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Sandia National Laboratories

The Schwarz Alternating Method for Concurrent Multiscale Coupling in Solid Mechanics

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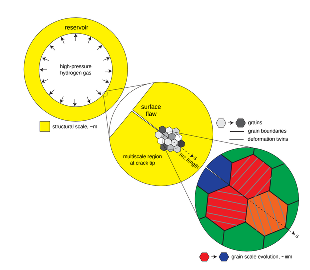
Motivation for Concurrent Multiscale Coupling

- ***Large scale*** structural ***failure*** frequently originates from ***small scale*** phenomena such as defects, microcracks, inhomogeneities and more, which grow quickly in unstable manner.
- Failure occurs due to ***tightly coupled interaction*** between small scale (stress concentrations, material instabilities, cracks, etc.) and large scale (vibration, impact, high loads and other perturbations).

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

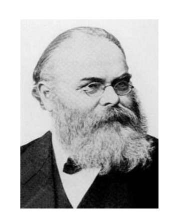
Concurrent multiscale methods are ***essential*** for understanding and prediction of behavior of engineering systems when a ***small scale failure*** determines the performance of the entire system.

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



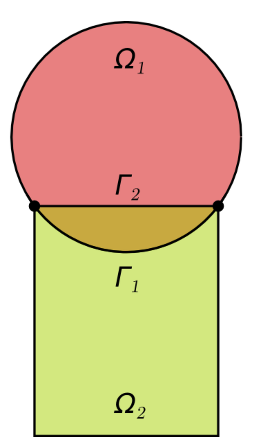
Schwarz Alternating Method for Domain Decomposition

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



H. Schwarz (1843 – 1921)

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



Basic Schwarz Algorithm

Initialize:

- Solve PDE by any method on Ω_1 w/ initial guess for Dirichlet BCs on Γ_1.

Iterate until convergence:

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

- Solve PDE by any method (can be different than for Ω_1) on Ω_2 w/ Dirichlet BCs on Γ_2 that are the values just obtained for Ω_1.
- Solve PDE by any method (can be different than for Ω_2) on Ω_1 w/ Dirichlet BCs on Γ_1 that are the values just obtained for Ω_2.

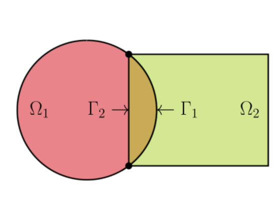
- Schwarz alternating method most commonly used as a ***preconditioner*** for Krylov iterative methods to solve linear algebraic equations.

Novel idea: using the Schwarz alternating as a ***discretization method*** for solving multi-scale partial differential equations (PDEs).

Schwarz Alternating Method for Multiscale Coupling

Pseudo-code for Quasistatics:

1: $\varphi^{(0)} \leftarrow \mathrm{id}_{\boldsymbol{X}}$ in Ω_2 ▷ initialize to zero displacement or a better guess in Ω_2
2: $n \leftarrow 1$
3: **repeat** ▷ Schwarz loop
4: $\varphi^{(n)} \leftarrow \chi$ on $\partial_{\varphi}\Omega_i$ ▷ Dirichlet BC for Ω_i
5: $\varphi^{(n)} \leftarrow P_{\Omega_j \to \Gamma_i}[\varphi^{(n-1)}]$ on Γ_i ▷ Schwarz BC for Ω_i
6: $\varphi^{(n)} \leftarrow \arg\min_{\varphi \in S_i} \Phi_i[\varphi]$ in Ω_i ▷ solve in Ω_i
7: $n \leftarrow n+1$
8: **until** converged



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

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Proof of Convergence for Finite-Deformation Solid Mechanics

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

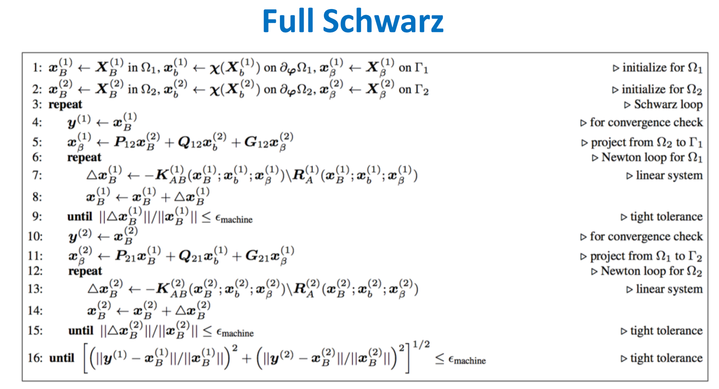
- S. L. Sobolev (1936): posed Schwarz method for ***linear elasticity*** in variational form and ***proved method's convergence*** by proposing a convergent sequence of energy functionals.
- S. G. Mikhlin (1951): ***proved convergence*** of Schwarz method for general linear elliptic PDEs.
- A. Mota, I. Tezaur, C. Alleman (2017)*: derived a ***proof of convergence*** of the alternating Schwarz method for the ***finite deformation quasistatic nonlinear PDEs*** (with ***quasi-convex*** energy functional $\boldsymbol{\Phi}[\boldsymbol{\varphi}]$ defined below), and determined a ***geometric convergence rate*** for the finite deformation quasistatic problem.

$$\boldsymbol{\Phi}[\boldsymbol{\varphi}] = \int_B W(\boldsymbol{F}, \boldsymbol{Z}, T)\, dV - \int_B \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_T B} \overline{\boldsymbol{T}} \cdot \boldsymbol{\varphi}\, dS$$
$$\nabla \cdot \boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$

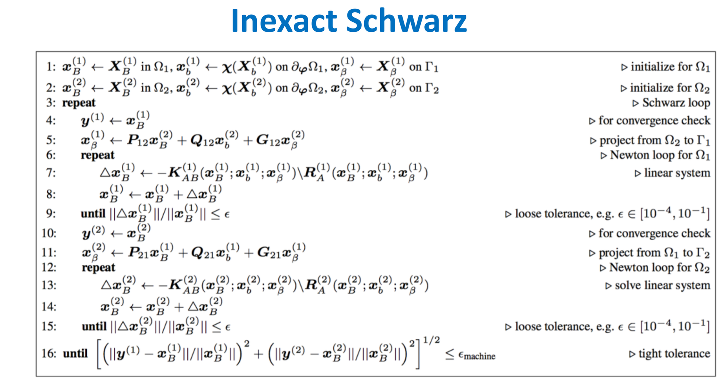
* A. Mota, I. Tezaur, C. Alleman. "The Schwarz Alternating Method in Solid Mechanics", *Comput. Meth. Appl. Mech. Engng.* 319 (2017), 19-51.

Four Variants of Schwarz Alternating Method for Quasistatics

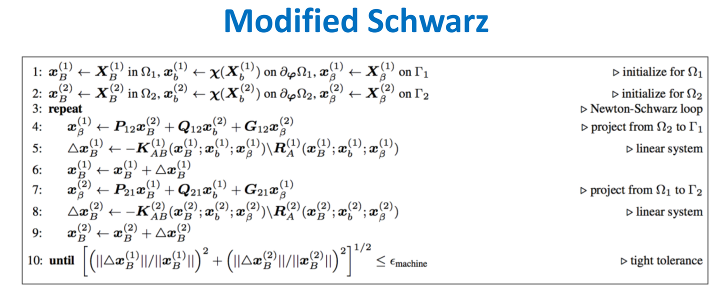
Full Schwarz



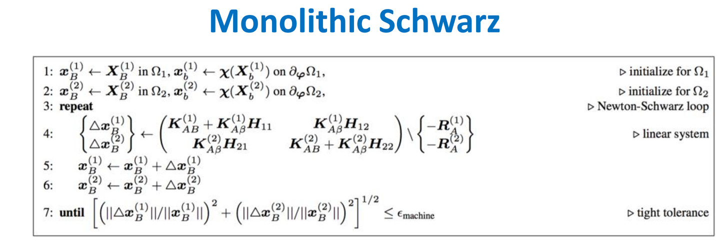
Inexact Schwarz



Modified Schwarz



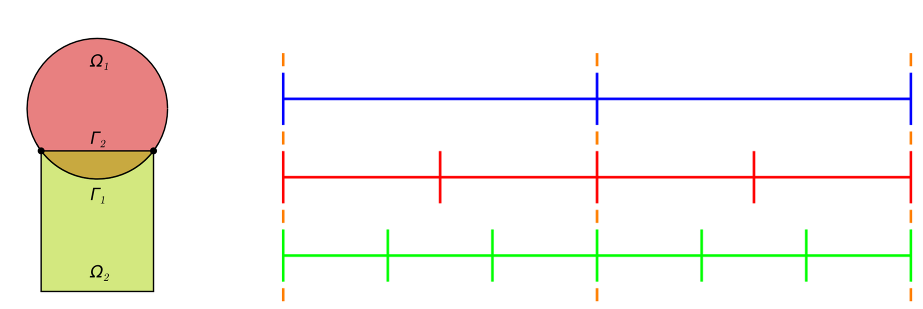
Monolithic Schwarz



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

Schwarz Alternating Method for Dynamics

- In literature, Schwarz method is applied to dynamics by using space-time discretizations – unfeasible given design of our current codes and size of simulations.
- Our extension of Schwarz coupling to ***dynamics*** uses a governing time stepping algorithm that ***controls*** time integrators within each domain.
- Can use ***different integrators*** (e.g., implicit, explicit) with different time steps in each domain.

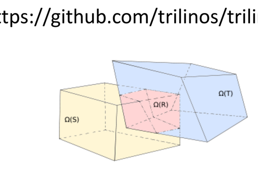


Implementation within Albany Finite Element Code

- ***Component-based*** design for rapid development of capabilities.
- Extensive use of libraries from the open-source ***Trilinos*** project.
  - Use of the ***Phalanx*** package to decompose complex problem into simpler problems with managed dependencies.
  - Use of the ***Sacado*** package for ***automatic differentiation.***
  - Use of ***Teko*** package for ***block preconditioning***.
  - Performance portability to GPUs and KNLs via ***Kokkos.***
- ***Parallel*** implementation of Schwarz uses the ***Data Transfer Kit*** (***DTK***).

https://github.com/gahansen/Albany

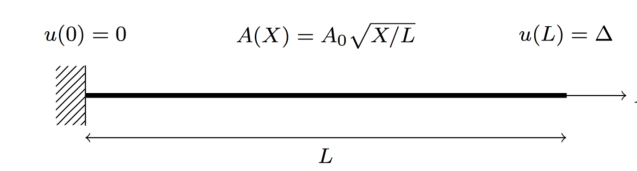
https://github.com/trilinos/trilinos

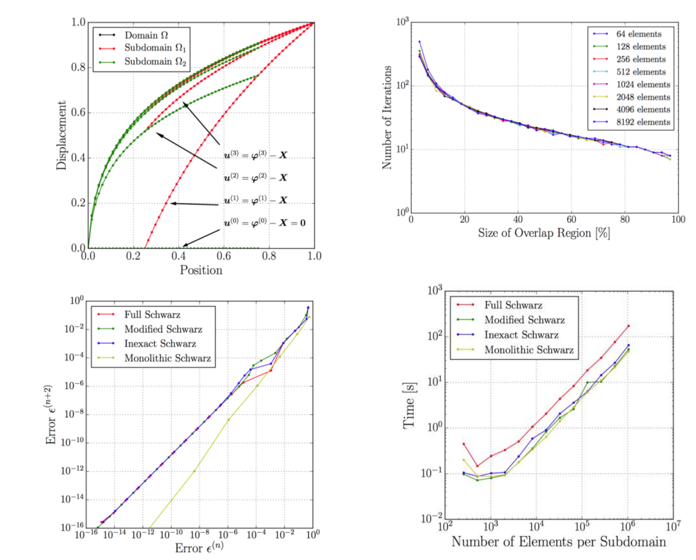


https://github.com/ORNL-CEES/DataTransferKit

Numerical Results: Quasistatics

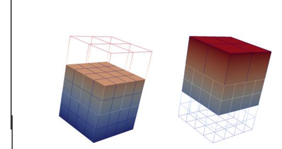
Foulk's Singular Bar



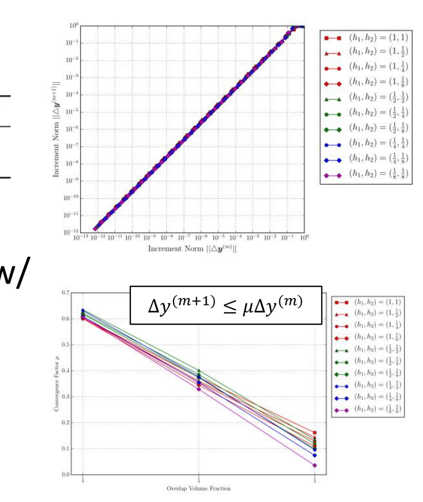


- ***1D bar*** with area proportional to square root of length with strong ***singularity*** on left end of bar and simple ***hyperelestic*** material model with no damage.
- **Test case goals**: explore viability of four variants of Schwarz alternating method, test convergence (expect ***faster convergence*** in ***fewer iterations*** with ***increased overlap***).

Cuboid

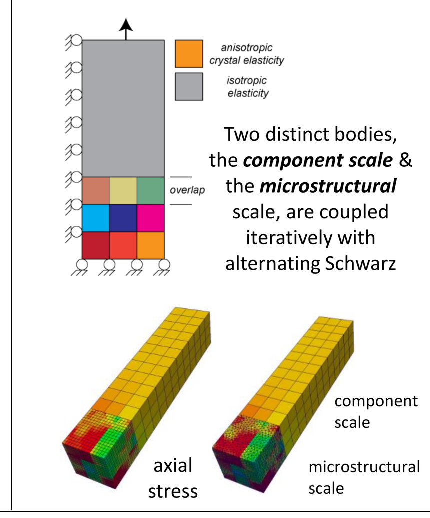


Subdomain	u_3 relative error	σ_{33} relative error
Ω_1	1.24×10^{-14}	2.31×10^{-13}
Ω_2	7.30×10^{-15}	3.06×10^{-13}

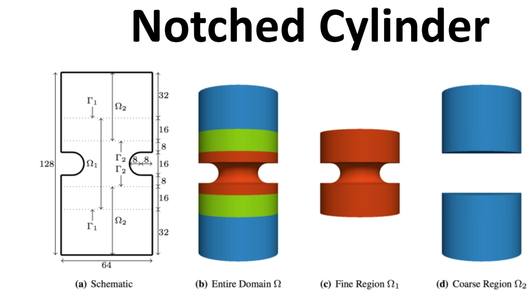


- Coupling of ***two cuboids*** with square base w/ ***Neohookean***-type material model.
- Schwarz alternating method converges ***linearly***.
- There is ***faster linear convergence*** with ***increasing*** overlap volume fraction.

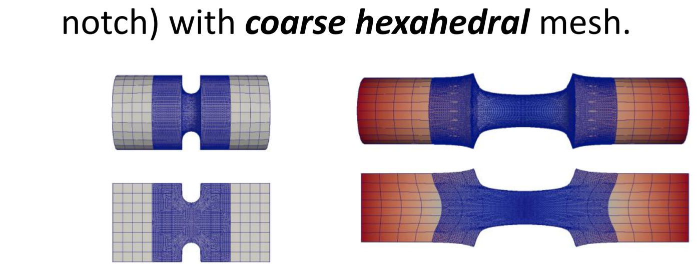
Rubik's Cube



Notched Cylinder

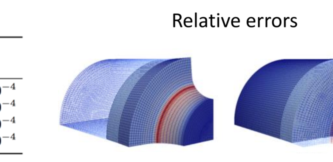


- ***Notched cylinder*** stretched along its axial direction, ***Neohookean***-type material model.
- Coupling of ***fine tetrahedral*** mesh (near notch) with ***coarse hexahedral*** mesh.



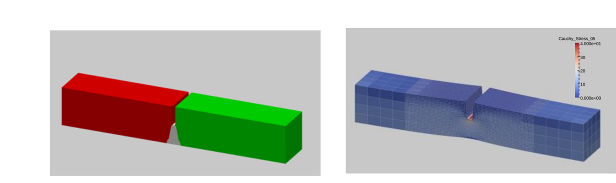
Absolute residual tolerance	u_3 relative error Ω_1	u_3 relative error Ω_2
1.0×10^{-8}	1.31×10^{-3}	4.45×10^{-4}
1.0×10^{-12}	1.30×10^{-3}	4.43×10^{-4}
1.0×10^{-14}	1.30×10^{-3}	4.43×10^{-4}
2.5×10^{-16}	1.30×10^{-3}	4.43×10^{-4}

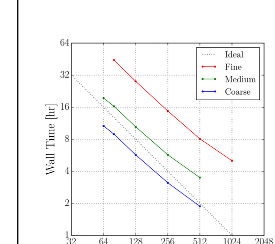
Relative errors



(a) Ω_1 (b) Ω_2

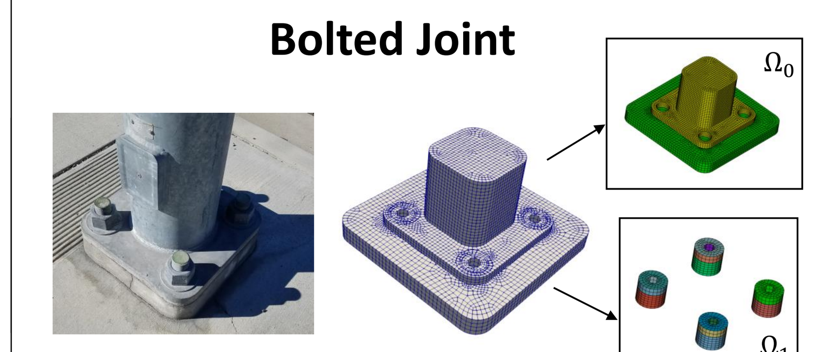
Laser Weld





- ***Isotropic elasticity*** & ***J2 plasticity*** with linear isotropic hardening.
- 3 subdomains.
- 50% reduction in problem size.
- Near perfect strong scaling.

Bolted Joint



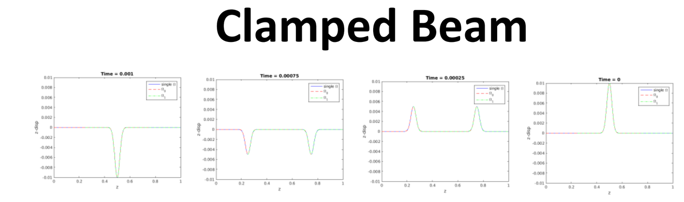
- Multi-scale problem of ***practical scale***: coupling 85K ***composite tet 10 element mesh*** (bolts, Ω_1) with 56K ***hex element mesh*** (parts, Ω_2).
- ***Neohookean*** material model: steel bolts, aluminum/steel parts.
- ***Lateral displacement load applied at top***: applies compression to 2 bolts, tension to

Nodal projection of 5th Cauchy stress

Acknowledgement: J. Foulk (Sandia National Labs) for creating mesh of this geometry.

Numerical Results: Dynamics

Clamped Beam

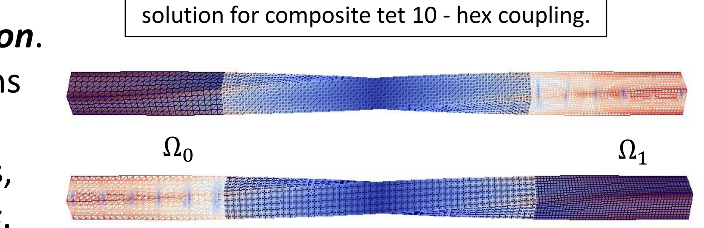


- Linear elastic ***clamped beam*** with Gaussian initial condition for the z-displacement.
- Coupling introduces ***no dynamic artifacts*** & ***energy is conserved*** throughout the simulation.

Torsion

- Nonlinear elastic bar subjected to high degree of ***torsion***.
- Dynamic Schwarz method is used to couple two regions of the bar using different mesh resolutions, different element types, and different time integration schemes, once more ***without introducing any dynamic artifacts***.

Relative errors are O(1%) w.r.t. reference solution for composite tet 10 - hex coupling.



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