The Schwarz Alternating Method for Dynamic Multiscale Coupling in Solid Mechanics

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Outline

This talk goes hand-in-hand with the previous talk in this MS: #2018677 - A. Mota, I. Tezaur, C. Alleman, “The Schwarz Alternating Method for Quasistatic Multiscale Coupling in Solid Mechanics”

1. Motivation and Background*.
2. Schwarz for Dynamic Multiscale Coupling.
4. Summary and Future Work.
5. References.
6. Appendix.

* Review from previous talk #2018677 by A. Mota.
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Motivation for Concurrent Multiscale Coupling

- Large scale structural failure frequently originates from small scale phenomena such as defects, microcracks, and inhomogeneities, 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 predicting the behavior of engineering systems when a small scale failure determines the performance of the entire system.

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

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.
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.

- 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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**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 $\Omega_2$.

**Requirement for convergence**: $\Omega_1 \cap \Omega_2 \neq \emptyset$
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Schwarz Alternating Method for Dynamic Multiscale Coupling

- In the literature the Schwarz method is applied to dynamics by using space-time discretizations.
Schwarz Alternating Method for Dynamic Multiscale Coupling

- In the literature the Schwarz method is applied to dynamics by using \textit{space-time discretizations}.

\textbf{Pro ☑️:} Can use \textit{non-matching} meshes and time-steps (see right figure).

\textbf{Con ☹️:} \textit{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

- 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.

**Our objective**: formulate dynamic Schwarz method for standard (non-space-time) discretizations (discretize in space, march forward in time).

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 $\Omega_2$
Schwarz Alternating Method for Dynamic Multiscale Coupling

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 $T_i + n\Delta t_1$. 

Integrate using $\Delta t_1$

Interpolate from $\Omega_2$ to $\Gamma_1$
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**Step 3:** Check for convergence at time $T_{i+1}$. 

Controller time stepper

Time integrator for $\Omega_1$

Time integrator for $\Omega_2$
Schwarz Alternating Method for Dynamic Multiscale Coupling

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**Diagram:**
- $\Omega_1$ and $\Omega_2$ are domains.
- $\Gamma_1$ and $\Gamma_2$ are interfaces.
- $T_1$ and $T_2$ are time points.
- $\Delta t_1$ and $\Delta t_2$ are time steps.
- Time integrator for $\Omega_1$ and $\Omega_2$.
- Interpolate from $\Omega_2$ to $\Gamma_1$.

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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].

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

(a) $\Phi[\tilde{\varphi}^{(0)}] \geq \Phi[\tilde{\varphi}^{(1)}] \geq \cdots \geq \Phi[\tilde{\varphi}^{(n-1)}] \geq \Phi[\tilde{\varphi}^{(n)}] \geq \cdots \geq \Phi[\varphi]$, where $\varphi$ is the minimizer of $\Phi[\varphi]$ over $S$.

(b) The sequence $\{\tilde{\varphi}^{(n)}\}$ defined in (39) converges to the minimizer $\varphi$ 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 $\tilde{\varphi}^{(0)}$.

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

• Quasistatic proof **extends naturally** assuming conformal meshes and the same time step is used in each Schwarz subdomain.

• Some analysis of Schwarz for evolution problems was performed in (Lions, 1988) and may be possible to **leverage**.

• Our numerical results suggest theoretical analysis is **possible**.
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Implementation within *Albany* Code

The proposed *dynamic alternating Schwarz method* has 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.
- Contains a wide variety of *constitutive models*.
- Extensive use of libraries from the open-source *Trilinos* project.
  - Use of the *Phalanx* package to decompose complex problem into simpler problems with managed dependencies.
  - Use of the *Sacado* package for *automatic differentiation*.
  - Use of *Tempus* package for *time-integration*.
- Parallel implementation of Schwarz alternating method uses the *Data Transfer Kit (DTK)*.
- All software available on [GitHub](https://github.com/gahansen/Albany)

*Current dynamic Schwarz implementation in Albany requires same $\Delta t$ in different subdomains.*
Example #1: Elastic Wave Propagation

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

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

**Time-discretizations**: Newmark-Beta (implicit, explicit) with same $\Delta t$.

**Meshes**: hexes, tets
Example #1: Elastic Wave Propagation

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

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

<table>
<thead>
<tr>
<th></th>
<th>Implicit-Implicit</th>
<th>Explicit(CM)-Implicit</th>
<th>Explicit(LM)-Implicit</th>
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</thead>
<tbody>
<tr>
<td>Conformal hex-hex</td>
<td>2.79e-3</td>
<td>7.32e-3</td>
<td>3.53e-3</td>
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<tr>
<td></td>
<td></td>
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<td>8.70e-3</td>
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<td>1.19e-2</td>
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<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
Example #1: Elastic Wave Propagation

Energy Conservation

For clamped beam problem, total energy \( TE = 0.5x^T K x + 0.5\dot{x}^T M \dot{x} \) 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: 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: \( \Omega_0 = (-0.025,0.025) \times (-0.025,0.025) \times (-0.5,0.25), \Omega_1 = (-0.025,0.025) \times (-0.25,0.025) \times (-0.25,0.5) \).

- **Time-discretizations:** Newmark-Beta (implicit, explicit) with same \( \Delta t \).

- **Meshes:** hexes, composite tet 10s.
Example #2: 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.

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

Velocity relative errors at final time ($T=0.002$)
Example #2: 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
Example #3: Tension Specimen

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

• Domain decomposition into \textit{two subdomains} (right): \( \Omega_0 = \) ends, \( \Omega_1 = \) 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.
Example #3: Tension Specimen

Average of ~7 Schwarz iterations/time step required for *convergence* to Schwarz tolerance of $1\times10^{-6}$.

*Nodal eqps = equivalent plastic strain computed via weighted volume average.*
Example #4: 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 $T = 1.0e^{-3}$ on top of parts.
- Run until $T = 5.0e^{-4}$ w/ $dt = 1e^{-5}$ + implicit Newmark with analytic mass matrix for composite tet 10s.
Example #4: Bolted Joint Problem

x-displacement

Single Ω

Schwarz
Example #4: Bolted Joint Problem

Nodal Equivalent Plastic Strain (eqps)

Time: 0.000000

Cross-section of bolts obtained via clip (right)
Example #4: Bolted Joint Problem

Some Performance Results

Schwarz / solver settings

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

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

The alternating Schwarz coupling method has been developed and implemented for concurrent multiscale 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.
Ongoing/Future Work

- Development of **theory** for dynamic alternating Schwarz formulation.

- **Journal article** on the work presented in this talk is in preparation.

- Extension of Albany/LCM implementation to allow for **different time steps** in different subdomains.

- Application of dynamic Schwarz for problems and test cases of interest to **production**.

- Implementation of alternating Schwarz method for concurrent multiscale coupling in Sandia **production codes** (Sierra Solid Mechanics), comparison to other methods (e.g., GFEM).

- Development of a **multi-physics coupling framework** based on variational formulations and the Schwarz alternating method.
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Appendix. Schwarz Alternating Method for Dynamic Multiscale Coupling

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

**Ingredients:**

- Controller time step $\Delta T \Rightarrow T_0 + n\Delta T$ are times at which Schwarz is synchronized
  - Convenient checkpoint to facilitate implementation
- Discretization + time-integrator for $\Omega_1$ with time-step $\Delta t_1$ (divides $\Delta T$)
- Discretization + time-integrator for $\Omega_2$ with time-step $\Delta t_2$ (divides $\Delta T$)

Can use *different integrators* with *different time steps* within each domain (w/o space-time discretization)!
Appendix. Dynamic Singular Bar (MATLAB)

- 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. Example #1: Elastic Wave

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. Example #2: 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. Example #4: Bolted Joint Problem

y-displacement

Time: 0.000000

Single Ω

Schwarz
Appendix. Example #4: Bolted Joint Problem

z-displacement

Single $\Omega$

Schwarz