The Schwarz Alternating Method for Dynamic Multiscale Coupling in Solid Mechanics

Irina Tezaur\textsuperscript{1}, Alejandro Mota\textsuperscript{1}, Greg Phlipot\textsuperscript{2}

\textsuperscript{1}Sandia National Laboratories, Livermore, CA, USA. \textsuperscript{2}California Institute of Technology, Pasadena, CA, USA.

WCCM 2018 New York, NY July 22-27, 2018
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.

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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.

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.
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 $\Omega_2$.

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

- 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 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

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**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

- 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).
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

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Time integrator for $\Omega_1$

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

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Schwarz Alternating Method for Dynamic Multiscale Coupling

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

**Controller time stepper** = convenient checkpoint to facilitate implementation. 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 $\tilde{\varphi}^{(0)}$.

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*.

*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>
</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
Example #1: Elastic Wave Propagation

Energy Conservation

- For clamped beam problem, total energy \( TE = 0.5\mathbf{x}^T \mathbf{K} \mathbf{x} + 0.5\dot{\mathbf{x}}^T \mathbf{M} \dot{\mathbf{x}} \) should be conserved.
- Total energy is calculated in 2 ways: with most of contribution from \( \Omega_0 \) and from \( \Omega_1 \).

Total energy is **conserved** and matches single-domain total energy.
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: \( \Omega_0 = (-0.025,0.025) \times (-0.025,0.025) \times (-0.5,0.25) \), \( \Omega_1 = (-0.025,0.025) \times (-0.025,0.025) \times (-0.25,0.5) \).

- **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.

Schwarz and single-domain results agree to almost *machine-precision*!
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 inelastic $J_2$ material model.

• Domain decomposition into two subdomains (right): $\Omega_0 = $ ends, $\Omega_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.
Example #3: 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 #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* 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)

Cross-section of bolts obtained via clip (right)
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%).
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: 0.0000000

Single $\Omega$

Schwarz
Appendix. Example #4: Bolted Joint Problem

z-displacement

Single $\Omega$

Schwarz