
2: & \quad x_B^{(2)} \leftarrow X_B^{(2)} \text{ in } \Omega_2, \, x_b^{(2)} \leftarrow \chi(X_b^{(2)}) \text{ on } \partial \Omega_2, \, x_\beta^{(2)} \leftarrow X_\beta^{(2)} \text{ on } \Gamma_2 \\
3: & \quad \text{repeat} \\
4: & \quad y^{(1)} \leftarrow x_B^{(1)} \\
5: & \quad x_\beta^{(1)} \leftarrow P_{12} x_B^{(2)} + Q_{12} x_b^{(2)} + G_{12} x_\beta^{(2)} \\
6: & \quad \text{repeat} \\
7: & \quad \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: & \quad x_B^{(1)} \leftarrow x_B^{(1)} + \Delta x_B^{(1)} \\
9: & \quad \text{until } \|\Delta x_B^{(1)}\|/\|x_B^{(1)}\| \leq \epsilon_{\text{machine}} \\
10: & \quad y^{(2)} \leftarrow x_B^{(2)} \\
11: & \quad x_\beta^{(2)} \leftarrow P_{21} x_B^{(1)} + Q_{21} x_b^{(1)} + G_{21} x_\beta^{(1)} \\
12: & \quad \text{repeat} \\
13: & \quad \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: & \quad x_B^{(2)} \leftarrow x_B^{(2)} + \Delta x_B^{(2)} \\
15: & \quad \text{until } \|\Delta x_B^{(2)}\|/\|x_B^{(2)}\| \leq \epsilon_{\text{machine}} \\
16: & \quad \text{until } \left[ \left( \|y^{(1)} - x_B^{(1)}\|/\|x_B^{(1)}\| \right)^2 + \left( \|y^{(2)} - x_B^{(2)}\|/\|x_B^{(2)}\| \right)^2 \right]^{1/2} \leq \epsilon_{\text{machine}}
\end{align*}
Appendix. Inexact Schwarz Method

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

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

\textit{init}ialize for \(\Omega_1\)
\textit{init}ialize for \(\Omega_2\)
\textit{S}chwarz loop
\textit{for} convergence check
\textit{p}roject from \(\Omega_2\) to \(\Gamma_1\)
\textit{N}ewton loop for \(\Omega_1\)
\textit{l}inear system
\textit{l}oose tolerance, e.g. \(\epsilon \in [10^{-4}, 10^{-1}]\)
\textit{for} convergence check
\textit{p}roject from \(\Omega_1\) to \(\Gamma_2\)
\textit{N}ewton loop for \(\Omega_2\)
\textit{s}olve linear system
\textit{l}oose tolerance, e.g. \(\epsilon \in [10^{-4}, 10^{-1}]\)
\textit{t}ight tolerance
Appendix. Monolithic Schwarz Method

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

1: \( \mathbf{x}_B^{(1)} \leftarrow \mathbf{X}_B^{(1)} \) in \( \Omega_1 \), \( \mathbf{x}_b^{(1)} \leftarrow \chi(\mathbf{X}_b^{(1)}) \) on \( \partial \varphi \Omega_1 \),
2: \( \mathbf{x}_B^{(2)} \leftarrow \mathbf{X}_B^{(2)} \) in \( \Omega_2 \), \( \mathbf{x}_b^{(2)} \leftarrow \chi(\mathbf{X}_b^{(2)}) \) on \( \partial \varphi \Omega_2 \),
3: repeat
4: \[
\begin{bmatrix}
\triangle \mathbf{x}_B^{(1)} \\
\triangle \mathbf{x}_B^{(2)}
\end{bmatrix} \leftarrow \begin{bmatrix}
K_{AB}^{(1)} + K_{A\beta}^{(1)} H_{11} & K_{A\beta}^{(1)} H_{12} \\
K_{A\beta}^{(2)} H_{21} & K_{AB}^{(2)} + K_{A\beta}^{(2)} H_{22}
\end{bmatrix} \begin{bmatrix}
-R_A^{(1)} \\
-R_A^{(2)}
\end{bmatrix}
\]
▷ linear system
5: \( \mathbf{x}_B^{(1)} \leftarrow \mathbf{x}_B^{(1)} + \triangle \mathbf{x}_B^{(1)} \)
6: \( \mathbf{x}_B^{(2)} \leftarrow \mathbf{x}_B^{(2)} + \triangle \mathbf{x}_B^{(2)} \)
7: until \[
\left( \frac{\| \triangle \mathbf{x}_B^{(1)} \| / \| \mathbf{x}_B^{(1)} \|}{\| \triangle \mathbf{x}_B^{(2)} \| / \| \mathbf{x}_B^{(2)} \|} \right)^2 \leq \epsilon_{\text{machine}}
\]
▷ tight tolerance

**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 \textit{since Newton-Schwarz loop}, with \textit{Schwarz boundaries} at \textit{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 $\partial \Omega_1$, $x_\beta^{(1)} \leftarrow X_\beta^{(1)}$ 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: $x_\beta^{(1)} \leftarrow P_{12}x_B^{(2)} + Q_{12}x_b^{(2)} + G_{12}x_\beta^{(2)}$
5: $\Delta x_B^{(1)} \leftarrow -K_{AB}^{(1)}(x_B^{(1)}; x_b^{(1)}; x_\beta^{(1)}) \setminus R_A^{(1)}(x_B^{(1)}; x_b^{(1)}; x_\beta^{(1)})$
6: $x_B^{(1)} \leftarrow x_B^{(1)} + \Delta x_B^{(1)}$
7: $x_\beta^{(2)} \leftarrow P_{21}x_B^{(1)} + Q_{21}x_b^{(1)} + G_{21}x_\beta^{(1)}$
8: $\Delta x_B^{(2)} \leftarrow -K_{AB}^{(2)}(x_B^{(2)}; x_b^{(2)}; x_\beta^{(2)}) \setminus R_A^{(2)}(x_B^{(2)}; x_b^{(2)}; x_\beta^{(2)})$
9: $x_B^{(2)} \leftarrow x_B^{(2)} + \Delta x_B^{(2)}$
10: until $\left(\frac{\|\Delta x_B^{(1)}\|}{\|x_B^{(1)}\|}\right)^2 + \left(\frac{\|\Delta x_B^{(2)}\|}{\|x_B^{(2)}\|}\right)^2 \leq \epsilon_{\text{machine}}$

\begin{itemize}
  \item By-passes Schwarz loop.
  \item No diagonal coupling (conventional linear solver can be used in each subdomain).
\end{itemize}

\textbf{Least-intrusive variant}: by-passes Schwarz iteration, no need for block solver.
Appendix. Convergence Proof
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

1 Processor, $2.5 \times 10^3$ DOF / proc

8 Processors, $2.1 \times 10^3$ DOF / proc

64 Processors, $1.9 \times 10^3$ DOF / proc

![Graph showing total time vs. number of processors](image)

Total Time (s) vs. Number of Processors
Appendix. Parallelization via DTK: Strong Scaling on Cubes Problem

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

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

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

Cauchy Stress 11

-5.0
-27.5
-60.0
-92.5
-125.0
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: \( \omega = 0.01 \)

Macroscale

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

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

Fix microstructure, investigate ensembles

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

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
Appendix. Tensile Bar: Results

Reduction in cross-sectional area over time

![Graph showing reduction in cross-sectional area over time](image-url)
Appendix. Schwarz Alternating Method for Dynamics

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

Overlapping non-matching meshes and time steps in dynamics.
Appendix. A Schwarz-like Time Integrator

- We developed an **extension of Schwarz coupling** to **dynamics** using a governing time stepping algorithm that controls time integrators within each domain.

- Can use **different integrators** with **different time steps** within each domain.

- 1D results show **smooth coupling without numerical artifacts** such as spurious wave reflections at boundaries of coupled domains.
Appendix. Dynamic Singular Bar

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