

Accelerating mod/sim workflows through hybrid domain decomposition-based models and the Schwarz alternating method









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# Outline

- 1. Schwarz Alternating Method for Coupling of Full Order Models (FOMs) in Solid Mechanics
  - Motivation & Background
  - Quasistatic Formulation
    - Numerical Examples
  - Extension to Dynamics
    - Numerical Examples
- 2. Schwarz Alternating Method for FOM-ROM\* and ROM-ROM Coupling
  - Motivation & Background
  - Formulation
  - Numerical Examples
- 3. Summary and Future Work







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# Motivation for Coupling in Solid Mechanics

#### **Concurrent multiscale coupling for predicting failure**

- 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

#### Simplification of mesh generation

Creating a *high-quality mesh* for a *single component* can take *weeks*, making it "the single biggest bottleneck in analyses" [Sandia Lab News, 2020]!

<u>Goal</u>: develop a *concurrent multiscale coupling method* that is *minimally-intrusive* to implement into large HPC codes and can *simplify* the task of *meshing* complex geometries.



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



Schematic of difficult-to-mesh ratcheting mechanism with multiple threaded fasteners. From Parish *et al.*, 2024.

# **Requirements for Multiscale Coupling Method**

- Coupling is *concurrent* (two-way)
- *Ease of implementation* into existing massively-parallel HPC codes
- *"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
- Scalable, fast, robust (we target real engineering problems, e.g., analyses involving failure of bolted components!)
- Coupling does not introduce *nonphysical artifacts*
- *Theoretical* convergence properties/ guarantees



- 6 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 transmission BCs on  $\Gamma_1$ . Iterate until convergence:
- Solve PDE by any method on  $\Omega_2$  w/ transmission BCs on  $\Gamma_2$  based on values just obtained for  $\Omega_1$ .
- Solve PDE by any method on  $\Omega_1$  w/ transmission BCs on  $\Gamma_1$  based on values just obtained for  $\Omega_2$ .





 Schwarz alternating method most commonly used as a *preconditioner* for Krylov iterative methods to solve linear algebraic equations.

Idea behind this work: using the Schwarz alternating method as a *discretization method* for solving multi-scale or multi-physics partial differential equations (PDEs).

## 7 How We Use the Schwarz Alternating Method



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# **Quasistatic Solid Mechanics Formulation**

• Energy functional defining weak form of the governing PDEs

$$\Phi[\boldsymbol{\varphi}] \coloneqq \int_{\Omega} A(\boldsymbol{F}, \boldsymbol{Z}) dV - \int_{\Omega} \rho \boldsymbol{B} \cdot \boldsymbol{\varphi} dV$$

- ➤ A(F,Z): Helmholtz free-energy density
- →  $F := \nabla \varphi$ : deformation gradient
- $\succ$  Z: collection of internal variables (for plastic materials)
- $\succ$  *ρ*: density, *B*: body force, *P* = ∂*A*/∂*F*: Piola-Kirchhoff stress
- Euler-Lagrange equations, obtained by minimizing  $\Phi[\boldsymbol{\varphi}]$ :  $\begin{cases} \text{Div } \boldsymbol{P} + \rho \boldsymbol{B} = \boldsymbol{0}, \text{ in } \Omega \\ \boldsymbol{\varphi} = \boldsymbol{\chi}, & \text{ on } \partial \Omega \end{cases}$
- Quasistatics solves **sequence of problems** in which loading (body force) **B** is incremented **quasistatically** w.r.t. **pseudo time** t<sub>i</sub>:

For i = 1, ..., nSolve Div  $P + \rho B(t_i) = 0$  with appropriate boundary conditions (BCs) Increment pseudo time  $t_i$  to obtain  $t_{i+1}$ 

# Spatial Coupling via (Multiplicative) Alternating Schwarz

 $\Omega_2$ 

#### **Overlapping Domain Decomposition**

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$$\begin{cases} \operatorname{Div} \boldsymbol{P}_{1}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{1} \backslash \Gamma_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\varphi}_{2}^{(n)} & \text{ on } \Gamma_{2} \end{cases}$$
$$\begin{cases} \operatorname{Div} \boldsymbol{P}_{2}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{2} \backslash \Gamma_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\varphi}_{1}^{(n+1)} & \text{ on } \Gamma_{2} \end{cases}$$

 Dirichlet-Dirichlet transmission BCs [Schwarz, 1870; Lions, 1988]

#### Non-overlapping Domain Decomposition



- Relevant for multi-material and multi-physics coupling
- Alternating Dirichlet-Neumann transmission BCs [Zanolli *et al.*, 1987]
- Robin-Robin transmission BCs also lead to convergence [Lions, 1990]
- $\theta \in [0,1]$ : relaxation parameter (can help convergence)

# Spatial Coupling via (Multiplicative) Alternating Schwarz

#### **Overlapping Domain Decomposition**

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$$\begin{cases} \operatorname{Div} \boldsymbol{P}_{1}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{1} \backslash \Gamma_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\varphi}_{2}^{(n)} & \text{ on } \Gamma_{2} \end{cases}$$
$$\begin{cases} \operatorname{Div} \boldsymbol{P}_{2}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{2} \backslash \Gamma_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\varphi}_{1}^{(n+1)} & \text{ on } \Gamma_{2} \end{cases}$$

 Dirichlet-Dirichlet transmission BCs [Schwarz, 1870; Lions, 1988]

Part 1 of talk

#### Non-overlapping Domain Decomposition

$$\begin{cases} \operatorname{Div} \boldsymbol{P}_{1}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{1} \setminus \Gamma \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\lambda}_{n+1} & \text{ on } \Gamma \\ \begin{cases} \operatorname{Div} \boldsymbol{P}_{2}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{2} \setminus \Gamma \\ \boldsymbol{P}_{2}^{(n+1)} \boldsymbol{n} = \boldsymbol{P}_{2}^{(n+1)} \boldsymbol{n}, & \text{ on } \Gamma \end{cases} \\ \boldsymbol{\lambda}_{n+1} = \theta \boldsymbol{\varphi}_{2}^{(n)} + (1 - \theta) \boldsymbol{\lambda}_{n}, \text{ on } \Gamma, \text{ for } n \geq 1 \end{cases}$$

#### Part 2 of talk

 $\Omega_2$ 

- Relevant for multi-material and multi-physics coupling
- Alternating Dirichlet-Neumann transmission BCs [Zanolli *et al.*, 1987]
- Robin-Robin transmission BCs also lead to convergence [Lions, 1990]
- $\theta \in [0,1]$ : relaxation parameter (can help convergence)

#### **Multiplicative Overlapping Schwarz**

# $\begin{cases} \operatorname{Div} \boldsymbol{P}_{1}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{1} \backslash \Gamma_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\varphi}_{2}^{(n)} & \text{ on } \Gamma_{2} \end{cases}$ $\begin{cases} \operatorname{Div} \boldsymbol{P}_{2}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{2} \backslash \Gamma_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\varphi}_{1}^{(n+1)} & \text{ on } \Gamma_{2} \end{cases}$

#### Additive Overlapping Schwarz

 $\begin{cases} \operatorname{Div} \boldsymbol{P}_{1}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{1} \backslash \Gamma_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\varphi}_{2}^{(n)} & \text{ on } \Gamma_{2} \end{cases}$  $\begin{cases} \operatorname{Div} \boldsymbol{P}_{2}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{2} \backslash \Gamma_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\varphi}_{1}^{(n)} & \text{ on } \Gamma_{2} \end{cases}$ 

Model PDE:	
$\int \text{Div} \boldsymbol{P} + \rho \boldsymbol{B} =$	= ${f 0}$ , in $\Omega$
$ig( arphi = \chi,$	on $\partial \Omega$



- Multiplicative Schwarz: solves subdomain problems sequentially (in serial)
- Additive Schwarz: advance subdomains in parallel, communicate boundary condition data later
  - > Typically requires a few more **Schwarz iterations**, but does not degrade **accuracy**
  - > Parallelism helps balance additional cost due to Schwarz iterations
  - > Applicable to both **overlapping** and **non-overlapping** Schwarz

# Additional Parallelism via Additive Schwarz

#### Part 1 of talk Multiplicative Overlapping Schwarz

$$\begin{cases} \operatorname{Div} \boldsymbol{P}_{1}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{1} \backslash \Gamma_{1} \\ \boldsymbol{\varphi}_{1}^{(n+1)} = \boldsymbol{\varphi}_{2}^{(n)} & \text{ on } \Gamma_{2} \end{cases}$$
$$\begin{cases} \operatorname{Div} \boldsymbol{P}_{2}^{(n+1)} + \rho \boldsymbol{B}(t_{i}) = \boldsymbol{0} , \text{ in } \Omega_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\chi}, & \text{ on } \partial \Omega_{2} \backslash \Gamma_{2} \\ \boldsymbol{\varphi}_{2}^{(n+1)} = \boldsymbol{\varphi}_{1}^{(n+1)} & \text{ on } \Gamma_{2} \end{cases}$$

Part 2 of talkAdditive Overlapping Schwarz $\begin{cases} \text{Div } P_1^{(n+1)} + \rho B(t_i) = \mathbf{0} \text{, in } \Omega_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\chi}, & \text{on } \partial \Omega_1 \setminus \Gamma_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\varphi}_2^{(n)} & \text{on } \Gamma_2 \end{cases}$  $\begin{cases} \text{Div } P_2^{(n+1)} + \rho B(t_i) = \mathbf{0} \text{, in } \Omega_2 \\ \boldsymbol{\varphi}_2^{(n+1)} = \boldsymbol{\chi}, & \text{on } \partial \Omega_2 \setminus \Gamma_2 \\ \boldsymbol{\varphi}_2^{(n+1)} = \boldsymbol{\varphi}_1^{(n)} & \text{on } \Gamma_2 \end{cases}$ 



- Multiplicative Schwarz: solves subdomain problems sequentially (in serial)
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# Overlapping Schwarz 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.

# Convergence Proof\*

A. Moto, J. Tesure, C. Alleman Schwarz, Alternating Method in Solid Mechanics	A Mota, I. Taaur, C. Alleman Schwarz Alternating Method in Solid Mechanics	A. Monz, J. Tezane, C. Alleman Schwarz, Alternating Method in Solid Mechanics	A. Mota, I. Tezane, C. Alleman Schwarz Allemaning Method in Solid Mechanics
2 Formulation of the Schwarz Alternating Method		1: $\mathbf{x}_{12}^{(1)} \leftarrow \mathbf{X}_{2}^{(1)} \inf \Omega_1, \mathbf{x}_{2}^{(1)} \leftarrow \mathbf{\chi}(\mathbf{X}_{2}^{(1)}) \otimes \partial_{\mathbf{\mu}} \Omega_1,$ $\geq \mathbf{x}_{12}^{(2)} \leftarrow \mathbf{X}_{11}^{(1)} \inf \Omega_1, \mathbf{x}_{22}^{(2)} \leftarrow \mathbf{\chi}(\mathbf{X}_{12}^{(2)}) \otimes \partial_{\mathbf{\mu}} \Omega_1,$ $\geq \min \{\mathbf{x}_{12}^{(1)} \leftarrow \mathbf{x}_{12}^{(1)} \otimes \partial_{\mathbf{\mu}} \Omega_1,$ $\geq \min \{\mathbf{x}_{12}^{(1)} \leftarrow \mathbf{x}_{12}^{(1)} \otimes \partial_{\mathbf{\mu}} \Omega_1,$	Remark that [50]
We start by defining the standard finite deformation variational formulation to establish notation before presenting the formulation of the coupling method.	$\begin{pmatrix} m_1 & m_2 & m_1 \end{pmatrix}$ $r_1 & m_2$	3. reject 4. $\begin{bmatrix} \mathcal{K}_{10}^{(1)} \\ \mathcal{K}_{2}^{(2)} \end{bmatrix} = \begin{pmatrix} \mathcal{K}_{10}^{(1)} + \mathcal{K}_{20}^{(1)} H_{11} \\ \mathcal{K}_{20}^{(2)} H_{20} \\ \mathcal{K}_{20}^{(2)} H_{2$	$S_n = \varphi^{(n-1)} + V_1$ for $\varphi^{(n-1)} \in S_{n-1} \Rightarrow \varphi^{(n-1)} \in S_{n-1}$ . (60) <b>Theorem 1.</b> Assume that the energy functional $\Phi(\varphi)$ satisfies properties $1-5$ above. Consider the Schwarz domination method of factor $2 + \delta domination (0, 0, 0, 0)$ for the method of domination of the factor $2 + \delta domination (0, 0, 0)$ .
2.1 Variational Formulation on a Single Domain Consider a local statement of $C = \frac{1}{2}$ induces a consider the theorem in $\sigma = -\sigma(X) + 0$ , $\gamma \in \mathbb{R}^3$		$\begin{array}{cccccccccccccccccccccccccccccccccccc$	intermining theorem is because in section 2 influence by (9)-(1) and in equivalent form (39). There (a) $\Phi[\tilde{\varphi}^{(0)}] \ge \Phi[\tilde{\varphi}^{(1)}] \ge \cdots \ge \Phi[\tilde{\varphi}^{(n-1)}] \ge \Phi[\tilde{\varphi}^{(n)}] \ge \cdots \ge \Phi[\tilde{\varphi}^{(n)}]$
Consider a rowspace with equation in $C = 0$ undergoing a non-constrained by an inequality $\omega = \varphi(X)$ . If $X = V$ , $X \in \Omega$ . Assume that the boundary of the body is $\partial \Omega = \partial_{\Omega} \Omega = \partial_{\Omega} X$ where $\partial_{\Omega} \Omega$ , where $\partial_{\Omega} \Omega$ is a displacement boundary, $\partial_{T} \Omega$ is a traction boundary, and $\partial_{\omega} \Omega = \partial_{T} \Omega = \emptyset$ . The prescribed boundary	Figure 1: Two subdomains $T_0$ and $T_0$ and $T_0$ and $T_0$ and $T_0$ minimum for a standard standar	2: notif $\left[\left(\left \left(\Delta u_{B}^{(1)}\left \left \left \mathbf{k}'_{D}^{(1)}\right \right \right)^{*} + \left(\left \left \left(\Delta u_{B}^{(1)}\right \left \left \left \left u_{B}^{(2)}\right \right \right)^{*}\right]\right] \le \varepsilon_{mathins}$ is tight tolerance. Algorithm 5: Monoid his: Schwart Method	(b) the sequence $\{\tilde{\varphi}^{(n)}\}$ defined in (39) converges to the minimizer $\varphi$ of $\Phi[\varphi]$ in S.
deplucements or Dirichlet boundary conditions are $\chi : \partial_{\mu} \Omega \rightarrow \mathbb{R}^{3}$ . The prescribed boundary tractions or Neurann boundary conditions are $\pi : \partial_{\mu} \Omega \rightarrow \mathbb{R}^{3}$ . Let $F := \text{Grad} \varphi = \text{bt}$ deformation gradient. Let also $RB : \Omega \rightarrow \mathbb{R}^{3}$ be the body force, with $R$ the mass density in the reference configuration. Furthermore,	that is $i = 1$ and $j = 2$ if n is odd, and $i = 2$ and $j = 1$ if n is even. Introduce the following definitions for	[35, 34, 4]. Although we do not provide here formal convergence proofs for the remaining variants of the	(c) the Schwarz minimum values Φ[φ <sup>(m)</sup> ] converge monotonically to the minimum value Φ[φ] in S starting from any lotital gavers φ <sup>(0)</sup> .
introduce the energy functional $\Phi(a) = \int A(\mathbf{F}, \mathbf{Z}) dV = \int B\mathbf{F}_{ab} dV = \int -\mathbf{T}_{ab} dS$ (1)	each subdomain /: • Closure: ≅0 := ≅0 / @®0	Schwarz method, we offer some numerical results illustrating their convergence in Section 4. Consider the energy functional $\Phi[\phi]$ defined in (1). We will denote by $\langle \cdot, \cdot \rangle$ the usual $L^2$ inner product over $\Omega$ , they is the sector of	(d) if Φ <sup>(</sup> (φ) is Lipschitz continuous in a neighborhood of φ, thus the sequence (φ <sup>(n)</sup> ) converges geometrically to the winitidizer φ. <sup>1</sup>
$\tau_{pq_1,\cdots} \int_{\eta} n(\mathbf{r}, \omega) d\mathbf{r} = \int_{\eta} n\omega \cdot \varphi d\mathbf{r} = \int_{\partial p\eta} \omega \cdot \varphi d\omega,$ (1)	Dirichlet boundary: @ III) = @ III1 III).	$(\psi_1, \psi_2) := \int \psi_1 \cdot \psi_2  dV,$ (35)	Proof. See Appendix A.
in which $A(F, Z)$ is the Belmhöltz free-energy density and Z is a collection of internal variables. The weak form of the problem is obtained by minimizing the energy functional $\Phi(\varphi)$ over the Subblev space $W_{i}^{2}(\Omega)$ that is comprised of all functions that are square-integrable and have square-integrable first derivatives. Define	<ul> <li>Naumann boundary: @ ∞ := @ ∞ i. ∞.</li> <li>Schwarz boundary: Γ<sub>1</sub> := @ 0 i. ∞.</li> </ul>	for $\psi_1, \psi_2 \in W_2^1(\Omega)$ , with corresponding nerm $  \cdot  $ . The proof of the convergence of the Schwarz alternating method requires that the functional $\Phi[\varphi]$ satisfy the following properties over the space S defined in (2):	Finally, while most of works cired above present their analysis for the specific case of two subdomains, extension to multiple subdomains is in general straightforward. The case of multiple subdomains is considered specifically in Lisses [33], Badar [4], and Li-Shan and Evars [34].
$S := \{\varphi \in W_2^1(\Omega) : \varphi = \chi \text{ on } \partial_{\varphi}\Omega\}$ (2) and	Note that with these definitions we guarantee that $(0, \varpi) \downarrow (0, \varpi) \downarrow (1, \varpi)$ . Now define the spaces	<ol> <li>Φ[φ] is coercive.</li> <li>Φ[φ] is Fréchet differentiable, with Φ'[φ] denoting its Fréchet derivative.</li> </ol>	4 Numerical Examples
$V := \{\xi \in W_2(\Omega) : \xi = 0 \text{ on } \partial_{\varphi}\Omega\}$ (3) where $\xi \in V$ is a test function. The rotantial assume is minimized if and only if divid $\leq 0$ for $z \neq z\xi'$ for all	$S_i := \{' 2 W_2^j(00) : ' = \chi \text{ on } (0, 00) : - P_{0j-1}, ['(00)] \text{ on } \Gamma_i \}$ , (7)	<ol> <li>Φ(φ) is strictly convex.</li> </ol>	In this section, we present numerical examples of the behavior of the Schwarz alternating method for two
$\xi \in V$ and $e \in \mathbb{R}$ . It is straightforward to show that the minimum of $\Phi[\varphi]$ is the mapping $\varphi \in S$ that satisfies	and $V_i := \{ e 2 W_2^1(\overline{\omega}) : e = 0 \text{ on } \otimes \overline{\omega} \setminus \Gamma_i \}$ (8)	<ol> <li>Φ[φ] is lower semi-continuous.</li> </ol>	in the open-source ALBANY finite element code [32]. Next, we discuss the error measures used throughout
$D\Phi[\varphi](\xi) = \int_{\Omega} \mathbf{P} : \operatorname{Grad} \xi  dV - \int_{\Omega} R\mathbf{B} \cdot \xi  dV - \int_{\partial_{\varphi} \cdot \Omega} \mathbf{T} \cdot \xi  dS = 0,$ (4)	where the symbol $P_{0, \Gamma_1}[\cdot]$ denotes the projection from the subdomain $\mathbb{Z}_2^0$ onto the Schwarz boundary $\Gamma_1$ . This projection operator plays a central role in the Schwarz alternating method. Its form and implementation	5. $\Phi'[\varphi]$ is uniformly continuous on $K_B$ , where $K_B = -i_B \in S : \Phi(\alpha) < B, B \in B, B < \infty$ . (36)	the numerical examptes. Then, we commoe with four examples that demonstrate different features of the Schwarz alternating method and our implementations. The first example, a one-dimensional singular bar, is used to demonstrate the behavior of the four Schwarz variants of Schriften 2.4. The vacend example, a subsid
where $P = \partial A/\partial F$ denotes the first Fields Kirchhoff stress. The Euler-Lagrange equation corresponding to the variational statement (4) is	are discussed in a skeapart sections. For the moment it is adfinited to assume that the operator is able to project a field of incom one skeapartian to the Schwarz shouting of the other subdomain. The Schwarz alternating method solves a sequence of problems on 30 and 50. The solution * <sup>(a)</sup> for the	It can be shown that the energy functional $\Phi(q)$ defined in (1) is strictly constrained in $\mathcal{O}(p)$ and that the behavior that the constrained of $\Phi(q)$ defined in (1) is strictly constrained in $\mathcal{O}(p)$ and that the behavior that the constrained of the $\mathcal{O}(q)$ and the constrained in $\mathcal{O}(q)$ and the constrained in $\mathcal{O}(q)$ and	body of square base, aims to study the effect of the size of the overlap region on the convergence of the method. The objective of the third example, a models of sindice is so analyze the numerical error in the evaluation and the demonstrate the ability of the method to courted different element motoriosity. The base carried, a laser

**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) Φ[φ̃<sup>(0)</sup>] ≥ Φ[φ̃<sup>(1)</sup>] ≥ ··· ≥ Φ[φ̃<sup>(n-1)</sup>] ≥ Φ[φ̃<sup>(n)</sup>] ≥ ··· ≥ Φ[φ], where φ is the minimizer of Φ[φ] over S.
  (b) The sequence {φ̃<sup>(n)</sup>} defined in (39) converges to the minimizer φ of Φ[φ] 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  $\tilde{\varphi}^{(0)}$ .

Remark 1 By the coercivity of $\Phi[\phi]$ , it follows from the Lax-Milgram theorem that a unique minimizer to	A minimum (47) and the (46) in (40) he has	$\lim   \tilde{\varphi}^{(n)} - \tilde{\varphi}^{(n+1)}  ^2 = 0,  (69)$	$\left(\Phi'[\psi^{(n)}], \varphi - \psi^{(n)}\right) \leq \left(\Phi'[\psi^{(n)}], \varphi - \psi^{(n)}\right) + \alpha_R   \varphi - \psi^{(n)}   \leq \Phi \varphi  - \Phi[\psi^{(n)} $ (79)
this functional over S exists, i.e., the minimization of $\Psi(\varphi)$ is well-posed. Remark 2. By the Stampacobia theorem, the minimization of $\Psi(\varphi)$ in S is equivalent to finding $\varphi \in S$ such then	$(\Psi'[\hat{\phi}^{(n)}] - \Psi'[\hat{\phi}^{(n-1)}], \xi_2) = (\Psi'[\hat{\phi}^{(n)}], \xi) \le   \Psi'[\hat{\phi}^{(n)}] - \Psi'[\hat{\phi}^{(n-1)}]   \cdot   \xi_2  ,  (61)$	from which we can conclude that $\phi^{(n)} - \phi^{(n+2)} \rightarrow 0$ as $n \rightarrow \infty$ . We must now show that $\phi^{(n)}$ converges to $\phi$ , the minimizer of $\Phi(\phi)$ on $S$ . By (53) with $\psi_1 = \phi$ and	since $\alpha_H \ge 0$ . Now, by the Cauchy-Schwarz inequality followed by the application of the Lipshitz continuity of $\Phi^*(\varphi)$ (66) we can write
$(\Phi'[\phi], \xi - \phi) \ge 0$ (51)	and substituting (56) into (61) we finally obtain that	$\psi_2 = \hat{\varphi}^{(n)}$ , we have	$\left(\Psi'   \tilde{\varphi}^{(n)}  , \varphi - \tilde{\varphi}^{(n)} \right) \le   \Psi' (\tilde{\varphi}^{(n)})   \cdot   \varphi - \tilde{\varphi}^{(n)}   \le K   \varphi - \tilde{\varphi}^{(n)}  ^2.$ (80)
for all $\xi \in S$ .	$(\Phi'   \tilde{\varphi}^{(n)}), \xi) \le C_0   \Phi'   \tilde{\varphi}^{(n)}  - \Phi'   \tilde{\varphi}^{(n-1)}    \cdot   \xi  ,$ (62)	$  \varphi - \hat{\varphi}^{(n)}  ^2 \le \frac{1}{\alpha_R} \left\{ \Phi(\varphi) - \Phi[\hat{\varphi}^{(n)}] - \left( \Phi^{\dagger}[\hat{\varphi}^{(n)}], \varphi - \hat{\varphi}^{(n)} \right) \right\}.$ (70)	Hence, from (79),
Remark 3 Recall that the strict convexity property of $\Phi(\varphi)$ can be written as	$\forall \boldsymbol{\xi} \in \mathcal{S}.$	Since $\varphi$ is the minimum of $\Phi[\varphi]$ , by (a) we have that $\Phi[\varphi] \leq \Phi[\varphi^{(n)}]$ . It follows that	$\Psi[\varphi^{(n)}] = \Psi[\varphi] \le K   \varphi^{(n)} - \varphi  ^n$ . (81) Measure by (53) since $\theta'(n) = 0$ .
$\Phi[\psi_2] - \Phi[\psi_1] - (\Psi'[\psi_1], \psi_2 - \psi_1) \ge 0,$ (52)	Remark 8 For part (d) of Theorem 1, recall the definition of geometric convergence:	$\Phi[\phi] - \Phi[\bar{\phi}^{(n)}] - (\Phi'[\bar{\phi}^{(n)}], \phi - \bar{\phi}^{(n)}) \le - (\Phi'[\bar{\phi}^{(n)}], \phi - \bar{\phi}^{(n)}) = (\Phi'[\bar{\phi}^{(n)}], \bar{\phi}^{(n)} - \phi).$ (71)	$\Phi[\hat{\alpha}^{(n)}] - \Phi[\alpha] > \alpha \alpha   \hat{\alpha}^{(n)} - \alpha  ^2$ (87)
$\forall \psi_1, \psi_2 \in S$ . From (36), remark that if $\Phi(\varphi)$ is strictly convex over $S \forall R \in \mathbb{R}$ such that $R < \infty$ , we can find an $\alpha_R > 0$ such that $\forall \psi_1, \psi_2 \in \mathcal{K}_R$ we have	$E_{n+1} \le CE_n$ , (63)	Substituting (71) into (70) we have	$\Psi_{[\Psi^{-1}]} = \Psi_{[\Psi^{-1}]} \ge w_{[0]}  \Psi^{-1} - \Psi_{[0]} $ . (6.2) Using (81) and (82) we obtain
$\Phi[\psi_2] - \Phi[\psi_1] - (\Phi'[\psi_1], \psi_2 - \psi_3) \ge \alpha_B   \psi_2 - \psi_1  ^2.$ (53)	$\forall n \in \{0, 1, 2,\}$ for some $C > 0$ , where $E_n :=   \phi^{(n+1)} - \phi^{(n)}  ,$ (64)	$  \varphi - \bar{\varphi}^{(n)}  ^2 \le \frac{1}{\alpha_R} \left( \bar{\varphi}'[\bar{\varphi}^{(n)}], \bar{\varphi}^{(n)} - \varphi \right).$ (72)	$\left(\Phi[\tilde{\varphi}^{(n)}] - \Phi[\varphi]\right) - \left(\Phi[\tilde{\varphi}^{(n+1)}] - \Phi[\varphi]\right) \le K   \tilde{\varphi}^{(n)} - \varphi  ^2 - \alpha_K   \tilde{\varphi}^{(n+1)} - \varphi  ^2.$ (83)
Remark 4 By property 5, the uniform continuity of $\Phi'[\phi]$ , there exists a modulus of continuity $\omega > 0$ , with	<ul> <li>A both of a set o</li></ul>	Now by (62) (Remark 7),	Combining (83) and (78) leads to
$\omega : \kappa_R \rightarrow \kappa_R$ , such that $  \Psi'(\psi_1) - \Psi'(\psi_2)   \le \omega \langle   \psi_1 - \psi_2   \rangle$ , (54)	Remark 9 Recall from the deminion of continuity that if $\Psi(\varphi)$ is Lipstitz continuous at $\varphi^{-n}$ near $\varphi$ , then there exists a constant $K \ge 0$ such that	$(\Phi'   \hat{\varphi}^{(n)}  , \hat{\varphi}^{(n)} - \varphi) \le C_0   \Phi'   \hat{\varphi}^{(n)}   - \Phi'   \hat{\varphi}^{(n-1)}    \cdot    \hat{\varphi}^{(n)} - \varphi   .$ (73)	$\frac{\alpha_R}{C}   \hat{\varphi}^{(n)} - \varphi  ^2 \le \left(\Phi[\hat{\varphi}^{(n)}] - \Phi[\varphi]\right) - \left(\Phi[\hat{\varphi}^{(n+1)}] - \Phi[\varphi]\right) \le K   \hat{\varphi}^{(n)} - \varphi  ^2 - \alpha_R   \hat{\varphi}^{(n+1)} - \varphi  ^2.$
$\forall \psi_1, \psi_2 \in K_R$ . By definition, $\omega(\epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$ .	$  \Psi'[\phi^{(n)}] - \Psi'[\phi]   \le \kappa$ (65)	Substituting (73) into (72) leads to	(84)
Remark 5 It was shown in [35] that in the case $\Omega_1 \cap \Omega_2 \neq \emptyset$ , $\forall \varphi \in S$ , there exist $\zeta_1 \in S_1$ and $\zeta_2 \in S_2$	$  \hat{\varphi}^{(n)} - \varphi   \ge n$ . (65)	$  \bar{\varphi}^{(n)} - \varphi   \le \frac{C_0}{2\pi}   \Phi' \bar{\varphi}^{(n)}  - \Phi' \bar{\varphi}^{(n-1)}   .$ (74)	$  \phi^{(n+1)} - \phi   \le B   \phi^{(n)} - \phi  $ (85)
such that $\varphi = \zeta_1 + \zeta_2,$ (55)	Considering that $\Psi'[\varphi] = 0$ since $\varphi$ is the minimizer of $\Phi[\varphi]$ , (65) is equivalent to	Applying the uniform continuity assumption (54), we obtain	with $B := \sqrt{\frac{K}{-1}}$ . (86)
and $\max(  \zeta_1  ,   \zeta_2  ) \le C_0  \varphi  $ , (56)	$  \psi  \varphi^{(-)}   \le K   \varphi^{(-)} - \varphi  .$ (66)	$  \hat{\varphi}^{(n)} - \varphi   \le \frac{C_0}{\omega} \omega \left(   \hat{\varphi}^{(n)} - \hat{\varphi}^{(n-1)}   \right).$ (75)	$\gamma \alpha_R = C_1$ and $R \in \mathbb{R}$ as we choose $C_1 > \alpha_{n-1}(K)$ . Burthermore, since the second conditional $(A^{(n)})$ , comparison monotonically to
for some $C_0 > 0$ independent of $\varphi$ .	Proof of Theorem 1	By (60) $  \hat{\alpha}^{(n)}  \rightarrow \hat{\alpha}^{(n-1)}   \rightarrow 0$ as $n \rightarrow \infty$ . From this we obtain the result assume that $\hat{\alpha}^{(n)} \rightarrow \infty$ is	the minimizer $\varphi$ of $\Phi(\varphi)$ by (b) and (c), it follows that $B \in (0, 1)$ . Define $C := 1 - B \in (0, 1)$ , then (85)
Remark 6 Note that (39) can be written as	Proof of (a). Let $\tilde{\psi}^{(1)} = \arg \min_{\psi \in \tilde{S}_1} \Phi(\varphi)$ . By (40), $\tilde{\varphi}^{(1)} \in \tilde{S}_2$ . Let $\tilde{\psi}^*$ be the minimizer of $\Phi[\varphi]$ over $\tilde{S}_2$ and $\varphi$ much $\tilde{\Phi}(\tilde{S}_1) = \Phi(\tilde{S}_1)$ . Using the intermediation drawn we have $\tilde{G}_2 = \tilde{G}_1^{(1)}$ . Hence it remarks to	$n \to \infty$ .	can be recast as $  \hat{\phi}^{(n+1)} - \hat{\phi}^{(n)}   \le C   \hat{\phi}^{(n)} - \hat{\phi}^{(n-1)}  $ (87)
$(\Phi'[\tilde{\varphi}^{(n)}], \xi^{(i)}) = 0, \text{ for } \tilde{\varphi}^{(n)} \in \tilde{S}_n, \forall \xi^{(i)} \in S_i,$ (57)	that $\mathfrak{s}[\tilde{\varphi}^{(1)}] < \mathfrak{s}[\tilde{\varphi}^{(2)}]$ where $\tilde{\varphi}^{(2)} = \arg \min_{\varphi \in \mathcal{S}_{0}} \mathfrak{s}[\varphi]$ . It follows by induction that	Proof of (c). This follows immediately from (a) and (b).	whereupon the claim is proven.
for $i \in \{1, 2\}$ and $n \in \{0, 1, 2,\}$ (recall from (6) the relation between $i$ and $n$ ). This is due to the uniqueness of the solution to each minimization problem over $\hat{S}_n$ and the definition of $\hat{\varphi}^{(n)}$ as the minimizer of $\Phi[\varphi]$ over	$\Psi[\hat{\varphi}^{(\alpha)}] \le \Psi[\hat{\varphi}^{(\alpha-1)}]$ (67)	Proof of (d). By (b) , for large enough n, there exists some $C_1 > 0$ independent of n such that $  \hat{\omega}^{(n_1)} = \varphi_1  ^2 \le C_1   \hat{\varphi}^{(n+1)} = \hat{\varphi}^{(n)}  ^2.$ (76)	B Analytic Solution for Linear-Elastic Singular Bar
$S_n$ . Remark 7 Let $\phi^{(n)} \in \hat{S}_n$ , and let $\xi \in S$ . By Remark 5, there exist $\zeta_1 \in S_1$ and $\zeta_2 \in S_2$ such that	tor $n \in \{1, 2, 3,\}$ . Now let $\varphi$ be the minimizer of $\Phi[\varphi]$ over $S$ . Since the problem is well-posed $\varphi$ is unique. Hence $\Phi[\varphi] \leq \Phi[\varphi^{(\alpha)}]$ for all $n \in \{1, 2, 3,\}$ .	Let us choose $C_1$ such that $C_1 > \alpha_R/K$ , where K is the Lipshitz continuity constant in (66). Combining (68) with (76) leads to	As reference, herein we provide the solution of the singular bar of Section 4.3 for linear elasticity. The equilibrium equation is
$(\Phi'[\hat{\varphi}^{(n)}], \xi) = (\Phi'[\hat{\varphi}^{(n)}], \zeta_1 + \zeta_2).$ (58)		$\frac{1}{\alpha_R} \left( \Phi[\tilde{\varphi}^{(n)}] - \Phi[\tilde{\varphi}^{(n+1)}] \right) \ge \ \tilde{\varphi}^{(n+1)} - \tilde{\varphi}^{(n)}\ ^2 \ge \frac{1}{C_1} \ \tilde{\varphi}^{(n)} - \varphi\ ^2.  (77)$	$P = \sigma(X)A(X) = \text{const.}$ $\sigma(X) = E_1(X),  e(X) := u'(X),  A(X) = A_0\left(\frac{X}{L}\right)^{\frac{1}{2}},$ (88)
	15	36	

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

# Implementation in Albany-LCM and Sierra/SM HPC Codes

The overlapping Schwarz alternating method has been implemented in two Sandia HPC codes: Albany-LCM and Sierra/SM

#### **Albany-LCM**<sup>1</sup>

- Open-source parallel, C++, multi-physics, finite element code that relies heavily on Trilinos<sup>2</sup> libraries
- Parallel implementation of Schwarz alternating method uses the Data Transfer Kit (DTK)<sup>3</sup>

#### Sierra/Solid Mechanics (Sierra/SM)

- Sandia proprietary production *Lagrangian 3D code* for finite element analysis of solids & structures
- Schwarz alternating method was "implemented" in Sierra/SM using Arpeggio iterative coupling framework

We did **not** have to write any **code** in Sierra/SM to implement Schwarz!







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## Cuboid Problem



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



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#### Schwarz Iteration

# Cuboid Problem: Convergence and Accuracy

- Top right: convergence of the cuboid problem for different mesh sizes and fixed overlap volume fraction. The Schwarz alternating method converges linearly.
- Bottom right: convergence factor μ as a function of overlap volume and different mesh. There is *faster linear convergence* with increasing *overlap volume fraction*.

 $\Delta y^{(m+1)} \le \mu \Delta y^{(m)}$ 

• **Below:** *relative errors* in displacement and stress w.r.t. single-domain reference solution. Errors are on the order of *machine precision*.

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



### Notched Cylinder



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

# Notched Cylinder: TET - HEX Coupling

- The Schwarz alternating method is capable of coupling *different mesh topologies*.
- The notched region, where stress concentrations are expected, is *finely* meshed with *tetrahedral* elements.
- The top and bottom regions, presumably of less interest, are meshed with *coarser hexahedral* elements.



# Notched Cylinder: TET - HEX Coupling

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 Relative errors in displacement w.r.t. single-domain reference solution are dominated by geometric (rather than coupling) error.

# Laser Weld (Albany/LCM)



Albany

# Single domain discretization



Coupled Schwarz discretization (50% reduction in model size)



- Problem of *practical scale*.
- *Isotropic elasticity* and *J*<sup>2</sup> *plasticity* with linear isotropic hardening.
- *Identical parameters* for weld and base materials for proof of concept, to become independent models.

# Laser Weld (Albany/LCM): Strong Scalability of Parallel Schwarz with DTK



• Near-ideal linear speedup (64-1024 cores).









# Laser Weld (Sierra/SM): Uniaxial Tension-Test Models



- The domains for Schwarz coupling are **meshed independently**
- This provides the ability to try different meshing schemes for each subdomain
- No need to re-mesh entire domain

- Schwarz gives accurate prediction of stress states if tight enough Schwarz tolerance is used
  - Tight Schwarz tolerance needed due to large disparity between element sizes
- For now, Schwarz is **slower** on this problem, but we are optimizing this



# 26 Tensile Bar

350

300

stress (MPa)

true s 200

150

# The alternating Schwarz method can be used as part of a *homogenization* (upscaling) process to bridge gap b/w *microscopic* and *macroscopic* regions

- *Microstructure* embedded in ASTM tensile geometry (right).
- Fix microstructure, investigate *ensemble* of uniaxial loads.
- Fit flow curves with a *macroscale* J<sub>2</sub> plasticity model (below).

100 0.000 0.005 0.010 0.015 0.020 0.025 0.030 0.035 0.040

equivalent plastic strain(mm/mm)

ensembles



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# Solid Dynamics Formulation

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• Kinetic energy:  $T(\dot{\varphi}) \coloneqq \frac{1}{2}$ 

$$T(\dot{\boldsymbol{\varphi}}) \coloneqq \frac{1}{2} \int_{\Omega} \rho \dot{\boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} \, dV$$

- Potential energy:  $V(\boldsymbol{\varphi}) \coloneqq \int_{\Omega} A(\boldsymbol{F}, \boldsymbol{Z}) dV \int_{\Omega} \rho \boldsymbol{B} \cdot \boldsymbol{\varphi} dV$
- Lagrangian:  $L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) \coloneqq T(\dot{\boldsymbol{\varphi}}) V(\boldsymbol{\varphi})$
- Action functional:  $S[\boldsymbol{\varphi}] \coloneqq \int_{T} L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) dt$
- Euler-Lagrange equations:  $\begin{cases}
  \text{Div } \boldsymbol{P} + \rho \boldsymbol{B} = \rho \boldsymbol{\ddot{\varphi}}, & \text{in } \Omega \times I \\
  \boldsymbol{\varphi}(\boldsymbol{X}, t_0) = \boldsymbol{x}_0, & \text{in } \Omega \\
  \boldsymbol{\dot{\varphi}}(\boldsymbol{X}, t_0) = \boldsymbol{v}_0, & \text{in } \Omega \\
  \boldsymbol{\varphi}(\boldsymbol{X}, t) = \boldsymbol{v}_0, & \text{on } \partial \Omega \times I
  \end{cases}$
- Semi-discrete problem following FEM discretization in space:

$$M\ddot{u} + f_{\rm int}(u, \dot{u}) = f_{\rm ext}$$

# <sup>29</sup> Time-Advancement Within the Schwarz Framework



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

Controller time stepper

Time integrator for  $\Omega_1$ 

Time integrator for  $\Omega_2$ 

**Model PDE:** 
$$\begin{cases} M\ddot{u} + f_{int}(u, \dot{u}) = f_{ext} \\ u(x, 0) = u_0 \end{cases}$$

# <sup>30</sup> Time-Advancement Within the Schwarz Framework



Controller time stepper

Time integrator for  $\Omega_1$ 

Time integrator for  $\Omega_2$ 

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

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

**Model PDE:** 
$$\begin{cases} M\ddot{u} + f_{int}(u, \dot{u}) = f_{ext} \\ u(x, 0) = u_0 \end{cases}$$

# Time-Advancement Within the Schwarz Framework



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

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

<u>Step 2</u>: Advance  $\Omega_2$  solution from time  $T_i$  to time  $T_{i+1}$  using time-stepper in  $\Omega_2$  with time-step  $\Delta t_2$ , using solution in  $\Omega_1$  interpolated to  $\Gamma_2$  at times  $T_i + n\Delta t_2$ .

Model PDE:  $\begin{cases} M\ddot{u} + f_{int}(u, \dot{u}) = f_{ext} \\ u(x, 0) = u_0 \end{cases}$ 

# Time-Advancement Within the Schwarz Framework



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Controller time stepper

Time integrator for  $\Omega_1$ 

Time integrator for  $\Omega_2$ 

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

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

**<u>Step 2</u>**: Advance  $\Omega_2$  solution from time  $T_i$  to time  $T_{i+1}$  using time-stepper in  $\Omega_2$  with time-step  $\Delta t_2$ , using solution in  $\Omega_1$  interpolated to  $\Gamma_2$  at times  $T_i + n\Delta t_2$ .

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

Model PDE:  $\begin{cases} M\ddot{u} + f_{int}(u, \dot{u}) = f_{ext} \\ u(x, 0) = u_0 \end{cases}$ 

# <sup>33</sup> Time-Advancement Within the Schwarz Framework



Controller time stepper

Time integrator for  $\Omega_1$ 

Time integrator for  $\Omega_2$ 

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

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

<u>Step 2</u>: Advance  $\Omega_2$  solution from time  $T_i$  to time  $T_{i+1}$  using time-stepper in  $\Omega_2$  with time-step  $\Delta t_2$ , using solution in  $\Omega_1$  interpolated to  $\Gamma_2$  at times  $T_i + n\Delta t_2$ .

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

If unconverged, return to Step 1.

**Model PDE:**  $\begin{cases} M\ddot{u} + f_{int}(u, \dot{u}) = f_{ext} \\ u(x, 0) = u_0 \end{cases}$ 

# <sup>34</sup> Time-Advancement Within the Schwarz Framework



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

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

<u>Step 2</u>: Advance  $\Omega_2$  solution from time  $T_i$  to time  $T_{i+1}$  using time-stepper in  $\Omega_2$  with time-step  $\Delta t_2$ , using solution in  $\Omega_1$  interpolated to  $\Gamma_2$  at times  $T_i + n\Delta t_2$ .

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

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

Can use *different integrators* with *different time steps* within each domain!

**Model PDE:** 
$$\begin{cases} M\ddot{u} + f_{int}(u, \dot{u}) = f_{ext} \\ u(x, 0) = u_0 \end{cases}$$

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# <sup>35</sup> Time-Advancement Within the Schwarz Framework



Time-stepping procedure is **equivalent** to doing Schwarz on **space-time domain** [Mota *et al.* 2022].

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

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

<u>Step 2</u>: Advance  $\Omega_2$  solution from time  $T_i$  to time  $T_{i+1}$  using time-stepper in  $\Omega_2$  with time-step  $\Delta t_2$ , using solution in  $\Omega_1$  interpolated to  $\Gamma_2$  at times  $T_i + n\Delta t_2$ .

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

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

**Model PDE:** 
$$\begin{cases} M\ddot{u} + f_{int}(u, \dot{u}) = f_{ext} \\ u(x, 0) = u_0 \end{cases}$$

# Schwarz Alternating Method for Dynamic Multiscale Coupling: Theory



- Like for quasistatics, dynamic alternating Schwarz method converges provided each singledomain problem is *well-posed* and *overlap region* is *non-empty*, under some *conditions* on  $\Delta t$ .
- Well-posedness for the dynamic problem requires that action functional  $S[\boldsymbol{\varphi}]\coloneqq$

 $\int_{I} \int_{\Omega} L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) dV dt \text{ be strictly convex or strictly concave, where } L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) \coloneqq T(\dot{\boldsymbol{\varphi}}) + V(\boldsymbol{\varphi}) \text{ is the Lagrangian.}$ 

> This is studied by looking at its second variation  $\delta^2 S[\boldsymbol{\varphi}_h]$ 

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• We can show assuming a *Newmark* time-integration scheme that for the *fully-discrete* problem:

$$\delta^2 S[\boldsymbol{\varphi}_h] = \boldsymbol{x}^T \left[ \frac{\gamma^2}{(\beta \Delta t)^2} \boldsymbol{M} - \boldsymbol{K} \right] \boldsymbol{x}$$

- $\geq \delta^2 S[\boldsymbol{\varphi}_h]$  can always be made positive by choosing a *sufficiently small*  $\Delta t$
- > Numerical experiments reveal that  $\Delta t$  requirements for *stability/accuracy* typically lead to automatic satisfaction of this bound.

\*A. Mota, I. Tezaur, G. Phlipot. "The Schwarz alternating method for dynamic solid mechanics", IJNME, 2022.
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### <sup>38</sup> Elastic Wave Propagation

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





*Time-discretizations:* Newmark (implicit, explicit).

*Meshes:* HEX, TET

### Elastic Wave: Different Integrators, Same $\Delta ts$



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

	Implicit-Implicit		Explicit(CM)-Implicit		Explicit(LM)-Implicit	
Conformal HEX - HEX	2.79e-3	7.32e-3	3.53e-3	8.70e-3	4.72e-3	1.19e-2
Nonconformal HEX - HEX	2.90e-3	7.10e-3	2.82e-3	7.29e-3	2.84e-3	7.33e-3
TET - HEX	2.79e-3	7.58e-3	3.52e-3	8.92e-3	4.72e-3	1.19e-2

### Elastic Wave: Different Integrators, Different $\Delta ts$



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**Figures above:** Plots of displacement, velocity and acceleration for the elastic wave propagation problem using different time integrators (implicit and explicit) and different time steps (1e-2s and 2e-7s) for each subdomain, superimposed over the analytic single domain solution.

The analytic solution is *indistinguishable* from Schwarz solutions (hidden behind the solutions for  $\Omega_0$  (red) and  $\Omega_1$  (green))!

### **Tension Specimen**

- Uniaxial aluminum cylindrical tensile specimen with *inelastic J<sub>2</sub> material model*.
- Domain decomposition into *two* subdomains (right):  $\Omega_0$  = ends,  $\Omega_1$  = gauge.
- Nonconformal HEX + composite TET10 coupling via Schwarz.
- *Implicit* Newmark time-integration with *adaptive time-stepping* algorithm employed in both subdomains.
- Slight *imperfection* introduced at center of gauge to force *necking* upon pulling in vertical direction.



### Tension Specimen: Expected Result

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LO



### Tension Specimen: Displacement & EQPS\*



### Bolted Joint Problem

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Problem of *practical scale*.

• Schwarz solution compared to single-domain solution on composite TET10 mesh.



- $\Omega_1 = \text{bolts}$  (Composite TET10),  $\Omega_2 = \text{parts}$  (HEX).
- Inelastic J<sub>2</sub> 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.





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### Bolted Joint Problem: Equivalent Plastic Strain (EQPS)





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### <sup>47</sup> Bolted Joint Problem: Convergence Rate



*Figure above*: Convergence behavior of the dynamic Schwarz algorithm for the bolted joint problem

	CPU times (64 procs*)	Avg # Schwarz iters	Max # Schwarz iters
Single Domain	3h 34m	—	—
Schwarz	2h 42m	3.22	4
Single Domain (finer)	17h 00m	_	_
Schwarz (finer mesh of bolts)	29h 29m	3.28	4



\* On SNL ascicgpu15, 16, 17 machines (Intel Skylake CPU processor), Schwarz tol = 1e-6.

	CPU times (64 procs*)	Avg # Schwarz iters	Max # Schwarz iters
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Schwarz (finer mesh of bolts)	29h 29m	3.28	4



- Despite its iterative nature, Schwarz can actually be *faster* than single domain run for discretizations having comparable # of elements in the bolts.
  - Even if the method is more computationally expensive for some resolutions, it may be preferred for its ability to *rapidly change* and *evaluate* a *variety* of *engineering designs* (our typical use case).

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	CPU times (64 procs*)	Avg # Schwarz iters	Max # Schwarz iters
Single Domain	3h 34m	—	—
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Single Domain (finer)	17h 00m	—	—
Schwarz (finer mesh of bolts)	29h 29m	3.28	4

- Despite its iterative nature, Schwarz can actually be *faster* than single domain run for discretizations having comparable # of elements in the bolts.
  - Even if the method is more computationally expensive for some resolutions, it may be preferred for its ability to *rapidly change* and *evaluate* a *variety* of *engineering designs* (our typical use case).
- Dynamic Schwarz converges in between 2-4 Schwarz iterations per time-step despite the overlap region being very small for this problem.



\* On SNL ascicgpu15, 16, 17 machines (Intel Skylake CPU processor), Schwarz tol = 1e-6.

# Outline

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    - Numerical Examples
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- 3. Summary and Future Work







### <sup>53</sup> Motivation for ROM-ROM/ROM-FOM Couplings

The past decades have seen tremendous investment in **simulation frameworks** for **coupled multi-scale** and **multi-physics** problems.

- Frameworks rely on established mathematical theories to couple physics components.
- Most existing coupling frameworks are based on traditional discretization methods.



#### Complex System Model

- PDEs, ODEs
- Nonlocal integral
- Classical DFT
- Atomistic, ...

#### **Traditional Methods**

 $N_{2}$ 

- Mesh-based (FE, FV, FD)
- Meshless (SPH, MLS)
- Implicit, explicit

 $N_3$ 

• Eulerian, Lagrangian...

#### **Coupled Numerical Model**

Monolithic (Lagrange multipliers)

 $N_{4}$ 

 $N_{s}$ 

(EAM)

E<sup>3</sup>SI

Ocean (MPAS-

Land (ELM)

Land Ice (MALI) Sea Ice (MPAS-

- Partitioned (loose) coupling
- Iterative (Schwarz, optimization)

# <sup>54</sup> Motivation for ROM-ROM/ROM-FOM Couplings

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#### **Traditional Methods**

- Mesh-based (FE, FV, FD)
- Meshless (SPH, MLS)
- Implicit, explicit
- Eulerian, Lagrangian, ...



#### **Coupled Numerical Model**

- Monolithic (Lagrange multipliers)
- Partitioned (loose) coupling
- Iterative (Schwarz, optimization)



- PINNs
- Neural ODEs
- Projection-based ROMs, ...
- There is currently a big push to integrate **data-driven methods** into modeling & simulation toolchains.

Unfortunately, existing algorithmic and software infrastructures are **ill-equipped** to handle plug-and-play integration of **non-traditional**, **data-driven models**!

# 55 Flexible Heterogeneous Numerical Methods (fHNM) Project

#### Principal research objective:

• **Discover mathematical principles** guiding the assembly of **standard** and **data-driven** numerical models in stable, accurate and physically consistent ways.

### Principal research challenges: we lack mathematical and algorithmic understanding of how to

• "Mix-and-match" standard and data-driven models from three-classes

Class A: projection-based reduced order models (ROMs) This talk.

- Class B: machine-learned models, i.e., Physics-Informed Neural Networks (PINNs)
- > Class C: flow map approximation models, i.e., dynamic model decomposition (DMD) models

This talk.

- Ensure well-posedness & physical consistency of resulting heterogeneous models.
- Solve such heterogeneous models efficiently.

#### Three coupling methods:

- Alternating Schwarz-based coupling
- Optimization-based coupling
- Coupling via generalized mortar methods





### Projection-Based Model Order Reduction via the POD/LSPG\* Method

Full Order Model (FOM):  $\frac{\partial q}{\partial t} = f(q, t; \mu)$ 

\*Least-Squares Petrov-Galerkin



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ROM = projection-based Reduced Order Model



HROM = Hyper-reduced ROM

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# Schwarz Extensions to FOM-ROM and ROM-ROM Couplings

#### Choice of domain decomposition

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- **Overlapping** vs. **non-overlapping** domain decomposition?
  - > Non-overlapping more flexible but typically requires more Schwarz iterations
- FOM vs. ROM subdomain assignment?
  - > Do not assign ROM to subdomains where they have no hope of approximating solution

#### Snapshot collection and reduced basis construction

• Are subdomains **simulated independently** in each subdomains or together?

#### Enforcement of boundary conditions (BCs) in ROM at Schwarz boundaries

- Strong vs. weak BC enforcement?
  - > Strong BC enforcement difficult for some models (e.g., cell-centered finite volume, PINNs)
- **Optimizing parameters** in Schwarz BCs for non-overlapping Schwarz?

### Choice of hyper-reduction

- What hyper-reduction method to use?
  - > Application may require particular method (e.g., ECSW for solid mechanics problems)
- How to **sample Schwarz boundaries** in applying hyper-reduction?
  - > Need to have enough sample mesh points at Schwarz boundaries to apply Schwarz

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# 60 2D Inviscid Burgers Equation

Popular analog for fluid problems where **shocks** are possible, and particularly **difficult** for conventional projection-based ROMs

$$\frac{\partial u}{\partial t} + \frac{1}{2} \left( \frac{\partial (u^2)}{\partial x} + \frac{\partial (uv)}{\partial y} \right) = 0.02 \exp(\mu_2 x)$$
$$\frac{\partial v}{\partial t} + \frac{1}{2} \left( \frac{\partial (vu)}{\partial x} + \frac{\partial (v^2)}{\partial y} \right) = 0$$
$$u(0, y, t; \boldsymbol{\mu}) = \mu_1$$
$$u(x, y, 0) = v(x, y, 0) = 1$$



#### Problem setup:

- $\Omega = (0, 100)^2, t \in [0, 25]$
- Two parameters  $\boldsymbol{\mu} = (\mu_1, \mu_2)$ . Training: uniform sampling of = [4.25, 5.50] × [0.015, 0.03] by a 3 × 3 grid. Testing: query unsampled point  $\boldsymbol{\mu} = [4.75, 0.02]$

#### FOM discretization:

- Spatial discretization given by a Godunov-type scheme with N = 250 elements in each dimension
  - Implicit **trapezoidal method** with fixed  $\Delta t = 0.05$



# Schwarz Coupling Details

### Choice of domain decomposition

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- Overlapping DD of  $\Omega$  into 4 subdomains coupled via multiplicative Schwarz
- Solution in  $\Omega_1$  is **most difficult** to capture by ROM

### Snapshot collection and reduced basis construction

• Single-domain FOM on  $\Omega$  used to generate snapshots/POD modes

#### Enforcement of boundary conditions (BCs) in ROM at Schwarz boundaries

• BCs imposed strongly using Method 1 of [Gunzburger et al., 2007] at indices i<sub>Dir</sub>

 $\boldsymbol{q}(t)\approx \overline{\boldsymbol{q}}+\boldsymbol{\Phi}\widehat{\boldsymbol{q}}(t)$ 

> POD modes made to satisfy homogeneous DBCs:  $\Phi(i_{\text{Dir}},:) = 0$ 

→ BCs imposed by modifying  $\overline{q}$ :  $\overline{q}(i_{\text{Dir}}) \leftarrow \chi_q$ 

#### Choice of hyper-reduction

- Energy Conserving Sampling & Weighting (ECSW) method for hyper-reduction
- All points on Schwarz boundaries are included in the sample mesh





# FOM-HROM-HROM-HROM Coupling



 $\Omega_1$ 

 $\Omega_2$ 

 $\Omega_{2}$ 

 $\Omega_4$ 

1 SD

- FOM in  $\Omega_1$  as this is "hardest" subdomain for ROM
- HROMs in  $\Omega_2$ ,  $\Omega_3$ ,  $\Omega_4$  capture 99% snapshot energy
- Method converges in **3 Schwarz iterations** per controller time-step
- Errors O(0.1%) with 0 error in  $\Omega_1$
- 2.26× speedup achieved over all-FOM coupling

Further **speedups** possible via **code optimizations**, **additive Schwarz** and **reduction** of # **sample mesh points**.



# <sup>63</sup> 2D Shallow Water Equations (SWE)

Hyperbolic PDEs modeling **wave propagation** below a pressure surface in a fluid (e.g., atmosphere, ocean).

$$\frac{\partial h}{\partial t} + \frac{\partial (hu)}{\partial x} + \frac{\partial (hv)}{\partial y} = 0$$
$$\frac{\partial (hu)}{\partial t} + \frac{\partial}{\partial x} \left( hu^2 + \frac{1}{2}gh^2 \right) + \frac{\partial}{\partial y} (huv) = -\mu v$$
$$\frac{\partial (hv)}{\partial t} + \frac{\partial}{\partial x} (huv) + \frac{\partial}{\partial y} \left( hv^2 + \frac{1}{2}gh^2 \right) = \mu u$$

#### Problem setup:

- $\Omega = (-5,5)^2$ ,  $t \in [0, 10]$ , Gaussian initial condition
- Coriolis parameter  $\mu \in \{-4, -3, -2, -1, 0\}$  for training, and  $\mu \in \{-3.5, -2.5, -1.5, -0.5\}$  for testing

#### FOM discretization:

- Spatial discretization given by a first-order **cell-centered finite volume** discretization with N = 300 elements in each dimension
- Implicit first order temporal discretization: **backward Euler** with fixed  $\Delta t = 0.01$
- Implemented in Pressio-demoapps (<u>https://github.com/Pressio/pressio-demoapps</u>)



Figure above: FOM solutions to SWE for  $\mu = -0.5$  (left) and  $\mu = -3.5$  (right).



\*https://github.com/Pressio/pressio-demoapps

#### **Green:** different from Burgers' problem

- Non-overlapping DD of  $\Omega$  into 4 subdomains coupled via additive Schwarz
  - OpenMP parallelism with 1 thread/subdomain
- All-ROM or All-HROM coupling via Pressio\*

Schwarz Coupling Details

Choice of domain decomposition

### Snapshot collection and reduced basis construction

• Single-domain FOM on  $\Omega$  used to generate snapshots/POD modes

### Enforcement of boundary conditions (BCs) in ROM at Schwarz boundaries

- BCs are imposed approximately by fictitious ghost cell states
  - Implementing Neumann and Robin BCs is challenging
- Ghost cells introduce some overlap even with non-overlapping DD
  - Dirichlet-Dirichlet non-overlapping Schwarz is stable/convergent!
- Choice of hyper-reduction

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- Collocation for hyper-reduction: min residual at small subset DOFs
- Assume fixed budget of sample mesh points at Schwarz boundaries





Figure above: sample mesh (yellow) and stencil (white) cells





### Schwarz All-ROM Domain Overlap Study

Study of Schwarz convergence for all-ROM coupling as a function of N<sub>o</sub> := cell width of overlap region (not including ghost cells).



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Movie above: FOM (left), 4 subdomain ROM coupled via non-overlapping Schwarz (middle), and 4 subdomain ROM coupled via overlapping Schwarz (right) for predictive SWE problem with  $\mu = -0.5$ . All ROMs have K = 80 POD modes.

- Schwarz iterations decrease (very roughly) with  $N_o^{0.25}$  (figure, right) whereas evaluating r(q) scales with  $N_o^2$ 
  - ➤ ⇒ there is no reason not to do nonoverlapping coupling for this problem

 Dirichlet-Dirichlet coupling with no-overlap (N<sub>o</sub>= 0) performs well with no convergence issues (movie, left) and errors comparable to Dirichlet-Dirichlet coupling with overlap (figure below, left)



Figures above: relative error and average # Schwarz iterations as a function of  $\mu$  and  $N_o$ . Black  $\mu$ : training, red  $\mu$ : testing.

# Schwarz Boundary Sampling for All-HROM Coupling

<u>Key question</u>: how many Schwarz boundary points need to be included in sample mesh when performing HROM coupling?

• Naive/sparsely-sampled Schwarz boundary results in failure to transmit coupling information during Schwarz





Movie above: FOM (left), all HROM with  $N_b = 5\%$  (middle) and all HROM with  $N_b = 10\%$  (left). ROMs have K = 100 modes and  $N_s = 0.5\%N$  sample mesh points.

Figure above: example sample mesh with sampling rate  $N_b = 10\%$ 

- Including too many Schwarz boundary points (Nb) in sample mesh given fixed budget of Ns sample mesh
  points may lead to too few sample mesh points in interior
- For SWE problem, we can get away with ~10% boundary sampling (movie above, right-most frame)

### Coupled HROM Performance

#### Water Height, $\mu = -0.5$ Water Height Mono PROM, various K 10<sup>0</sup> $N_b = 5$ Mono HPROM, K = 80 $V_{b} = 10$ Schwarz PROM, various K $N_{b} = 15$ Schwarz HPROM, K = 80 $10^{-1}$ $10^{-3}$ Relative l<sup>2</sup> error Relative l<sup>2</sup> error 10-2 $N_{\rm s} = 0.5\% N$ Solid: Dashed: $N_s = 1\% N$ 10-3 $10^{-4}$ $10^{-4}$ $10^{-5}$ $10^{-1}$ 100 101 102 -2.5 -0.50.0 -4.0-3.5-<u>3</u>.0 -2.0-1.5-1.0Speedup vs. Monolithic FOM

- For a fixed ROM dimension, Schwarz delivers lower error and comparable cost!
- There are noticeable **cost savings** relative to **monolithic FOM**!
- Accuracy similar for **predictive**  $\mu$  (red) and **non-predictive**  $\mu$  (black) cases.

### <sup>68</sup> Teaser: 2D Euler Equations Riemann Problem



$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ (E+p)u \end{pmatrix} + \frac{\partial}{\partial y} \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ (E+p)v \end{pmatrix} = \mathbf{0}$$
$$p = (\gamma - 1) \left( \rho E - \frac{1}{2} \rho (u^2 + v^2) \right)$$



#### Problem setup:

- $\Omega = (0,1)^2$ ,  $t \in [0,0.8]$ , homogeneous Neumann BCs
- Fix  $\rho_1 = 1.5$ ,  $u_1 = v_1 = 0$ ,  $p_3 = 0.029$
- Vary  $p_1$ ; IC from compatibility conditions\*
  - ▶ Training:  $p_1 \in [1.0, 1.25, 1.5, 1.75, 2.0]$
  - ▶ Testing:  $p_1 \in [1.125, 1.375, 1.625, 1.875]$

### Preliminary results:

- Schwarz can **stabilize** unstable monolithic ROM for fixed dimension *K* (above)
- Since shock traverses all parts of domain, achieving speedups with Schwarz is more difficult

#### FOM discretization:

- Spatial discretization given by a first-order **cell-centered finite volume** discretization with N = 300 or N = N = 100 elements in each dimension
- Implicit first order temporal discretization: **backward Euler** with fixed  $\Delta t = 0.005$
- Implemented in **Pressio-demoapps** (<u>https://github.com/Pressio/pressio-demoapps</u>)

\*Schulz-Rinne, 1993.

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The Schwarz alternating method has been developed for concurrent multi-scale coupling of conventional and data-driven models.

- ☺ Coupling is *concurrent* (two-way).
- ③ *Ease of implementation* into existing massively-parallel HPC codes.
- ③ "*Plug-and-play*" *framework*: simplifies task of meshing complex geometries!
  - ③ Ability to couple regions with different non-conformal meshes, different element types and different levels of refinement.
  - Obility to use different solvers (including ROM/FOM) and time-integrators in different regions.
- ③ Scalable, fast, robust on real engineering problems
- © Coupling does not introduce *nonphysical artifacts*.
- ③ *Theoretical* convergence properties/guarantees.

# Ongoing & Future Work

- Development fundamentally new approach for simulating multiscale **mechanical contact** using the Dirichlet-Neumann **Schwarz alternating method** 
  - Contact constraints are replaced with boundary conditions applied iteratively at contact boundaries
- Implementation of **non-overlapping** Schwarz in Sierra/SM
- Working with analysts to apply Schwarz to problems of interest to Sandia missions
  - Laser welds

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- Fastener modeling for joints
- > Salt caverns for **oil storage**
- **Rigorous analysis** of why Dirichlet-Dirichlet BC "work" when employing non-overlapping Schwarz with discretizations that employ ghost cells
- Extension to coupling of **non-intrusive ROMs** (dynamic mode decomposition, operator inference, neural networks)
- Development of automated criteria to determine appropriate use of less refined or reduced-order models w/o sacrificing accuracy, enabling real-time transitions between different model fidelities



From Murugesan et al., 2020.



Impact of two 3D beams having different meshes with Schwarz contact method. From [Mota et al., 2023].





### 72 Team & Acknowledgments











Irina Tezaur

Joshua Barnett

Alejandro Mota

Chris Wentland

Francesco Rizzi





Coleman Alleman



Greg Phlipot


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# Start of Backup Slides

#### **Theoretical Foundation**

Using the Schwarz alternating as a *discretization method* for PDEs is natural idea with a sound *theoretical foundation*.

- <u>S.L. Sobolev (1936)</u>: posed Schwarz method for *linear elasticity* in variational form and *proved method's convergence* by proposing a convergent sequence of energy functionals.
- <u>S.G. Mikhlin (1951):</u> *proved convergence* of Schwarz method for general linear elliptic PDEs.
- <u>P.-L. Lions (1988):</u> studied convergence of Schwarz for *nonlinear monotone elliptic problems* using max principle.
- <u>A. Mota, I. Tezaur, C. Alleman (2017)</u>: proved *convergence* of the alternating Schwarz method for *finite deformation quasi-static nonlinear PDEs* (with energy functional  $\Phi[\varphi]$ ) with a *geometric convergence rate*.

$$\boldsymbol{\Phi}[\boldsymbol{\varphi}] = \int_{B} A(\boldsymbol{F}, \boldsymbol{Z}) \, dV - \int_{B} \boldsymbol{B} \cdot \boldsymbol{\varphi} \, dV$$
$$\nabla \cdot \boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



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S.L. Sobolev (1908 - 1989)





S.G. Mikhlin (1908 - 1990)

P.- L. Lions (1956-)



A. Mota, I. Tezaur, C. Alleman

#### 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.

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• 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*.



Albany

Overlap far from notch.

Overlap near notch.

# Single Domain Predictive ROM

- Uniform sampling of  $\mathcal{D} = [4.25, 5.50] \times [0.015, 0.03]$  by a 3 × 3 grid  $\Rightarrow$  9 training parameters characterized by  $\Delta \mu_1 = 0.625$ ,  $\Delta \mu_2 = 0.0075$ 
  - > 200 POD modes required to capture 99% snapshot energy
- Queried but **unsampled parameter** point  $\mu = [4.75, 0.02]$
- Reduced mesh resulting from solving non-negative least squares problem defining ECSW gives  $n_e = 5,689$  elements (9.1% of  $N_e = 62,500$  elements).



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*Figure above:* Reduced mesh of single domain HROM



*Figure above*: HROM and FOM results at various time steps



% SV Energy	М	MSE* (%)	CPU time* (s)
95	69	1.1	138
99	177	0.17	447

\* Numbers in table are w/o hyper-reduction



# All-ROM Coupling

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- Method converges in only 3
  Schwarz iterations per controller time-step
- Errors O(1%) or less
- **1.47**× **speedup** over all-FOM coupling for 95% SV energy retention case

	95% SV Energy			99% SV Energy		
Subdomains	М	MSE (%)	CPU time (s)	М	MSE (%)	CPU time (s)
$\Omega_1$	57	1.1	85	146	0.18	295
$\Omega_2$	44	1.2	56	120	0.18	216
$\Omega_3$	24	1.4	43	60	0.16	89
$\Omega_4$	32	1.9	61	66	0.25	100
Total			245			700



*Key question*: how many Schwarz boundary points need to be included in sample mesh when performing HROM coupling?

<u>Key question</u>: how many Schwarz boundary points need to be included in sample mesh when performing HROM coupling?

• Naïve/sparsely-sampled Schwarz boundary results in failure to transmit coupling information during Schwarz



Movie above: FOM (left) and all HROM with  $N_b = 5\%$  (right). ROMs have K = 100 modes and  $N_s = 0.5\%N$  sample mesh points.

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Figure above: example sample mesh with sampling rate  $N_b = 5\%$ .

<u>Key question</u>: how many Schwarz boundary points need to be included in sample mesh when performing HROM coupling?

• Naive/sparsely-sampled Schwarz boundary results in failure to transmit coupling information during Schwarz



ROMs have K = 100 modes and  $N_s = 0.5\% N$  sample mesh points.

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Figure above: example sample mesh with sampling rate  $N_b = 0$ .

 Including too many Schwarz boundary points (Nb) in sample mesh given fixed budget of Ns sample mesh points may lead to too few sample mesh points in interior

<u>Key question</u>: how many Schwarz boundary points need to be included in sample mesh when performing HROM coupling?

• Naive/sparsely-sampled Schwarz boundary results in failure to transmit coupling information during Schwarz





Movie above: FOM (left) and all HROM with  $N_b = 5\%$  (right). ROMs have K = 100 modes and  $N_s = 0.5\%N$  sample mesh points.

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Figure above: example sample mesh with sampling rate  $N_b = 5\%$ .

 Including too many Schwarz boundary points (N<sub>b</sub>) in sample mesh given fixed budget of N<sub>s</sub> sample mesh points may lead to too few sample mesh points in interior

<u>Key question</u>: how many Schwarz boundary points need to be included in sample mesh when performing HROM coupling?

• Naive/sparsely-sampled Schwarz boundary results in failure to transmit coupling information during Schwarz



Movie above: FOM (left) and all HROM with  $N_b = 5\%$  (right). ROMs have K = 100 modes and  $N_s = 0.5\%N$  sample mesh points.

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Figure above: example sample mesh with sampling rate  $N_b = 10\%$ .

 Including too many Schwarz boundary points (N<sub>b</sub>) in sample mesh given fixed budget of N<sub>s</sub> sample mesh points may lead to too few sample mesh points in interior

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<u>Key question</u>: how many Schwarz boundary points need to be included in sample mesh when performing HROM coupling?

• Naive/sparsely-sampled Schwarz boundary results in failure to transmit coupling information during Schwarz



Figure above: example sample mesh with sampling rate  $N_b = 15\%$ .

- Movie above: FOM (left) and all HROM with  $N_b = 5\%$  (right). ROMs have K = 100 modes and  $N_s = 0.5\% N$  sample mesh points.
- Including too many Schwarz boundary points (Nb) in sample mesh given fixed budget of Ns sample mesh points may lead to too few sample mesh points in interior



#### <sup>86</sup> Model Problem 3: 2D Euler Equations Riemann Problem



$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ (E+p)u \end{pmatrix} + \frac{\partial}{\partial y} \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ (E+p)v \end{pmatrix} = \mathbf{0}$$
$$p = (\gamma - 1) \left( \rho E - \frac{1}{2} \rho (u^2 + v^2) \right)$$

#### Problem setup:

- $\Omega = (0,1)^2$ ,  $t \in [0,0.8]$ , homogeneous Neumann BCs
- Fix  $\rho_1 = 1.5$ ,  $u_1 = v_1 = 0$ ,  $p_3 = 0.029$
- Vary  $p_1$ ; IC from compatibility conditions\*
  - ▶ Training:  $p_1 \in [1.0, 1.25, 1.5, 1.75, 2.0]$
  - ▶ Testing:  $p_1 \in [1.125, 1.375, 1.625, 1.875]$



Figure above: FOM solutions to Euler Riemann problem for  $p_1 = 0.875$  (left) and  $p_1 = 1.5$  (right).

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Preliminary results (WIP)

#### FOM discretization:

- Spatial discretization given by a first-order **cell-centered finite volume** discretization with N = 300 or N = N = 100 elements in each dimension
- Implicit first order temporal discretization: **backward Euler** with fixed  $\Delta t = 0.005$
- Implemented in **Pressio-demoapps** (<u>https://github.com/Pressio/pressio-demoapps</u>)

\*Schulz-Rinne, 1993.

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# Schwarz Coupling Details

#### Choice of domain decomposition

- Overlapping and non-overlapping DD of Ω into 4 subdomains coupled via additive/multiplicative Schwarz
- All-ROM or All-HROM coupling via Pressio\*

#### Snapshot collection and reduced basis construction

• Single-domain FOM on  $\Omega$  used to generate snapshots/POD modes

# Enforcement of boundary conditions (BCs) in ROM at Schwarz boundaries

- BCs are imposed **approximately** by fictitious ghost cell states
- Dirichlet-Dirichlet BCs for both overlapping and non-overlapping

#### Choice of hyper-reduction

- Collocation and gappy POD for hyper-reduction
- Assume fixed budget of sample mesh points at Schwarz boundaries



Figure above: DD of  $\Omega$  into 4 subdomains



*Figure above*: Slow decay of POD energy for Euler problem



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#### Model Problem 3: All-ROM Coupling + Overlapping Schwarz

- For smaller basis sizes and larger  $p_1$ , monolithic ROM is **unstable** whereas **Schwarz ROM** gives **accurate solution**!
- Increased overlap degrades accuracy (top right)

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- Shock transmission error significantly increases with overlap
- ~4.4 average # Schwarz iterations with additive Schwarz vs.
  ~3.6 for multiplicative Schwarz
- With **additive Schwarz**, can achieve **lower error** than monolithic ROM for **same CPU time** (bottom right)



Movie above: FOM (left), K = 50 monolithic ROM (middle), and K = 50 overlapping Schwarz ROM with  $N_o = 4$  (left) for  $p_1 = 1.875$ .



# Model Problem 3: All-HROM Coupling + Non-Overlapping Schwarz

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- Hyper-reduction via collocation works better than gappy POD
- Schwarz can give **improved accuracy** relative to monolithic ROM
- Achieving **cost-savings** w.r.t. monolithic FOM is WIP

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Movie above: FOM (left), HROM (middle) and Schwarz All-HROM (right) solution. HROMs have 5% sampling rate and 200 POD modes.

#### Preliminary results (WIP)



*Figure above:* collocation and gappy POD relative errors for K=200, 1% sampling rate.



*Figure above:* monolithic vs. decomposed HROM errors with 5% sampling rate no overlap.

- 90 Energy-Conserving Sampling and Weighting (ECSW)
  - **Project-then-approximate** paradigm (as opposed to approximate-then-project)

$$r_{k}(q_{k}, t) = W^{T}r(\tilde{u}, t)$$
$$= \sum_{e \in \mathcal{E}} W^{T}L_{e}^{T}r_{e}(L_{e}+\tilde{u}, t)$$

- $L_e \in \{0,1\}^{d_e \times N}$  where  $d_e$  is the **number of degrees of freedom** associated with each mesh element (this is in the context of meshes used in first-order hyperbolic problems where there are  $N_e$  mesh elements)
- $L_{e^+} \in \{0,1\}^{d_e \times N}$  selects degrees of freedom necessary for flux reconstruction
- Equality can be **relaxed**



Augmented reduced mesh:  $\odot$  represents a selected node attached to a selected element; and  $\otimes$  represents an added node to enable the full representation of the computational stencil at the selected node/element

# 91 ECSW: Generating the Reduced Mesh and Weights

- Using a subset of the same snapshots  $u_i, i \in 1, ..., n_h$  used to generate the state basis V, we can train the reduced mesh
- Snapshots are first **projected** onto their associated basis and then **reconstructed**

$$\begin{split} c_{se} &= W^T L_e^T r_e \left( L_{e^+} \left( u_{ref} + V V^T \left( u_s - u_{ref} \right) \right), t \right) \in \mathbb{R}^n \\ d_s &= r_k (\tilde{u}, t) \in \mathbb{R}^n, \quad s = 1, \dots, n_h \end{split}$$

• We can then form the **system** 

$$\boldsymbol{C} = \begin{pmatrix} c_{11} & \dots & c_{1N_e} \\ \vdots & \ddots & \vdots \\ c_{n_h 1} & \dots & c_{n_h N_e} \end{pmatrix}, \quad \boldsymbol{d} = \begin{pmatrix} d_1 \\ \vdots \\ d_{n_h} \end{pmatrix}$$

- Where  $C\xi = d, \xi \in \mathbb{R}^{N_e}, \xi = 1$  must be the solution
- Further relax the equality to yield **non-negative least-squares problem**:

 $\boldsymbol{\xi} = \arg\min_{\boldsymbol{x}\in\mathbb{R}^n} ||\boldsymbol{C}\boldsymbol{x} - \boldsymbol{d}||_2$  subject to  $\boldsymbol{x} \geq \boldsymbol{0}$ 

 Solve the above optimization problem using a non-negative least squares solver with an early termination condition to promote sparsity of the vector ξ