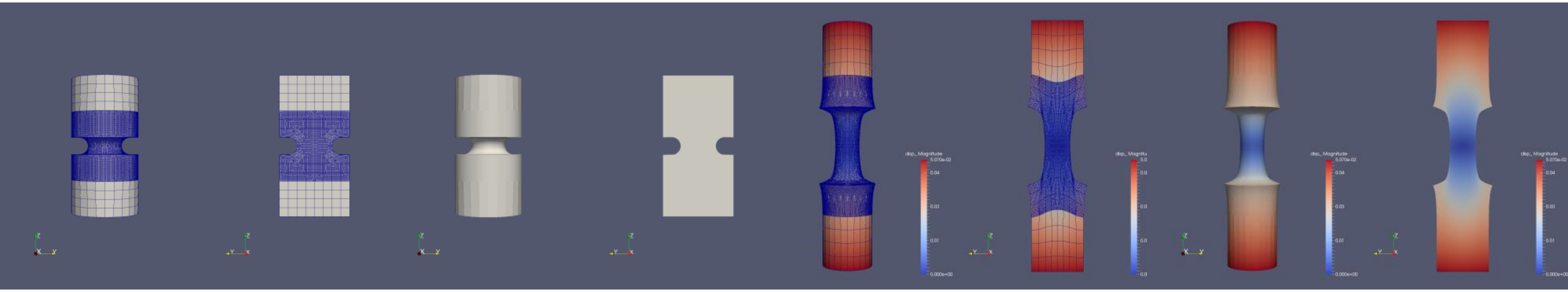

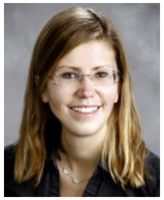

The Schwarz Alternating Method for Dynamic Multiscale Coupling in Solid Mechanics

Irina Tezaur[1], Alejandro Mota[1], Greg Phlipot[2]

[1]Sandia National Laboratories, Livermore, CA, USA. [2]California Institute of Technology, Pasadena, CA, USA.

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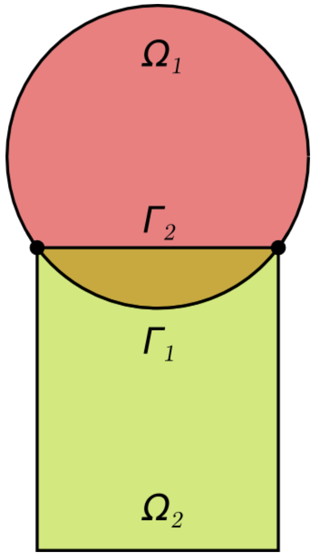
Outline

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



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3. Numerical Examples.
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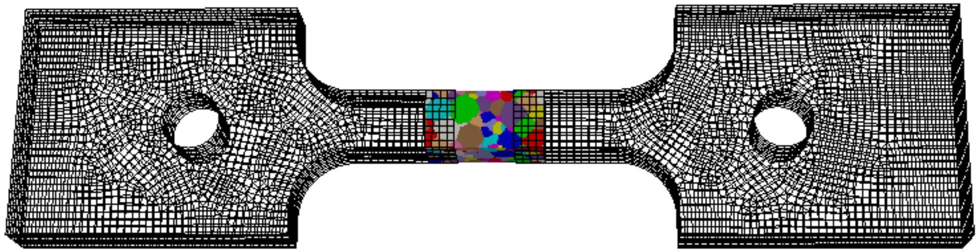

* Review from previous talk #2018677 by A. Mota.

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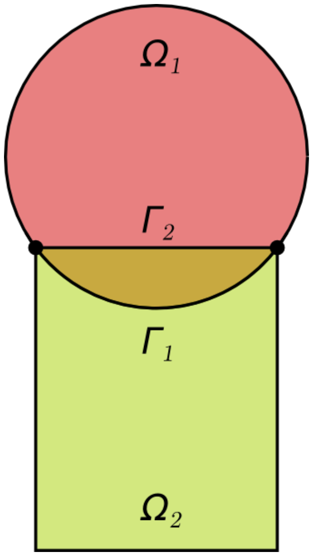

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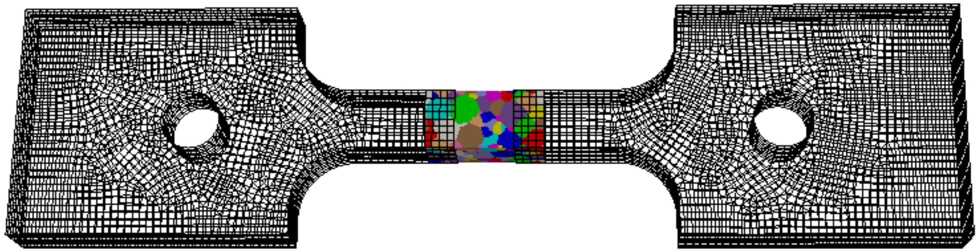


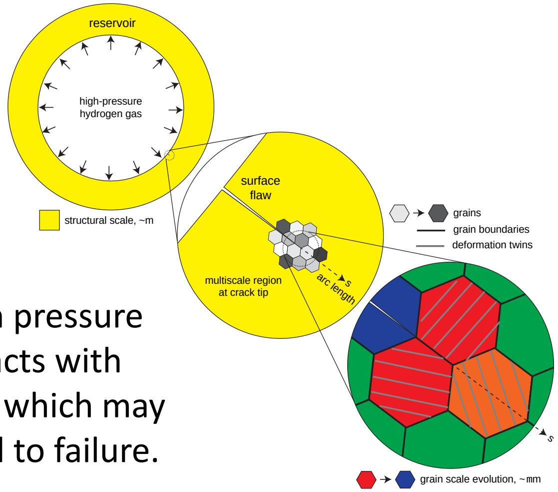
Motivation for Concurrent Multiscale Coupling

- ***Large scale*** structural ***failure*** frequently originates from ***small scale*** phenomena such as defects, microcracks, and inhomogeneities, which grow quickly in unstable manner.

- Failure occurs due to ***tightly coupled interaction*** between small scale (stress concentrations, material instabilities, cracks, etc.) and large scale (vibration, impact, high loads and other perturbations).

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

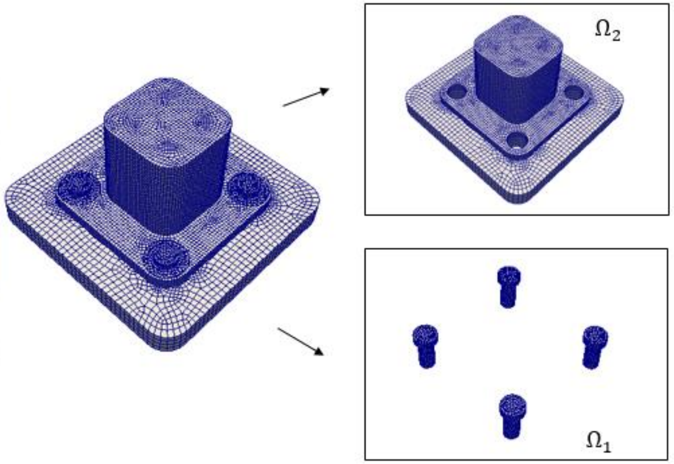
Roof failure of Boeing 737 aircraft due to fatigue cracks. From *imechanica.org*



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

Requirements for Multiscale Coupling Method

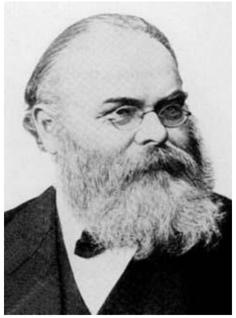
- Coupling is ***concurrent*** (two-way).
- ***Ease of implementation*** into existing massively-parallel HPC codes.
- ***Scalable, fast, robust*** (we target ***real*** engineering problems, e.g., analyses involving failure of bolted components!).
- ***"Plug-and-play" framework***: simplifies task of meshing complex geometries!
  - Ability to couple regions with ***different non-conformal meshes***, ***different element types*** and ***different levels of refinement.***
  - Ability to use ***different solvers/time-integrators*** in different regions.
- Coupling does not introduce ***nonphysical artifacts.***
- ***Theoretical*** convergence properties/guarantees.



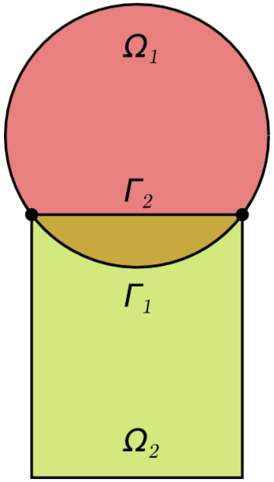
Schwarz Alternating Method for Domain Decomposition

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

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



H. Schwarz (1843 – 1921)



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 multiscale partial differential equations (PDEs).

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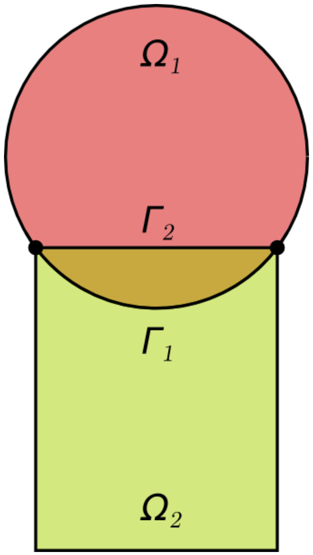

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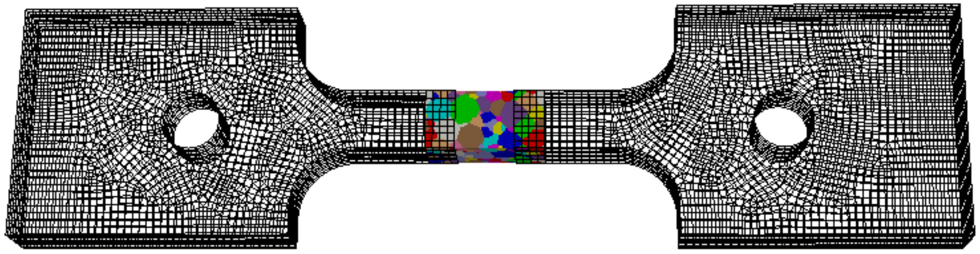
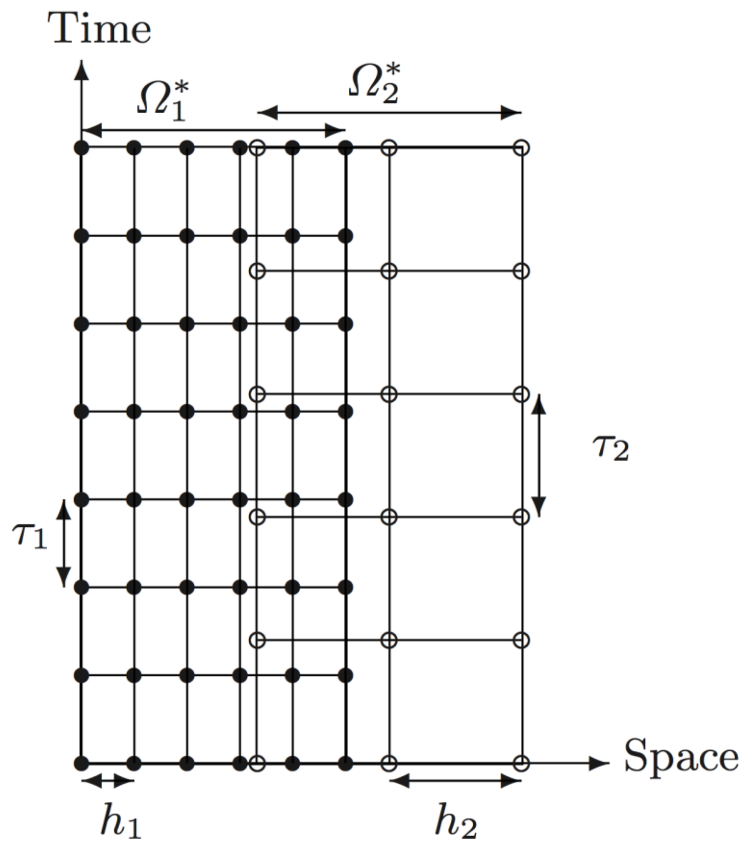


Schwarz Alternating Method for Dynamic Multiscale Coupling

- In the literature the Schwarz method is applied to dynamics by using ***space-time discretizations***.



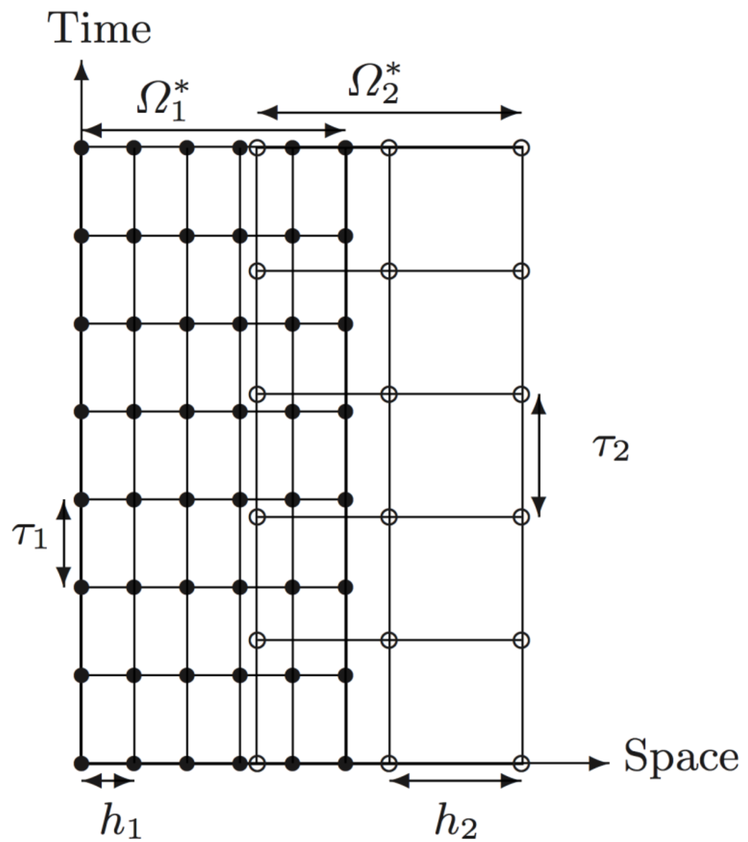
Overlapping non-matching meshes and time steps in dynamics.

Schwarz Alternating Method for Dynamic Multiscale Coupling

- In the literature the Schwarz method is applied to dynamics by using ***space-time discretizations***.

Pro ☺: Can use ***non-matching*** meshes and time-steps (see right figure).

Con ☹: ***Unfeasible*** given the design of our current codes and size of simulations.



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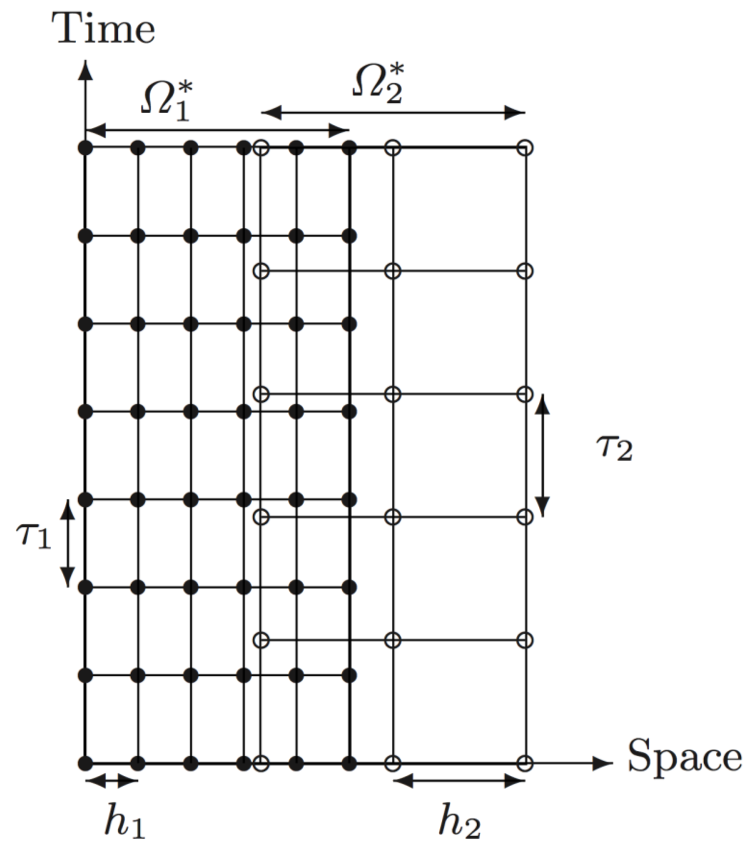
Schwarz Alternating Method for Dynamic Multiscale Coupling

- In the literature the Schwarz method is applied to dynamics by using ***space-time discretizations***.

Pro ☺: Can use ***non-matching*** meshes and time-steps (see right figure).

Con ☹: ***Unfeasible*** given the design of our current codes and size of simulations.

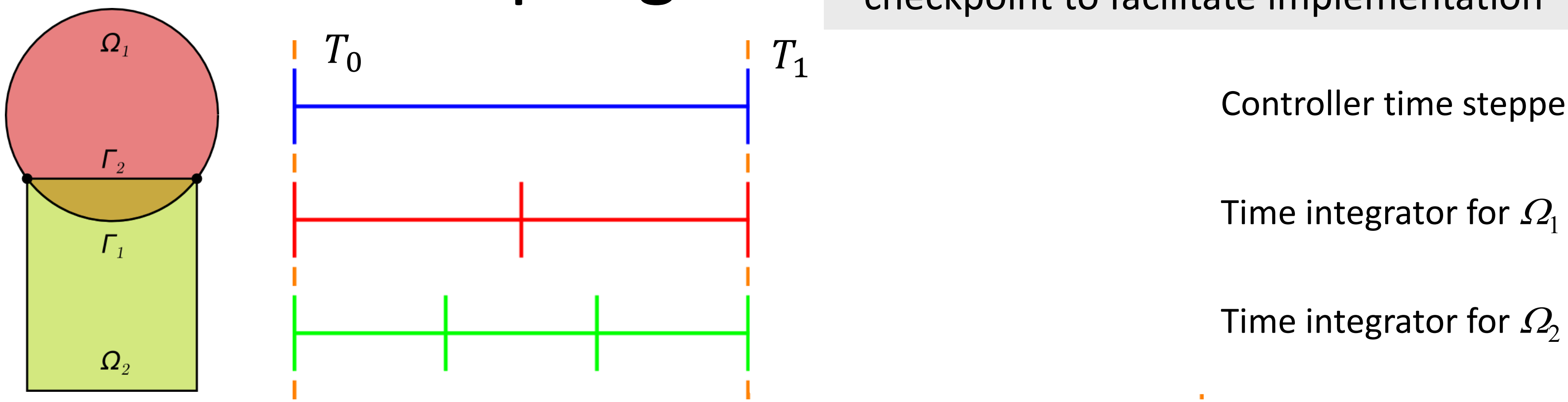
Our objective: formulate dynamic Schwarz method for standard (non-space-time) discretizations (discretize in space, march forward in time).



Overlapping non-matching meshes and time steps in dynamics.

Schwarz Alternating Method for Dynamic Multiscale Coupling

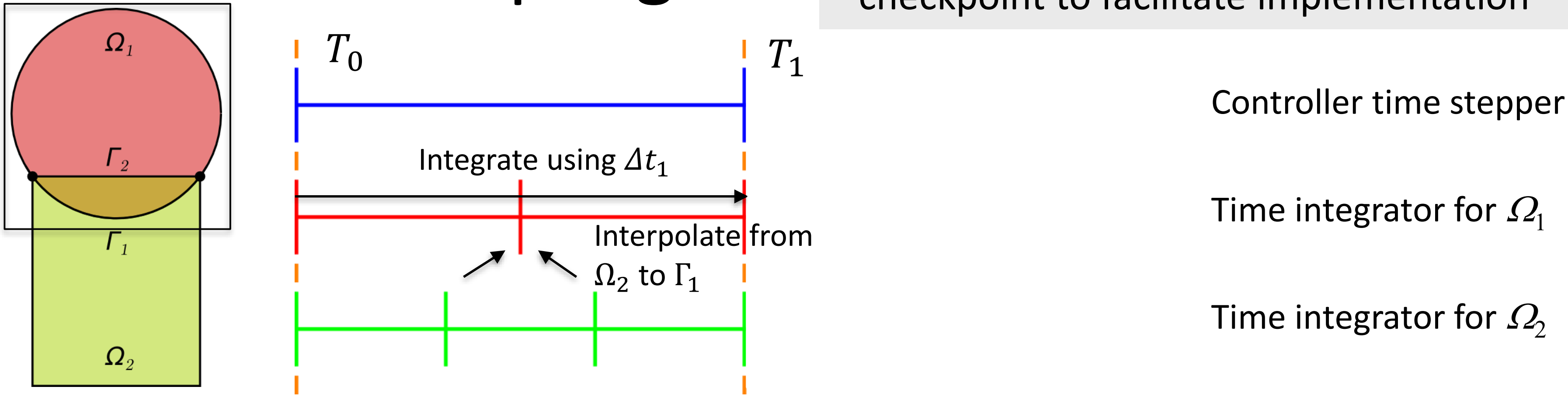
Controller time stepper = convenient checkpoint to facilitate implementation



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

Schwarz Alternating Method for Dynamic Multiscale Coupling

Controller time stepper = convenient checkpoint to facilitate implementation



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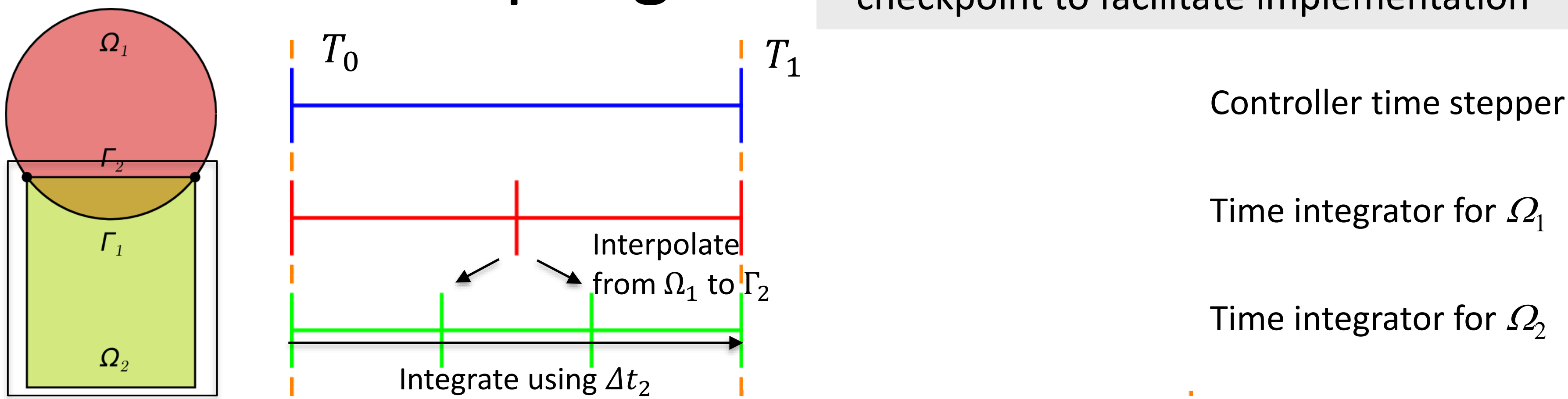

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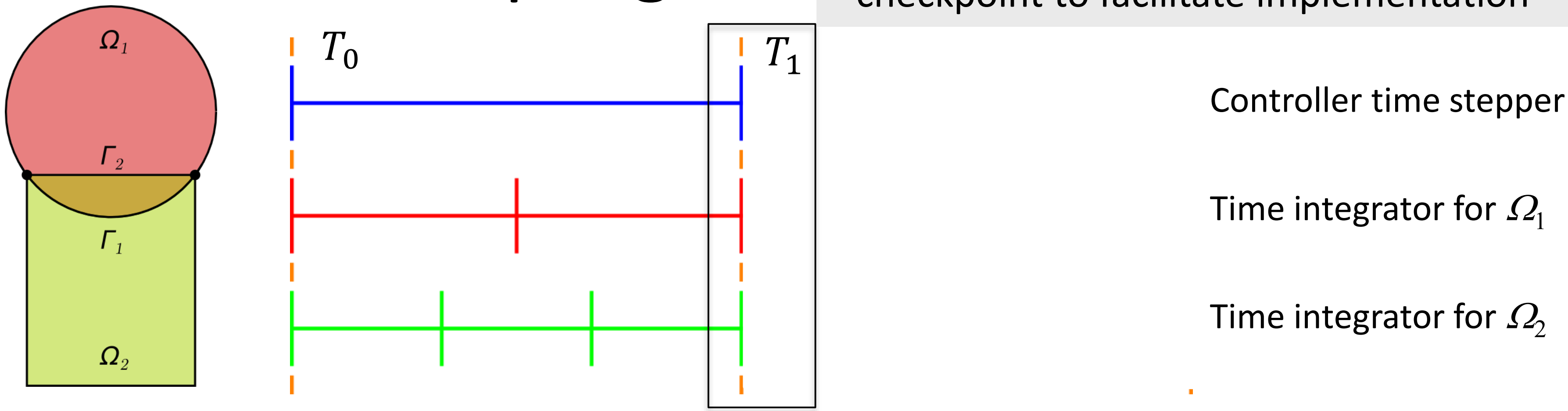

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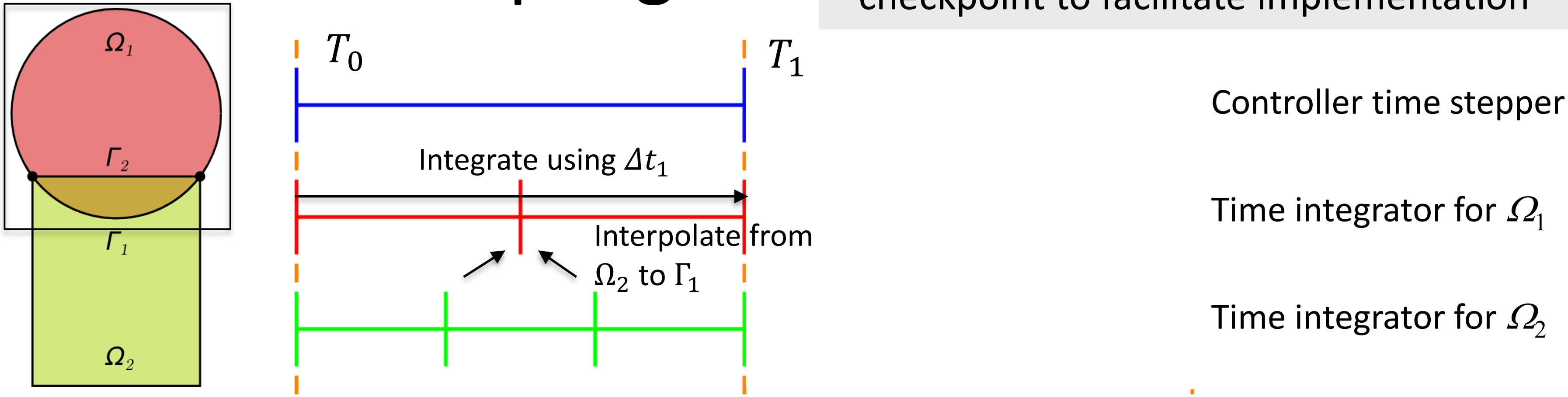

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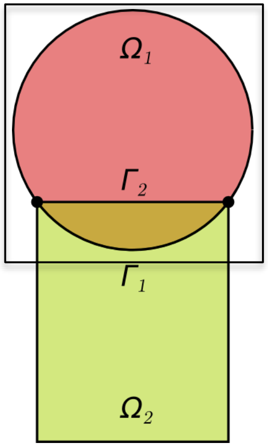
Schwarz Alternating Method for Dynamic Multiscale Coupling



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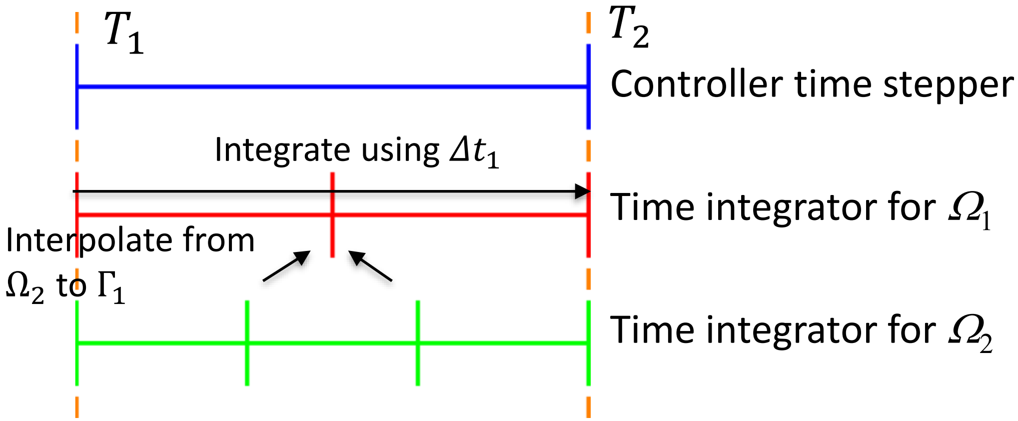

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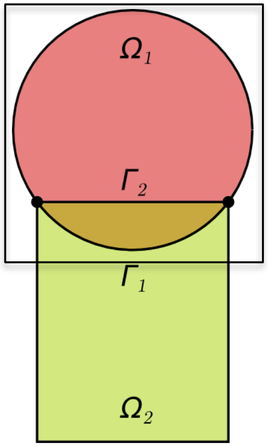
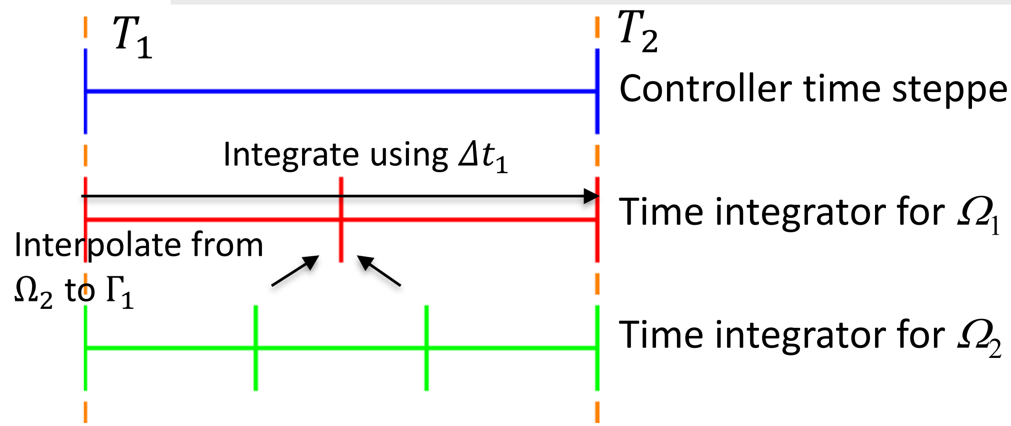
Schwarz Alternating Method for Dynamic Multiscale Coupling

Controller time stepper = convenient checkpoint to facilitate implementation





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

Schwarz Alternating Method for Dynamic Multiscale Coupling: Theory

Sandia National Laboratories

- For quasistatics, we derived a ***proof of convergence*** of the alternating Schwarz method for the ***finite deformation*** problem, and determined a ***geometric convergence rate*** [(Mota, Tezaur, Alleman, *CMAME,* 2017) and previous talk].

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

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

(b) *The sequence $\{\tilde{\varphi}^{(n)}\}$ defined in (39) converges to the minimizer φ of $\Phi[\varphi]$ in $\mathcal{S}$.*

(c) *The Schwarz minimum values $\Phi[\tilde{\varphi}^{(n)}]$ converge monotonically to the minimum value $\Phi[\varphi]$ in $\mathcal{S}$ starting from any initial guess $\tilde{\varphi}^{(0)}$.*

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

- Quasistatic proof ***extends naturally*** assuming conformal meshes and the same time step is used in each Schwarz subdomain.
- Some analysis of Schwarz for evolution problems was performed in (Lions, 1988) and may be possible to ***leverage***.
- Our numerical results suggest theoretical analysis is ***possible***.

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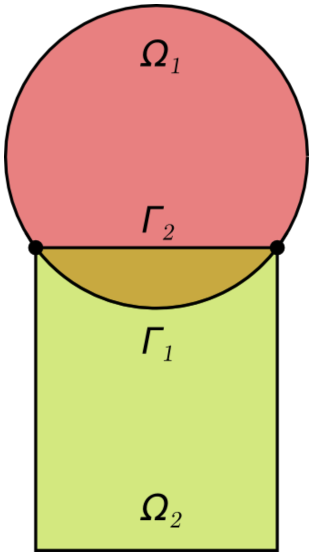

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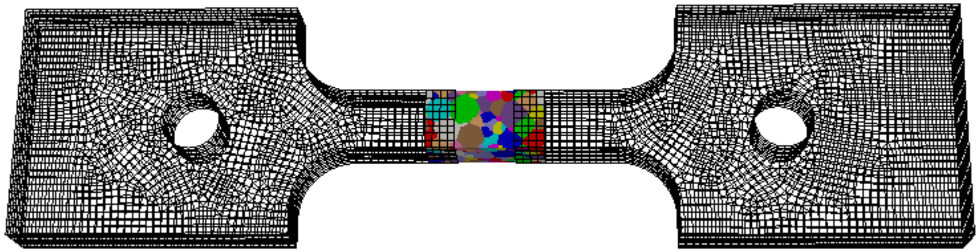


* Review from previous talk #2018677 by A. Mota.

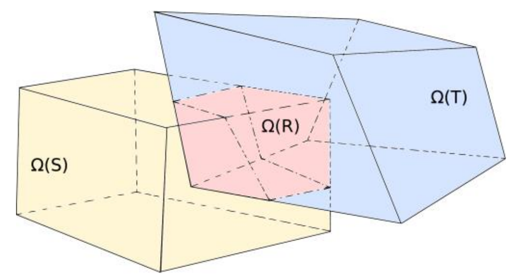
Implementation within *Albany* Code

The proposed ***dynamic alternating Schwarz method*** has been implemented within the ***LCM project*** in Sandia's open-source parallel, C++, multi-physics, finite element code, ***Albany***.

- ***Component-based*** design for rapid development of capabilities.
- Contains a wide variety of ***constitutive models***.
- Extensive use of libraries from the open-source ***Trilinos*** project.
  - Use of the ***Phalanx*** package to decompose complex problem into simpler problems with managed dependencies.
  - Use of the ***Sacado*** package for ***automatic differentiation.***
  - Use of ***Tempus*** package for ***time-integration****.
- ***Parallel*** implementation of Schwarz alternating method uses the ***Data Transfer Kit*** (***DTK***).
- All software available on ***GitHub***.

https://github.com/gahansen/Albany

https://github.com/trilinos/trilinos

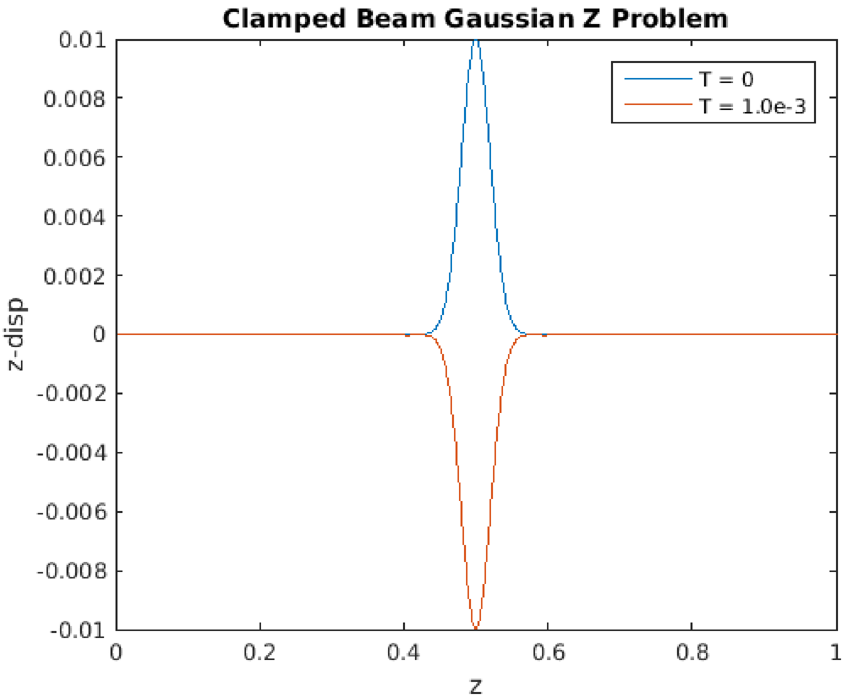


https://github.com/ORNL-CEES/DataTransferKit

* Current dynamic Schwarz implementation in Albany requires same Δt in different subdomains.

Example #1: Elastic Wave Propagation

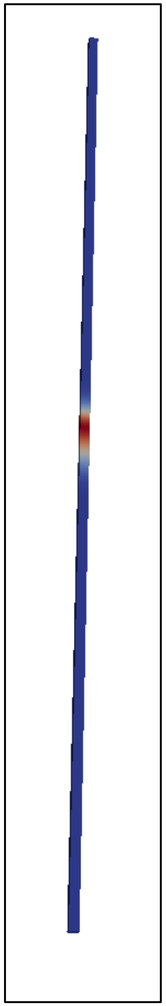
- Linear elastic ***clamped beam*** with Gaussian initial condition for the z-displacement (see figures to the right and below).
- Simple problem with analytical exact solution but very ***stringent test*** for discretization methods.
- Test Schwarz with ***2 subdomains***: $\Omega_0 = (0{,}0.001) \times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



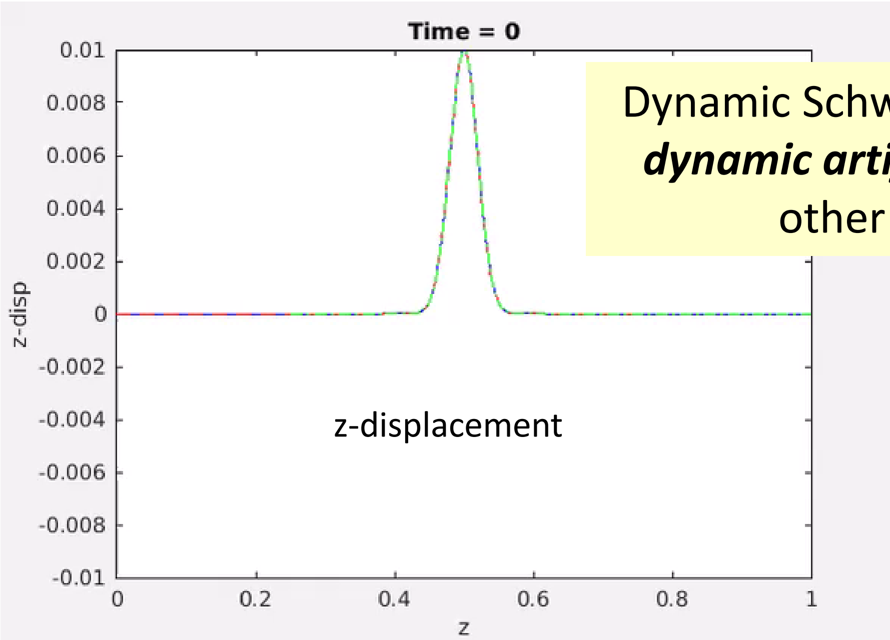
Left: Initial condition (blue) and final solution (red). Wave profile is negative of initial profile at time T = 1.0e-3.

Time-discretizations: Newmark-Beta (implicit, explicit) with same Δt.

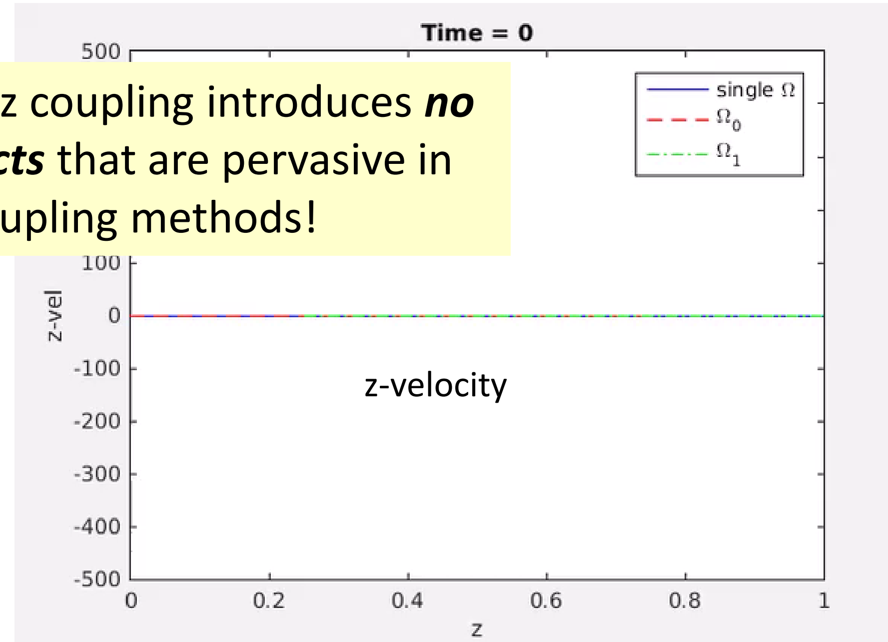
Meshes: hexes, tets



Example #1: Elastic Wave Propagation



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



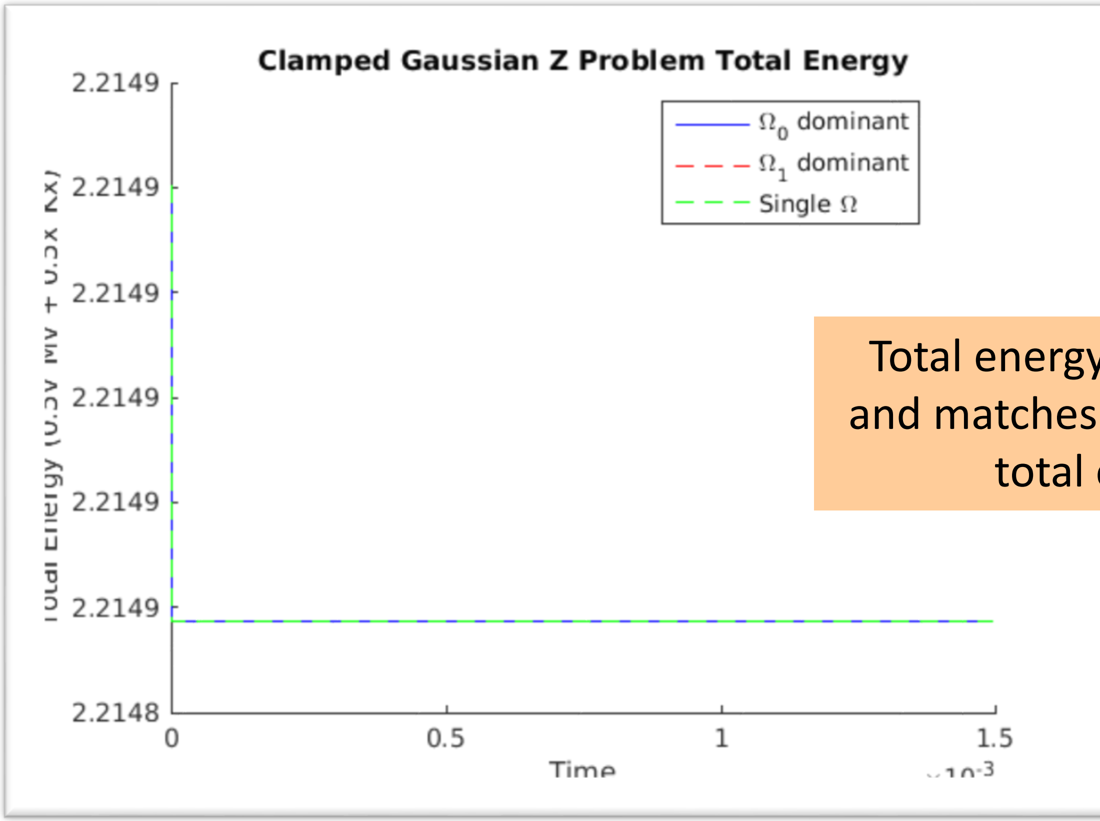
<u>Table 1:</u> Averaged (over times + domains) relative errors in **z–displacement** (blue) and **z-velocity** (green) for several different Schwarz couplings, 50% overlap volume fraction

	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

LM = Lumped Mass, CM = Consistent Mass

Example #1: Elastic Wave Propagation

Energy Conservation



Total energy is **conserved** and matches single-domain total energy.

- For clamped beam problem, total energy (TE = $0.5\boldsymbol{x}^T\boldsymbol{K}\boldsymbol{x} + 0.5\dot{\boldsymbol{x}}^T\boldsymbol{M}\dot{\boldsymbol{x}}$) should be conserved.
- Total energy is calculated in 2 ways: with most of contribution from Ω_0 and from Ω_1.

Example #2: Torsion

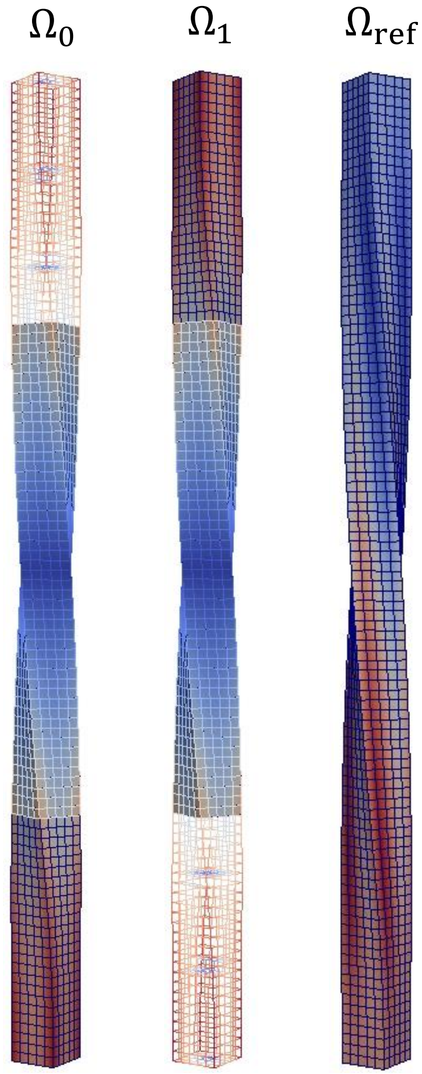
- Nonlinear elastic bar (Neohookean material model) subjected to a high degree of ***torsion***.

- The ***domain*** is $\Omega = (-0.025,0.025) \times (-0.025,0.025) \times (-0.5,0.5)$.

- We evaluate ***dynamic Schwarz*** with 2 subdomains: $\Omega_0 = (-0.025,0.025) \times (-0.025,0.025) \times (-0.5,0.25), \Omega_1 = (-0.025,0.025) \times (-0.025,0.025) \times (-0.25,0.5)$.

- ***Time-discretizations***: Newmark-Beta (implicit, explicit) with same Δt.

- ***Meshes:*** hexes, composite tet 10s.



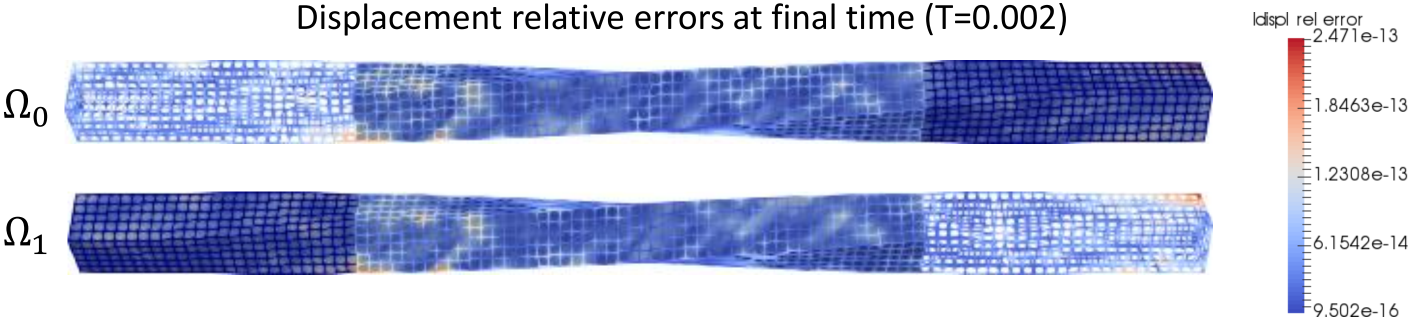
Example #2: Torsion

Schwarz and single-domain results agree to almost ***machine-precision***!

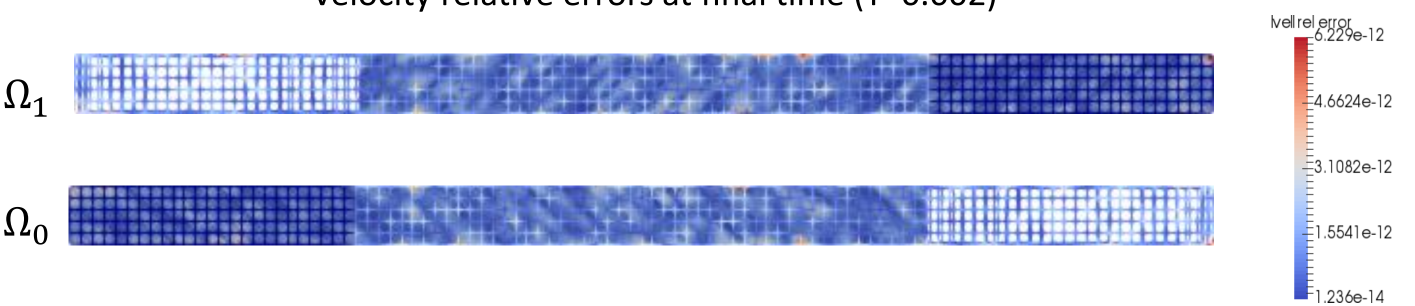
Conformal Hex + Hex Coupling

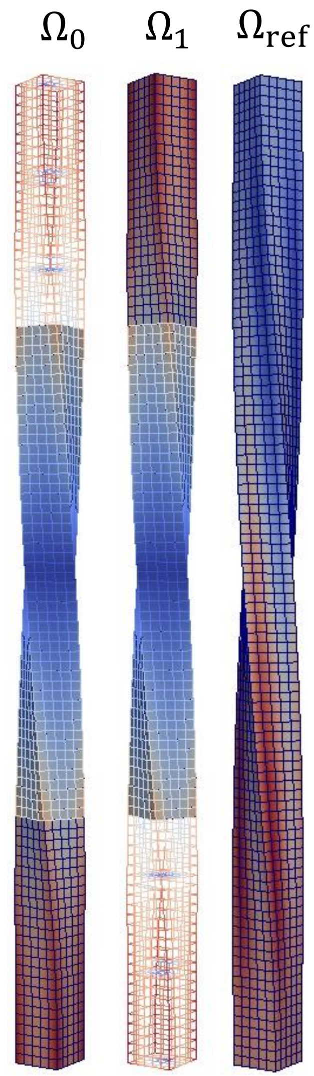
- Each subdomain discretized using **uniform hex mesh** with $\Delta x_i = 0.01$, and advanced in time using implicit Newmark-Beta scheme with Δt =1e-6.
- Results compared to single-domain solution on mesh **conformal** with Schwarz domain meshes.

Displacement relative errors at final time (T=0.002)



Velocity relative errors at final time (T=0.002)





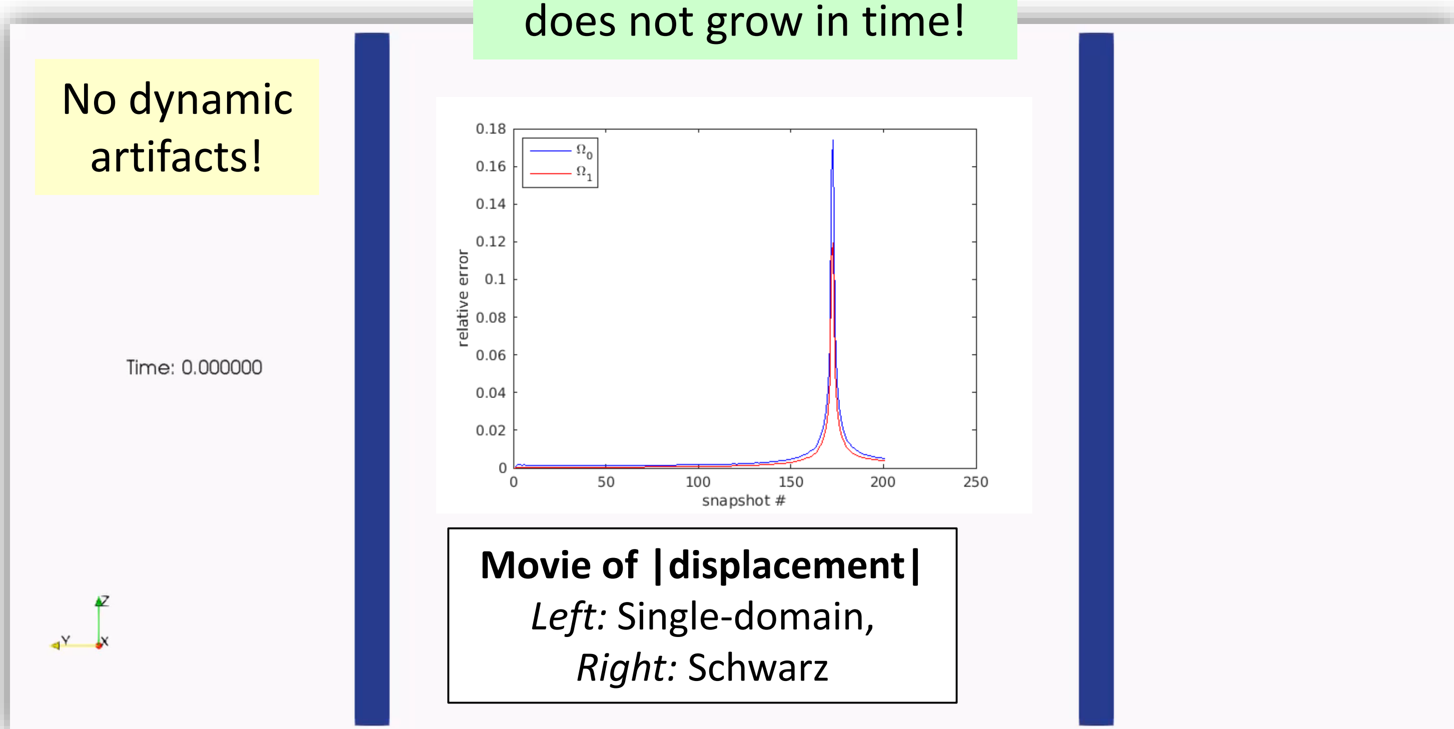
Example #2: Torsion

Hex + Composite Tet 10 Coupling

- Coupling of composite tet 10s + explicit Newmark with consistent mass in Ω_0 with hexes + implicit Newmark in Ω_1.
- Reference solution is computed on fine hex mesh + implicit Newmark Ω_{ref}

Relative error <1% and does not grow in time!

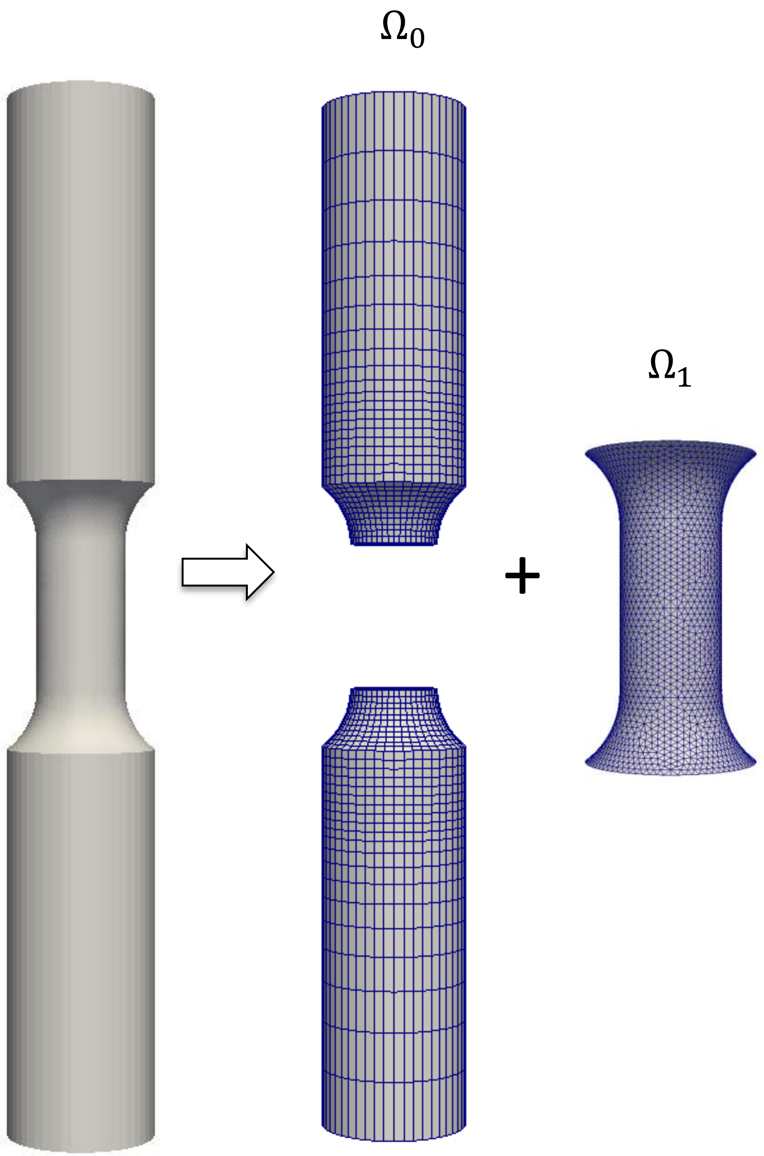
No dynamic artifacts!



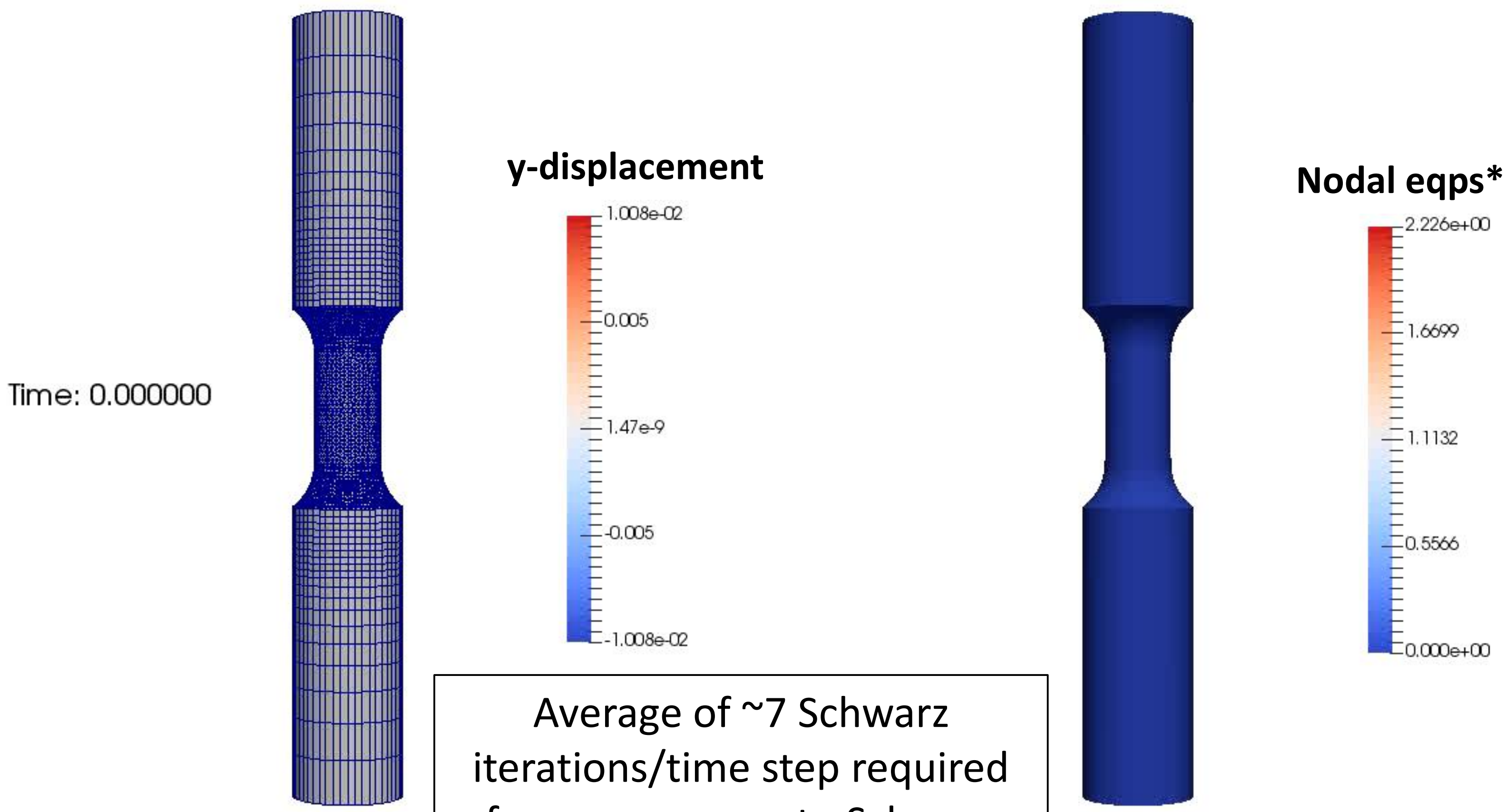
Movie of |displacement|
Left: Single-domain,
Right: Schwarz

Example #3: Tension Specimen

- Uniaxial aluminum cylindrical tensile specimen with ***inelastic J_2 material model***.
- Domain decomposition into ***two subdomains*** (right): Ω_0 = ends, Ω_1 = gauge.
- ***Nonconformal hex + composite tet 10*** coupling via Schwarz.
- ***Implicit*** Newmark time-integration with ***adaptive time-stepping*** algorithm employed in both subdomains.
- Slight ***imperfection*** introduced at center of gauge to force ***necking*** upon pulling in vertical direction.



Example #3: Tension Specimen



Average of ~7 Schwarz iterations/time step required for ***convergence*** to Schwarz tolerance of 1e-6.

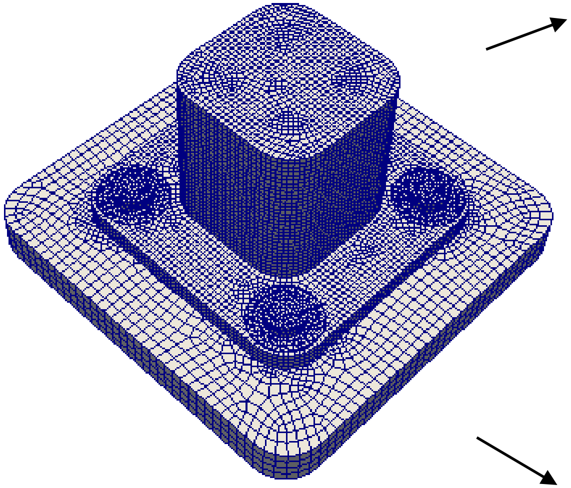
*Nodal eqps = equivalent plastic strain computed via weighted volume average.

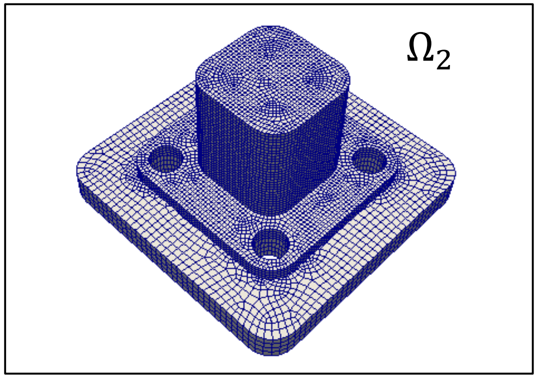
Example #4: Bolted Joint Problem

Sandia National Laboratories

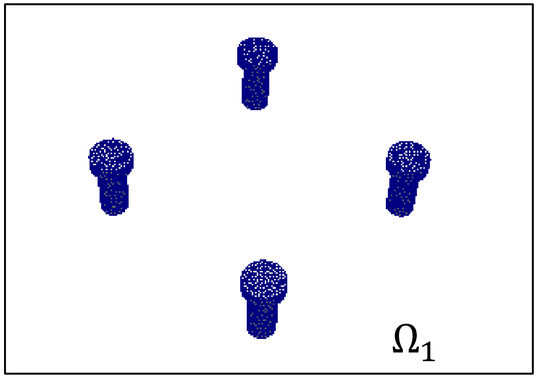
Problem of *practical scale*.

- Schwarz solution compared to single-domain solution on composite tet 10 mesh.





- 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.

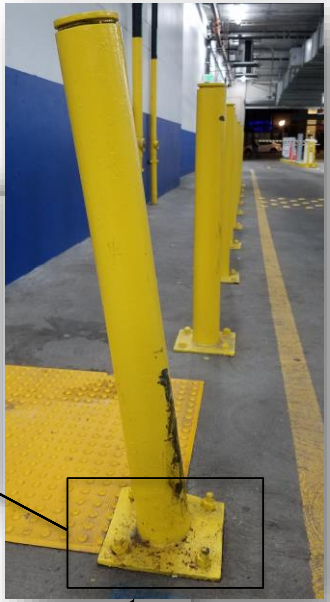


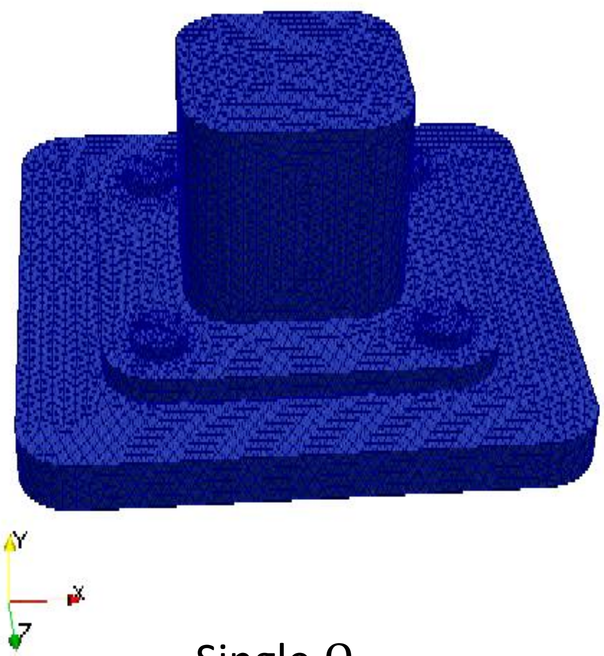
- Ω_1 = bolts (composite tet 10), Ω_2 = parts (hex).
- ***Inelastic J_2 material model*** in both subdomains.
  - Ω_1: steel
  - Ω_2: steel component, aluminum (bottom) plate

Example #4: Bolted Joint Problem

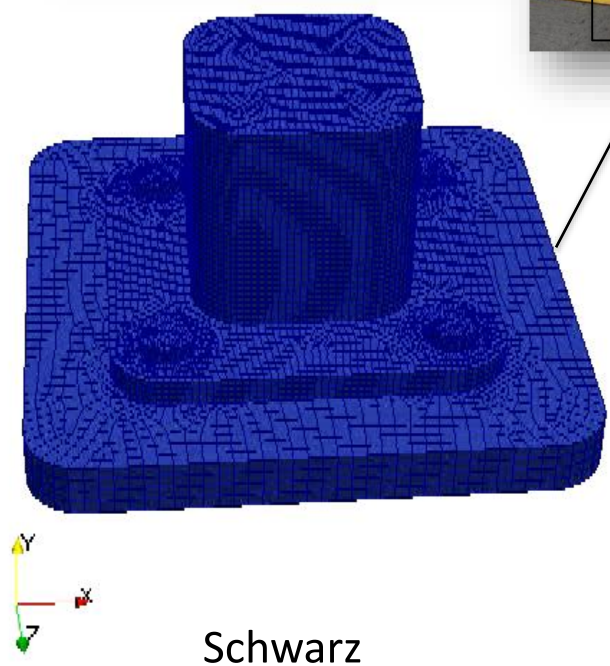
Time: 0.000000

x-displacement



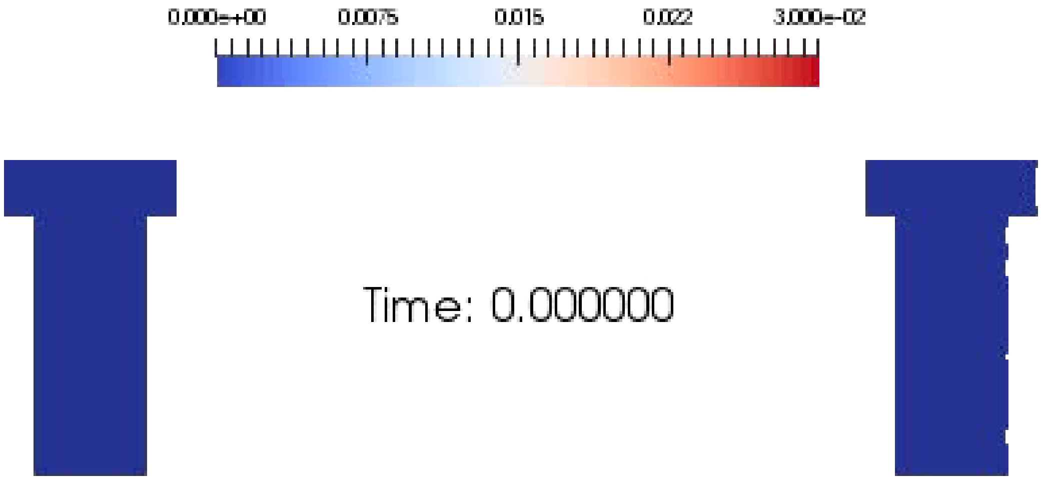
Single Ω



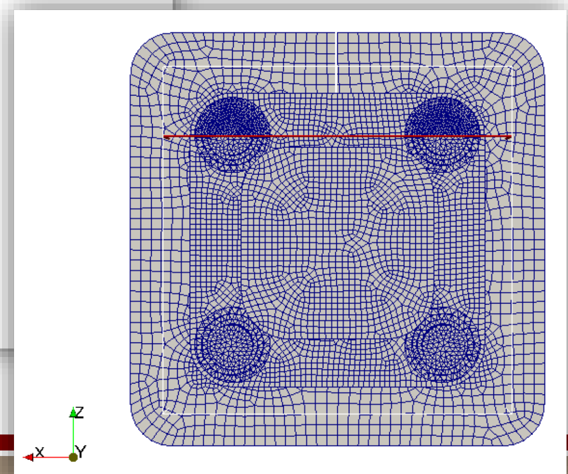
Schwarz

Example #4: Bolted Joint Problem

Nodal Equivalent Plastic Strain (eqps)



Cross-section of bolts obtained via clip (right)

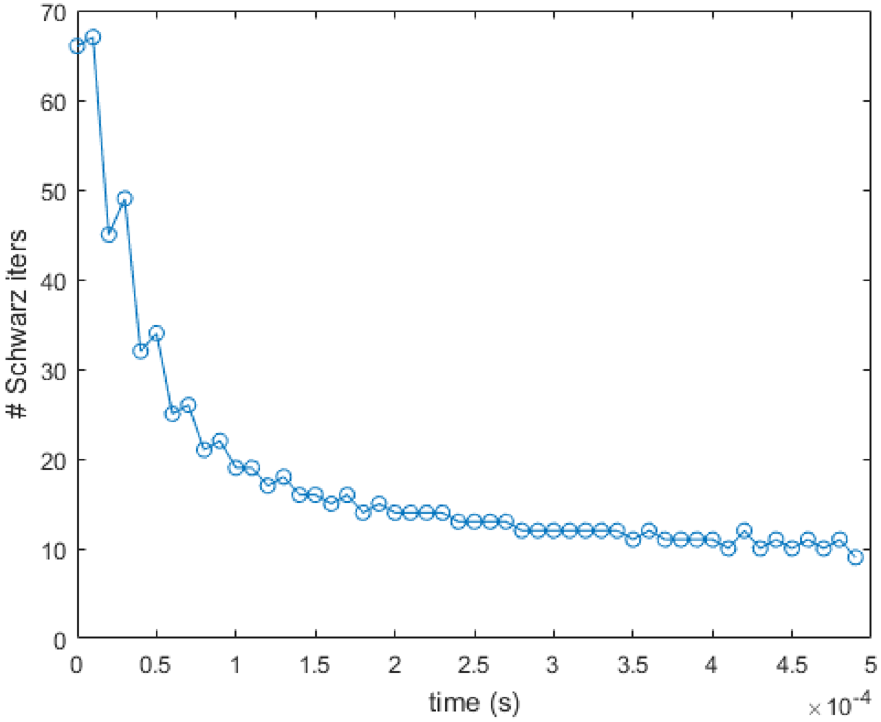


Example #4: Bolted Joint Problem

Some Performance Results

Schwarz / solver settings

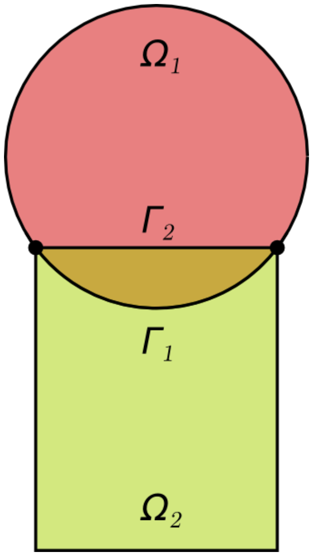
- Relatively loose Schwarz tolerances were used:
  - Relative Tolerance: 1.0e-3.
  - Absolute Tolerance: 1.0e-4.
- Newton tolerance on NormF: 1e-8
- Linear solver tolerance: 1e-5
- MueLu preconditioner



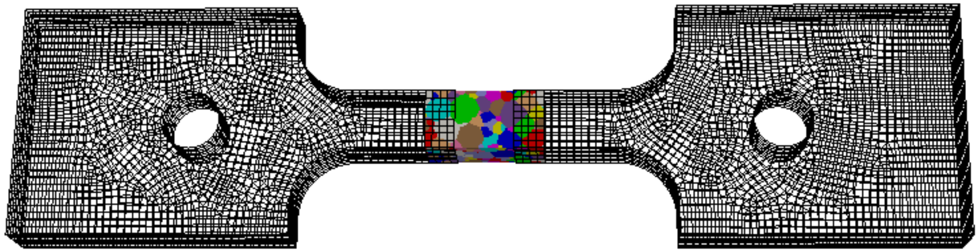
- ***Top right plot:*** # Schwarz iterations for each time step.
  - After start-up, # Schwarz iterations / time step is ~9-10. This is not bad given how small is the size of the overlap region for this problem.

Outline

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



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



* Review from previous talk #2018677 by A. Mota.

Summary

The **alternating Schwarz** coupling method has been developed and implemented for **concurrent multiscale dynamic modeling** in Sandia's Albany/LCM code.

☺ Coupling is ***concurrent*** (two-way).

☺ ***Ease of implementation*** into existing massively-parallel HPC codes.

☺ ***Scalable, fast, robust*** (we target ***real*** engineering problems, e.g., analyses involving failure of bolted components!).

☺ ***"Plug-and-play" framework***: simplifies task of meshing complex geometries!

- ☺ Ability to couple regions with ***different non-conformal meshes***, ***different element types*** and ***different levels of refinement.***
- ☺ Ability to use ***different solvers/time-integrators*** in different regions.

☺ Coupling does not introduce ***nonphysical artifacts.***

😐 ***Theoretical*** convergence properties/guarantees.

Ongoing/Future Work

- Development of ***theory*** for dynamic alternating Schwarz formulation.
- ***Journal article*** on the work presented in this talk is in preparation.
- Extension of Albany/LCM implementation to allow for ***different time steps*** in different subdomains.
- Application of dynamic Schwarz for problems and test cases of interest to ***production***.
- Implementation of alternating Schwarz method for concurrent multiscale coupling in Sandia ***production codes*** (Sierra Solid Mechanics), comparison to other methods (e.g., GFEM).
- Development of a ***multi-physics coupling framework*** based on variational formulations and the Schwarz alternating method.

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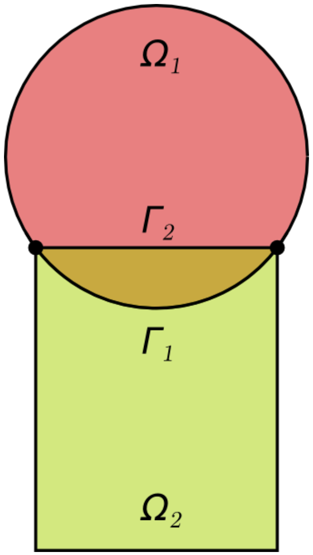

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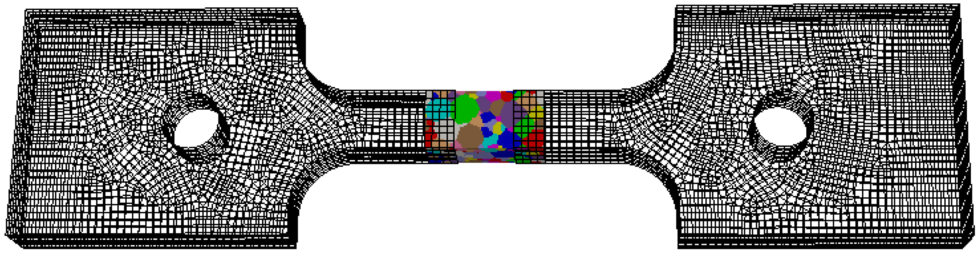

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[5] S. Mikhlin. "On the Schwarz algorithm". In: Proceedings of the USSR Academy of Sciences (in Russian) 77 (1951), pp. 569–571.

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[8] A. Mota, **I. Tezaur**, C. Alleman. "The Schwarz Alternating Method in Solid Mechanics", *Comput. Meth. Appl. Mech. Engng.* 319 (2017), 19-51. [http://www.sandia.gov/~ikalash/journal.html].

[9] A. Mota, **I. Tezaur**. "The Schwarz alternating method for dynamic solid mechanics", in preparation for submission to *Comput. Meth. Appl. Mech. Engng.*

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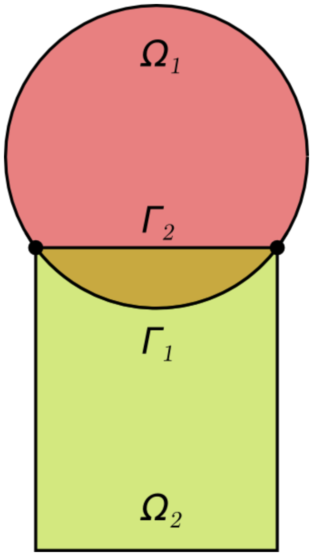

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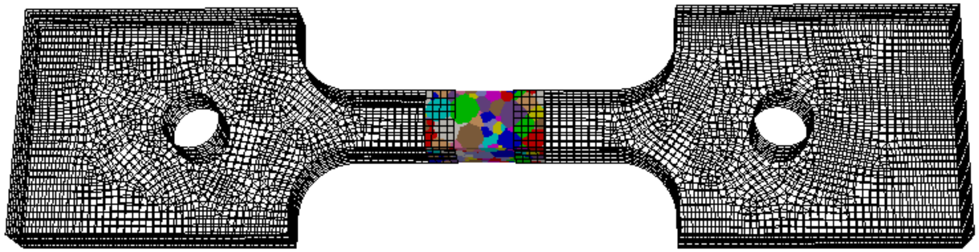

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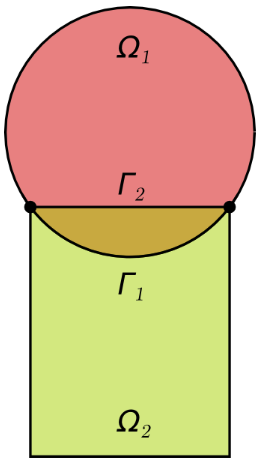
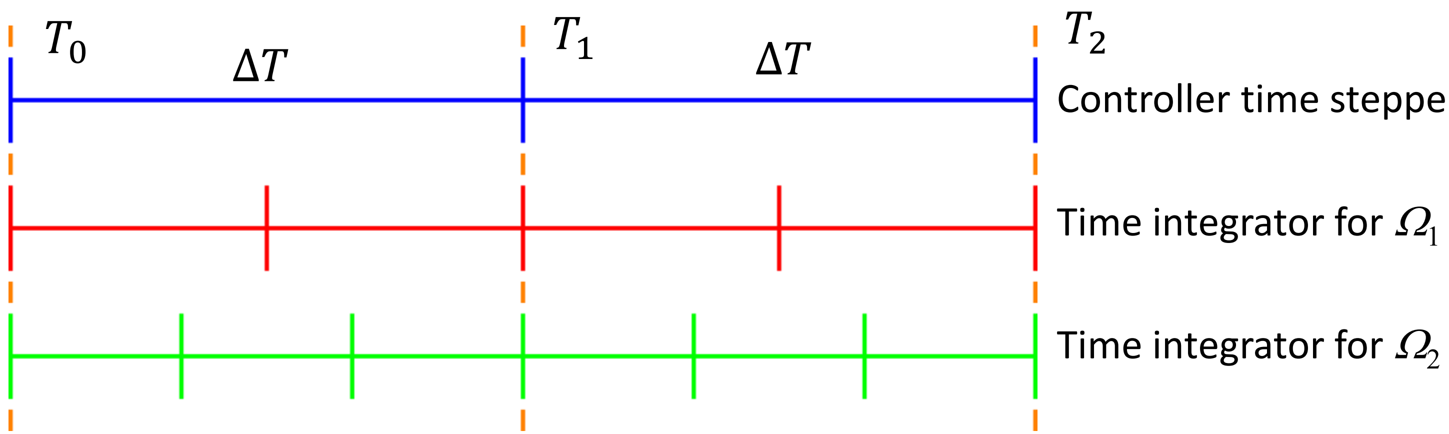
Appendix. Schwarz Alternating Method for Dynamic Multiscale Coupling

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





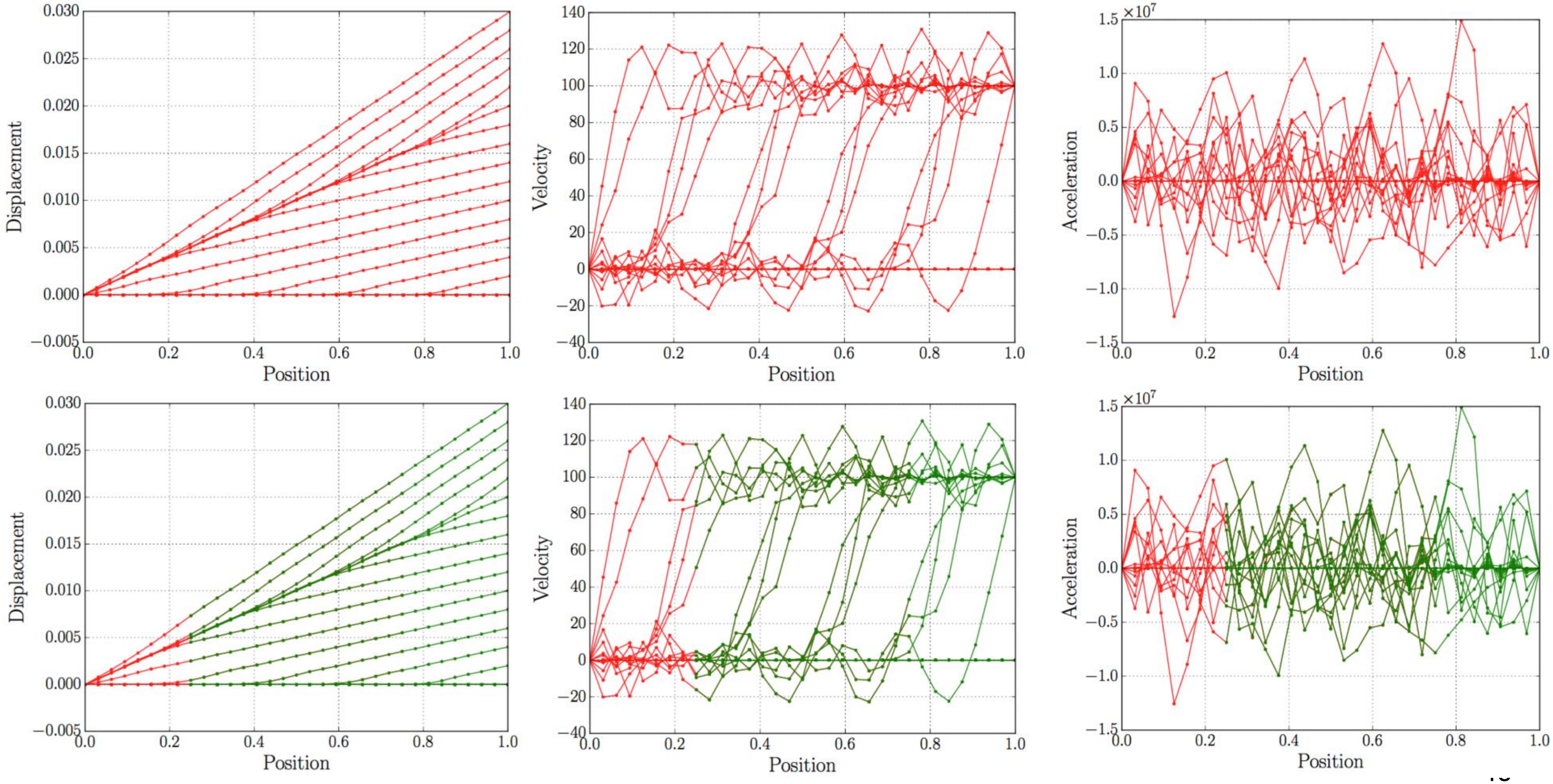
Can use ***different integrators*** with ***different time steps*** within each domain (w/o space-time discretization)!

Ingredients:

- Controller time step $\Delta T \Rightarrow T_0 + n\Delta T$ are times at which Schwarz is synchronized
  - Convenient checkpoint to facilitate implementation
- Discretization + time-integrator for Ω_1 with time-step Δt_1 (divides ΔT)
- Discretization + time-integrator for Ω_2 with time-step Δt_2 (divides ΔT)

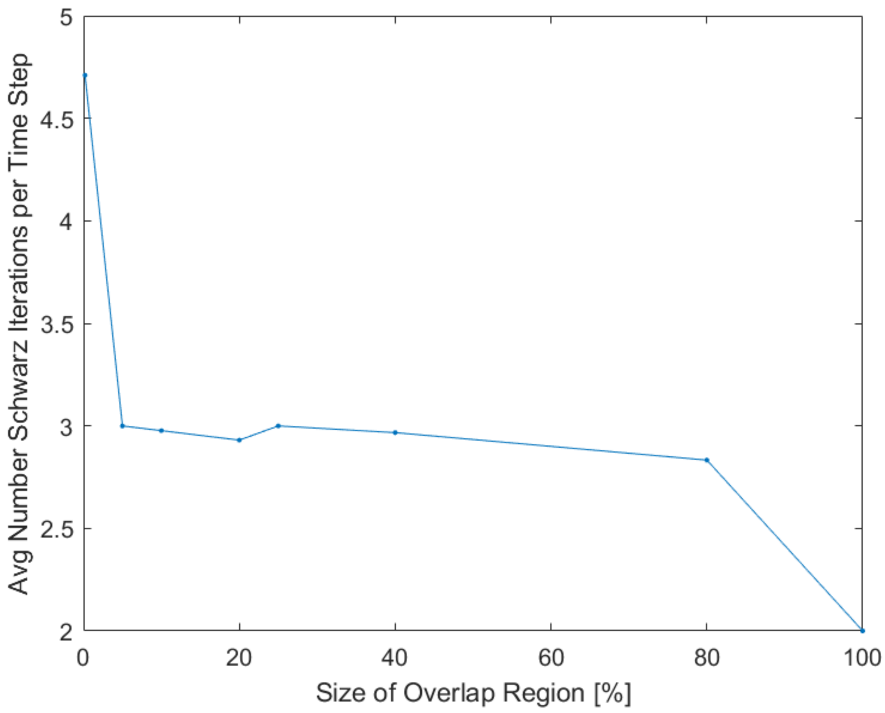
Appendix. Dynamic Singular Bar (MATLAB)

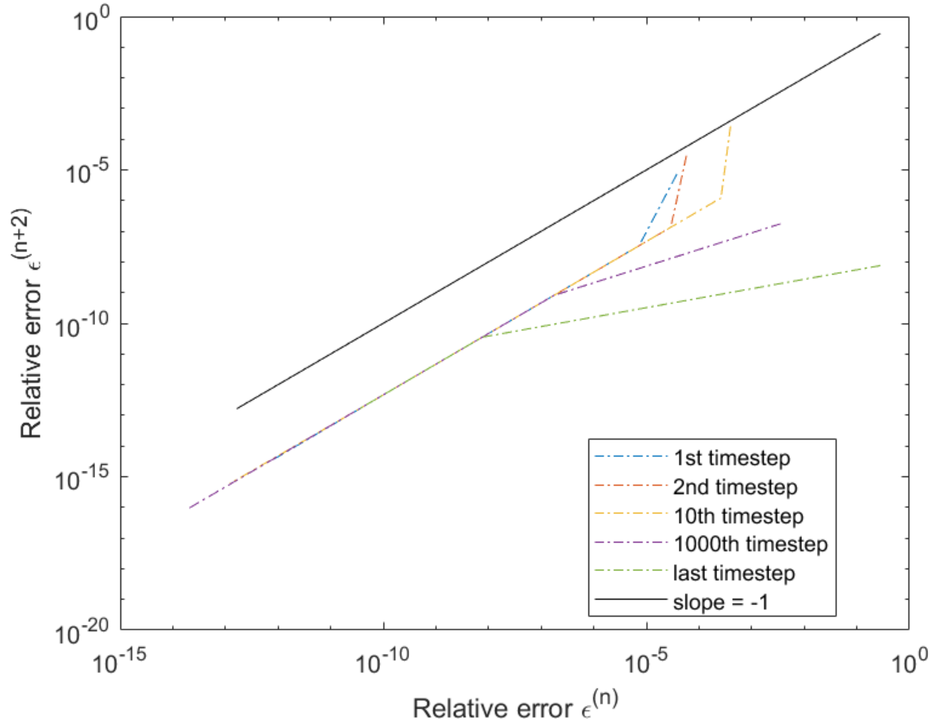
- Inelasticity masks problems by introducing energy dissipation.
- Schwarz does not introduce numerical artifacts.
- Can couple domains with different time integration schemes (Explicit-Implicit below).



Appendix. Example #1: Elastic Wave

Some Performance Results

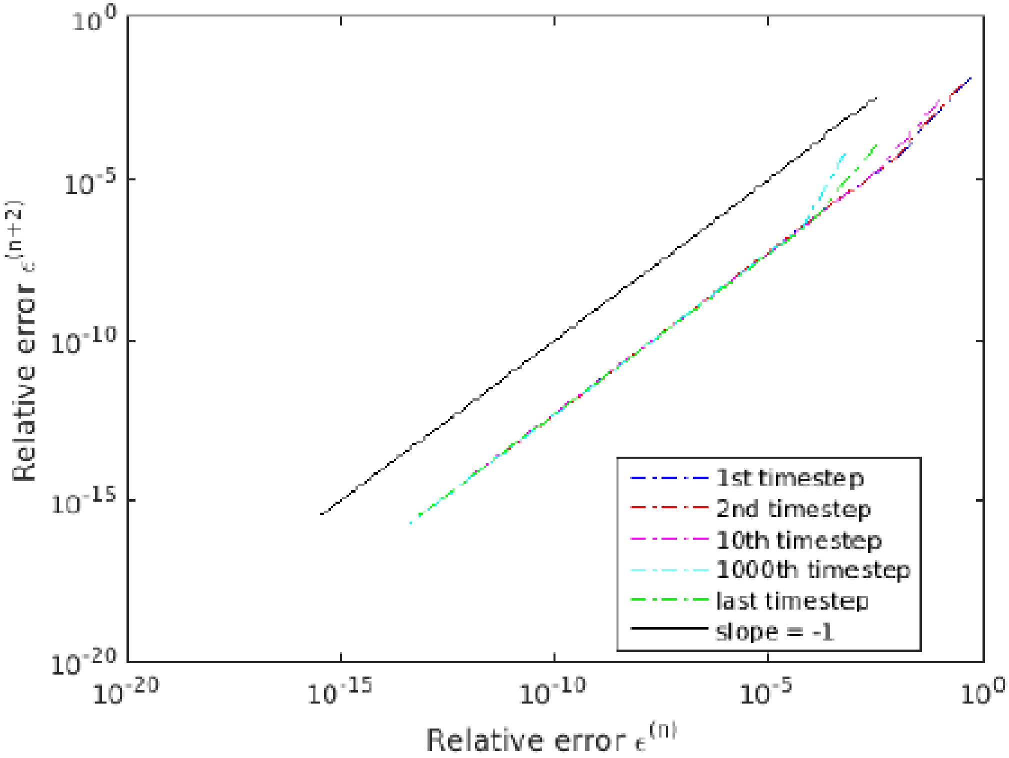




- Left figure shows ***# of iterations*** as a function of ***overlap region size*** for 2 subdomains. The method does not converge for 0% overlap. If the overlap is 100% then the single-domain solution is recovered for each of the subdomains.
- Right figure shows ***linear convergence rate*** of dynamic Schwarz implementation (for small overlap fraction of 0.2%).

Appendix. Example #2: Torsion

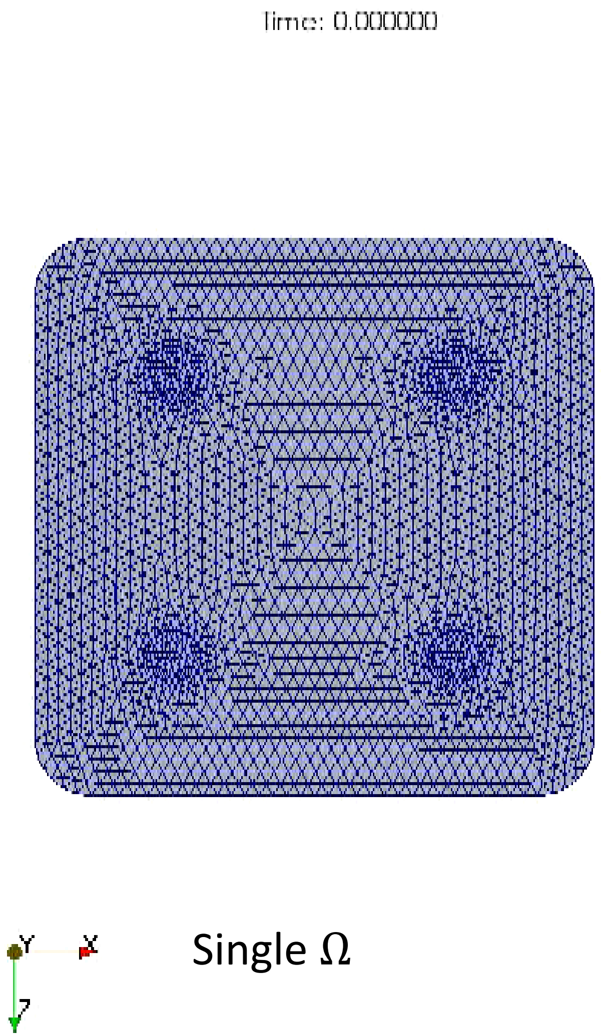
Some Performance Results



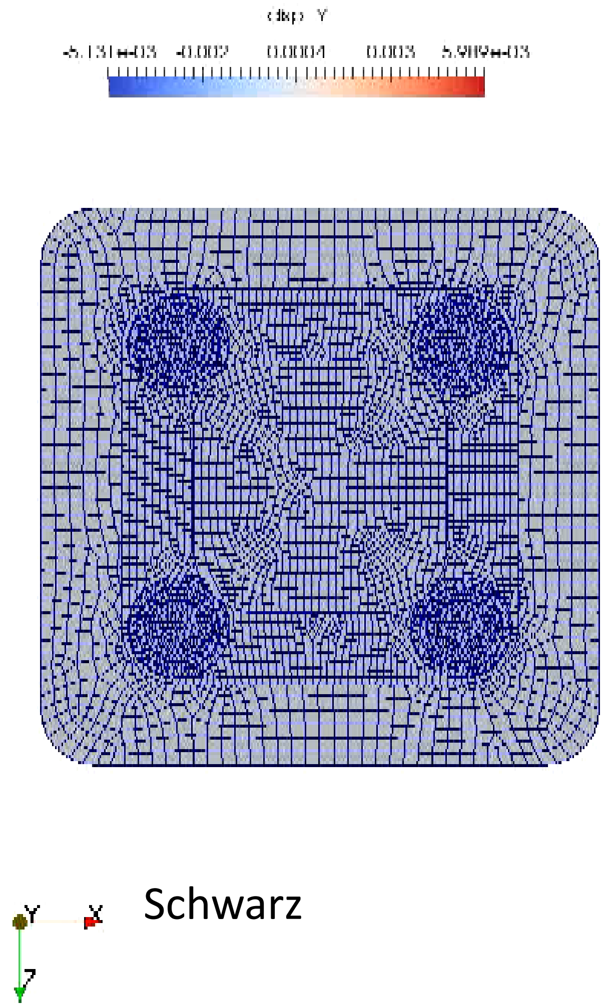
- Convergence behavior of the dynamic Schwarz algorithm for the torsion problem for small overlap volume fraction (2%) in which each subdomain is discretized using a hexahedral mesh. The plot shows that a ***linear convergence rate*** is achieved.

Appendix. Example #4: Bolted Joint Problem

y-displacement



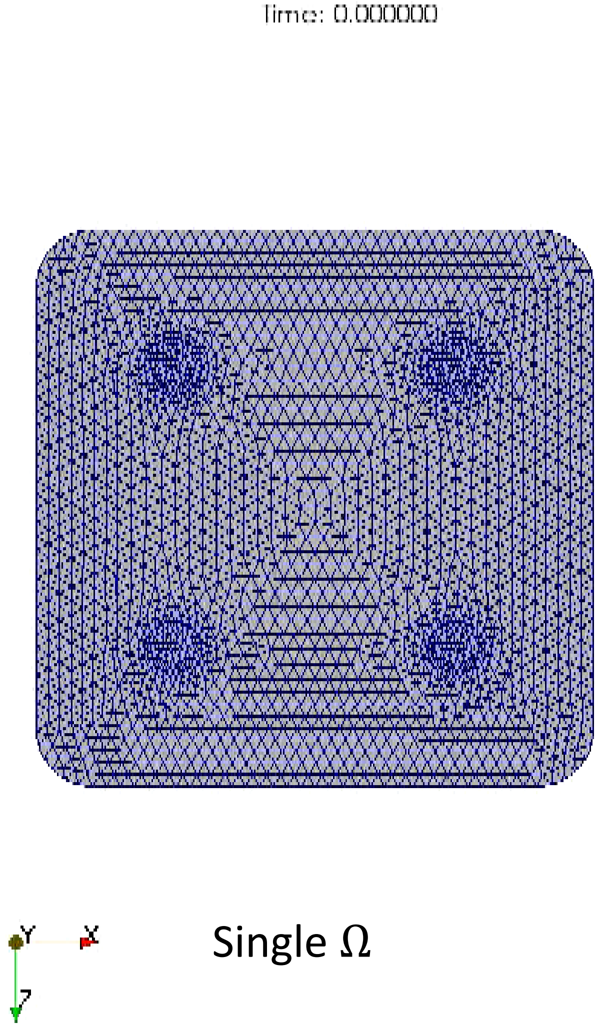
Single Ω



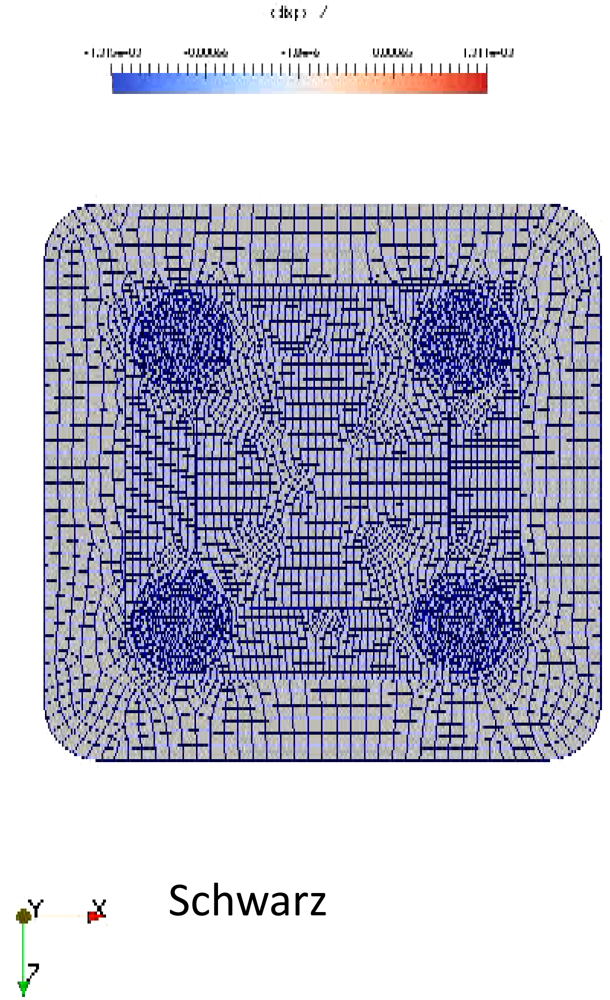
Schwarz

Appendix. Example #4: Bolted Joint Problem

z-displacement



Single Ω



Schwarz