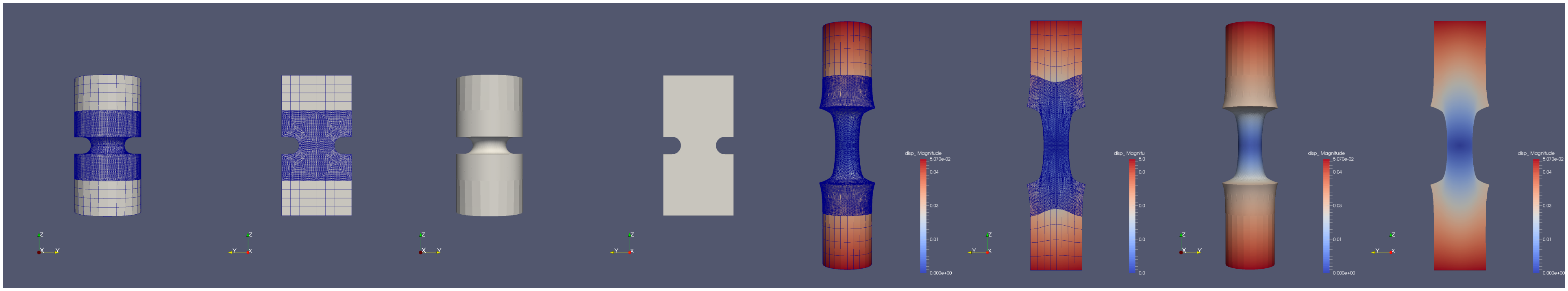
SAND2015-5927C

Sandia National Laboratories



The Alternating Schwarz Method for Concurrent Multiscale in Finite Deformation Solid Mechanics

Alejandro Mota, Irina Tezaur

Sandia National Laboratories, Livermore, CA

U.S. DEPARTMENT OF ENERGY

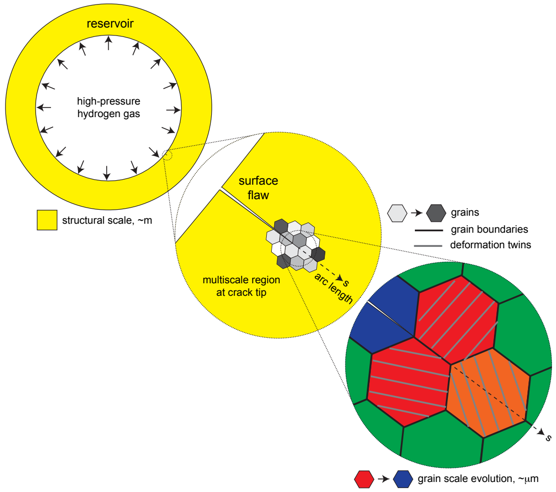
NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

Concurrent Multiscale Coupling

- Large scale structural failure frequently originates from very small scale phenomena such as defects, microcracks, inhomogeneites and more.
- Failure occurs due to the tightly coupled interaction between what is occurring at the small scale (stress concentrations, material instabilities, cracks, etc.) and the large scale (vibration, impact, high loads and other perturbations).
- Concurrent multiscale methods for solid mechanics are essential for the understanding and prediction of behavior of engineering systems when a small scale event will eventually determine the performance of the entire system.

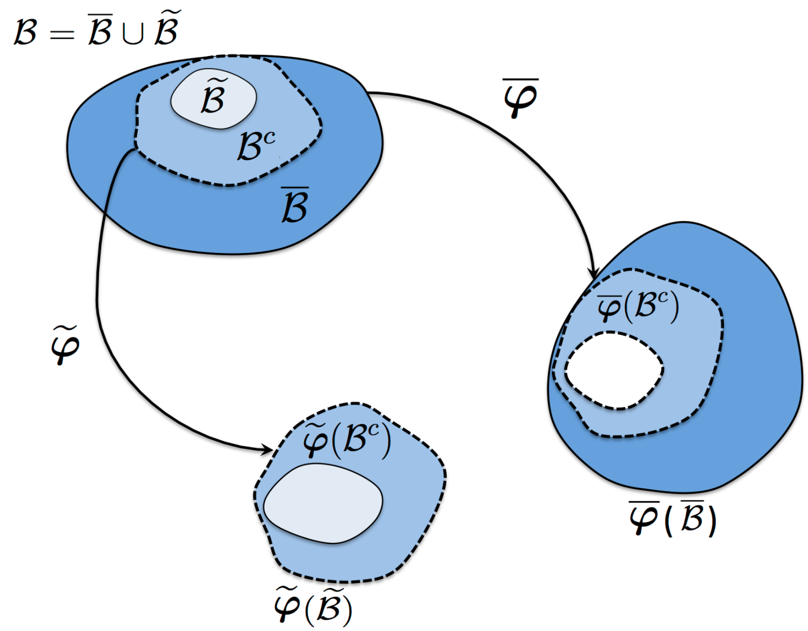
Roof failure (large scale) of Boeing 737 aircraft due to fatigue cracks (small scale). From *imechanica.org*



Surface flaw in pressure vessel.

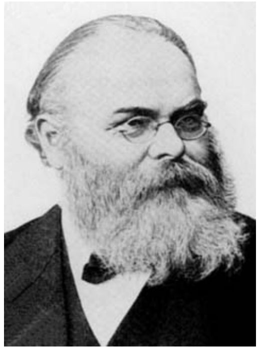
Schwarz Coupling: Concurrent Multiscale

- The Schwarz coupling method has been adapted and implemented for use in concurrent multiscale modeling in Sandia's open-source Albany/LCM code, thus allowing the study of models where information is exchanged back and forth between small and large scales.
- The coupling of the primary fields on overlapping regions will enable information to flow between scales. Both scales will converge to a *single solution*. This intimate coupling is termed **concurrent multiscale coupling**.

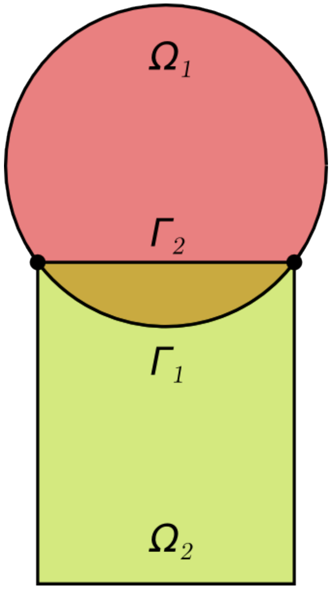


Alternating Schwarz for Domain Decomposition

- First developed in 1870 for solving Laplace's equation in irregularly shaped domains.
- Simple idea: if the solution is known in regularly shaped domains, use those as puzzle pieces to iteratively build a solution for the more complex domain.
- Later generalized for any elliptic PDE.
- Guaranteed to converge to the global solution.



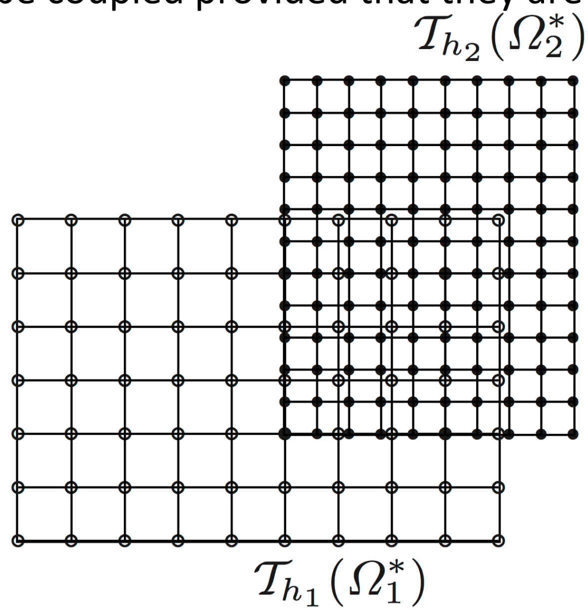
Karl Hermann Amandus Schwarz (1843 – 1921). Source: *bibmath.net*



- Initialize:
  - Solve PDE by any method on Ω_1 using an initial guess for Dirichlet BCs on Γ_1.
- Iterate until convergence:
  - Solve PDE by any method (can be different than for Ω_1) on Ω_2 using 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 using Dirichlet BCs on Γ_1 that are the values just obtained for Ω_2.

Alternating Schwarz for Multiscale Coupling in Quasistatics

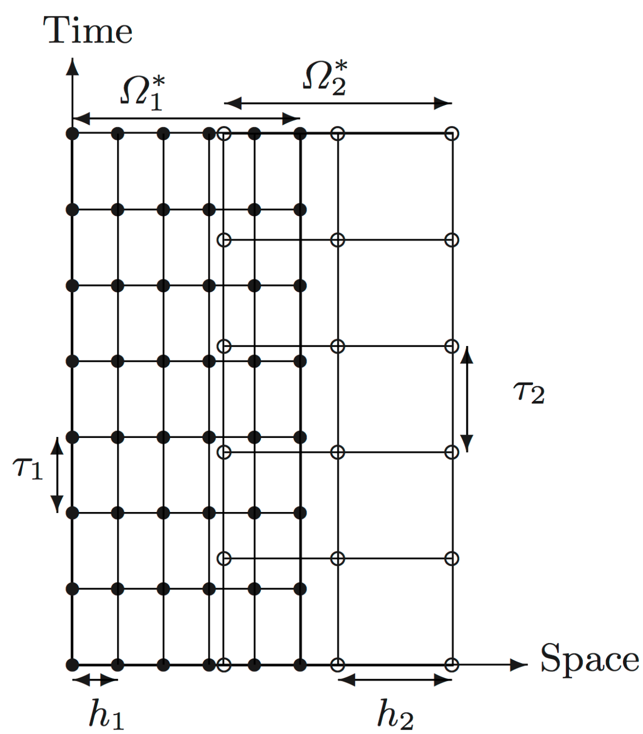
- The Alternating Schwarz Method is a technique that we have adopted for concurrent multiscale coupling.
- It allows the coupling of regions with different meshes, for example, different element types, levels of refinement and non-conforming.
- Information is exchanged among the different regions (there could be more than two) so the coupling is 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.
- Conceptually very simple.



Overlapping non-matching meshes in quasi-statics.

Alternating Schwarz for Multiscale Coupling in Dynamics

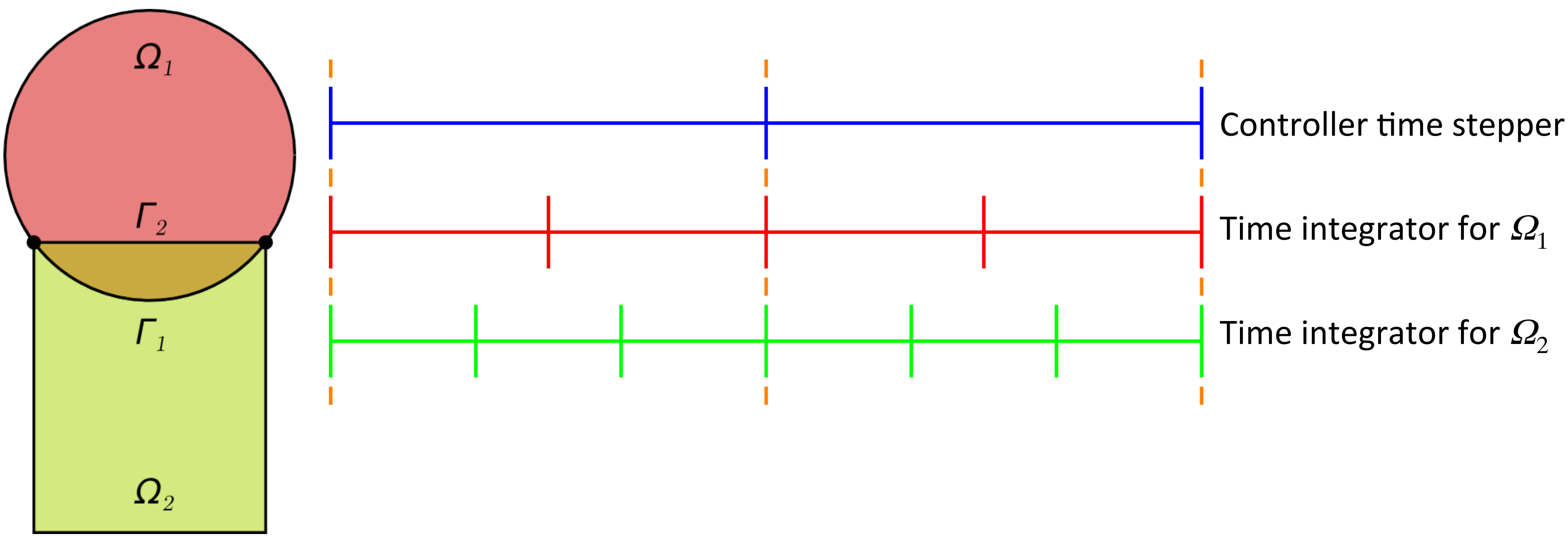
- In the literature the Schwarz method is applied to dynamics by using space-time discretizations.
- This was deemed unfeasible given the design of our current codes and size of simulations.



Overlapping non-matching meshes
and time steps in dynamics.

A Schwarz-like time integrator.

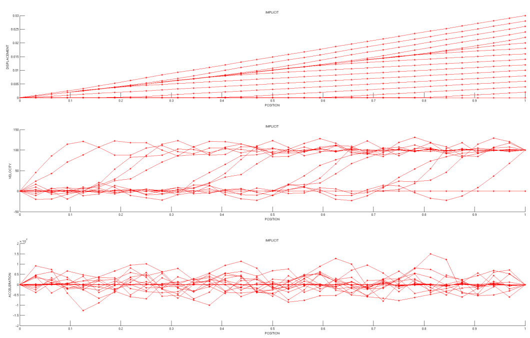
- We developed an extension to Schwarz coupling to dynamics using a governing time stepping algorithm that controls time integrators within each domain.
- Can use different integrators with different time steps within each domain.
- 1D results show smooth coupling without numerical artifacts such as spurious wave reflections at boundaries of coupled domains.



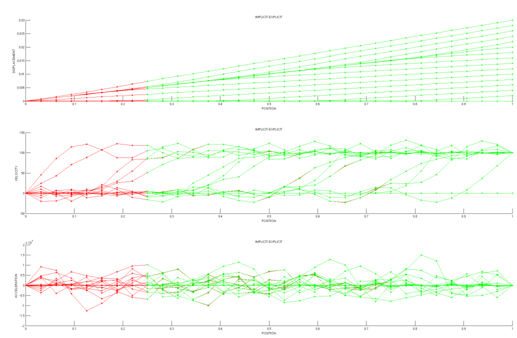
1D Elastic Bar

Schwarz alternating coupling results for elastic bar.

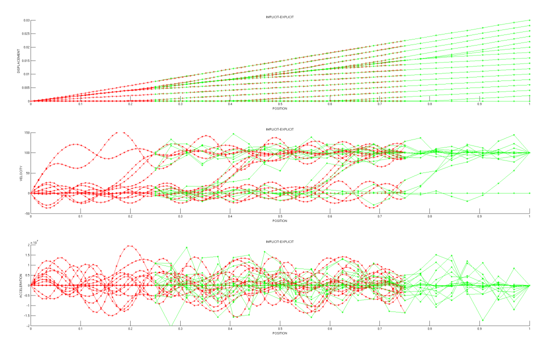
- In dynamics, elasticity is more difficult because defects in time integration schemes are exposed by the need for energy conservation. Inelasticity masks problems by introducing energy dissipation.
- Verification of 1D problem shows that Schwarz does not introduce numerical artifacts. Solutions (a) and (b) below match for same level of refinement, as expected, even using different integrators.
- Can couple domains with different levels of refinement and different time integration schemes as shown in (c) below. The coarse domain uses an explicit time integrator and its stable time step is used for the implicit time integrator in the fine domain. Thus avoid using an extremely small time step that would be dictated by the fine domain if not using coupling.



(a) Reference single-domain solution



(b) Two-domain implicit-explicit solution equal to (a). No dynamic artifacts.



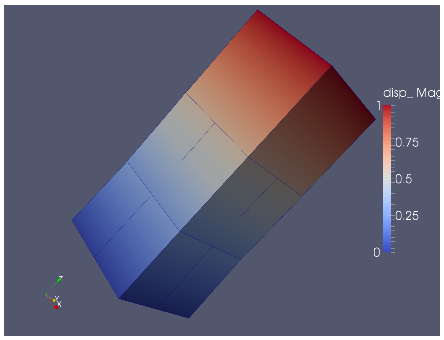
(c) Fine-coarse implicit-explicit coupling

Simple Examples in Albany/LCM

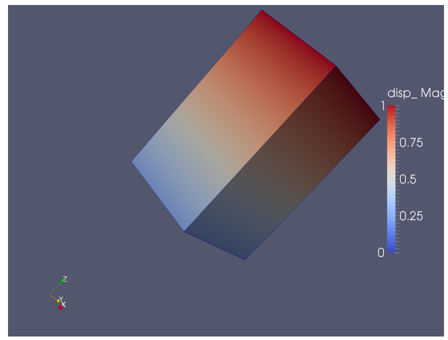
Sandia National Laboratories

Two simple examples of coupling using the Alternating Schwarz Method, both with overlap region.

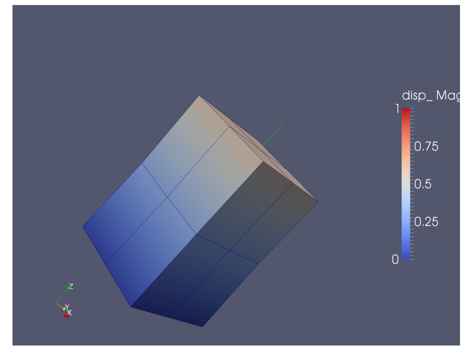
- Two cubes with different levels of mesh refinement.



Coupled meshes

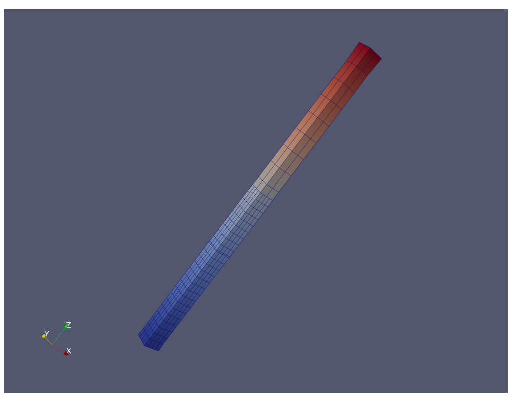


Coarse mesh

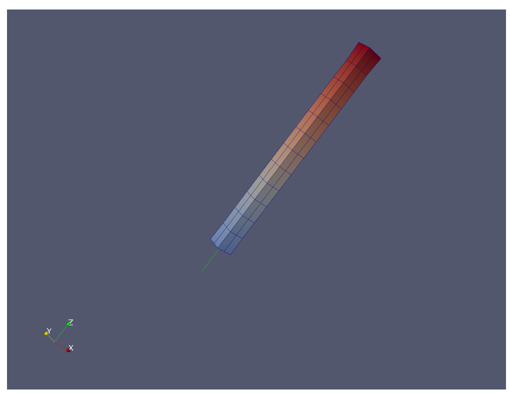


Fine mesh

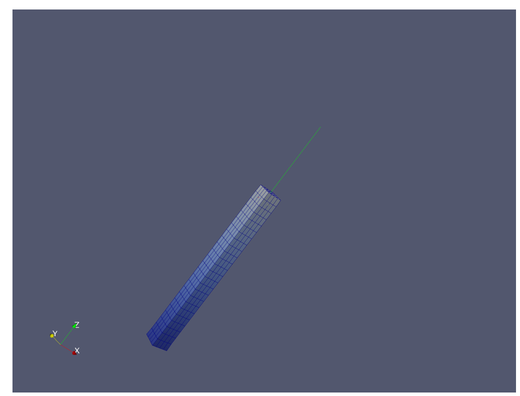
- Bar with square cross section stretched to twice its original length.



Coupled meshes



Coarse mesh

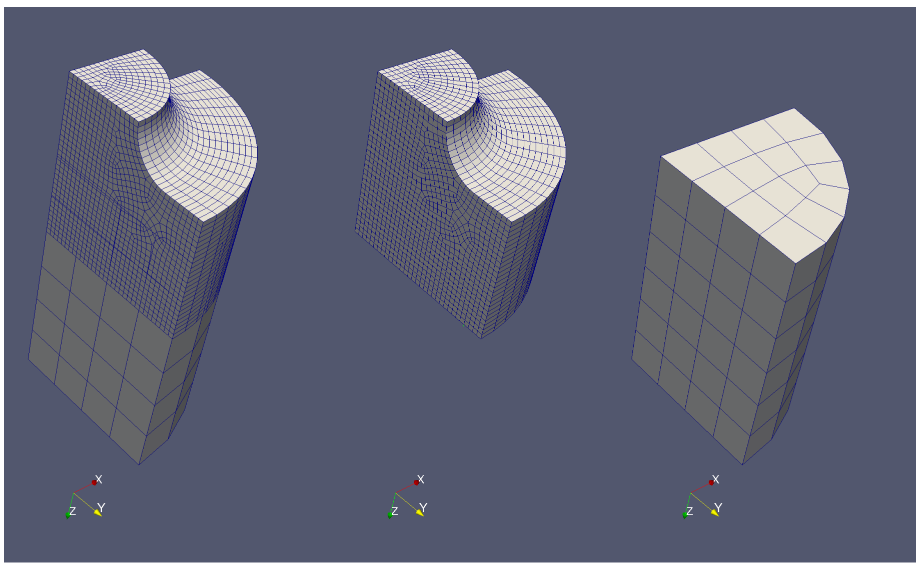


Fine mesh

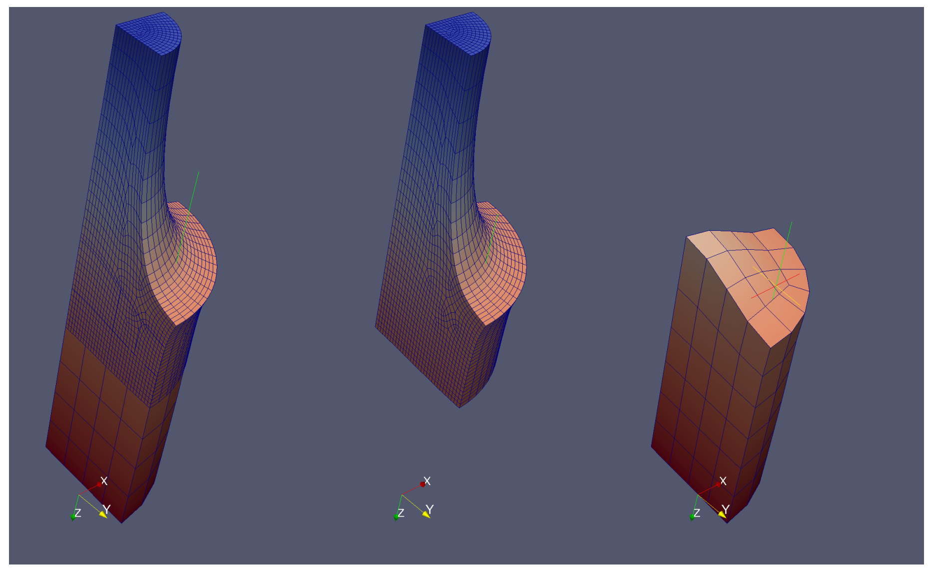
Hyperelastic Notched Cylinder

A nontrivial example of the Schwarz Alternating Coupling method.

Notched cylinder stretched to twice its original height. Stress concentrations and strain localization in the notch require a higher level of mesh refinement. The fine and coarse region overlap but the solutions are computed separately. Communication is effected through specialized Dirichlet boundary conditions and goes from coarse to fine and from fine to coarse as well (concurrent multiscale).



Notched cylinder section. Reference configuration with coupled, fine and coarse meshes. Note the overlap region on the left.



Deformed configuration colored with displacement magnitude. Smooth field transition even when the meshes do not match.

Coupling of two material models with Schwarz

Coupling of two material models with Schwarz:

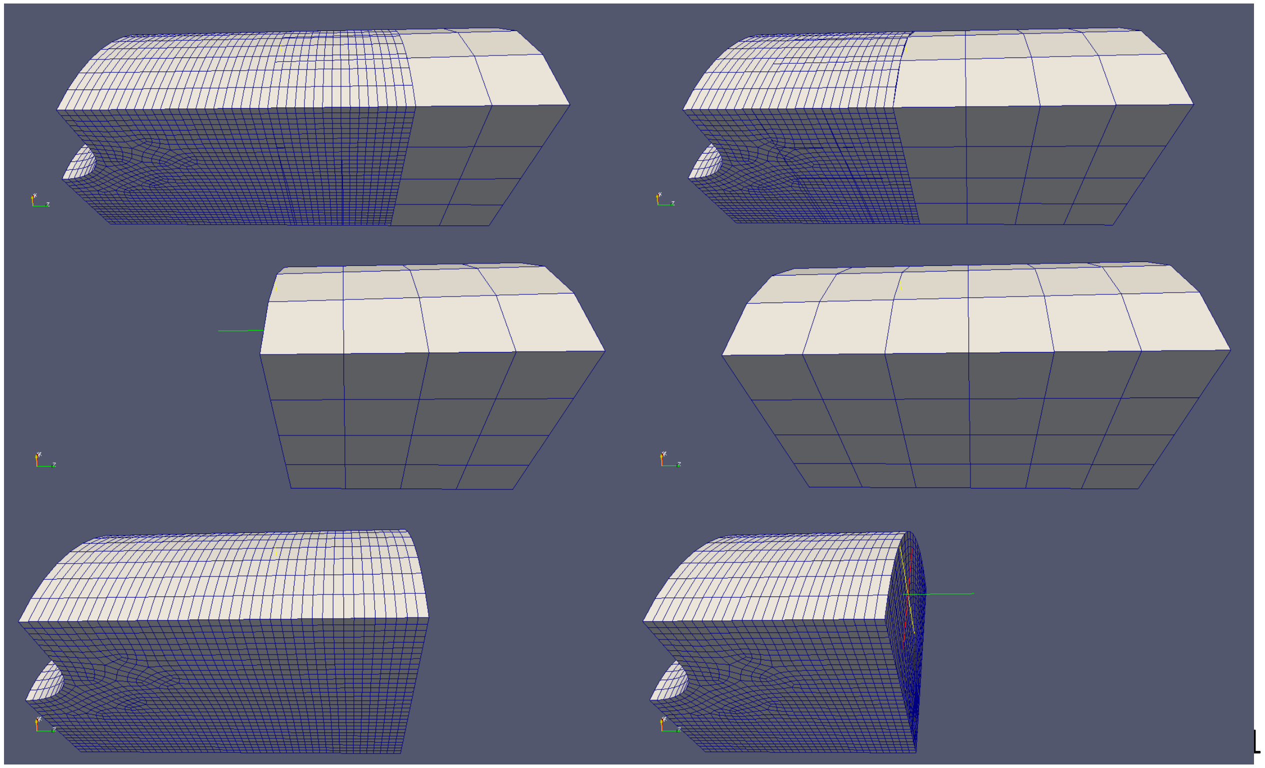
- Notched cylinder subjected to tensile load with an elastic and J2 elasto-plastic regions.
- Coarse region is elastic and fine region is elasto-plastic. The overlap region in the first mesh is nearer the notch, where plastic behavior is expected.

Overlap far from notch. Overlap near notch.

Coupled regions

Coarse, elastic region

Fine, elasto-plastic region

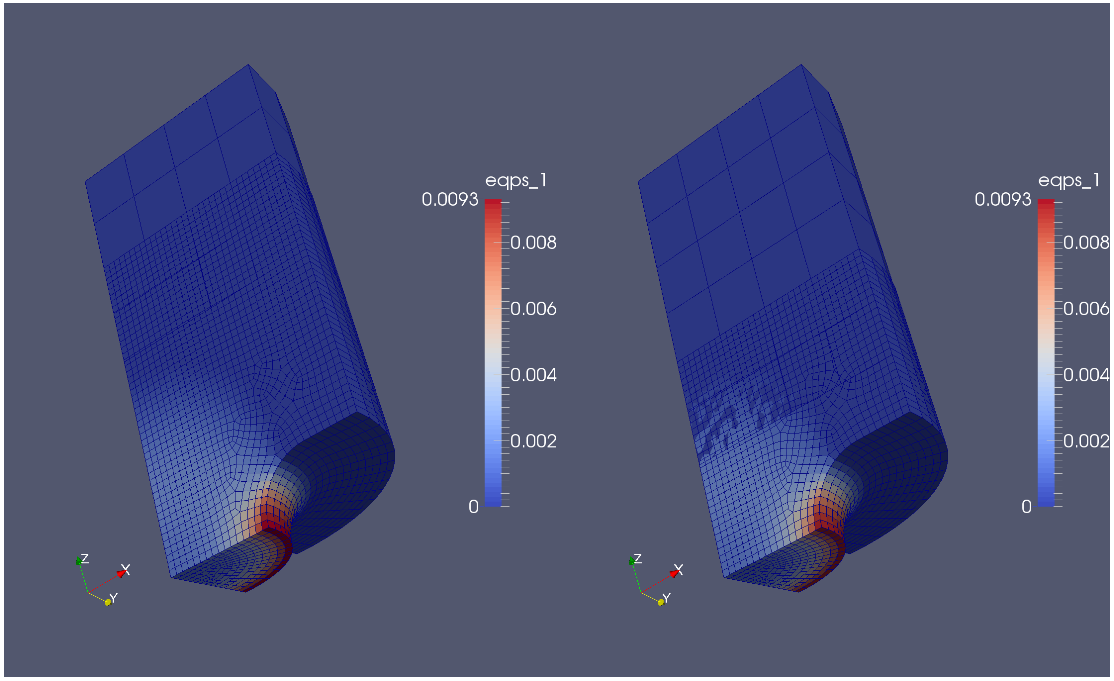


Coupling of two material models with Schwarz

Coupling of two material models with Schwarz:

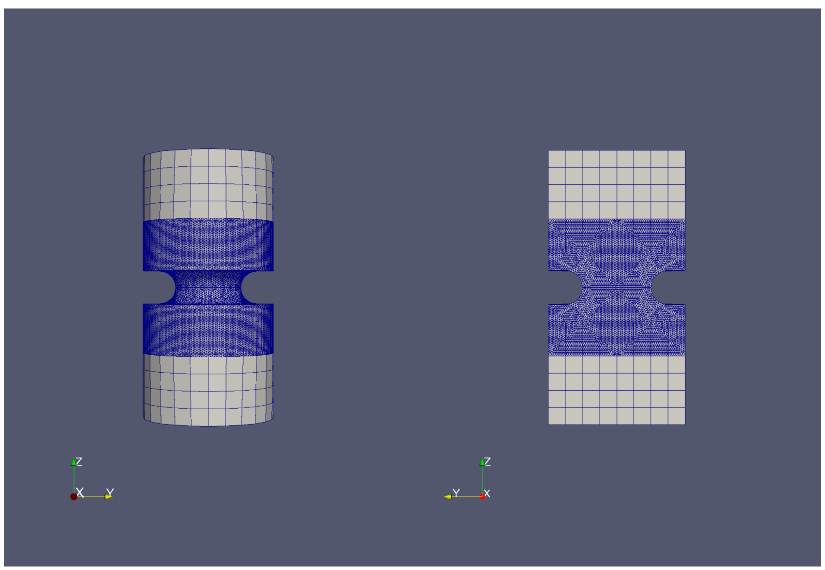
- The Schwarz method is capable of coupling regions with different material models.
- When the overlap region is far from the notch, no plastic deformation exists in it: the coarse and fine regions predict the same behavior there.
- When the overlap region is near the notch, plastic deformation spills onto it and the two models predict different behavior, affecting convergence adversely. Independent of any method, this kind of solution is questionable.

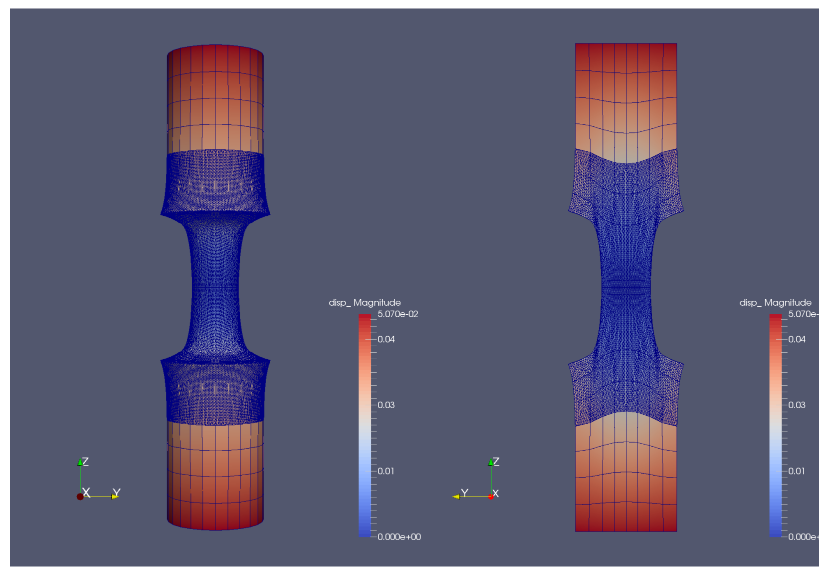
Overlap far from notch.   Overlap near notch.



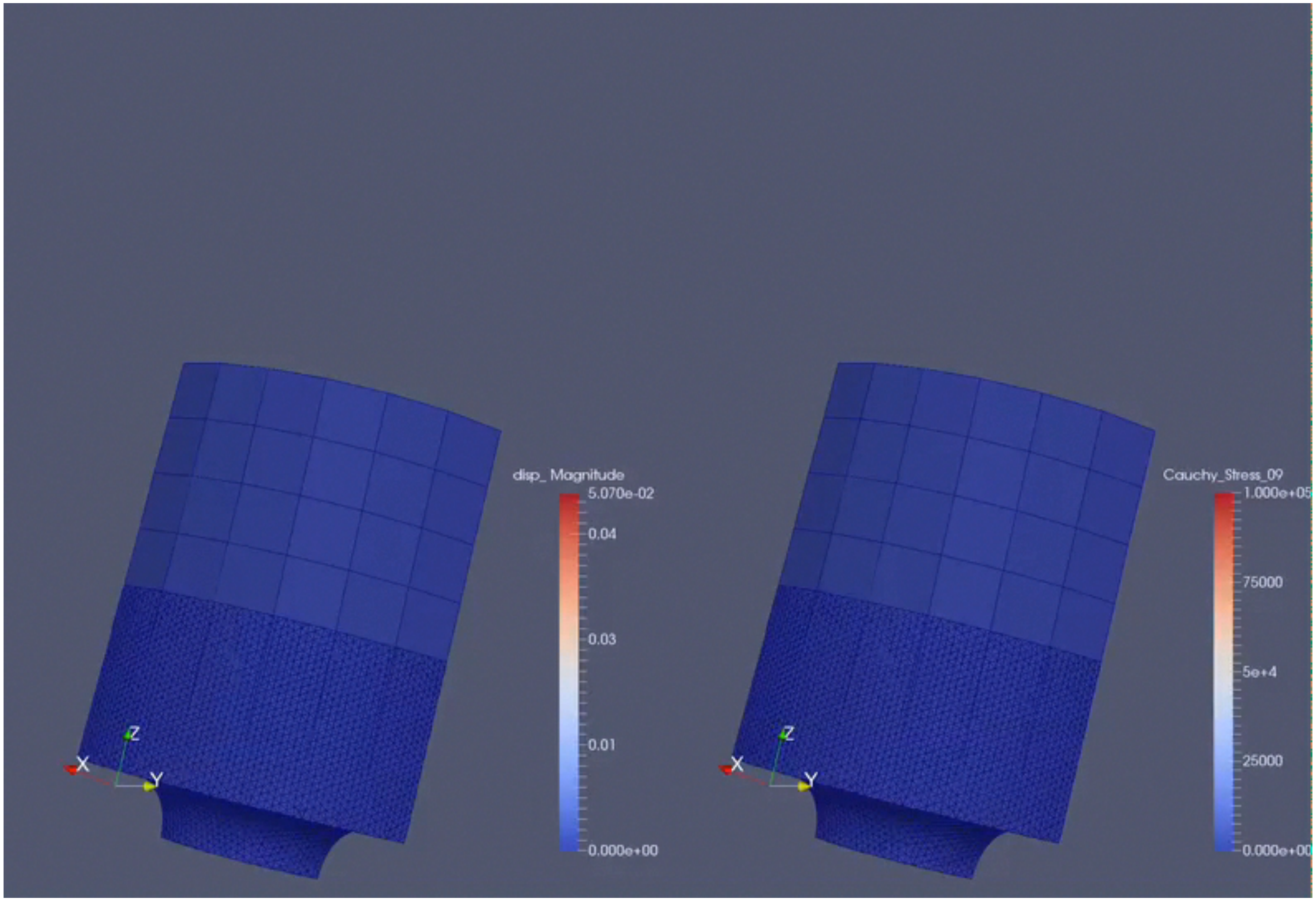
Schwarz Coupling: Notched Cylinder

- The method is capable of coupling different mesh topologies.
- The figure below shows the results of pulling on a notched cylinder.
- 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.
- This provides the flexibility of using more refined meshes in critical regions of complex geometry and phenomena where tetrahedral meshers excel, and less refined meshes away from critical regions that can be meshed by hexahedra that are traditionally less amenable to very complex geometries.





Schwarz Coupling: Movie of Half Notched Cylinder



Schwarz Coupling: Summary of Findings

- Preconditioners for Schwarz: the method works with a variety of preconditioners provided with Trilinos, or none at all for very simple problems. To obtain the best performance, however, Trilinos provides a block system preconditioner package called Teko. The Schwarz method can be formulated as a block system of equations, and therefore the best preconditioner to use is Teko.
- Now that each mesh is its own independent application from the point of view of Albany, this opens the possibility of using different discretizations altogether for each, as shown.
- This demonstration calculation used linear tetrahedral elements for the fine region and trilinear hexahedra for the coarse region.
- It is known that linear tetrahedra are notoriously bad at representing stress, specially under large distortion, thus the non-smooth stress field near the notch in this demonstration calculation. The emphasis here is in the ability to couple different mesh topologies, which is a first for Albany.
- We have started preliminary performance studies of Albany under Kokkos using OpenMP. Kokkos can use a variety of alternate accelerators such as OpenMP, Cuda, Intel Phi, etc.