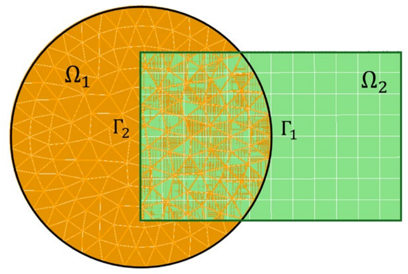
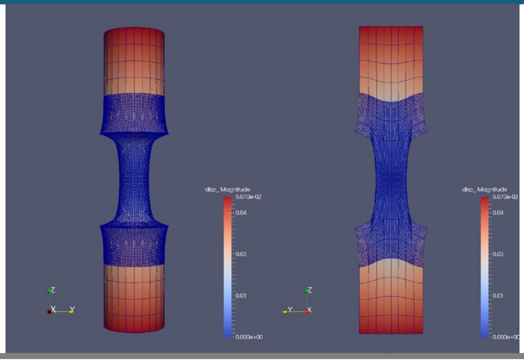
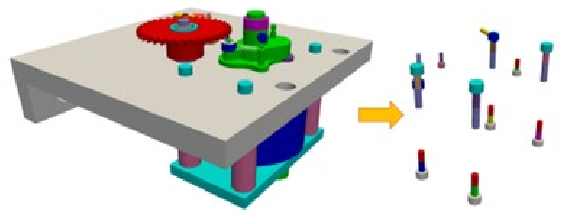
Accelerating modeling and simulation workflows via the Schwarz alternating method for multiscale coupling and contact







Irina Tezaur

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SAND2025-13500C

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Team & Acknowledgements (Over Almost 11 Years!)


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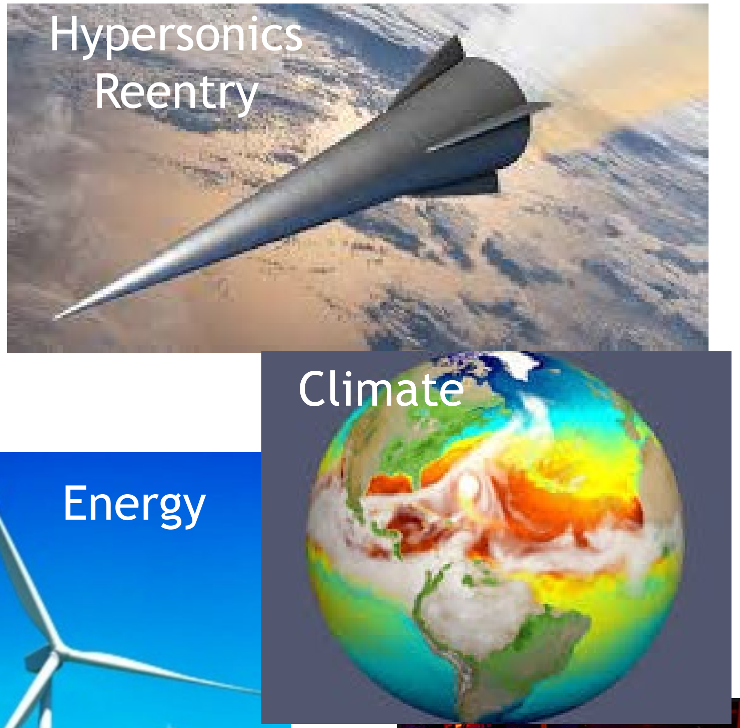

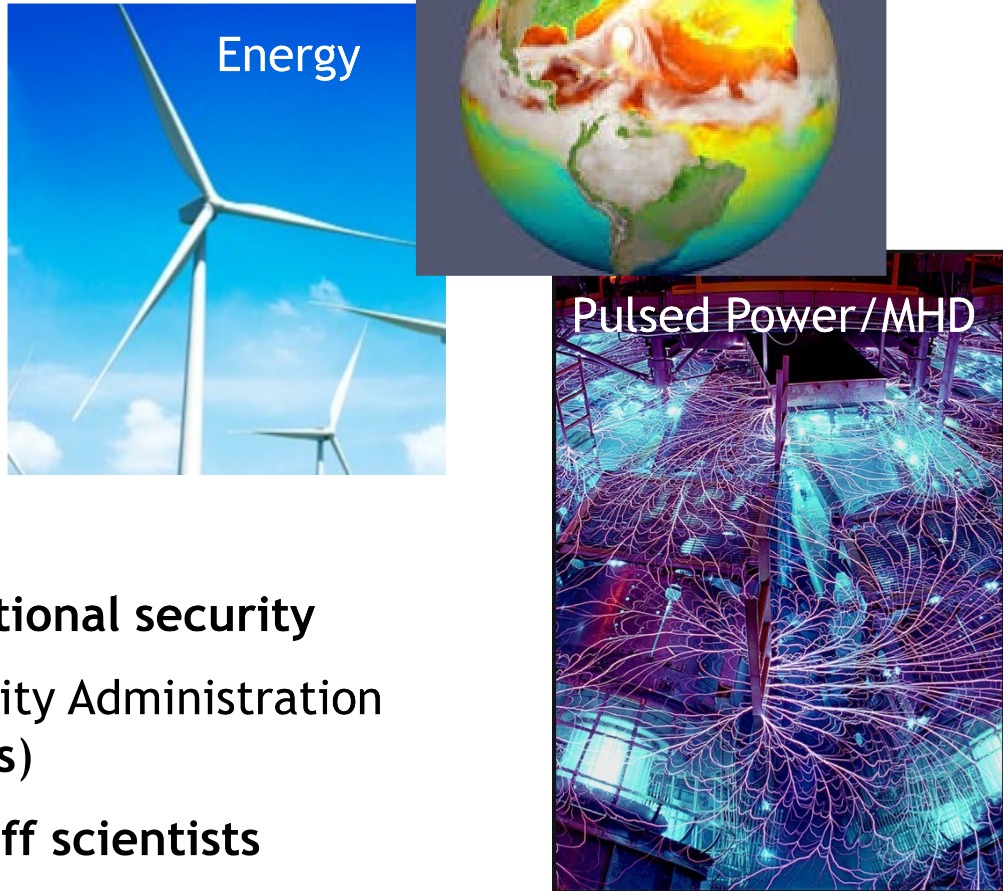

- Sandia is a **multi-mission** national lab aimed at advancing **U.S. national security**
- 1 of 3 U.S. Department of Energy's (**DOE's**) National Nuclear Security Administration (**NNSA**) R&D labs (along with **Lawrence Livermore** and **Los Alamos**)
- **Two main sites** (Albuquerque, NM and Livermore, CA), **17,000 staff scientists**

Outline

Fundamental **method development** in a **mission-**

1. Schwarz Alternating Method (SAM) for Coupling of Full Order Models (FOMs) in Solid Mechanics
   - Motivation & Background
   - Formulation
   - Numerical Examples
2. SAM for FOM-ROM* and ROM-ROM Coupling in Solid Mechanics
   - Motivation & Background
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   - Numerical Examples
3. SAM as a Novel Contact Enforcement Metho
   - Motivation & Background
   - Formulation
   - Numerical Examples
4. Summary

Outline

Insights, lessons learned, practical

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Motivation for Coupling in Solid Mechanics

Concurrent multiscale coupling for predicting failure

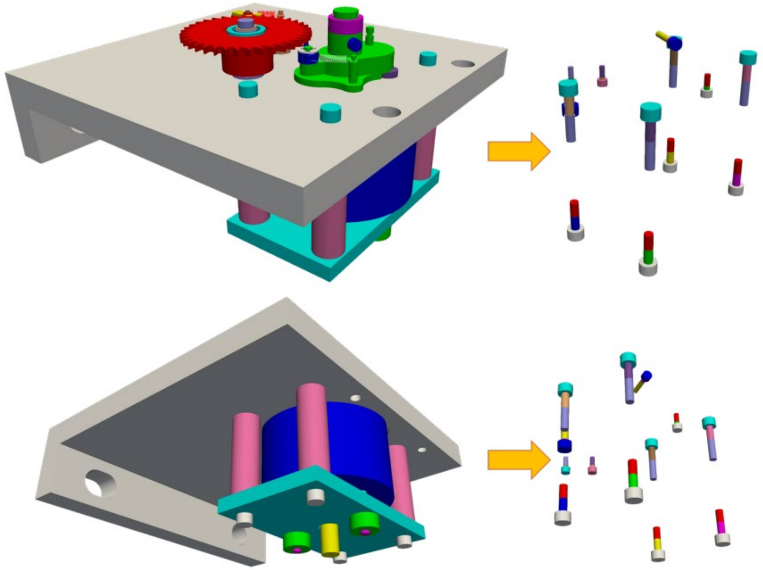
- ***Large scale*** structural ***failure*** frequently originates from ***small scale*** phenomena such as defects, microcracks, inhomogeneities and more, which grow quickly in unstable manner
- Failure occurs due to ***tightly coupled interaction*** between small scale (stress concentrations, material 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 [mod/sim] analyses" [Sandia Lab News, 2020]!

Goal: 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.

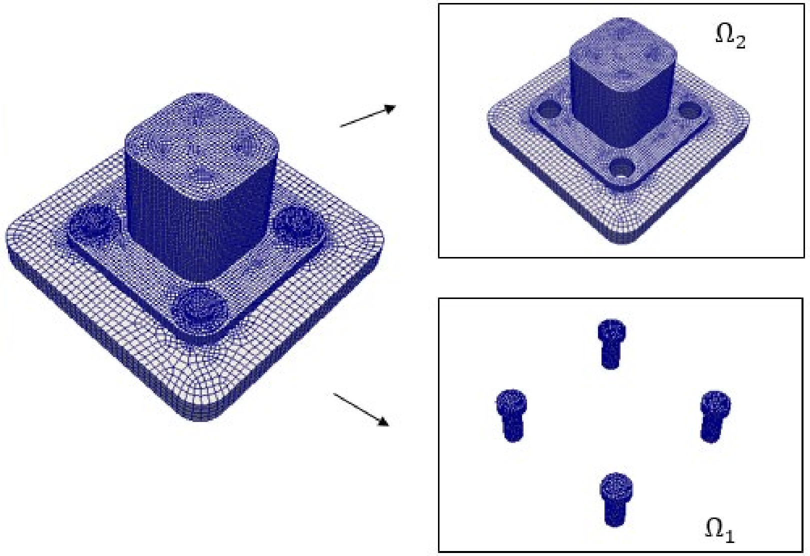
Roof failure of Boeing 737 aircraft due to fatigue cracks. From *imechanica.org*.



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)
- ***"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
- ***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!)
- Coupling does not introduce ***nonphysical artifacts***
- ***Theoretical*** convergence properties/ guarantees



Requirements for Multiscale Coupling Method

A great method theoretically may not make it if it is too difficult to implement in production codes.*

- Coupling is ***concurrent*** (two-way)
- ***"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***
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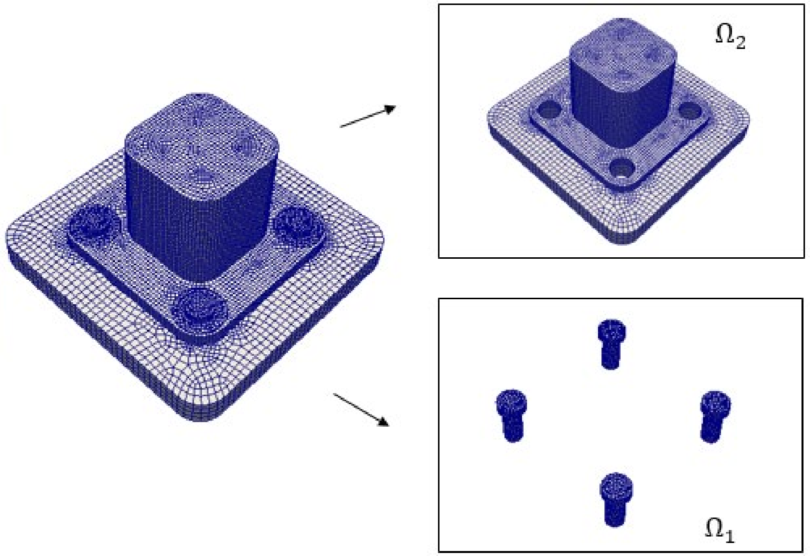

* W. Sun, A. Mota. "A multiscale overlapped coupling formulation for large-deformation strain localization", *Comp. Mech.* 2014.

Requirements for Multiscale Coupling Method

Our customers are most excited about the Schwarz method's potential to simplify meshing.

- Coupling is ***concurrent*** (two-way)
- ***"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
- ***Ease of implementation*** into existing massively-parallel HPC codes
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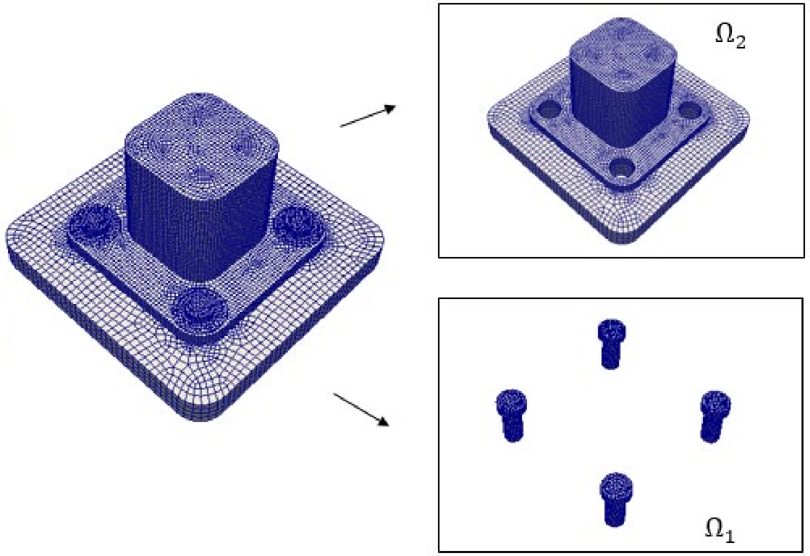

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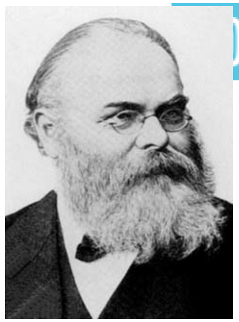
Schwarz Alternating Method for Domain Decomposition (DD)



H. Schwarz
(1843-1921)

- 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

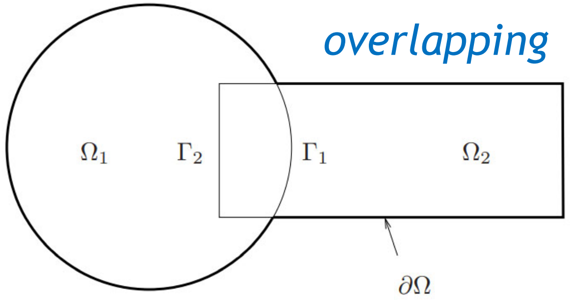
Initialize:

- Solve PDE by any method on Ω_1 w/ initial guess for transmission boundary conditions (BCs) on Γ_1.

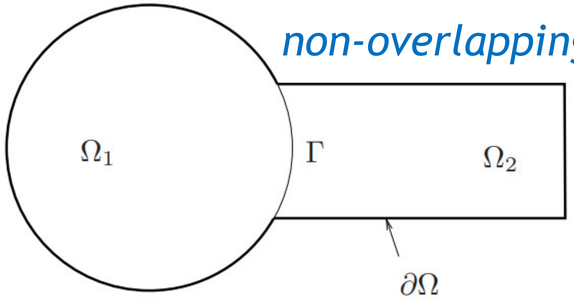
Iterate until convergence:

- Solve PDE by any method in Ω_2 w/ BCs on Γ_2 from just-obtained Ω_1 solution.
- Solve PDE by any method in Ω_1 w/ BCs on Γ_1 from just-obtained Ω_2 solution.

overlapping



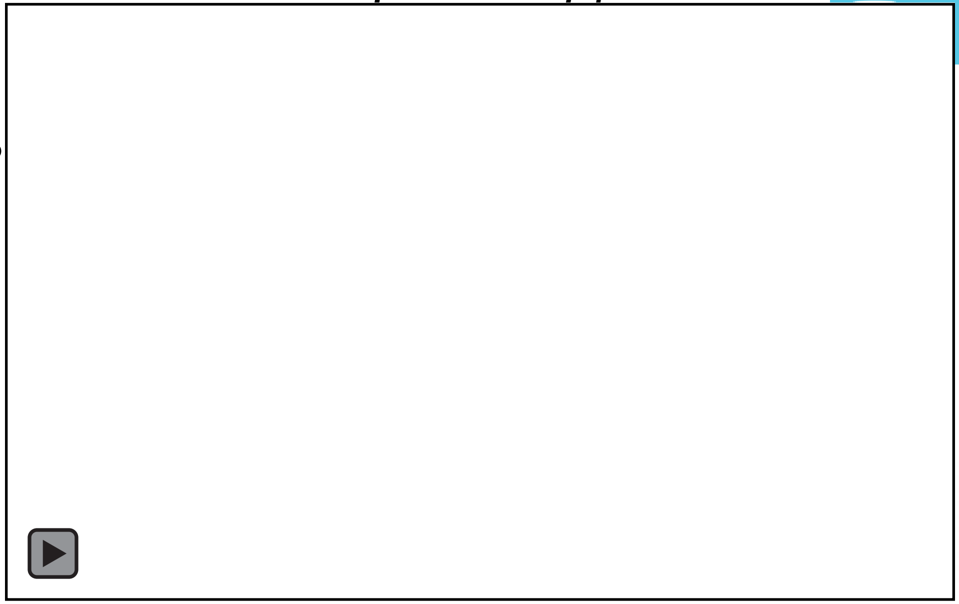
non-overlapping



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

<u>Idea behind this work</u>: using the Schwarz alternating method as a ***discretization method*** for solving multiscale or multiphysics partial differential equations (PDEs).

Quasistatic Solid Mechanics Formulation



- **Energy functional** defining weak form of the governing PDEs

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

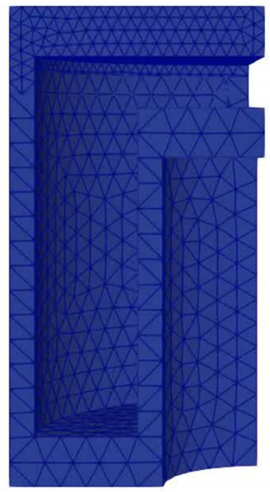
  - $A(\boldsymbol{F}, \boldsymbol{Z})$: Helmholtz free-energy density
  - $\boldsymbol{F} := \nabla \boldsymbol{\varphi}$: deformation gradient
  - $\boldsymbol{Z}$: collection of internal variables (for plastic materials)
  - ρ: density, $\boldsymbol{B}$: body force, $\boldsymbol{P} = \partial A / \partial \boldsymbol{F}$: Piola-Kirchhoff stress

- **Euler-Lagrange equations**, obtained by minimizing $\Phi[\boldsymbol{\varphi}]$: $\begin{cases} \mathrm{Div}\, \boldsymbol{P} + \rho \boldsymbol{B} = \boldsymbol{0}, & \text{in } \Omega \\ \boldsymbol{\varphi} = \boldsymbol{\chi}, & \text{on } \partial\Omega \end{cases}$

- Quasistatics solves **sequence of problems** in which loading (body force) $\boldsymbol{B}$ is incremented **quasistatically** w.r.t. **pseudo time** t_i:

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

Pressure vessel



Spatial Coupling via (Multiplicative) Alternating Schwarz

Model PDE:

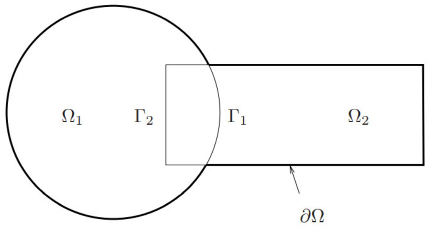
$$\begin{cases} \text{Div}\, \boldsymbol{P} + \rho \boldsymbol{B} = \boldsymbol{0}\ , \text{ in } \Omega \\ \boldsymbol{\varphi} = \boldsymbol{\chi}, \quad \text{on } \partial\Omega \end{cases}$$

Overlapping Domain Decomposition

$$\begin{cases} \text{Div}\, \boldsymbol{P}_1^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\ , \text{ in } \Omega_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\chi}, \quad \text{on } \partial\Omega_1 \backslash \Gamma_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\varphi}_2^{(n)} \quad \text{on } \Gamma_2 \end{cases}$$

$$\begin{cases} \text{Div}\, \boldsymbol{P}_2^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\ , \text{ in } \Omega_2 \\ \boldsymbol{\varphi}_2^{(n+1)} = \boldsymbol{\chi}, \quad \text{on } \partial\Omega_2 \backslash \Gamma_2 \\ \boldsymbol{\varphi}_2^{(n+1)} = \boldsymbol{\varphi}_1^{(n+1)} \quad \text{on } \Gamma_2 \end{cases}$$

*Easier **implementation** and **faster convergence***



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

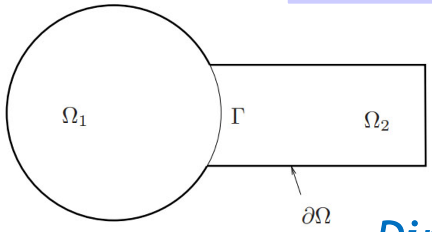
Non-overlapping Domain Decomposition

$$\begin{cases} \text{Div}\, \boldsymbol{P}_1^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\ , \text{ in } \Omega_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\chi}, \quad \text{on } \partial\Omega_1 \backslash \Gamma \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\lambda}_{n+1} \quad \text{on } \Gamma \end{cases}$$

$$\begin{cases} \text{Div}\, \boldsymbol{P}_2^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\ , \text{ in } \Omega_2 \\ \boldsymbol{\varphi}_2^{(n+1)} = \boldsymbol{\chi}, \quad \text{on } \partial\Omega_2 \backslash \Gamma \\ \boldsymbol{P}_2^{(n+1)} \boldsymbol{n} = \boldsymbol{P}_1^{(n+1)} \boldsymbol{n}, \quad \text{on } \Gamma \end{cases}$$

$$\boldsymbol{\lambda}_{n+1} = \theta \boldsymbol{\varphi}_2^{(n)} + (1-\theta)\boldsymbol{\lambda}_n, \text{on } \Gamma, \text{for } n \geq 1$$

*More **flexible** but **slower** to converge*



Dirichlet-Neumann variant preferred since BCs are readily available in SM codes

- 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)

Additional Parallelism via Additive Schwarz

This talk

Multiplicative Overlapping Schwarz

$$\begin{cases} \text{Div } \boldsymbol{P}_1^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\ , & \text{in } \Omega_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\chi}, & \text{on } \partial\Omega_1 \backslash \Gamma_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\varphi}_2^{(n)} & \text{on } \Gamma_2 \end{cases}$$

$$\begin{cases} \text{Div } \boldsymbol{P}_2^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\ , & \text{in } \Omega_2 \\ \boldsymbol{\varphi}_2^{(n+1)} = \boldsymbol{\chi}, & \text{on } \partial\Omega_2 \backslash \Gamma_2 \\ \boldsymbol{\varphi}_2^{(n+1)} = \boldsymbol{\varphi}_1^{(n+1)} & \text{on } \Gamma_2 \end{cases}$$

Additive Overlapping Schwarz

$$\begin{cases} \text{Div } \boldsymbol{P}_1^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\ , & \text{in } \Omega_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\chi}, & \text{on } \partial\Omega_1 \backslash \Gamma_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\varphi}_2^{(n)} & \text{on } \Gamma_2 \end{cases}$$

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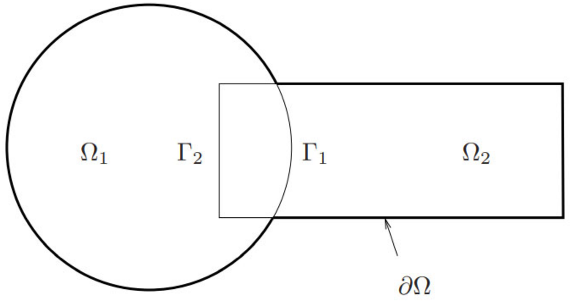
Model PDE:

$$\begin{cases} \text{Div } \boldsymbol{P} + \rho \boldsymbol{B} = \boldsymbol{0}\ , & \text{in } \Omega \\ \boldsymbol{\varphi} = \boldsymbol{\chi}, & \text{on } \partial\Omega \end{cases}$$

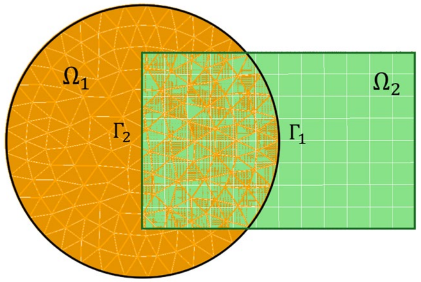


- **Multiplicative Schwarz:** solves subdomain problems **sequentially** (in serial)
- **Additive Schwarz:** advance subdomains in **parallel**, communicate boundary condition data later
  - Typically requires a few more **Schwarz iterations**, but does not degrade **accuracy**
  - **Parallelism** helps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

Overlapping Schwarz Coupling in Quasistatics

outer quasistatic loop

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

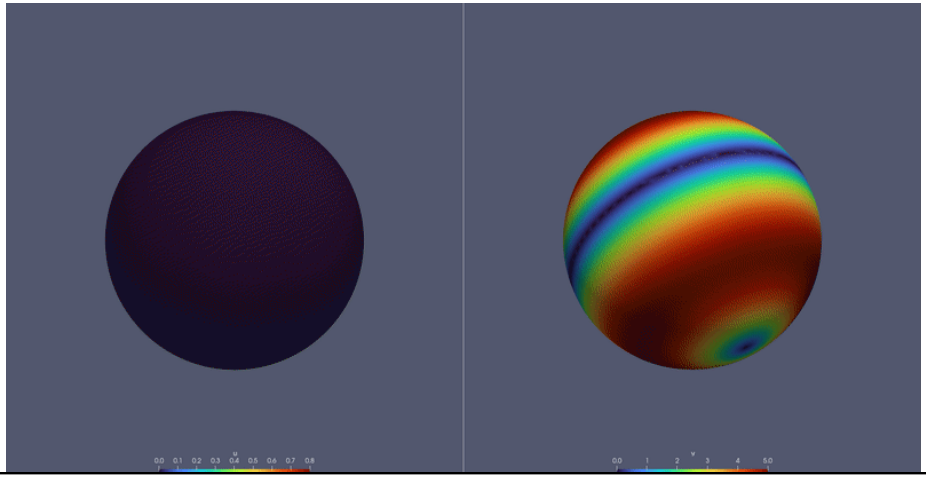


Advantages:

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

Solid Dynamics Formulation

Large-deformation vibration of a soft rubber ball



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

- 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: $S[\boldsymbol{\varphi}] \coloneqq \int_{I} L(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}})\, dt$

- Euler-Lagrange equations: $\begin{cases} \mathrm{Div}\,\boldsymbol{P} + \rho\boldsymbol{B} = \rho\ddot{\boldsymbol{\varphi}}, \\ \boldsymbol{\varphi}(\boldsymbol{X},t_0) = \boldsymbol{x}_0, \\ \dot{\boldsymbol{\varphi}}(\boldsymbol{X},t_0) = \boldsymbol{v}_0, \\ \boldsymbol{\varphi}(\boldsymbol{X},t) = \boldsymbol{\chi}, \end{cases}$

- Semi-discrete problem following FEM discretizati

$$\boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{f}_{\text{int}}(\boldsymbol{u}) = \boldsymbol{f}$$

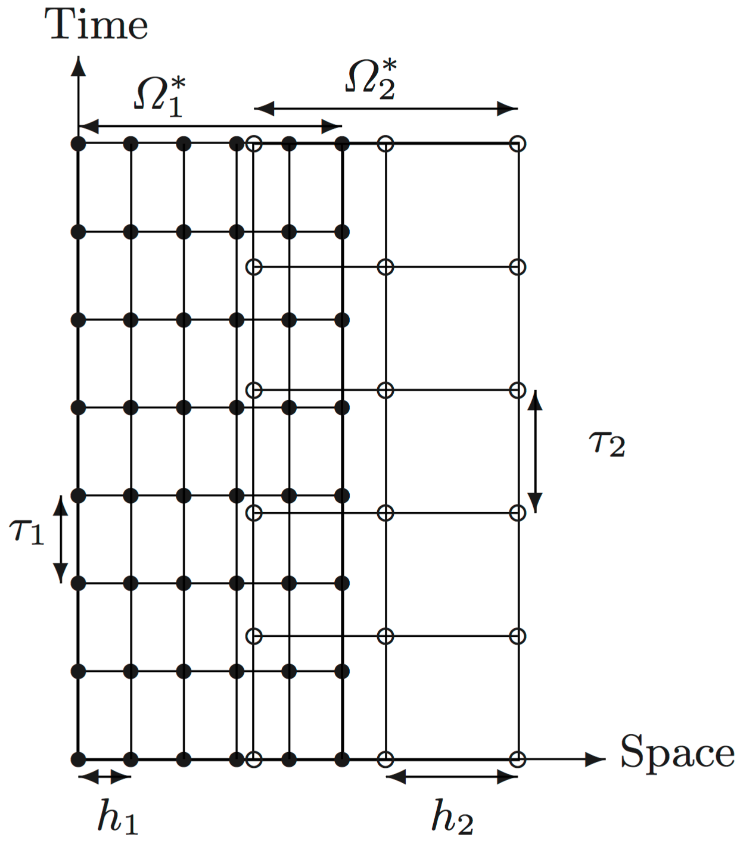
How to Apply Schwarz to Dynamics?

- 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).

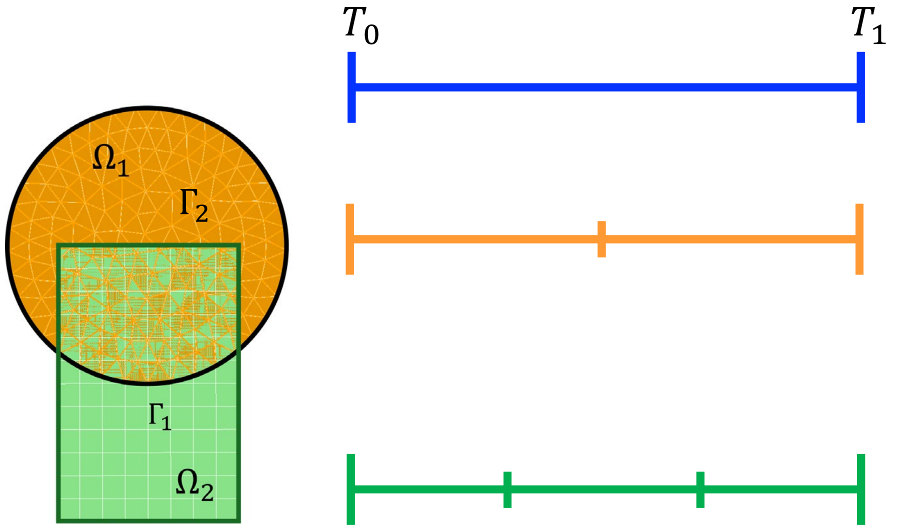
Con ☹: ***Unfeasible*** given the design of our current codes and size of simulations.

Ease of implementation is a very important requirement!



Overlapping non-matching meshes and time steps in dynamics.

Time-Advancement within the Schwarz Framework



Controller time stepper

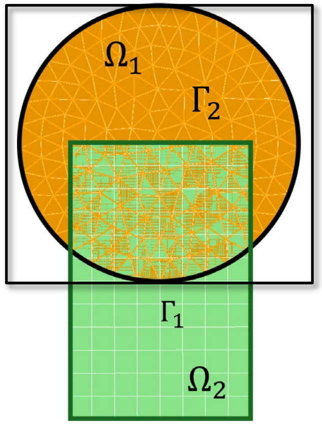
Time integrator in Ω_1

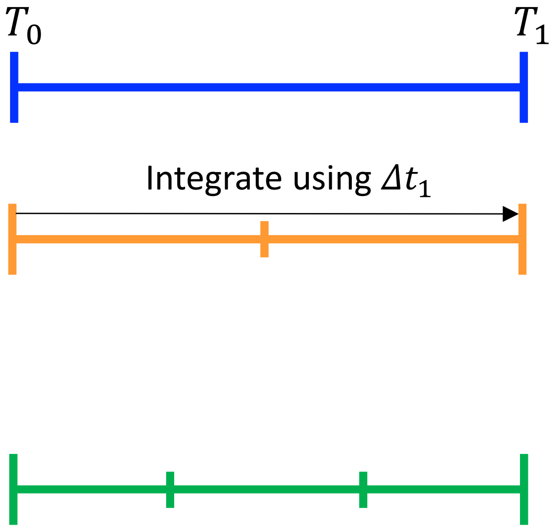
Time integrator in Ω_2

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

Model PDE: $\begin{cases} \boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{f}_{\text{int}}(\boldsymbol{u}, \dot{\boldsymbol{u}}) = \boldsymbol{f}_{\text{ext}} \\ \boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0 \end{cases}$

Time-Advancement within the Schwarz Framework





Controller time stepper

Time integrator in Ω_1

Time integrator in Ω_2

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

Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ_1 at times $T_i + n\Delta t_1$.

Model PDE: $\begin{cases} \boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{f}_{\text{int}}(\boldsymbol{u}, \dot{\boldsymbol{u}}) = \boldsymbol{f}_{\text{ext}} \\ \boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0 \end{cases}$

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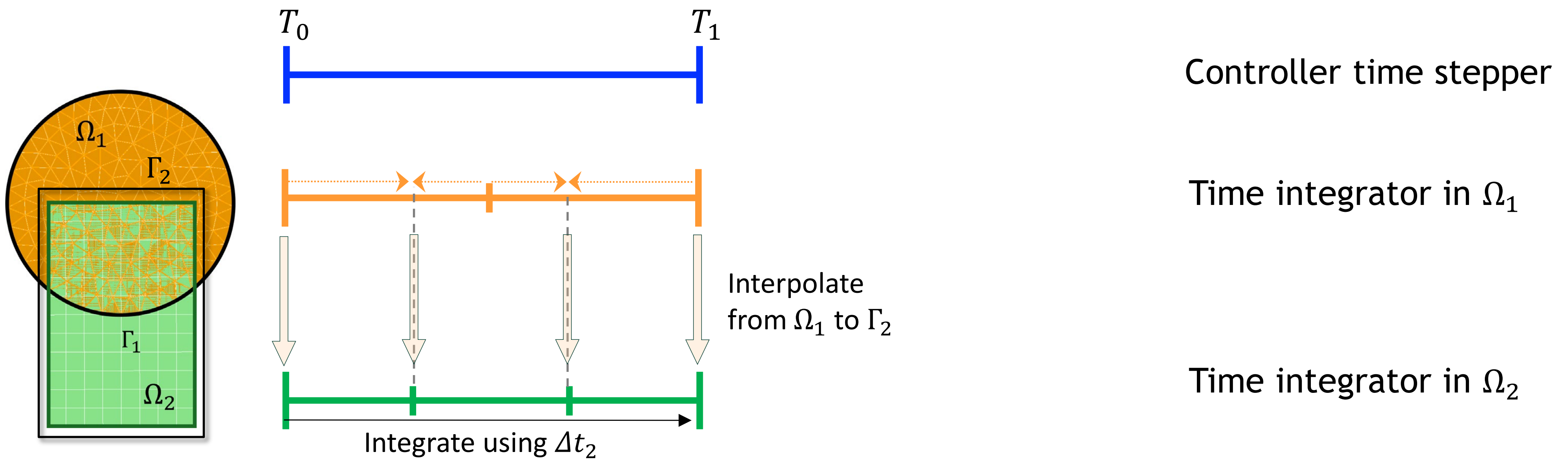

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Step 2: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ_2 at times $T_i + n\Delta t_2$.

.

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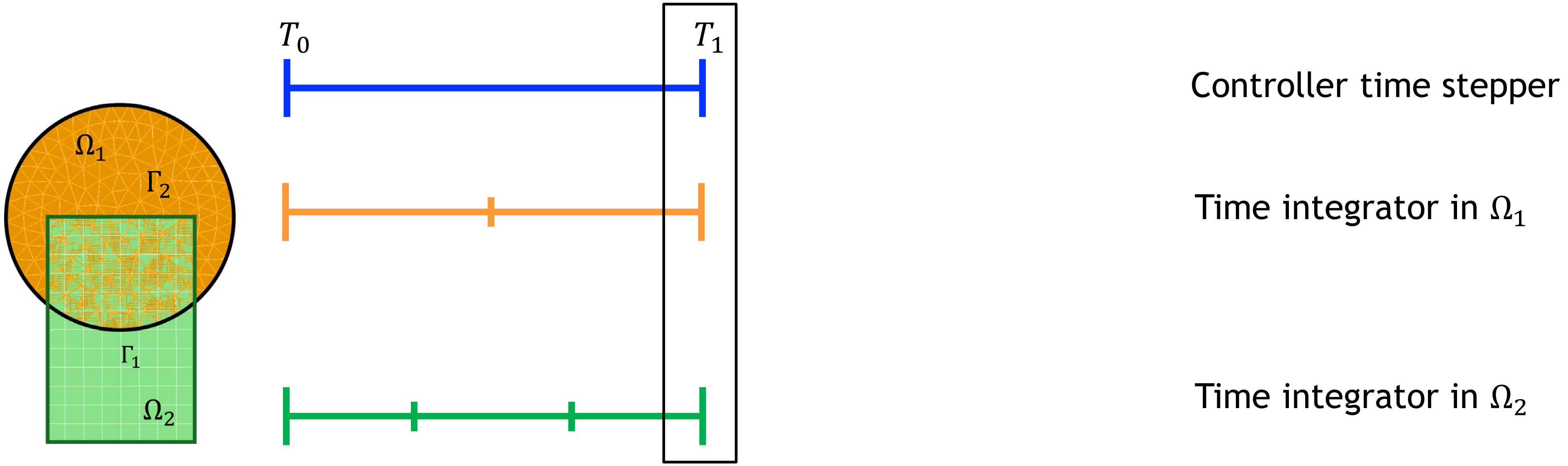

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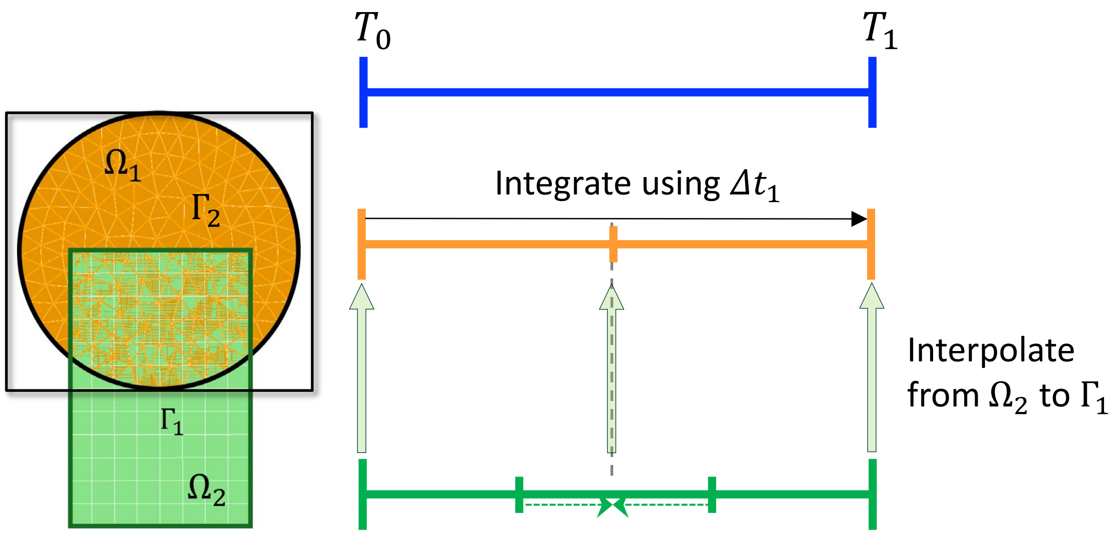
__Step 2__: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ_2 at times $T_i + n\Delta t_2$.

__Step 3__: Check for convergence at time T_{i+1}.

Model PDE: $\begin{cases} \boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{f}_{\text{int}}(\boldsymbol{u}, \dot{\boldsymbol{u}}) = \boldsymbol{f}_{\text{ext}} \\ \boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0 \end{cases}$

Time-Advancement within the Schwarz Framework



Controller time stepper

Time integrator in Ω_1

Time integrator in Ω_2

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

Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ_1 at times $T_i + n\Delta t_1$.

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- If unconverged, return to Step 1.

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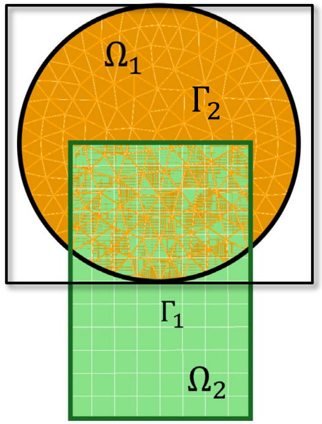
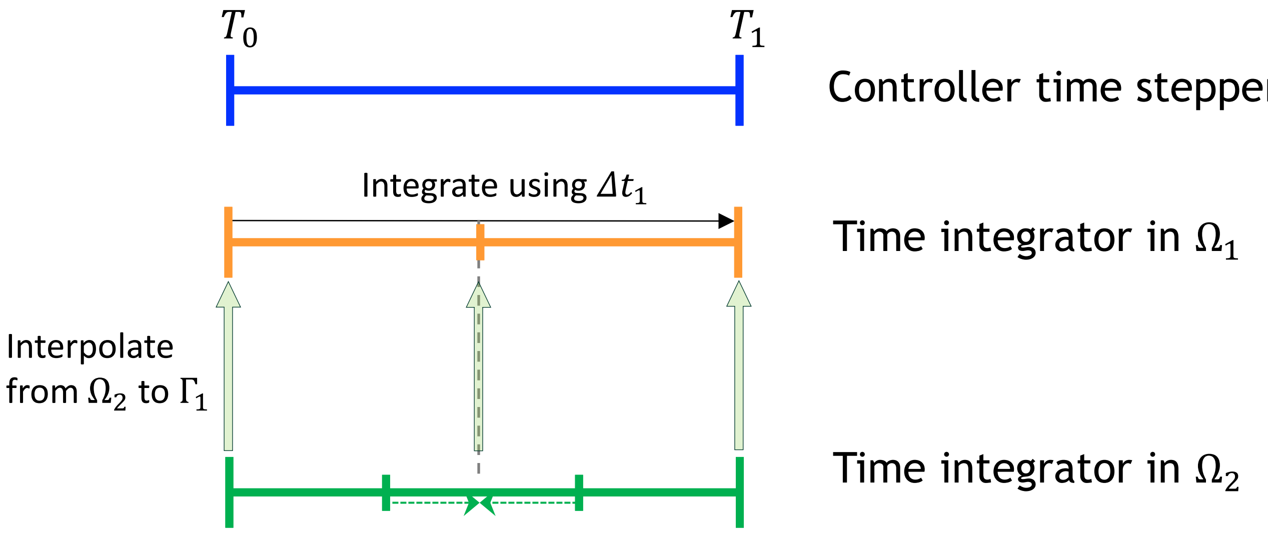
Time-Advancement within the Schwarz Framework





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

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

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

Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ_1 at times $T_i + n\Delta t_1$.

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Step 3: 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:
$$\begin{cases} \boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{f}_{\text{int}}(\boldsymbol{u}, \dot{\boldsymbol{u}}) = \boldsymbol{f}_{\text{ext}} \\ \boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0 \end{cases}$$

Outline

Insights, lessons learned, practical

1. **Schwarz Alternating Method (SAM) for Coupling Full Order Models (FOMs) in Solid Mechanics**
   - Motivation & Background
   - Formulation
   - **Numerical Examples**
2. SAM for FOM-ROM* and ROM-ROM Coupling in Solid Mechanics
   - Motivation & Background
   - Formulation
   - Numerical Examples
3. SAM as a Novel Contact Enforcement Metho
   - Motivation & Background
   - Formulation
   - Numerical Examples
4. Summary

From Prototyping to Production: Our Software Implementations of SAM

Exploration

Norma.jl is a Julia-based prototype for rapidly testing algorithms and ideas for domain coupling and contact in solid mechanics.

https://github.com/sandialabs/Norma.jl

HPC development

Albany-LCM (Laboratory for Computational Mechanics) is a research-grade, finite element code that targets multiphysics simulations on unstructured grids.

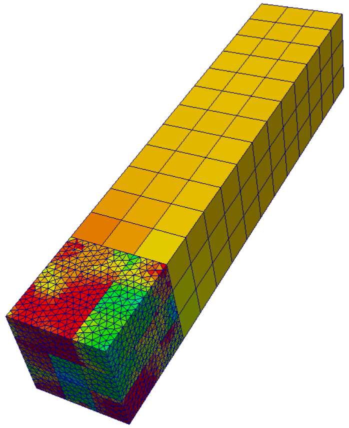
https://github.com/sandialabs/LCM

HPC production

SIERRA/Solid Mechanics (SM) is a 3D Lagrangian finite element code for static and dynamic analysis of solids and structures. It supports implicit and explicit time integration.

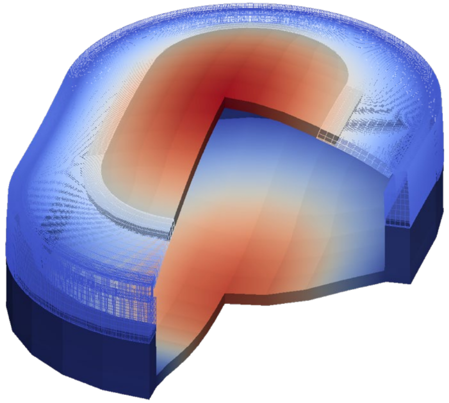
https://compsim.sandia.gov/adagio/index.html

From Prototyping to Production: Using the Schwarz Method

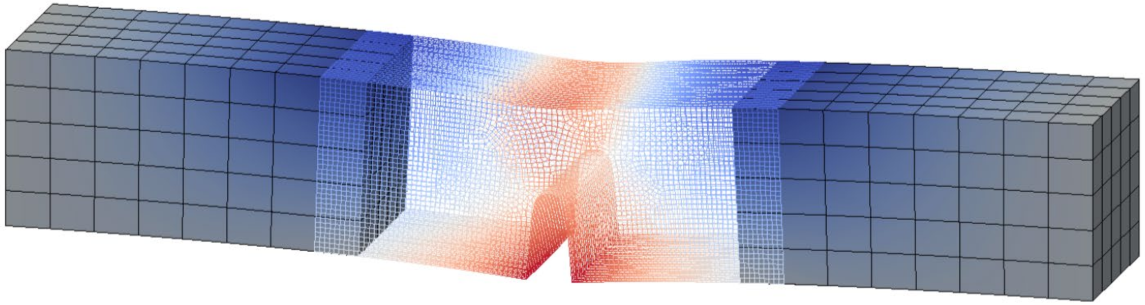


Rubik's Cube

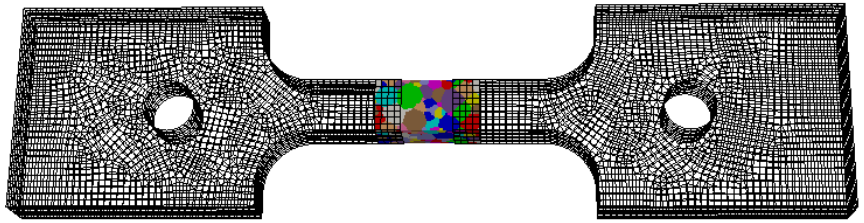
J. Foulk, D. Littlewood, C. Battaile, H. Lim



Tuna Can

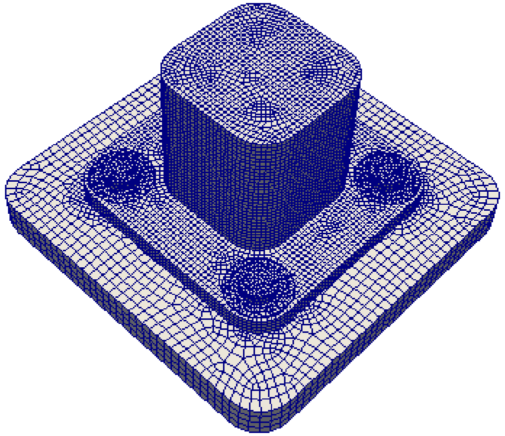


Laser Weld

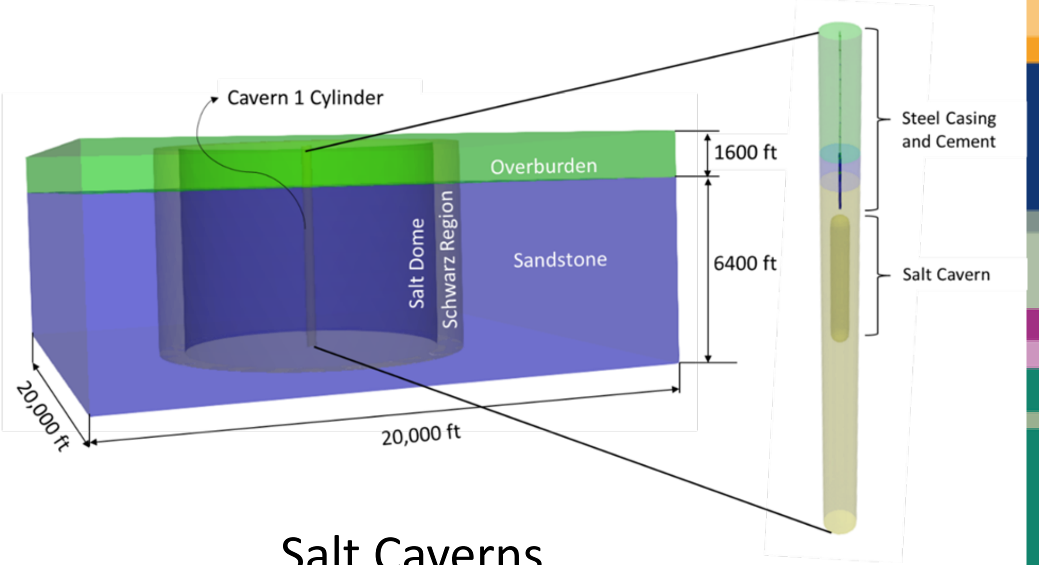


Tensile Bar

C. Alleman, J. Foulk, D. Littlewood, H. Lim, G. Bergel



Bolted Joint

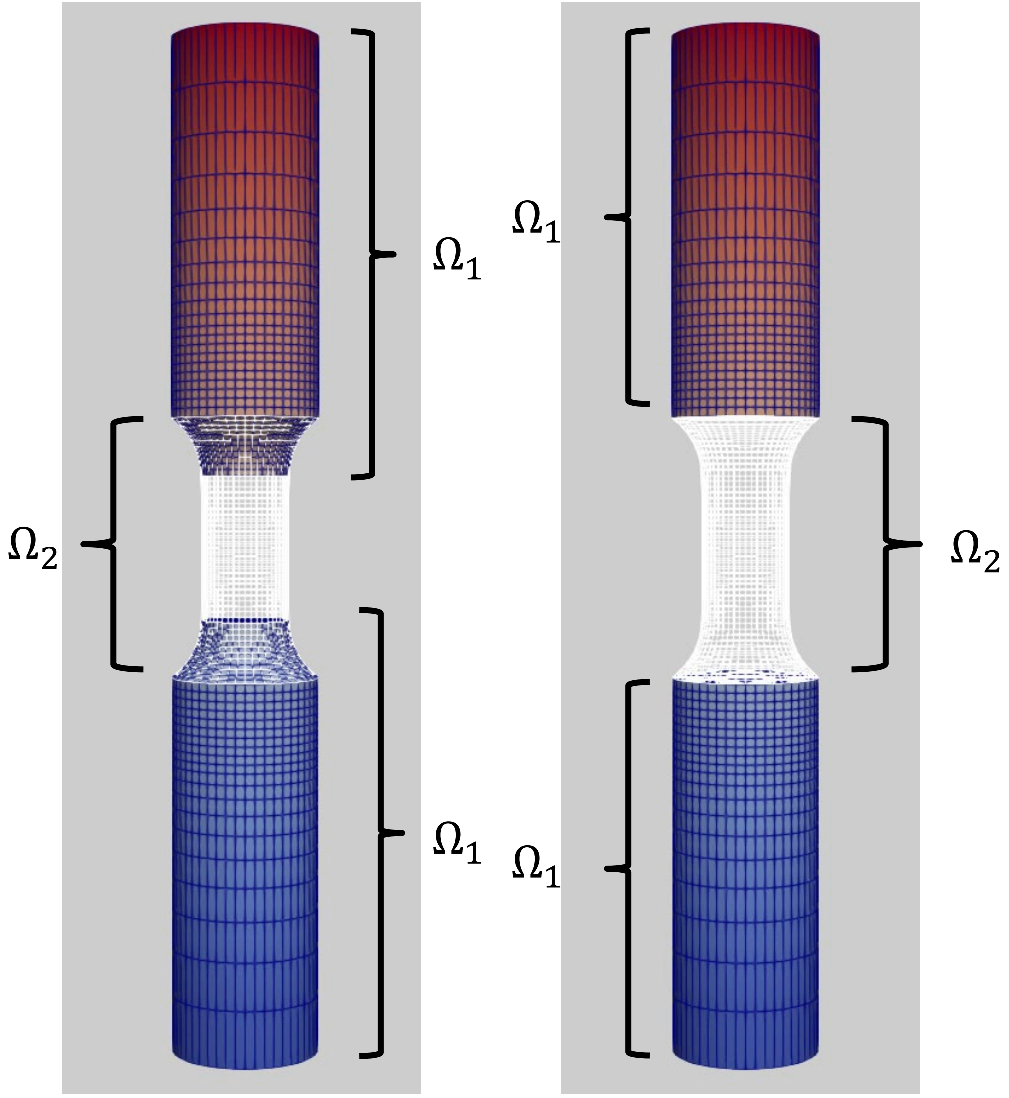


Salt Caverns

T. Ross

Tension Specimen (Overlapping & Non-Overlapping SAM)

- Uniaxial aluminum ***cylindrical tensile specimen*** with Sandia-internal ***plasticity model***, ***pulled*** from both ends
- Domain decomposition into ***two subdomains*** (right): Ω_1 = ends, Ω_2 = gauge.
- ***HEX8-HEX8*** coupling via ***overlapping*** and ***non-overlapping 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.



Overlap

Non-overlap

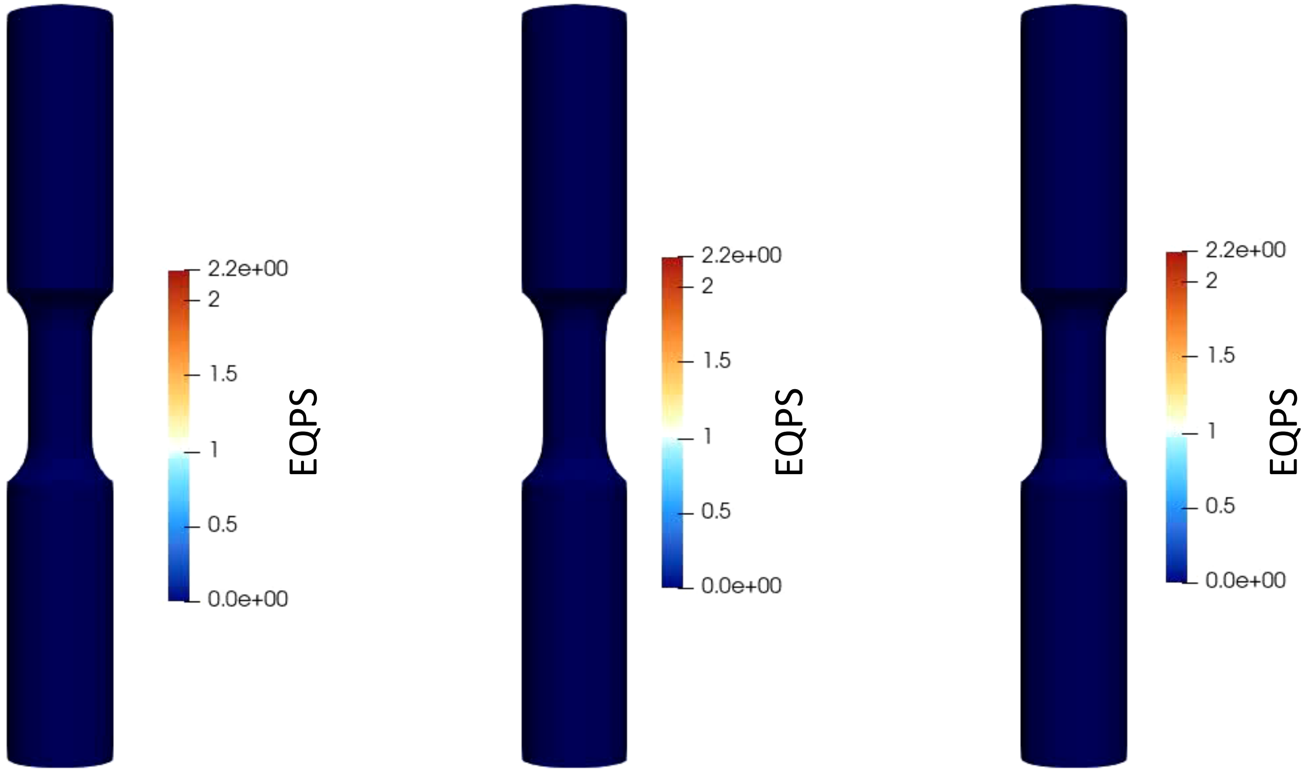
Tension Specimen: Equivalent Plastic Strain (EQPS)

M. Merewether

	Overlap	Non-overlap
Max rel error in Ω_1	1.3e-7	2.7e-7
Max rel error in Ω_2	1.9e-3	1.8e-3

Monolithic single *Ω* run **struggled** and required ***Δt*-cutting** but SAM cases did not

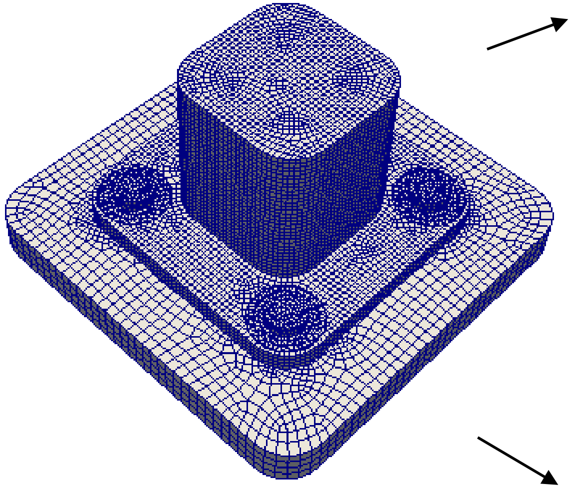
Why? Problem is **easier to converge** with **SAM:** single **difficult multiscale problem** in Ω replaced with two **easier mono-scale problems** in Ω_1 and Ω_2

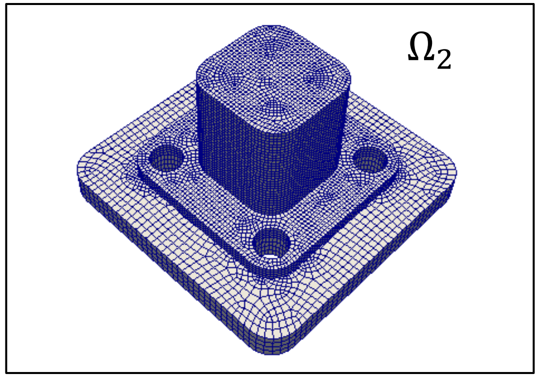


Single-Domain   Overlapping   Non-Overlapping

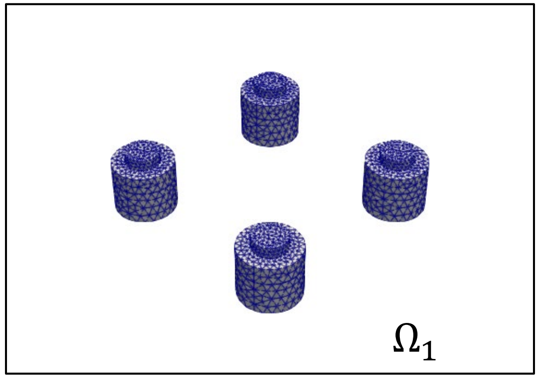
Bolted Joint (Overlapping SAM)

- Problem of **practical scale**
- Schwarz solution **compared** to single-domain solution on composite TET10 mesh.





- BC: x-displacement = 0.02 at T = 1.0e-3 on top of parts.
- Run until T = 5.0e-4 w/ Δt = 1e-5 + implicit Newmark with analytic mass matrix for composite tet 10s.



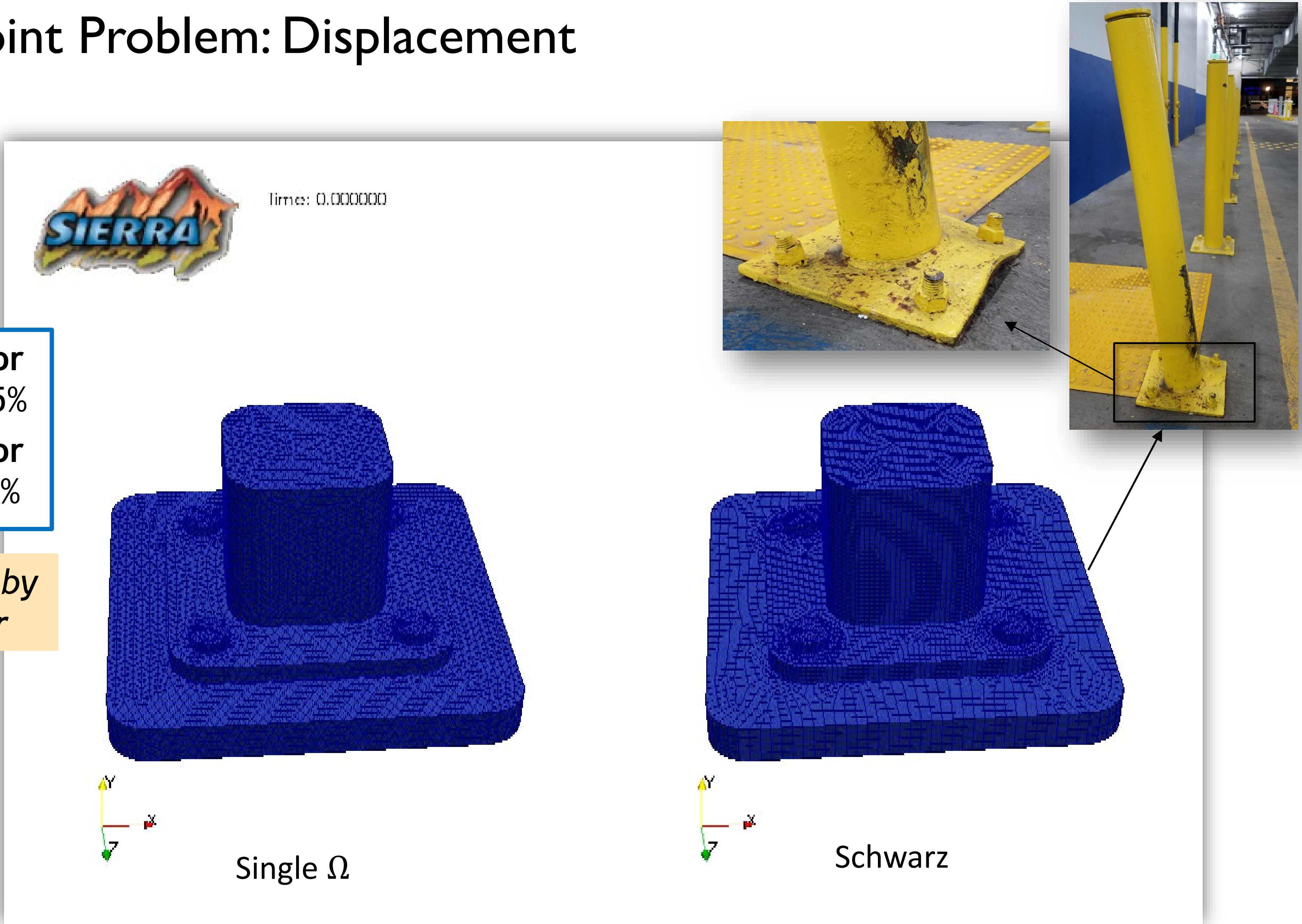
- Ω_1 = bolts (Composite TET10), Ω_2 = parts (HEX8).
- ***Inelastic J_2 material model*** in both subdomains.
  - Ω_1: steel
  - Ω_2: steel component, aluminum (bottom) plate

Bolted Joint Problem: Displacement

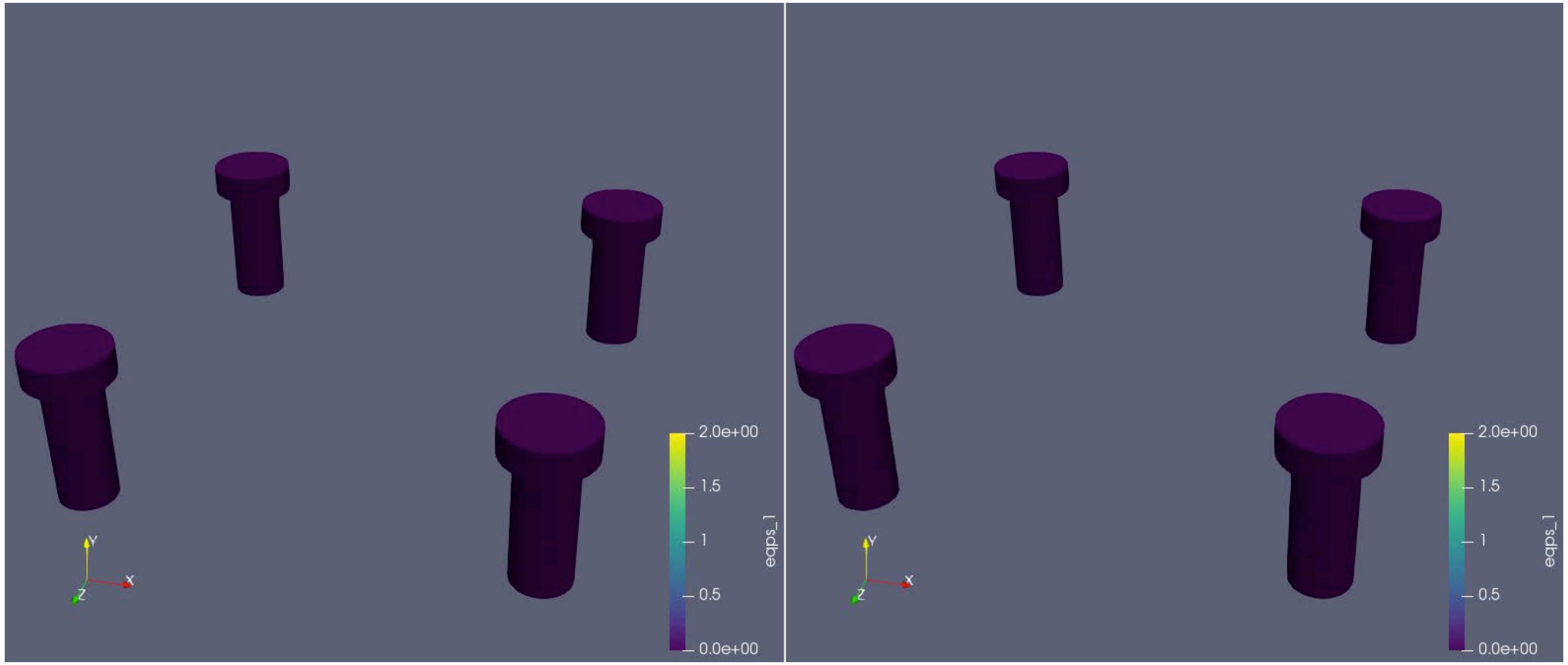
Max relative error in Ω_1 (bolts): 0.25%

Max relative error in Ω_2 (parts): 3.6%

Errors dominated by ***geometric error***



Bolted Joint Problem: Equivalent Plastic Strain (EQPS)



Single Ω

Schwarz

Bolted Joint Problem: Performance (Multiplicative Schwarz)

	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.

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Schwarz 36% faster than single domain

Despite its iterative nature, (even multiplicative) Schwarz can actually be ***faster*** than single domain run for discretizations having comparable # of elements in the bolts!

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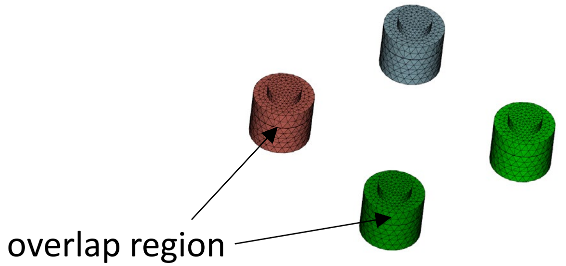
- (Multiplicative) Schwarz converges in just ***2-4 Schwarz iterations*** per time-step despite the ***small overlap***.



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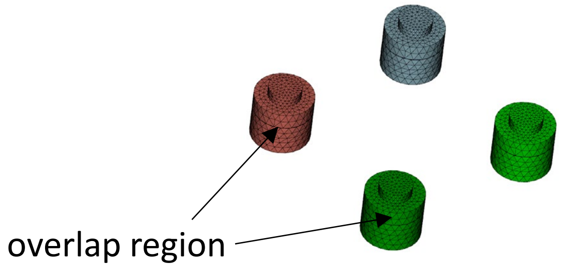
Schwarz 36% faster than single domain

Schwarz 73% slower than single domain

Despite its iterative nature, (even multiplicative) Schwarz can actually be ***faster*** than single domain run for discretizations having comparable # of elements in the bolts!



- (Multiplicative) Schwarz converges in just ***2-4 Schwarz iterations*** per time-step despite the ***small overlap***

- Schwarz is ***not always faster*** (as expected).

While we would like comparable CPU times, analysts are OK with slowdowns of as much as 3-4× if meshing is simplified significantly.

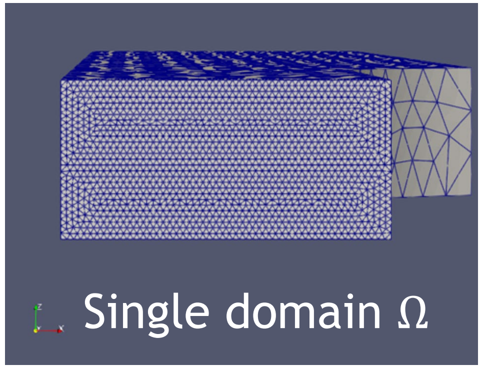
* On SNL ascicgpu15, 16, 17 machines (Intel Skylake CPU processor), Schwarz tol = 1e-6.

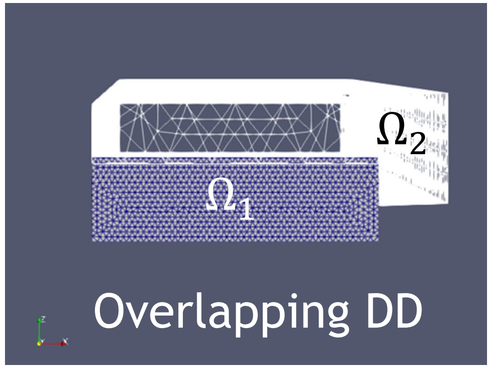
Laser Weld (Overlapping & Non-Overlapping SAM)

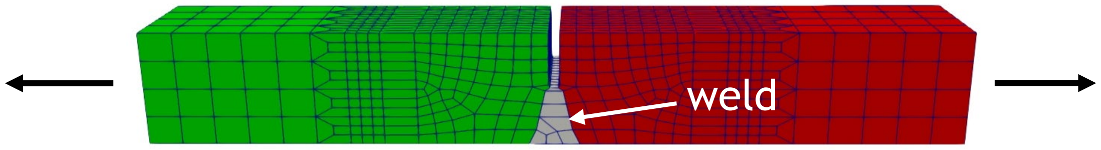
- Problem of **practical scale**
- Geometry is **pulled dynamically** from both ends
- **Two variants** of this problem to **demonstrate:**
  1. **Improving performance via mesh/DD design**
     - ➢ *Two subdomains (below)*: holder, gauge
     - ➢ *Overlapping* SAM + plastic
  2. **Overlapping & non-overlapping coupling of >2 subdomains**
     - ➢ *Three subdomains (right)*: two holders (yellow + blue) + gauge (white)
     - ➢ *Overlapping* & *non-overlapping* SAM + hyperelastic

NORMA.JL

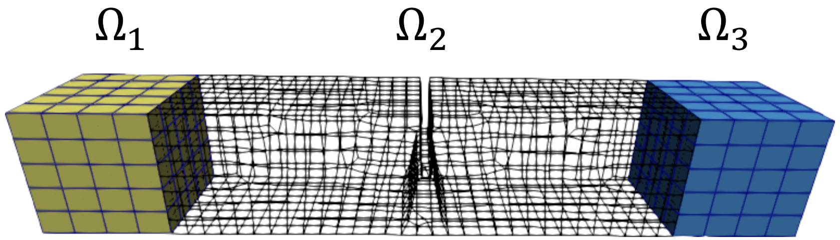
Goal: model **stress/strain localization** in the weld subject to **tension.**



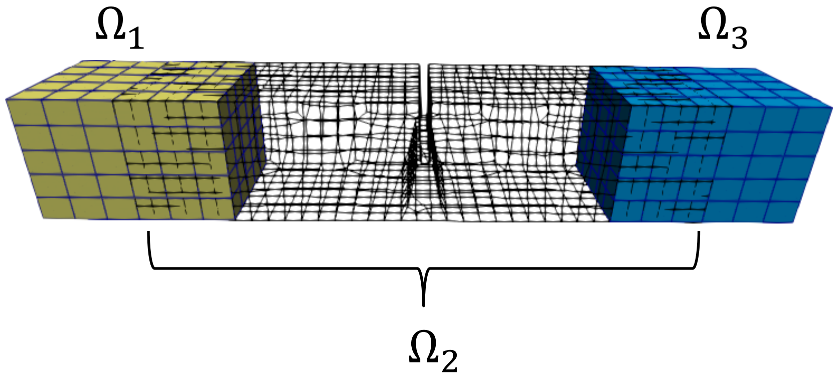




Single domain Ω



Non-overlapping DD

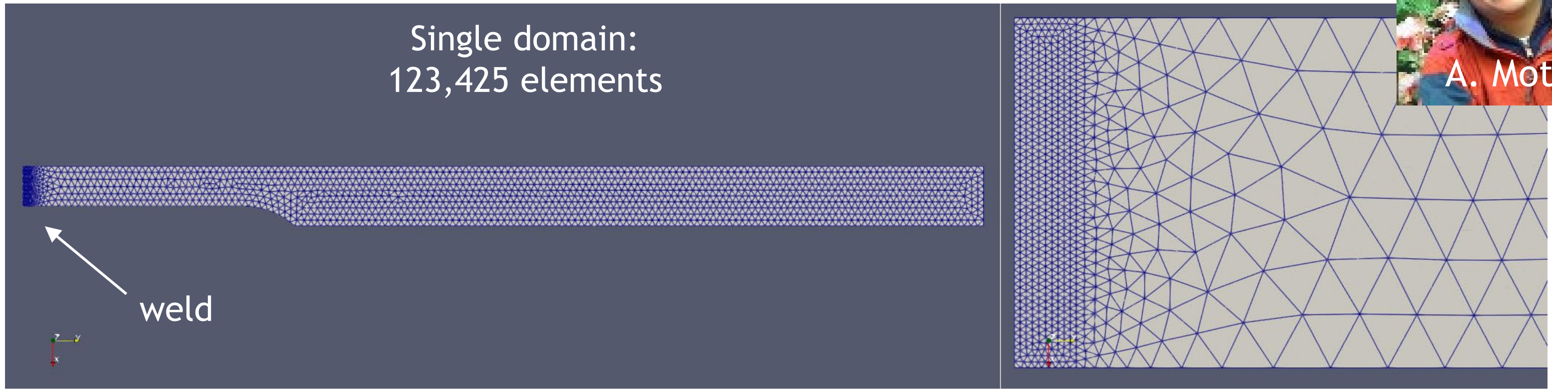


Overlapping DD

Illustration of geometry and DDs for simple variant (above) and more complex (left) variant of the laser weld problem.

Laser Weld: Improving Performance via Mesh/DD Design

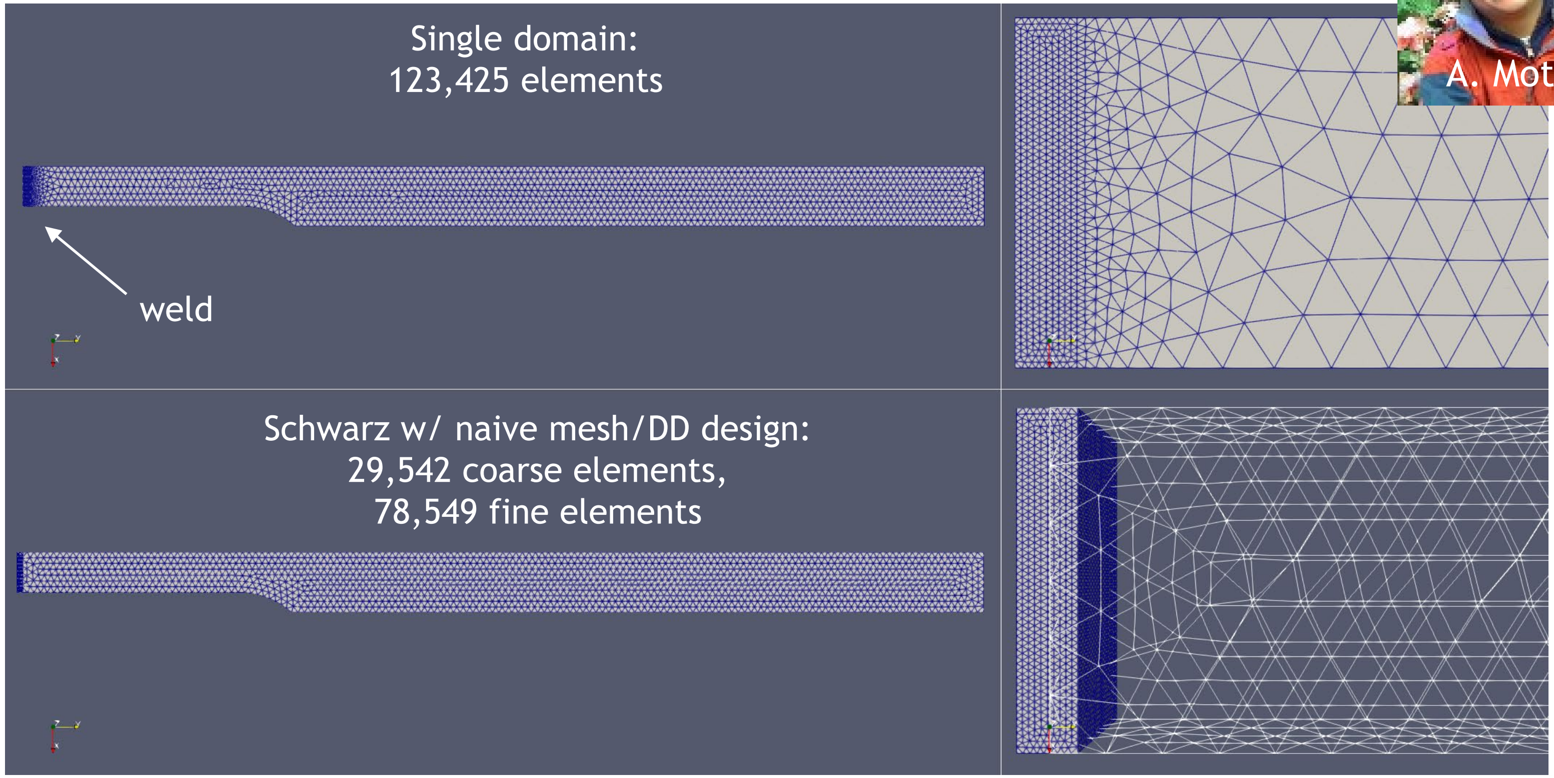
- **Production** laser weld problem in SIERRA/SM with plasticity



Simulation Type	Wall Time 64 procs
Single domain	3 hr 17 min

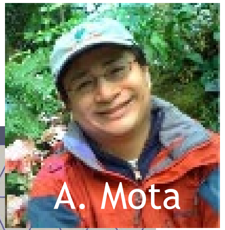
Laser Weld: Improving Performance via Mesh/DD Design

- **Production** laser weld problem in SIERRA/SM with plasticity
- **Overlapping** Schwarz with **naïve DD/meshing** takes ~**3**× longer to run than single Ω solve

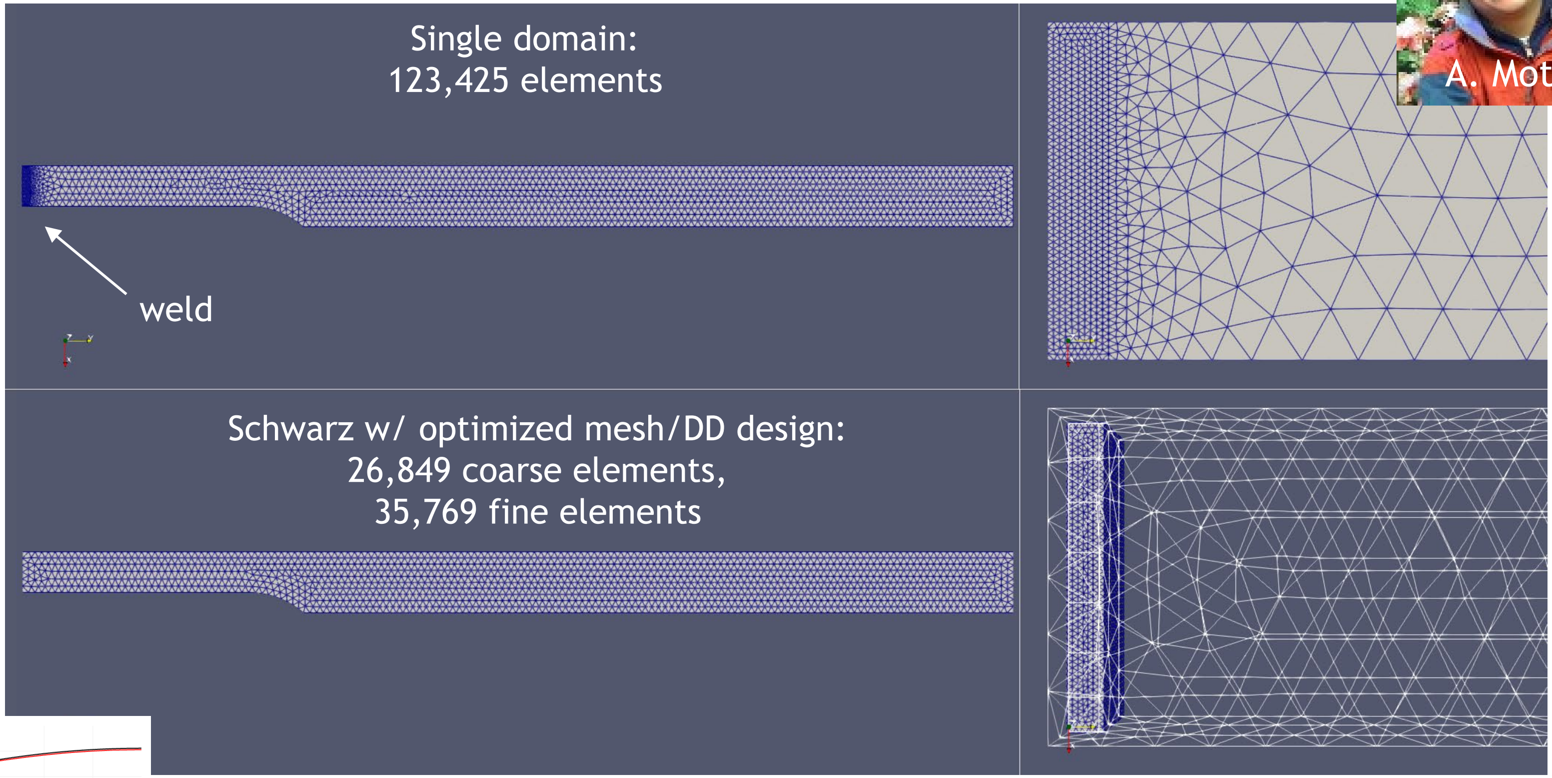


Simulation Type	Wall Time 64 procs
Single domain	3 hr 17 min
Overlapping SAM (16 iters, naïve DD and mesh design)	10 hr 14 min

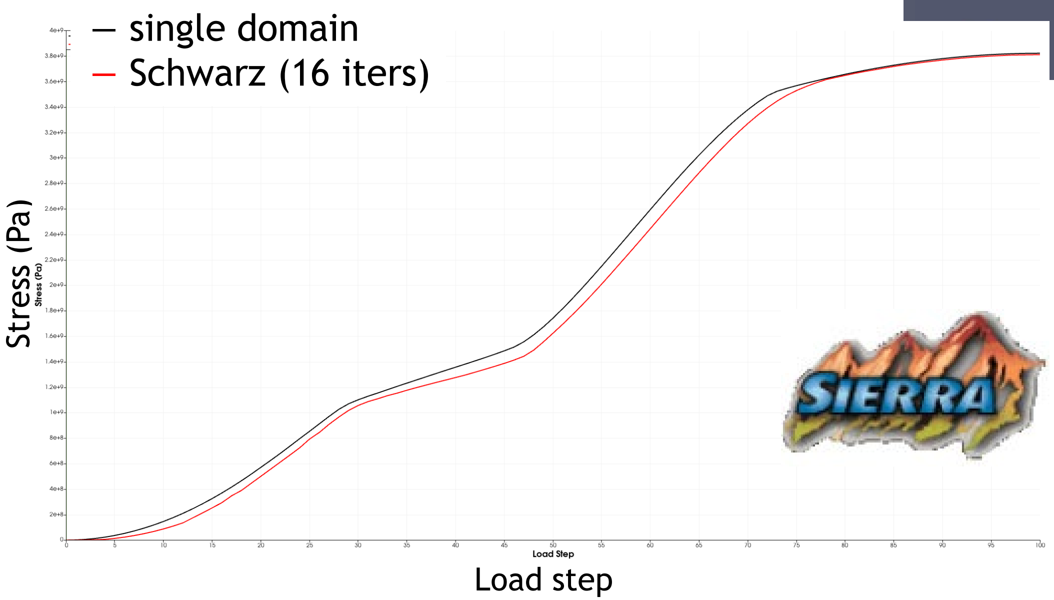
Laser Weld: Improving Performance via Mesh/DD Design



- **Production** laser weld problem in SIERRA/SM with plasticity
- **Overlapping** Schwarz with **naïve DD/meshing** takes $\sim$**3**$\times$ longer to run than single Ω solve



Schwarz performance can be **improved by** $\sim$**3**$\times$ while maintaining the **same accuracy** by **optimizing** the **mesh design**

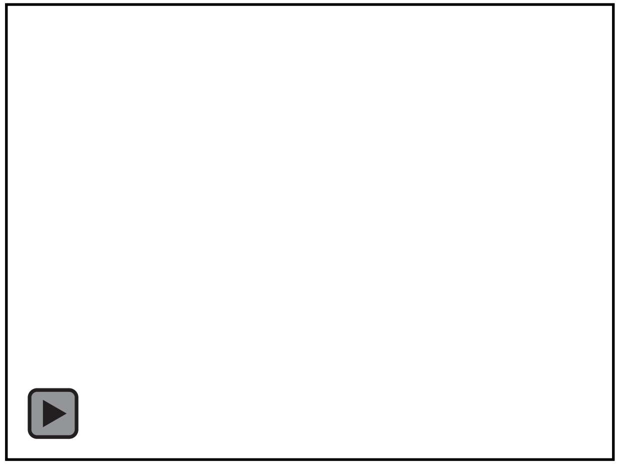


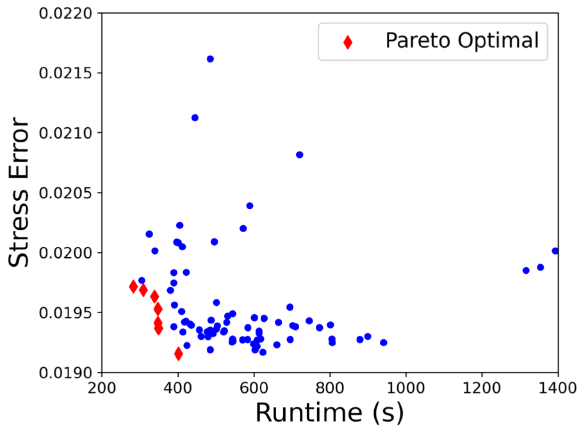
Simulation Type	Wall Time 64 procs
Single domain	3 hr 17 min
Overlapping SAM (16 iters, naïve DD and mesh design)	10 hr 14 min
Overlapping SAM (16 iters, optimized DD and mesh design)	3 hr 37 min

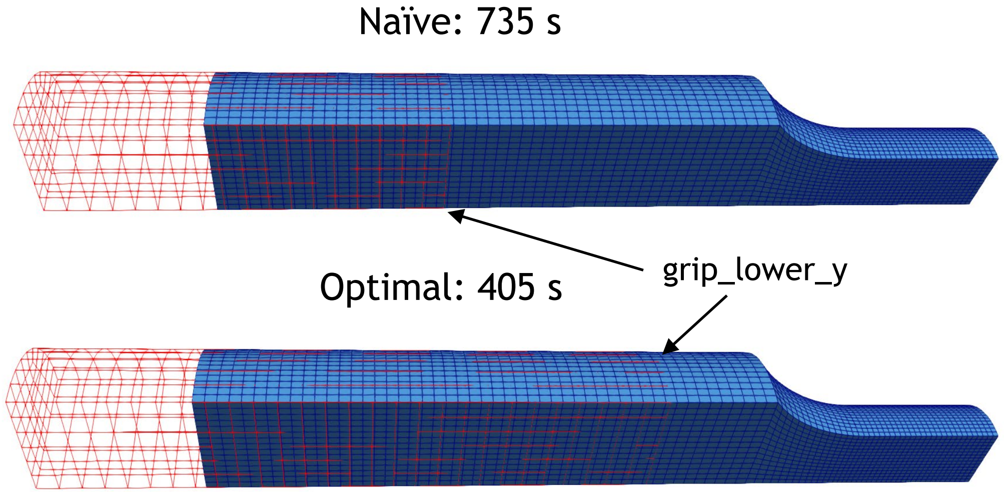
Work in Progress: Bayesian Optimization of SAM Parameters

C. Wentland

- **Risk:** Manual SAM DD **tuning** is often **expert-driven**, **trial-and-error**, **costly** and **tedious**
- **Mitigation: multi-objective (MO) optimization**
  - ➢ Minimize CPU time + stress recovery-based error indicator, two competing metrics
- **GPTune:** developed by Lawrence Berkeley Lab
  - ➢ **Bayesian, gradient-free optimization** of black box models (Norma.jl, Albany-LCM, SIERRA/SM)
  - ➢ Intelligently learns **interpretable Gaussian process (GP) surrogate** of model with baked-in UQ
  - ➢ **Reduces search time** w.r.t. grid/random search
  - ➢ **Balances total mesh size, SAM convergence speed** and **solution accuracy** with minimal user input
- **Optimization parameters:** interface location, subdomain count, overlap size, relaxation parameter







GPTune auto-tuning of Schwarz interface location can **reduce CPU time** by **>80%** without sacrificing accuracy.

Movie top right: parameter sampling for lower and upper boundary of tension specimen w/ MO target.
Plots bottom right: optimal interface placement (bottom) decreases cost by 25% over naïve interface placement (top).

oupling >2 Subdomains?

Our DDs are physic
motivated. We usu
have 3-4 subdoma
(5-10 max).

NORMA.JL

	Overlap	Non-over
Max rel error in gauge	6.2e-4	1.5e-4
Mean # Schwarz iters	11.1	36.7

Coupling >2 Subdomains?

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NORMA.JL

	Overlap	Non-over
Max rel error in gauge	6.2e-4	1.5e-4
Mean # Schwarz iters	11.1	36.7

- **Non-overlapping Schwarz** takes ~ **3.3× more Schwarz iteration** and is ~**2.8× slower** than overlapping Schwarz

We are exploring several mechanisms for **accelerating non-overlapping Schwarz.**

Work in Progress: Optimizing Non-Overlapping Schwarz via Transmission Condition Design


C. Rodriguez

- **Risk:** non-overlapping Schwarz can be **slow to converge** w/ **Dirichlet-Neumann TCs.**
- **Mitigation:** explore optimized **Robin-Robin** transmission conditions and **relaxation.**

General non-overlapping Schwarz formulation

$$\begin{cases} \boldsymbol{M}_1 \ddot{\boldsymbol{u}}_1^{(s+1)} + \boldsymbol{K}_1 \boldsymbol{u}_1^{(s+1)} = \boldsymbol{F}_1^{(s+1)} & \text{in } \Omega_1 \\ \boldsymbol{u}_1^{(s+1)} = \boldsymbol{u}_D & \text{on } \partial_\Psi \Omega_1 \backslash \Gamma \\ \boxed{\alpha_{12} \boldsymbol{T}_1^{(s+1)} + \beta_{12} \boldsymbol{u}_1^{(s+1)} = \boldsymbol{\lambda}_1^{(s+1)} \quad \text{on } \Gamma} \end{cases}$$

$$\begin{cases} \boldsymbol{M}_2 \ddot{\boldsymbol{u}}_2^{(s+1)} + \boldsymbol{K}_2 \boldsymbol{u}_2^{(s+1)} = \boldsymbol{F}_2^{(s+1)} & \text{in } \Omega_2 \\ \boldsymbol{u}_2^{(s+1)} = \boldsymbol{u}_D & \text{on } \partial_\Psi \Omega_2 \backslash \Gamma \\ \boxed{\alpha_{21} \boldsymbol{T}_2^{(s+1)} + \beta_{21} \boldsymbol{u}_2^{(s+1)} = \boldsymbol{\lambda}_2^{(s+1)} \quad \text{on } \Gamma} \end{cases}$$

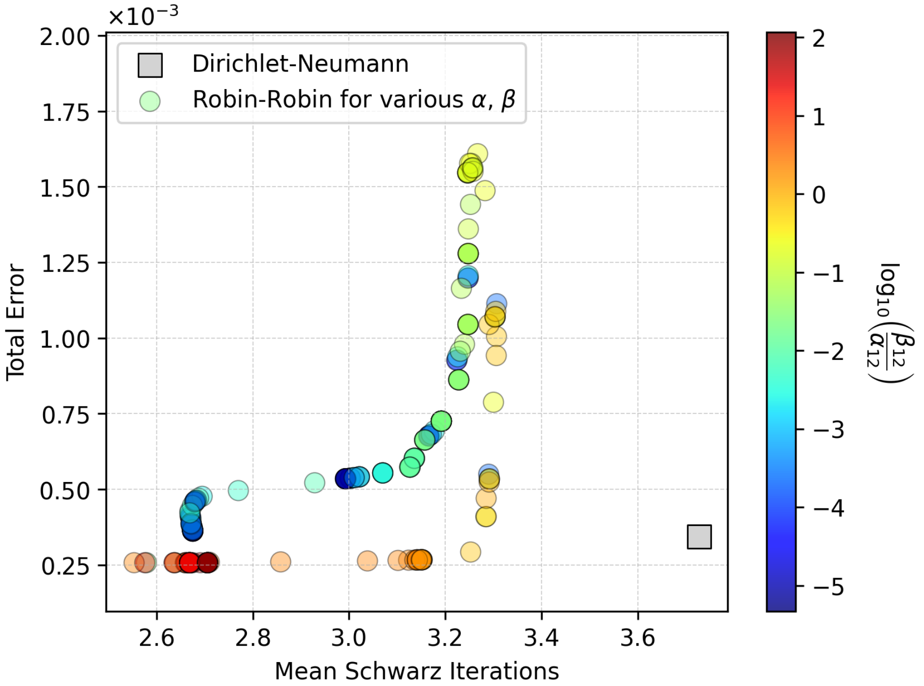
$$\boxed{\begin{aligned} \boldsymbol{\lambda}_1^{(s+1)} &= \theta_1 \left[\alpha_{12} \boldsymbol{T}_2^{(s)} + \beta_{12} \boldsymbol{u}_2^{(s)} \right] + (1-\theta_1)\, \boldsymbol{\lambda}_1^{(s)} \\ \boldsymbol{\lambda}_2^{(s+1)} &= \theta_2 \left[\alpha_{21} \boldsymbol{T}_1^{(s+1)} + \beta_{21} \boldsymbol{u}_1^{(s+1)} \right] + (1-\theta_2)\, \boldsymbol{\lambda}_2^{(s)} \end{aligned}}$$

Practical concern: Robin BCs not readily available in solid mechanics codes

General transmission conditions which can be **Dirichlet-Neumann** or **Robin-Robin**

Relaxation through parameters θ_i

Total Error vs. Mean Schwarz Iterations



Optimized Robin-Robin TCs can give to **faster convergence (29% less Schwarz iterations)** and **lower errors (by up to 25%)** than Dirichlet-Neumann TCs.

Work in Progress: Accelerating Non-Overlapping Schwarz


G. Sambataro

- **Risk:** non-overlapping Schwarz can be **slow to converge** w/ **Dirichlet-Neumann TCs.**
- **Mitigation:** explore accelerating Dirichlet-Neumann Schwarz via **Aitken** and **Anderson acceleration.**

Non-overlapping Dirichlet-Neumann Schwarz

$$\begin{cases} \mathrm{Div}\, \boldsymbol{P}_1^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\,, & \text{in } \Omega_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\chi}, & \text{on } \partial\Omega_1 \setminus \Gamma \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\lambda}_{n+1} & \text{on } \Gamma \end{cases}$$

$$\begin{cases} \mathrm{Div}\, \boldsymbol{P}_2^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\,, & \text{in } \Omega_2 \\ \boldsymbol{\varphi}_2^{(n+1)} = \boldsymbol{\chi}, & \text{on } \partial\Omega_2 \setminus \Gamma \\ \boldsymbol{P}_2^{(n+1)} \boldsymbol{n} = \boldsymbol{P}_2^{(n+1)} \boldsymbol{n}, & \text{on } \Gamma \end{cases}$$

Aitken acceleration can **reduce** the # of Schwarz iterations by **3**× and has virtually **no tuning knobs.**

Minimal tuning knobs improves usability.

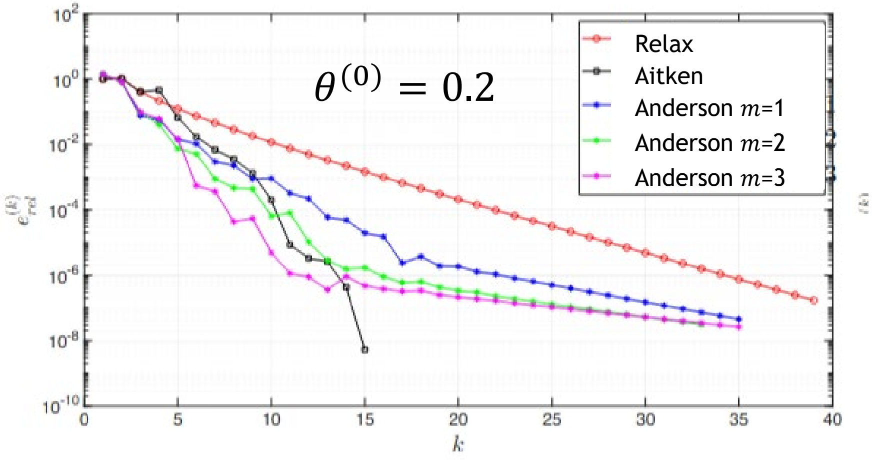
Classical relaxation: $\boldsymbol{\lambda}_{n+1} = \theta \boldsymbol{\varphi}_2^{(n)} + (1-\theta)\boldsymbol{\lambda}_n, \text{on } \Gamma, \text{for } n \geq 1$

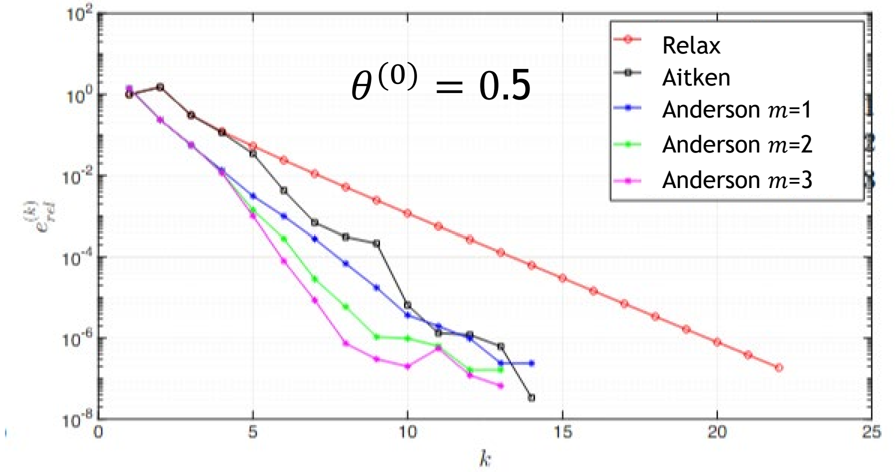
Aitken acceleration: $\boldsymbol{\lambda}_{n+1} = \boldsymbol{\varphi}_1^{(n)} + \theta^{(n-1)} \left(\boldsymbol{\varphi}_2^{(n-1)} - \boldsymbol{\varphi}_1^{(n-1)} \right)$

$$\theta^{(n)} = -\frac{\left(\boldsymbol{\varphi}_2^{(n)} - \boldsymbol{\varphi}_1^{(n)} - \boldsymbol{\varphi}_2^{(n-1)} - \boldsymbol{\varphi}_1^{(n-1)}\right) \cdot \left(\boldsymbol{\varphi}_1^{(n)} - \boldsymbol{\varphi}_1^{(n-1)}\right)}{\left\| \boldsymbol{\varphi}_2^{(n)} - \boldsymbol{\varphi}_1^{(n)} - \boldsymbol{\varphi}_2^{(n-1)} - \boldsymbol{\varphi}_1^{(n-1)} \right\|^2}$$

Anderson acceleration: $\boldsymbol{\lambda}_{n+1} = \sum_{j=0}^{m} \theta^{(n)} T(\boldsymbol{\lambda}_{k-m+j}),$

$\theta^{(n)}$ from optimization problem





References on SAM for FOM-FOM Coupling in Solid Mechanics

Quasistatic Schwarz:

- A. Mota, **I. Tezaur**, C. Alleman. “The Schwarz alternating method in solid mechanics”, *Comput. Meth. Appl. Mech. Engng.* 319 19-51, 2017.

Dynamic Schwarz:

- A. Mota, **I. Tezaur**, G. Phlipot. "The Schwarz alternating method for dynamic solid mechanics", *Int. J. Numer. Meth. Engng.* 123(21) 5036-5071, 2022.

Transmission Condition Design for Non-Overlapping Schwarz:

- C. Rodriguez**, I. Tezaur**, A. Mota, A. Gruber, E. Parish, C. Wentland. “Transmission Conditions for the Non-Overlapping Schwarz Coupling of Full Order and Operator Inference Models”, Computer Science Research Institute Summer Proceedings 2025, Sandia National Laboratories, 2025. https://arxiv.org/abs/2509.12228


I. Tezaur


A. Mota


C. Alleman


B. Phung


G. Phlipot


T. Shelton


C. Rodriguez


M. Merewether


G. Sambataro

Outline

Insights, lessons learned, practical

1. Schwarz Alternating Method (SAM) for Coupling of Full Order Models (FOMs) in Solid Mechanics
   - Motivation & Background
   - Formulation
   - Numerical Examples
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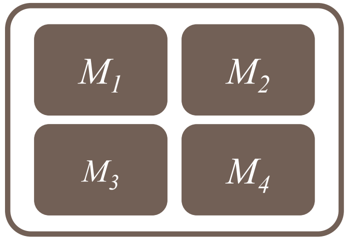
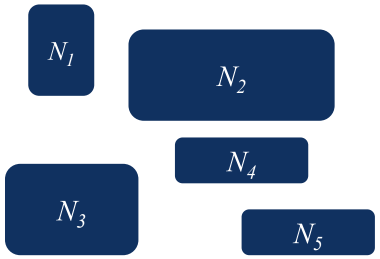
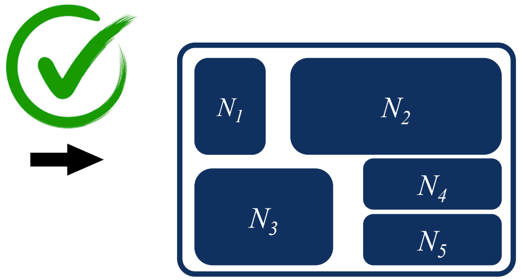
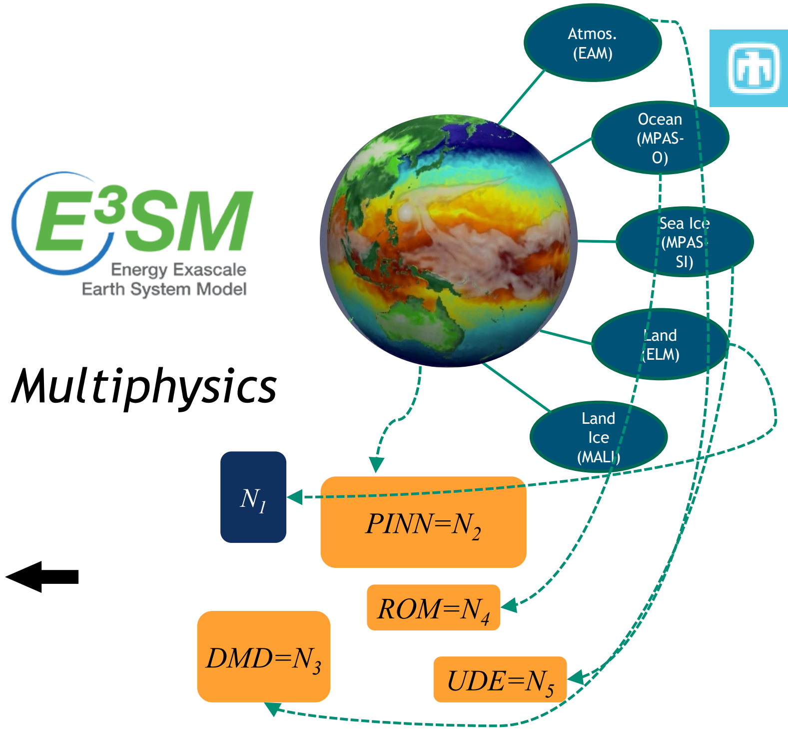
Motivation: Multiscale & Multiphysics Coupling for Predictive Digital Twins

There exist established **rigorous mathematical theories** for **coupling** multiscale/multiphysics components based on **traditional discretization methods** (FOM).









Complex System Model

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

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)

Traditional + Data-Driven Methods

- PINNs
- Neural ODEs
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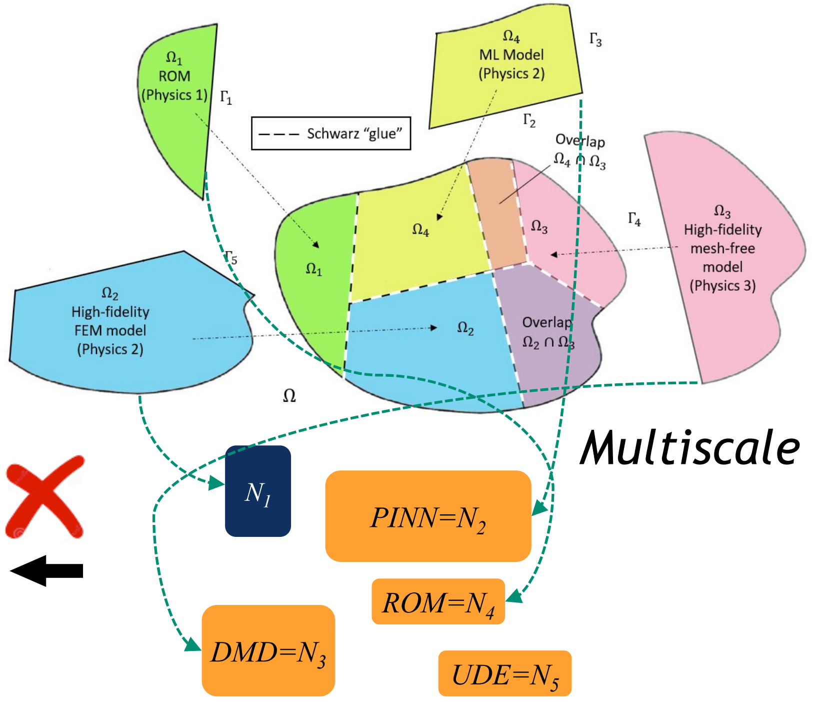

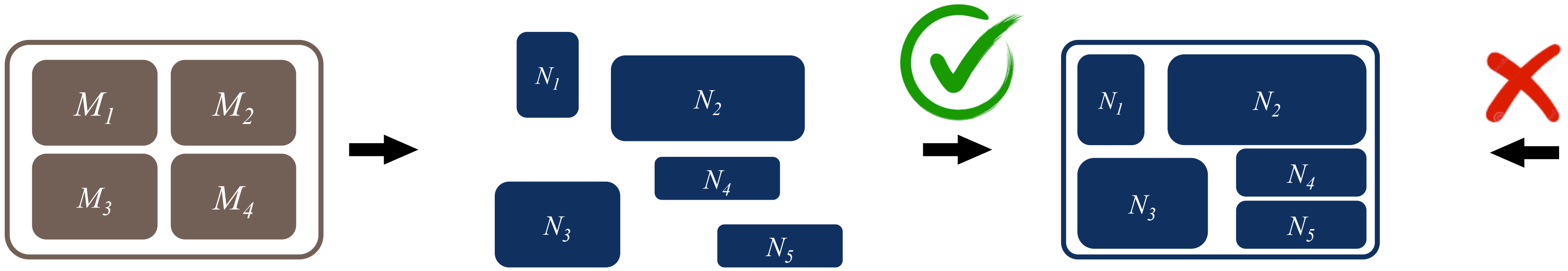

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- **Deficiencies of data-driven models and couplings involving them:**
  - ➢ Existing coupling methods for high-fidelity models **may not work** out-of-the-box when including **data-driven models**
  - ➢ **ROMs** can suffer from **lack of robustness**, **stability** and **accuracy,** and **cannot** be **easily refined** to achieve a specified accuracy

Fast + inaccurate ≠ good!

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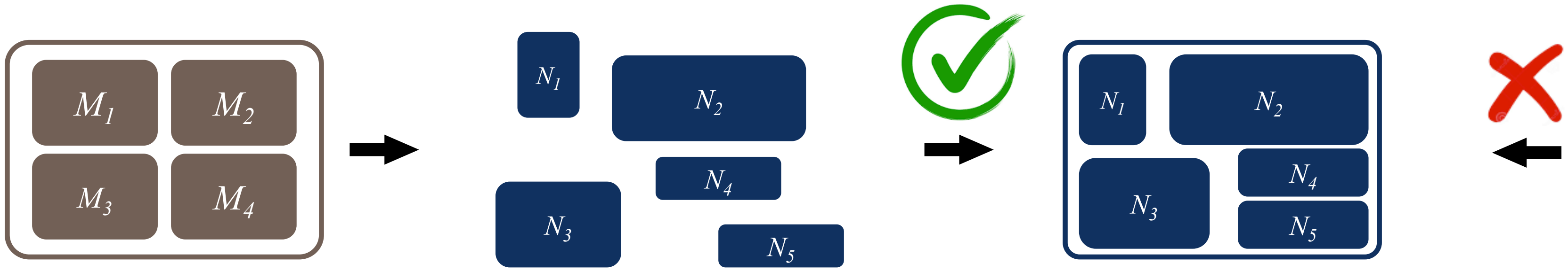

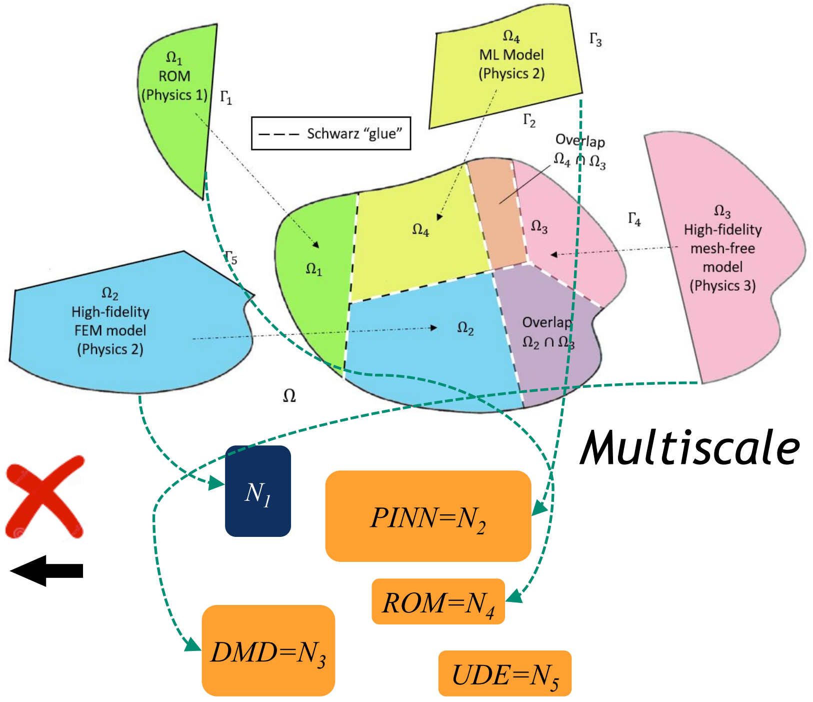

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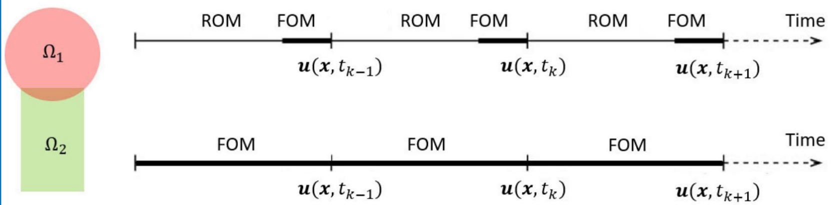
Proposed solution: Schwarz & (soon) online model switching



Projects on Coupling for Predictive Hybrid Models

Three projects:

- **FHNM**: Flexible Heterogeneous Numerical Methods [LDRD, FY22-FY24]
- **M2dt**: Multi-faceted Mathematics for Predictive Digital Twins [ASCR, FY23-FY27]
- **AHEAD**: Adaptive Hybrid modEls via domAin Decomposition [LDRD, FY25-FY27]

Principal research objective:

- Develop rigorous methods to enable the **"plug-and-play" coupling** of **standard** and **data-driven models** from the following classes
  - *Class A*: intrusive projection-based ROMs
  - *Class B*: machine-learned models
  - *Class C*: flow map approximation models, i.e., dynamic model decomposition (DMD)
  - *Class D*: non-intrusive operator inference (OpInf) ROMs

Three classes of coupling methods:

- Alternating **Schwarz**-based coupling [FHNM, M2dt, AHEAD]
- **Optimization**-based coupling [FHNM, M2dt]
- Coupling via **generalized mortar methods** [FHNM, M2dt]

Projects on Coupling for Predictive Hybrid Models

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$\int \mathcal{M}^2 dt$

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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  - ➢ *Class D*: non-intrusive operator inference (OpInf) ROMs → this talk

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Office of Science

Why? Less intrusive to integrate into **production codes.**

Three classes of coupling methods:

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- Coupling via **generalized mortar methods** [FHNM, M2dt]

! *Less intrusive methods are preferred!*

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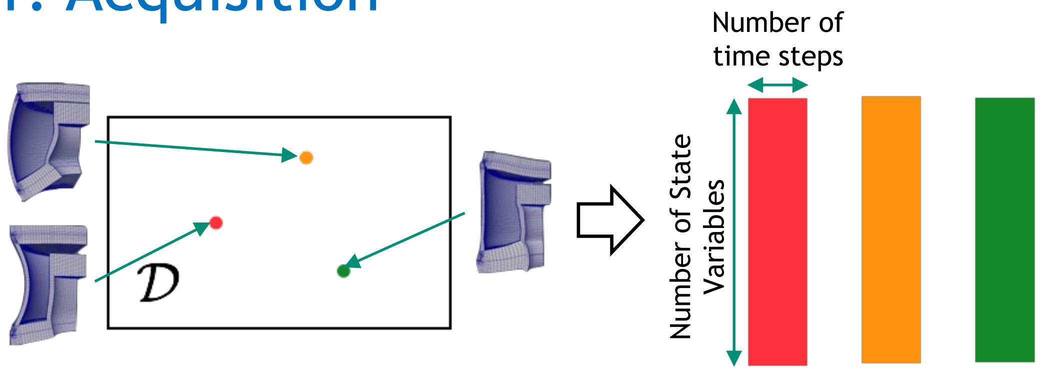
Projection-Based Model Order Reduction via the POD/Galerkin Method

Full Order Model (FOM): $\boldsymbol{M}\frac{d^2\boldsymbol{u}}{dt^2} + \boldsymbol{f}_{\text{int}}(\boldsymbol{u}) = \boldsymbol{f}_{\text{ext}}$

1. Acquisition

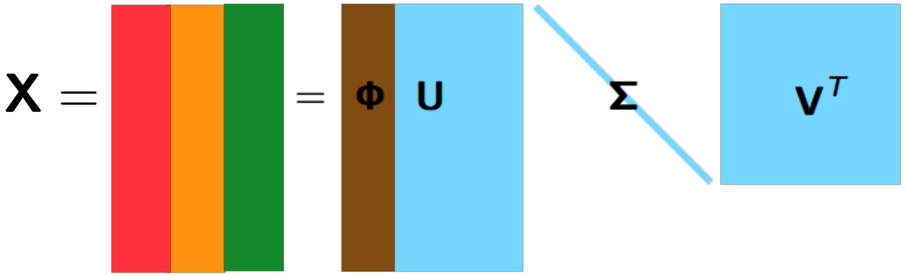


Solve ODE at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



ROM = projection-based Reduced Order Model

3. Projection-Based Reduction

Reduce the number of unknowns

$\boldsymbol{u}(t) \approx \tilde{\boldsymbol{u}}(t) = \boldsymbol{\Phi}\hat{\boldsymbol{u}}(t)$

Perform Galerkin projection

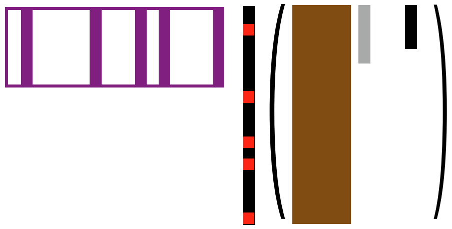
$\boldsymbol{\Phi}^T\boldsymbol{M}\boldsymbol{\Phi}\frac{d^2\hat{\boldsymbol{u}}}{dt^2} + \boldsymbol{\Phi}^T\boldsymbol{f}_{\text{int}}(\boldsymbol{\Phi}\hat{\boldsymbol{u}}) = \boldsymbol{\Phi}^T\boldsymbol{f}_{\text{ext}}$

***Disadvantage:** intrusive!*

Hyper-reduce nonlinear terms

$\boldsymbol{f}_{\text{int}}(\boldsymbol{\Phi}\hat{\boldsymbol{u}}) \approx \boldsymbol{A} \quad \boldsymbol{f}_{\text{int}}(\boldsymbol{\Phi}\hat{\boldsymbol{u}})$

Hyper-reduction/sample mesh



HROM = Hyper-reduced ROM

Non-Intrusive Model Order Reduction via OpInf*

Key Idea Behind OpInf: circumvent the burden of implementing intrusive ROMs in HPC codes by **combining projection-based ROM** and **machine learning (ML).**

Nuances:

- OpInf can be applied to **nonlinear problems** by transforming the nonlinear PDEs into PDEs with a polynomial functional form (**"lifting"** [Qian *et al.*, 2019]) or assuming a **polynomial functional form** for the ROM
- The OpInf least-squares (LS) minimization problem often requires **regularization** to be solvable, e.g., Tikhonov regularization
- **Structure preservation** (e.g., symmetry constraints) can be incorporated into the OpInf LS minimization problem

FOM:
$$\dot{\boldsymbol{q}} + \boldsymbol{A}\boldsymbol{q} + \boldsymbol{H}(\boldsymbol{q} \otimes \boldsymbol{q}) + \boldsymbol{B}\boldsymbol{u} = \boldsymbol{0}$$

snapshots of $\boldsymbol{q}$

Reduced basis $\boldsymbol{\Phi}$
(e.g., linear POD or quadratic manifold basis)

$$\min_{\widehat{\boldsymbol{A}},\widehat{\boldsymbol{H}},\widehat{\boldsymbol{B}}} \left\| \dot{\widehat{\boldsymbol{Q}}}^T + \widehat{\boldsymbol{Q}}^T \widehat{\boldsymbol{A}}^T + (\widehat{\boldsymbol{Q}} \otimes \widehat{\boldsymbol{Q}})^T \widehat{\boldsymbol{H}}^T + \widehat{\boldsymbol{U}}^T \widehat{\boldsymbol{B}}^T \right\|_F^2 + \gamma \left(\|\widehat{\boldsymbol{A}}\|_F + \|\widehat{\boldsymbol{H}}\|_F + \|\widehat{\boldsymbol{B}}\|_F \right)$$

$\widehat{\boldsymbol{Q}}$: snapshots generated from projected simulation data $\boldsymbol{q}$

$\widehat{\boldsymbol{A}}, \widehat{\boldsymbol{H}}, \widehat{\boldsymbol{B}}$: low-dimensional operators defining ROM dynamical system

OpInf ROM:
$$\dot{\widehat{\boldsymbol{q}}} + \widehat{\boldsymbol{A}}\widehat{\boldsymbol{q}} + \widehat{\boldsymbol{H}}(\widehat{\boldsymbol{q}} \otimes \widehat{\boldsymbol{q}}) + \widehat{\boldsymbol{B}}\boldsymbol{u} = \boldsymbol{0}$$

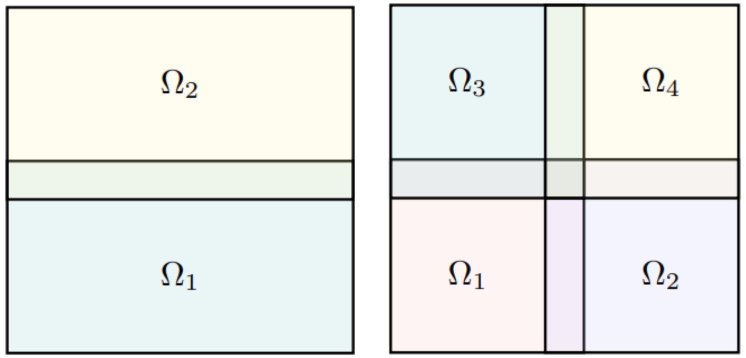
* [Peherstorfer & Willcox, 2016] + many subsequent refs

Less intrusive methods are preferred!

Overlapping SAM-based Coupling for Non-Intrusive OpInf ROMs

Offline stage:

- Create **DD** of Ω into d **overlapping subdomains** Ω_i
- Perform a SAM-coupled **all-FOM simulation** on $\cup_i \Omega_i$
- Compute **POD basis** $\boldsymbol{\Phi}_i$ on each Ω_i
- Assume a **functional form** for your ROM in Ω_i, informed by the functional form of the corresponding FOM
  - ➢ ***Key question***: *how to impose Schwarz BCs in OpInf ROMs?*



OpInf ROM in Ω_i:

$$\dot{\widehat{\boldsymbol{q}}}_i + \widehat{\boldsymbol{A}}_i \widehat{\boldsymbol{q}}_i + \widehat{\boldsymbol{H}}_i(\widehat{\boldsymbol{q}}_i \otimes \widehat{\boldsymbol{q}}_i) = \boldsymbol{0}$$

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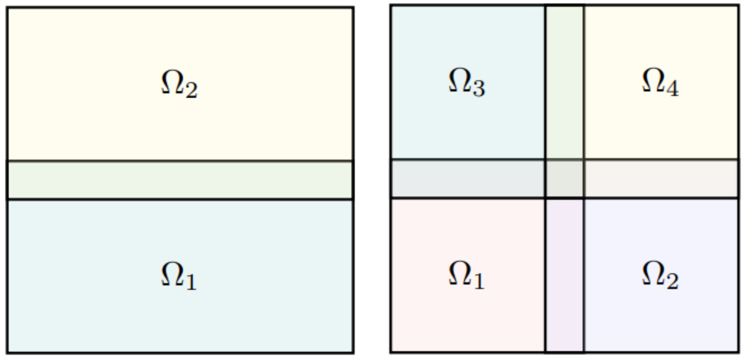

OpInf ROM + Schwarz BCs in Ω_i:

$$\dot{\hat{\boldsymbol{q}}}_i + \widehat{\boldsymbol{A}}_i \hat{\boldsymbol{q}}_i + \widehat{\boldsymbol{H}}_i(\hat{\boldsymbol{q}}_i \otimes \hat{\boldsymbol{q}}_i) + \underbrace{\widehat{\boldsymbol{B}}_i \boldsymbol{g}_i}_{\text{Schwarz Dirichlet BC term}} = \boldsymbol{0}$$

Motivated by implementation of **Dirichlet BCs** in **FEM**

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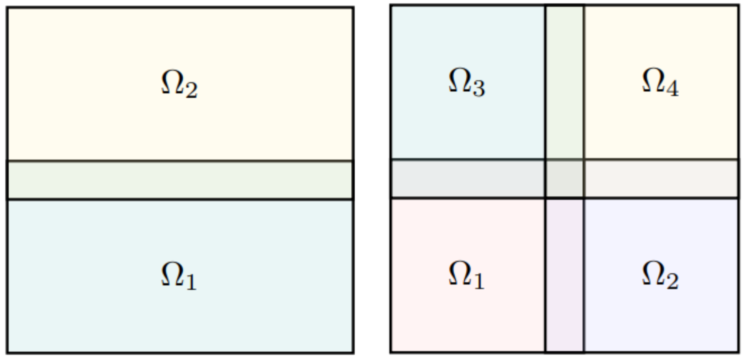

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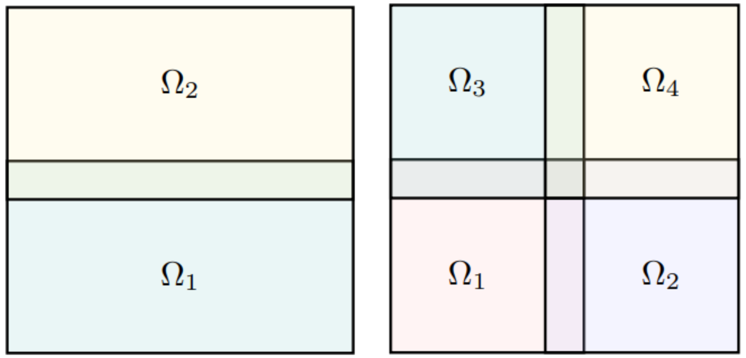

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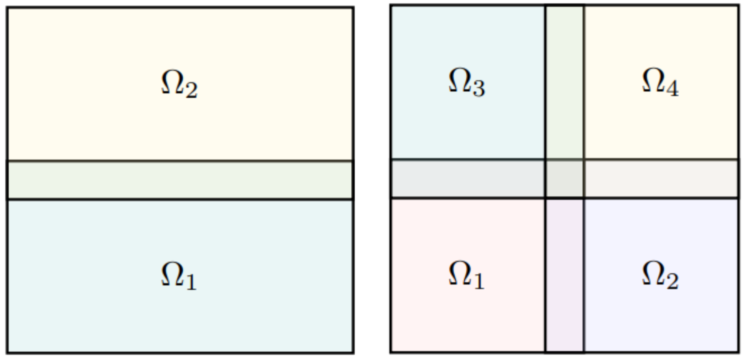

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Online stage:

- Apply **Schwarz iteration procedure**, with Schwarz BC transfer via pre-learned boundary contributions $\widetilde{\boldsymbol{B}}_i \boldsymbol{g}_i$

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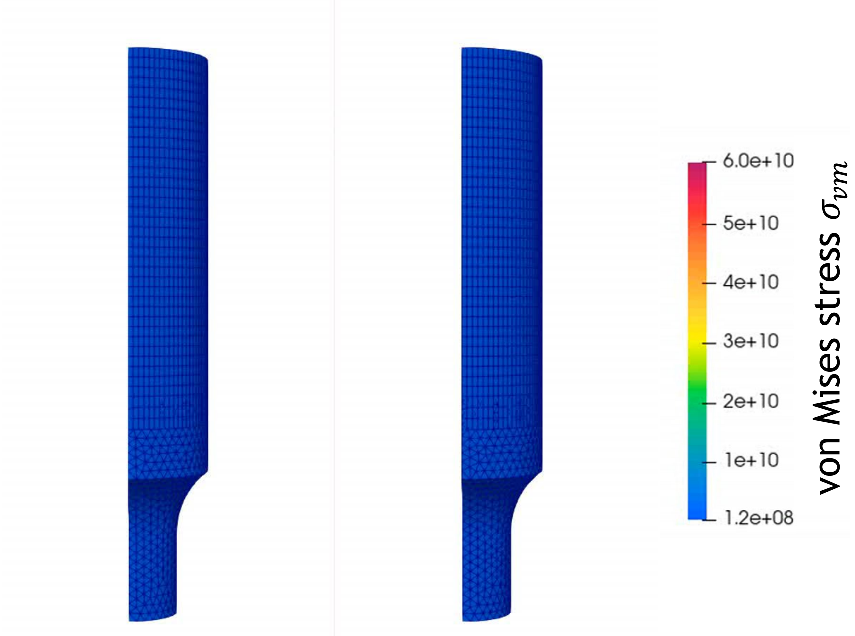
Tension Specimen (Overlapping SAM)

- **Hyperelastic** variant of previous problem (Neohookean material model)
- **TET10 - HEX8 overlapping** coupling with **implicit Newmark** with **same Δt**
- **QOpInf** models with M=2 POD modes, capturing 99.9999% snapshot energy
- All results are **predictive** w.r.t. DBC applied at top of holder

		FOM-FOM	FOM-QOpInf	QOpInf-QOpInf
Ω_1 rel errs	displacement	–	3.44e-4	5.73e-4
	velocity	–	1.72e-2	1.83e-2
	σ_{vm} stress	–	3.41e-4	8.53e-4
Ω_2 rel errs	displacement	–	2.50e-4	4.41e-4
	velocity	–	1.86e-2	1.96e-2
	σ_{vm} stress	–	2.40e-3	6.00e-3
CPU time	–	8h 19m 29.5s	1h 21m 25.9s	4m 42.1s
Mean/max # Schwarz iters	–	32.0/32	7.03/8	7.74/8



FOM-FOM FOM-QOpInf

QOpInf = Quadratic OpInf

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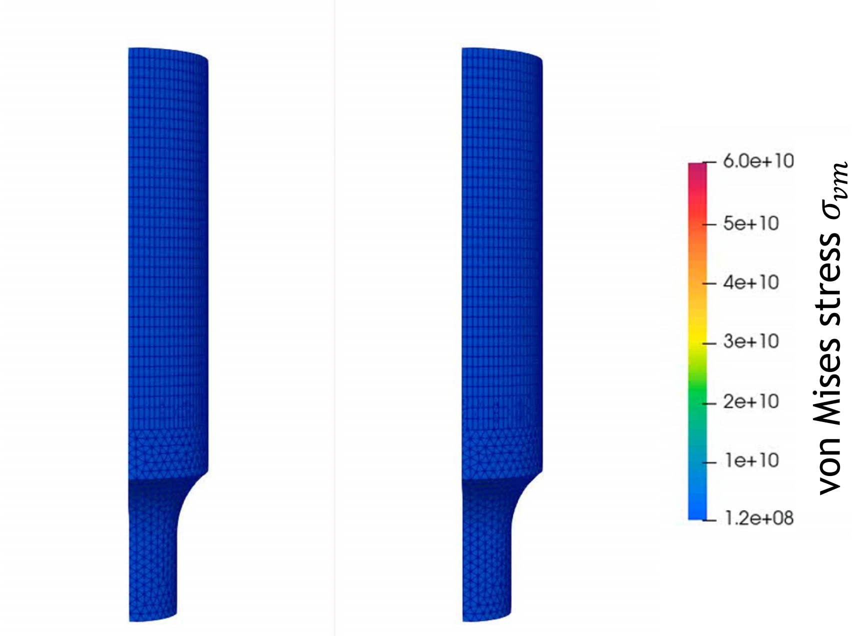
- **TET10 - HEX8 overlapping** coupling with **implicit Newmark** with **same** Δt
- **QOpInf** models with M=2 POD modes, capturing 99.9999% snapshot energy
- All results are **predictive** w.r.t. DBC applied at top of holder

		FOM-FOM	FOM-QOpInf	QOpInf-QOpInf
Ω_1 rel errs	displacement	–	3.44e-4	5.73e-4
	velocity	–	1.72e-2	1.83e-2
	σ_{vm} stress	–	3.41e-4	8.53e-4
Ω_2 rel errs	displacement	–	2.50e-4	4.41e-4
	velocity	–	1.86e-2	1.96e-2
	σ_{vm} stress	–	2.40e-3	6.00e-3
CPU time	–	8h 19m 29.5s	1h 21m 25.9s	4m 42.1s
Mean/max # Schwarz iters	–	32.0/32	7.03/8	7.74/8



FOM-FOM FOM-QOpInf

- Relative errors of $\boldsymbol{O}$**(1e-4)-**$\boldsymbol{O}$**(1e-3)** are achieved for the displacement and von Mises stress (σ_{vm})

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NORMA.JL

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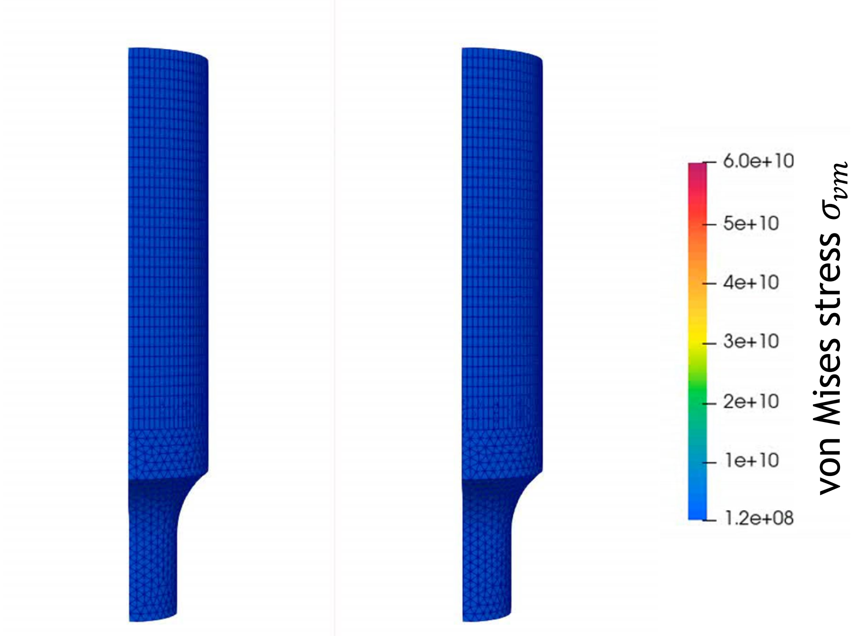

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Impressive **6.13**× and **106**× **speedups** are achieved via **FOM-QOpInf** and **QOpInf-QOpInf** couplings, respectively!

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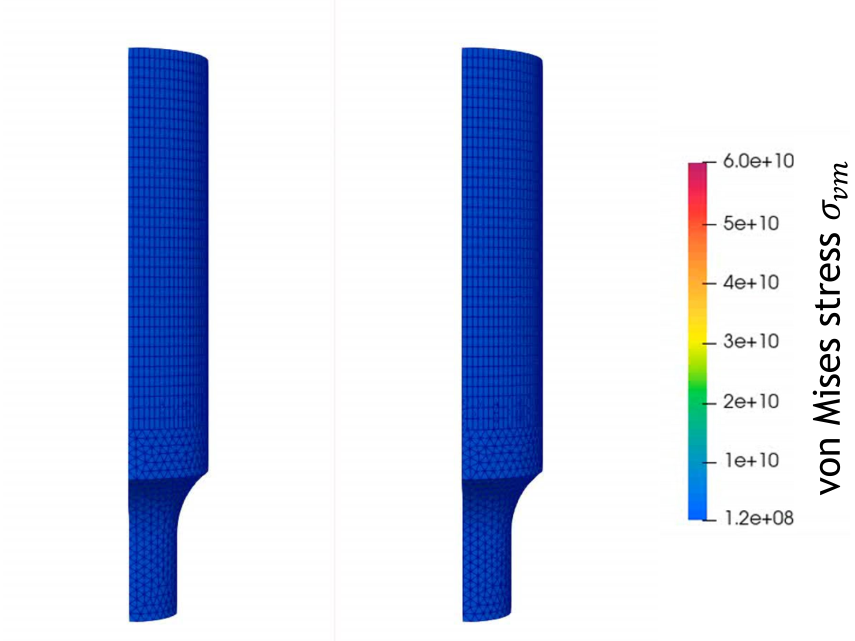

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Torsion (Overlapping SAM)

- **Neohookean** material model
- **TET4 - HEX8 overlapping** coupling with **implicit-explicit Newmark** having **different Δt**
- **QOpInf-FOM** coupled models with M=27 and M=30 POD modes, capturing 99.9999% snapshot energy
- **Prediction** w.r.t. **initial velocity** (rotation speed/direction)
- (Linear) **OpInf-FOM** coupling **insufficient**

		FOM-FOM	QOpInf-FOM reproductive	QOpInf-FOM predictive
Ω_1 rel errs	displacement	–	2.67e-3	4.32e-2
	velocity	–	3.56e-2	1.49e-1
Ω_2 rel errs	displacement	–	1.13e-3	2.44e-2
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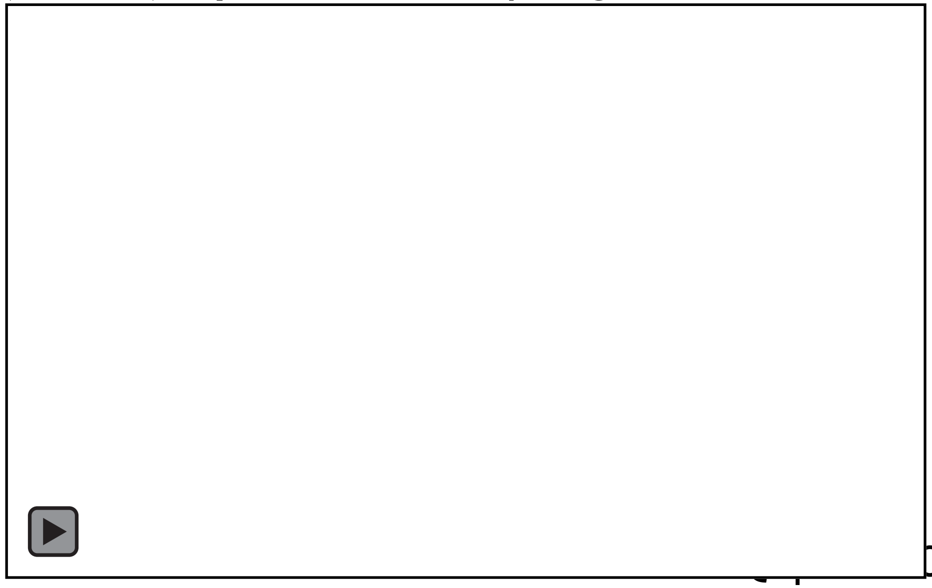

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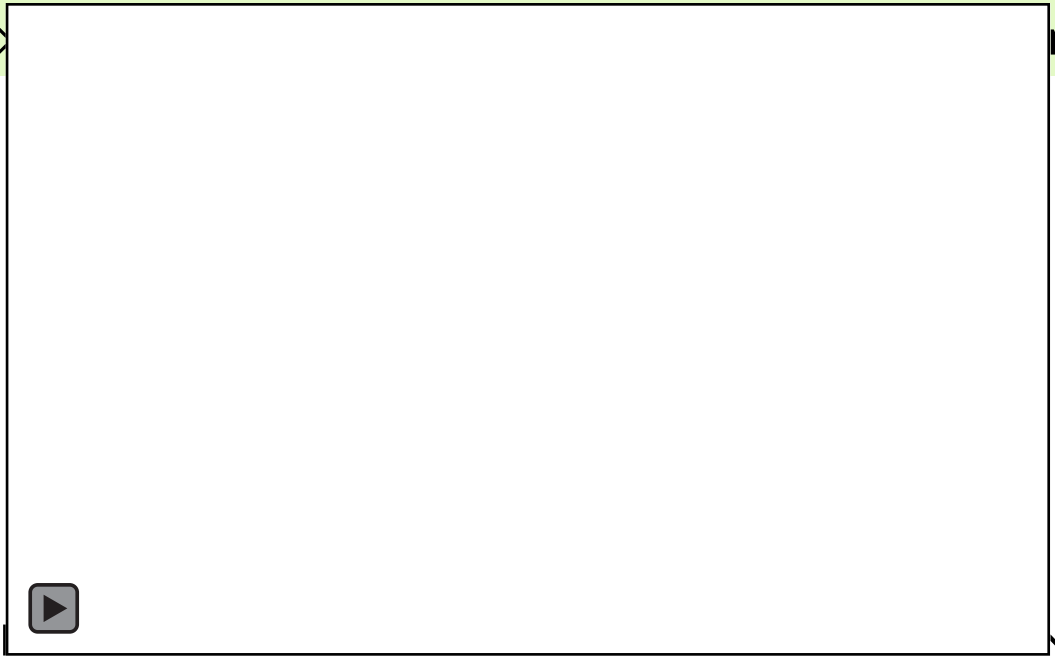
~**23.5**× ... ngs



Bolted Joint (Overlapping SAM)

- **Hyper-elastic** (Saint-Venant Kirchhoff) variant of previous problem with **TET10 - HEX8 meshes**
- **Cubic OpInf (COpInf)** coupled models
- Hybrid couplings require **fewer Schwarz iterations** to converge
- **Convergence** w.r.t. basis size is observed for reproductive FOM-QOpInf couplings

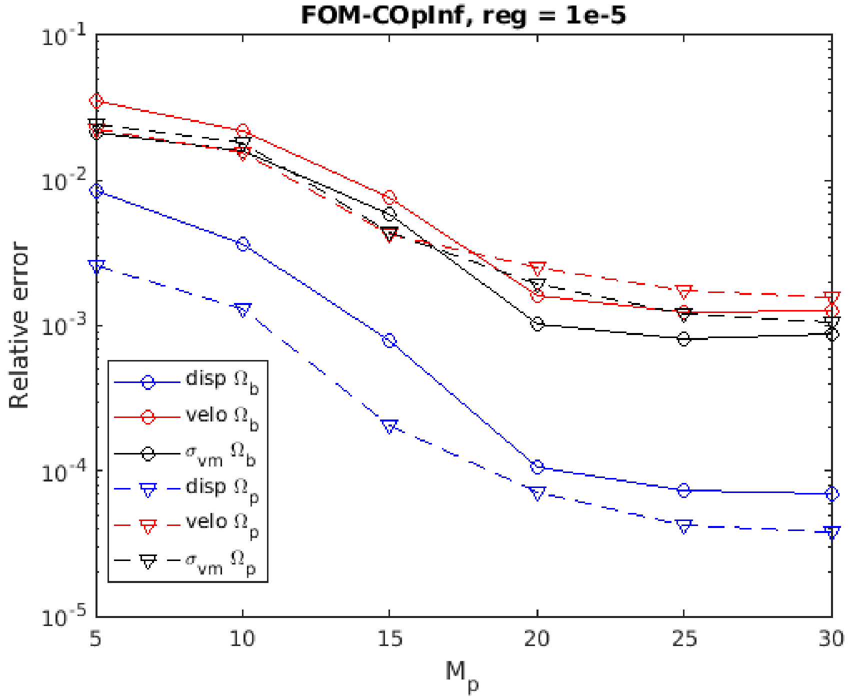
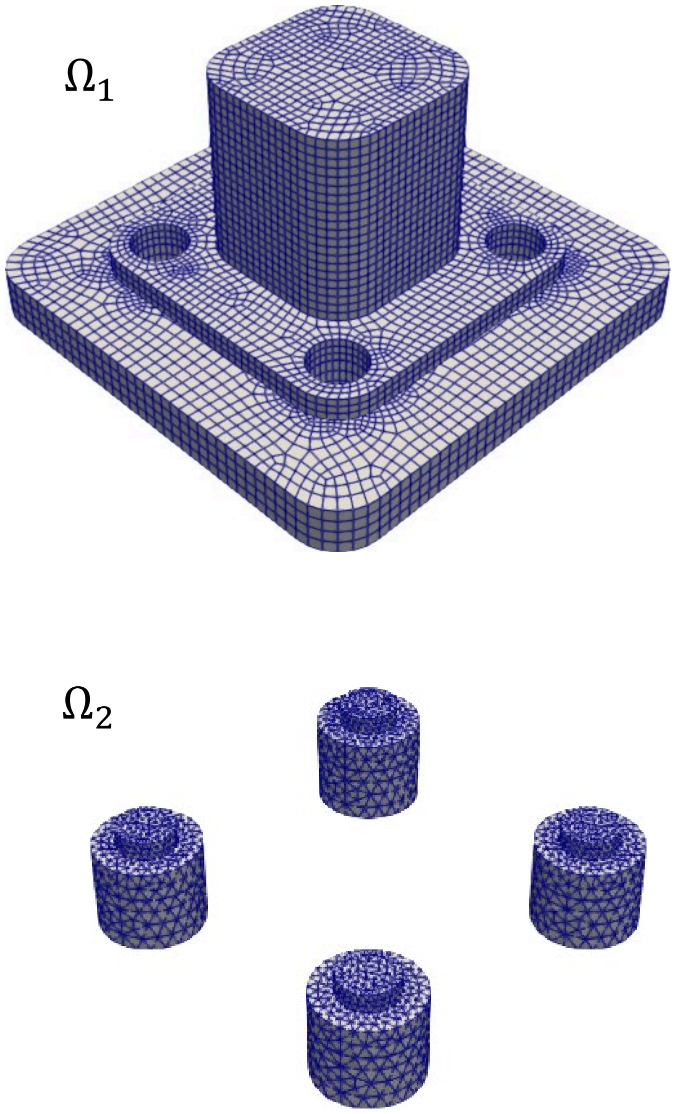
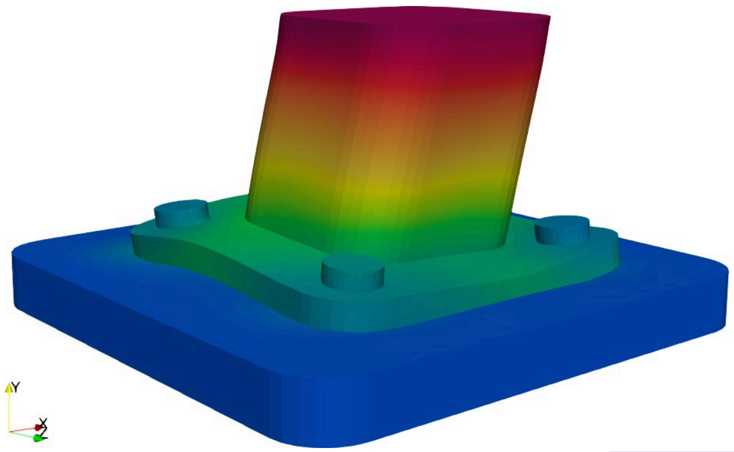


Figure left: convergence w.r.t. basis size for reproductive FOM-COpInf coupling

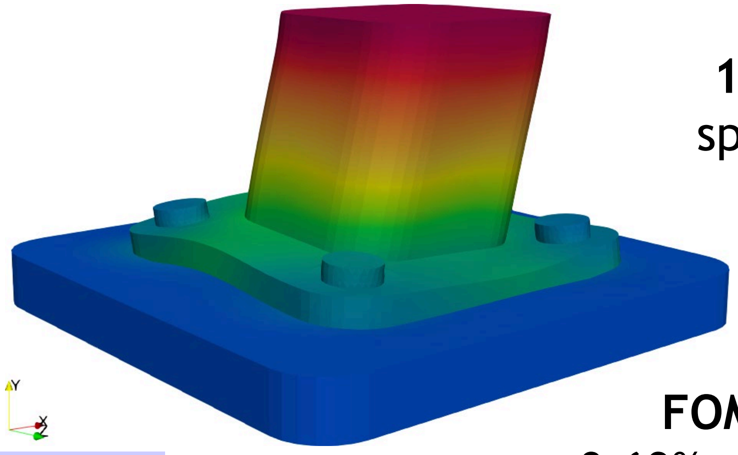


Bolted Joint (Overlapping SAM, Predictive): Displacements

COpInf = Cubic OpInf



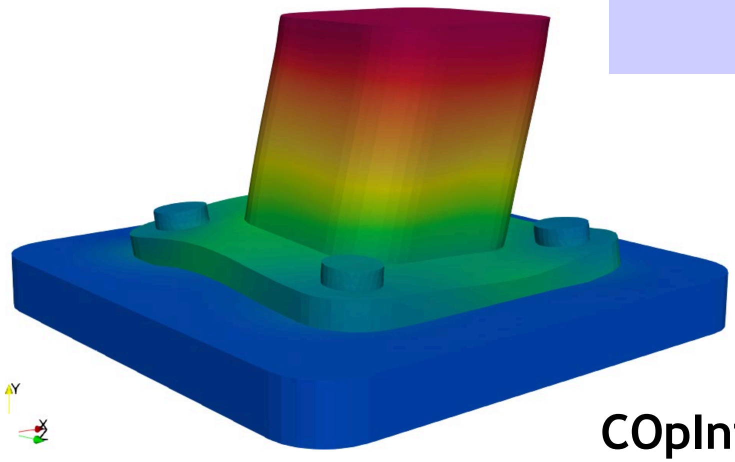
FOM-FOM



1.65×
speedup

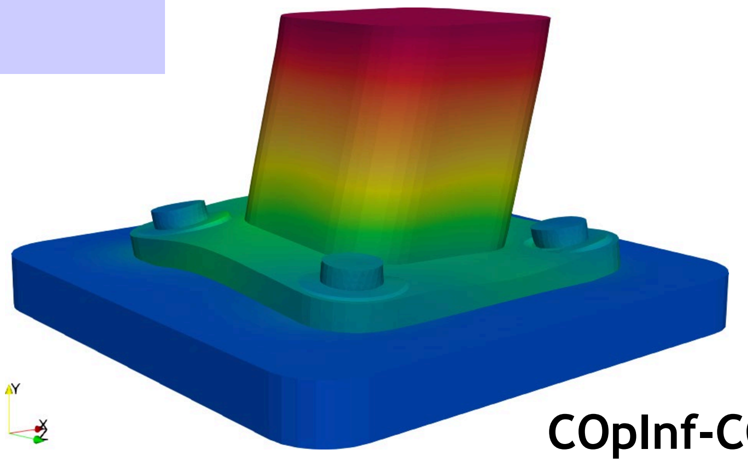
FOM-COpInf
0.69% rel err (parts)
3.51% rel err (bolts)

All models achieve **relative errors** of $\boldsymbol{O}$**(1%)** in **displacement.**



6.12×
speedup

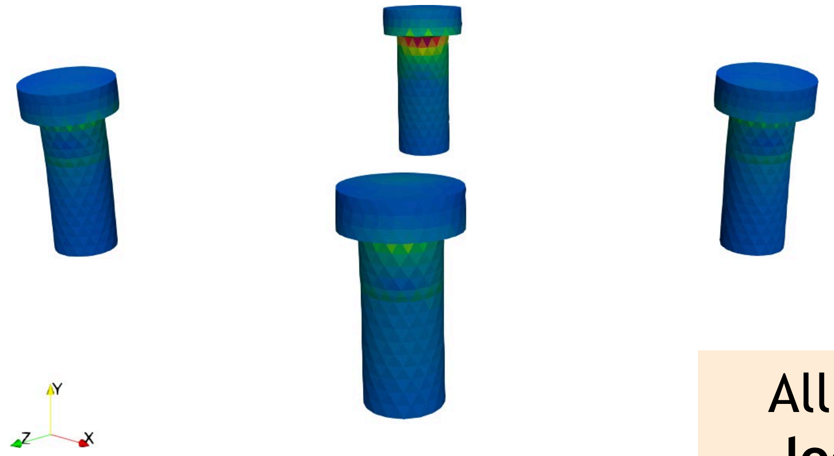
COpInf-COpInf (best)
0.98% rel err (parts)
4.41% rel err (bolts)



COpInf-COpInf (worst)
12.9% rel err (parts)
12.5% rel err (bolts)

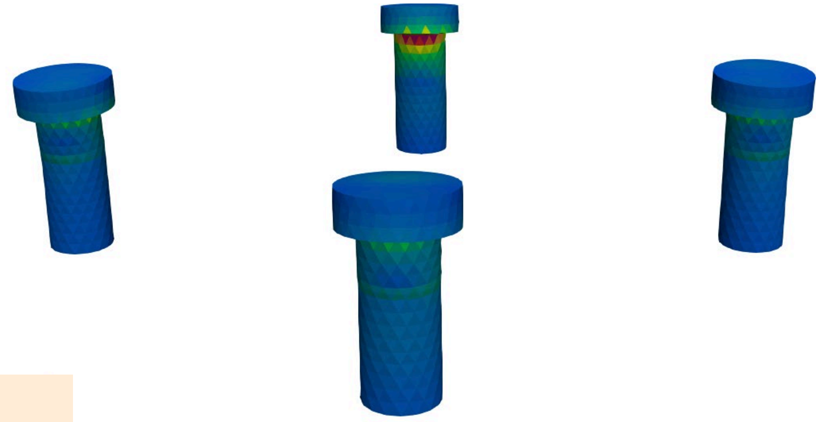
Bolted Joint (Overlapping SAM, Predictive): von Mises Stresses

COpInf = Cubic OpInf



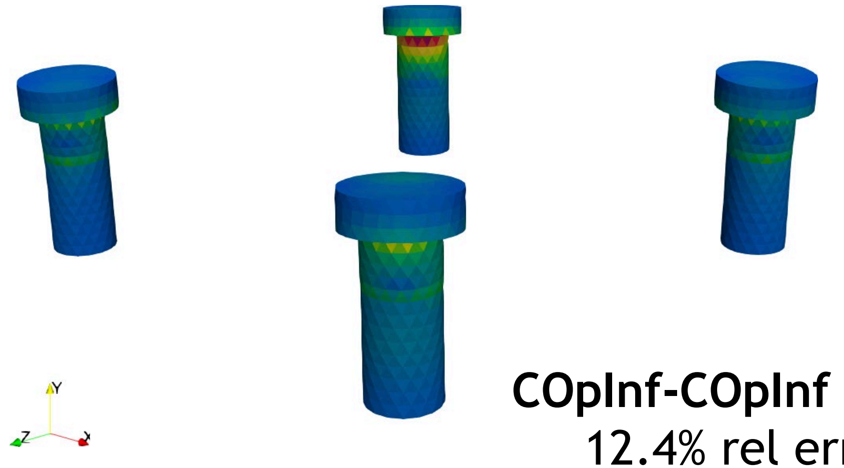
FOM-FOM

1.65× speedup



FOM-COpInf
7.74% rel err

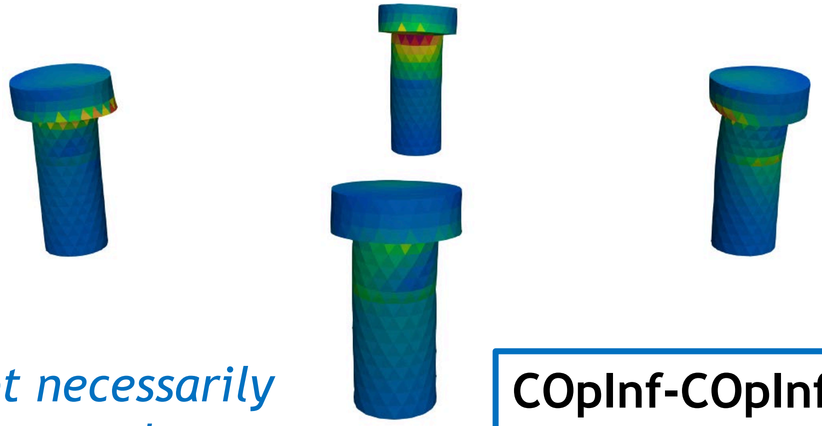
All models **correctly predict locations** of **maximum von Mises stress** (failure).



COpInf-COpInf (best)
12.4% rel error

6.12× speedup

High errors do not necessarily mean result cannot be informative. Know what QOIs are important!



COpInf-COpInf (worst)
30.9% rel error

Work in Progress: SAM-based Coupling for Non-Intrusive NN-based Models

E. Parish

A. Gruber

Motivation: finite deformation mechanics ***does not*** admit a ***polynomial structure***

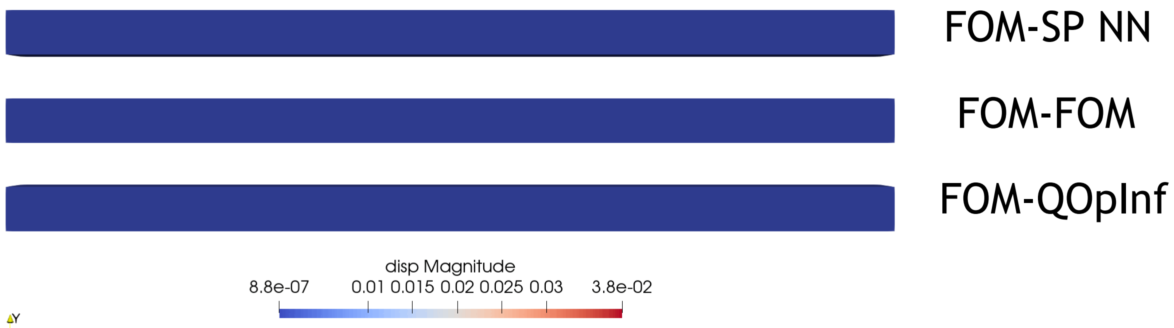
- Limits capacity of polynomial-based OpInf models

Approach: Develop a ***neural-network***-based ***OpInf*** model-reduction strategy

- Can represent ***general nonlinearities***
- Enforces ***structure*** by designing NN operators to parameterize a positive definite stiffness matrix
- ***Fully differentiable ML software*** enables standard and dynamics-constrained training

Pros: Enables accurate models for ***strong nonlinearities***

Cons: Higher ***offline cost***



NN modeling strategy

$$\ddot{\hat{\boldsymbol{q}}}^{NN} + \widehat{\boldsymbol{K}}(\hat{\boldsymbol{q}}^{NN}; \boldsymbol{w}_K) - \widehat{\boldsymbol{B}}(\boldsymbol{u}_i, \hat{\boldsymbol{q}}^{NN}; \boldsymbol{w}_B) = \boldsymbol{0}$$

$\widehat{\boldsymbol{K}}, \widehat{\boldsymbol{B}}$: NN models for stiffness and boundary forcings

$\boldsymbol{w}_K, \boldsymbol{w}_B$: Learnable parameters

Structure is enforced via SPD parameterization of stiffness:

$$\widehat{\boldsymbol{K}} = \hat{\boldsymbol{L}}\widehat{\boldsymbol{D}}\hat{\boldsymbol{L}}^T$$

Enforced structure significantly improves performance

Future work: Hamiltonian parameterizations

Training paradigms

Offline (traditional) training

$$min_{\boldsymbol{w}_K,\boldsymbol{w}_B} \sum_{i=1}^{N}(\ddot{\hat{\boldsymbol{q}}}_i + \widehat{\boldsymbol{K}}(\hat{\boldsymbol{q}}_i; \boldsymbol{w}_K) - \widehat{\boldsymbol{B}}(\boldsymbol{u}_i, \hat{\boldsymbol{q}}_i; \boldsymbol{w}_B))^2$$

Dynamics-constrained training (rollout)

$$min_{\boldsymbol{w}_K,\boldsymbol{w}_B} \sum_{i=1}^{N}(\hat{\boldsymbol{q}}(t_i) - \hat{\boldsymbol{q}}^{NN}(t_i))^2$$

$$\text{s.t. } \ddot{\hat{\boldsymbol{q}}}^{NN} + \widehat{\boldsymbol{K}}(\hat{\boldsymbol{q}}^{NN}; \boldsymbol{w}_K) - \widehat{\boldsymbol{B}}(\boldsymbol{u}_i, \hat{\boldsymbol{q}}^{NN}; \boldsymbol{w}_B) = \boldsymbol{0}$$

References on SAM for FOM-ROM and ROM-ROM Coupling

Schwarz Couplings Involving Non-Intrusive OpInf ROMs:

- I. Moore, C. Wentland, A. Gruber, **I. Tezaur.** "Domain decomposition-based coupling of Operator Inference reduced order models via the Schwarz alternating method", CSRI Summer Proceedings 2024, Sandia National Laboratories. https://arxiv.org/abs/2409.01433

Hot off the press/processor!

- **I. Tezaur,** E. Parish, A. Gruber, I. Moore, C. Wentland, A. Mota. "Hybrid coupling with operator inference and the overlapping Schwarz alternating method". Pre-print, 2025. https://www.sandia.gov/app/uploads/sites/127/2025/11/Schwarz_OpInf_Paper.pdf

- C. Rodriguez, **I. Tezaur**, A. Mota, A. Gruber, E. Parish, C. Wentland. "Transmission Conditions for the Non-Overlapping Schwarz Coupling of Full Order and Operator Inference Models", CSRI Summer Proceedings 2025, Sandia National Laboratories. https://arxiv.org/abs/2509.12228

First application of **non-overlapping** Schwarz to OpInf-FOM and OpInf-OpInf coupling (not in this talk).


I. Tezaur


J. Barnett


I. Moore


E. Parish


C. Wentland


A. Gruber


C. Rodriguez


W. Snyder


G. Sambataro

Outline

Insights, lessons
learned, practical

1. Schwarz Alternating Method (SAM) for Coupling of Full Order Models (FOMs) in Solid Mechanics
   - Motivation & Background
   - Formulation
   - Numerical Examples
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3. **SAM as a Novel Contact Enforcement Met**
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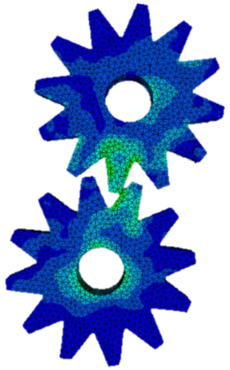
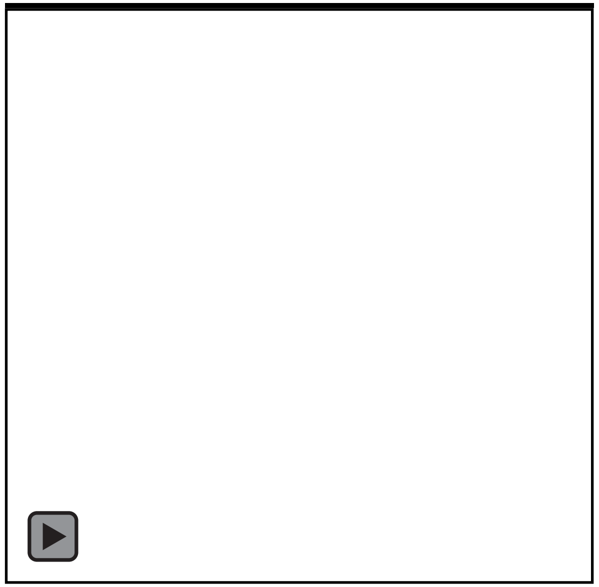
Motivation for Novel Contact Enforcement Algorithm Development

- Stable, accurate and robust methods for simulating **mechanical contact** are extremely important in computational solid mechanics
  - *Example scenarios where contact arises*: touching surfaces, sliding, tightened bolts, impact, …



Above: gears in contact within MEMS device. From *sandia.gov/media.*

Below: oblique cylinder impact simulated using Sandia's ALEGRA code.



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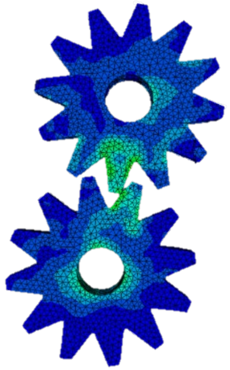

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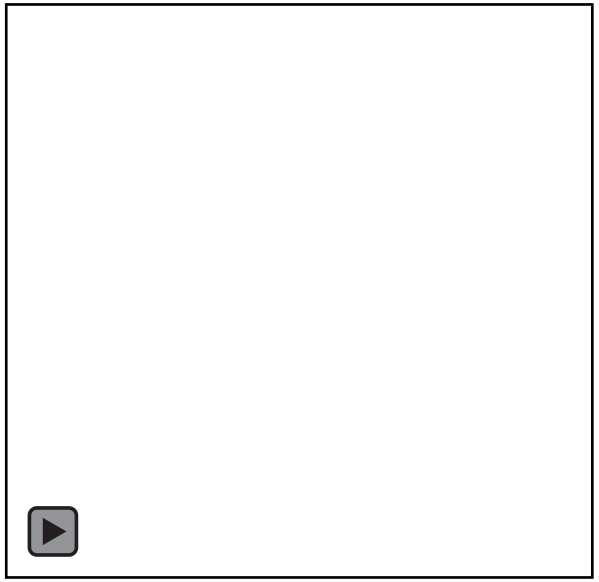

Two-step process to the computational simulation of contact:

1. **Proximity search**

2. **Contact enforcement step**

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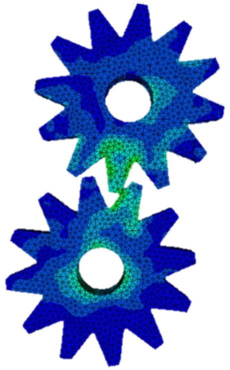

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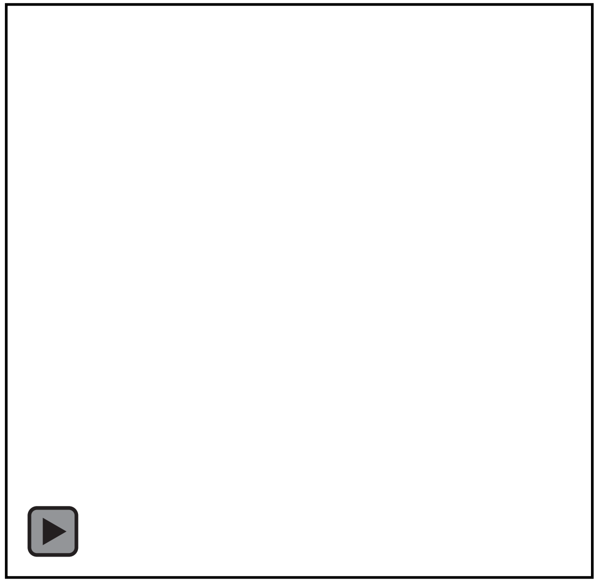

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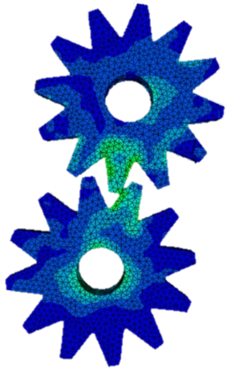

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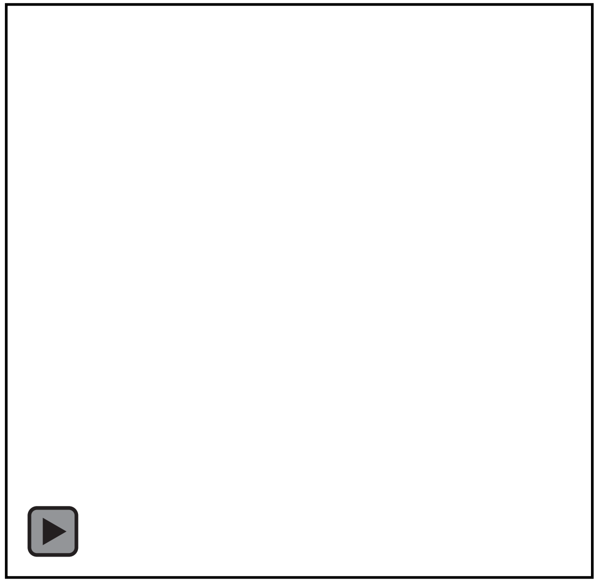

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   - Long simulation times
   - Lack of accuracy
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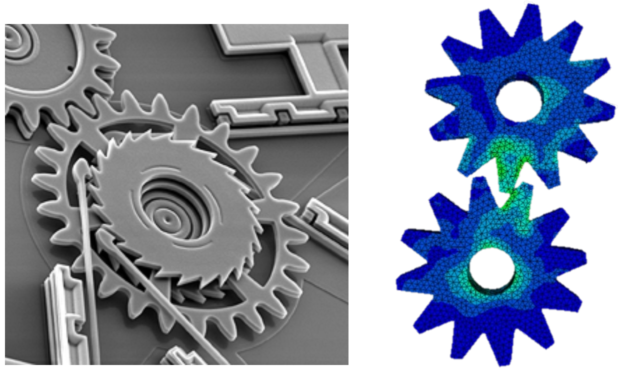

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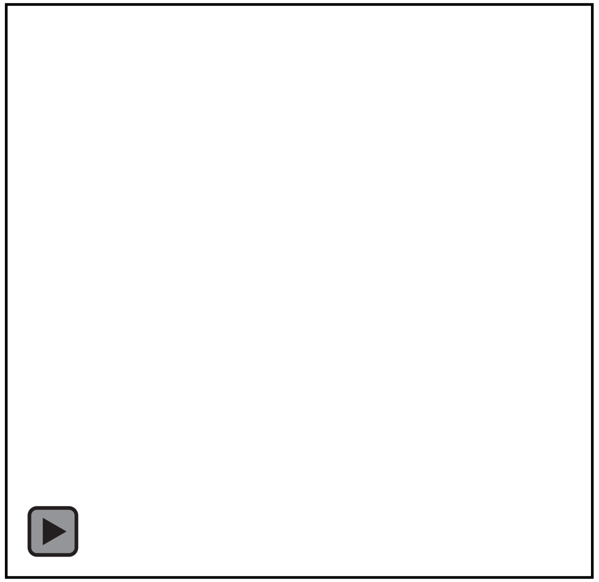

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! *Production codes do not always have the best, most robust methods.*

<u>This talk</u>: new approach for simulating multiscale mechanical contact using the **non-overlapping Schwarz alternating method.**

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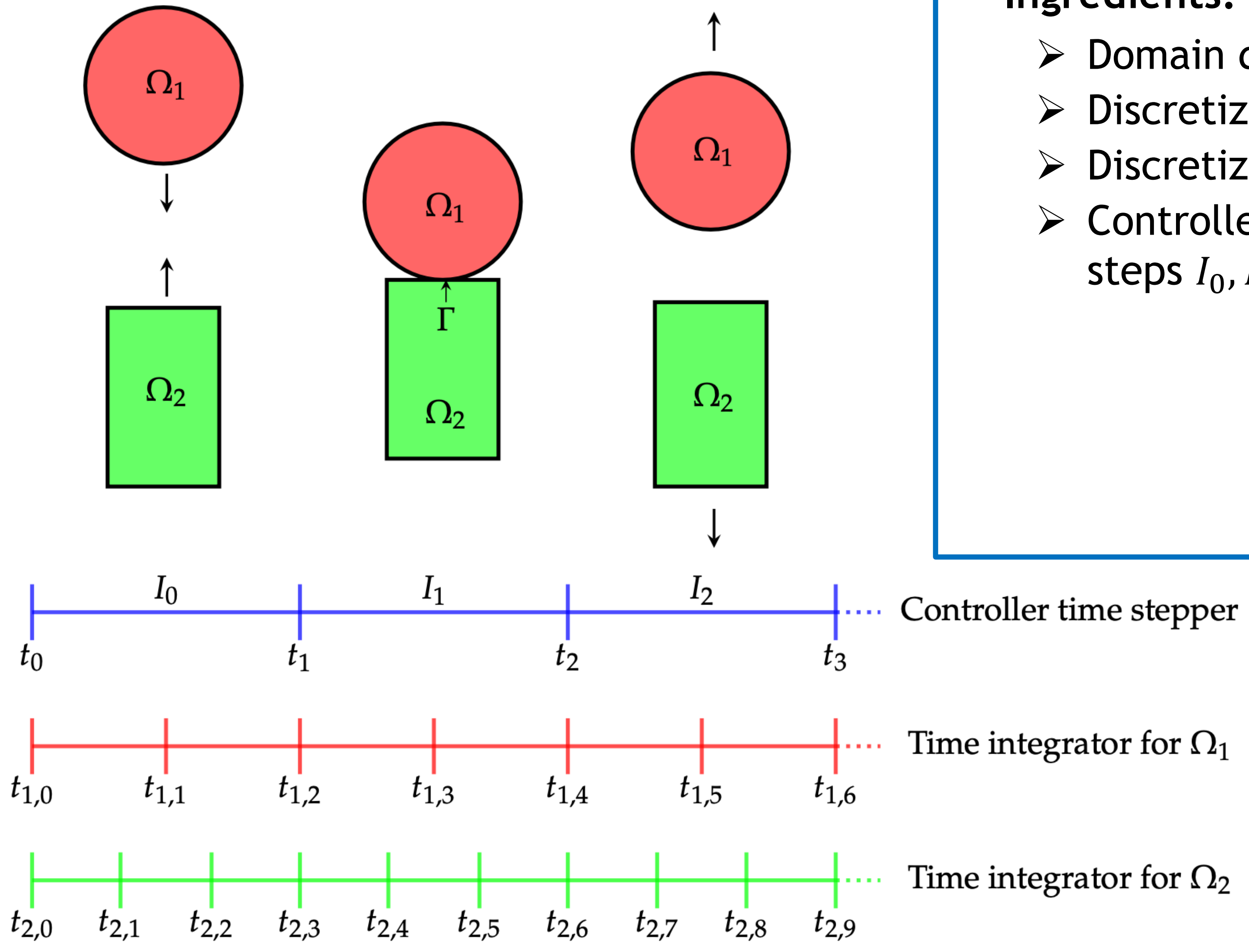
Non-Overlapping Schwarz Contact Formulation



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  - Domain decomposition
  - Discretization and time-stepper in Ω_1 (red)
  - Discretization and time-stepper in Ω_2 (green)
  - Controller time-stepper (blue): defines global time-steps $I_0, I_1, \ldots$ at which subdomains are synchronized

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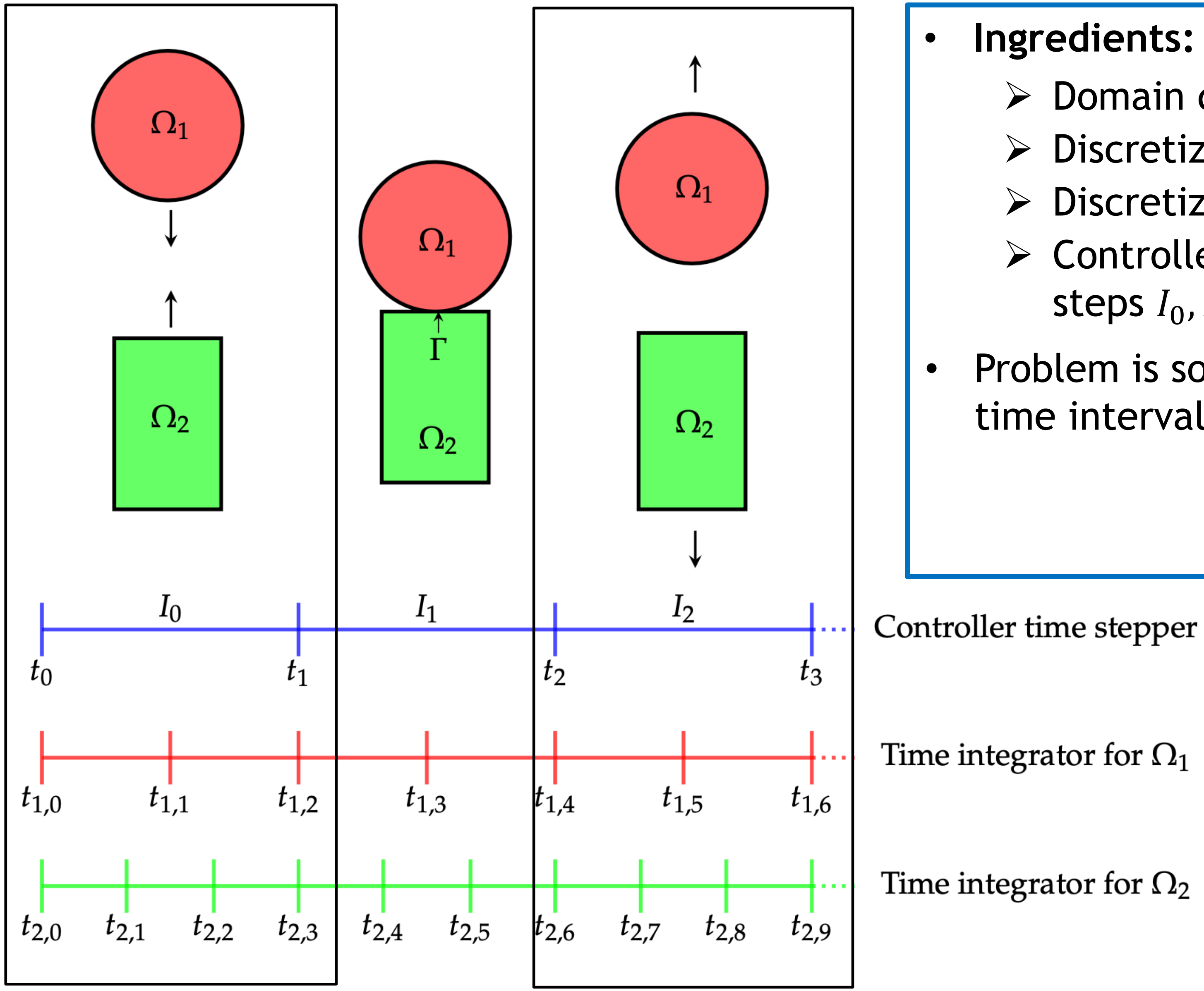

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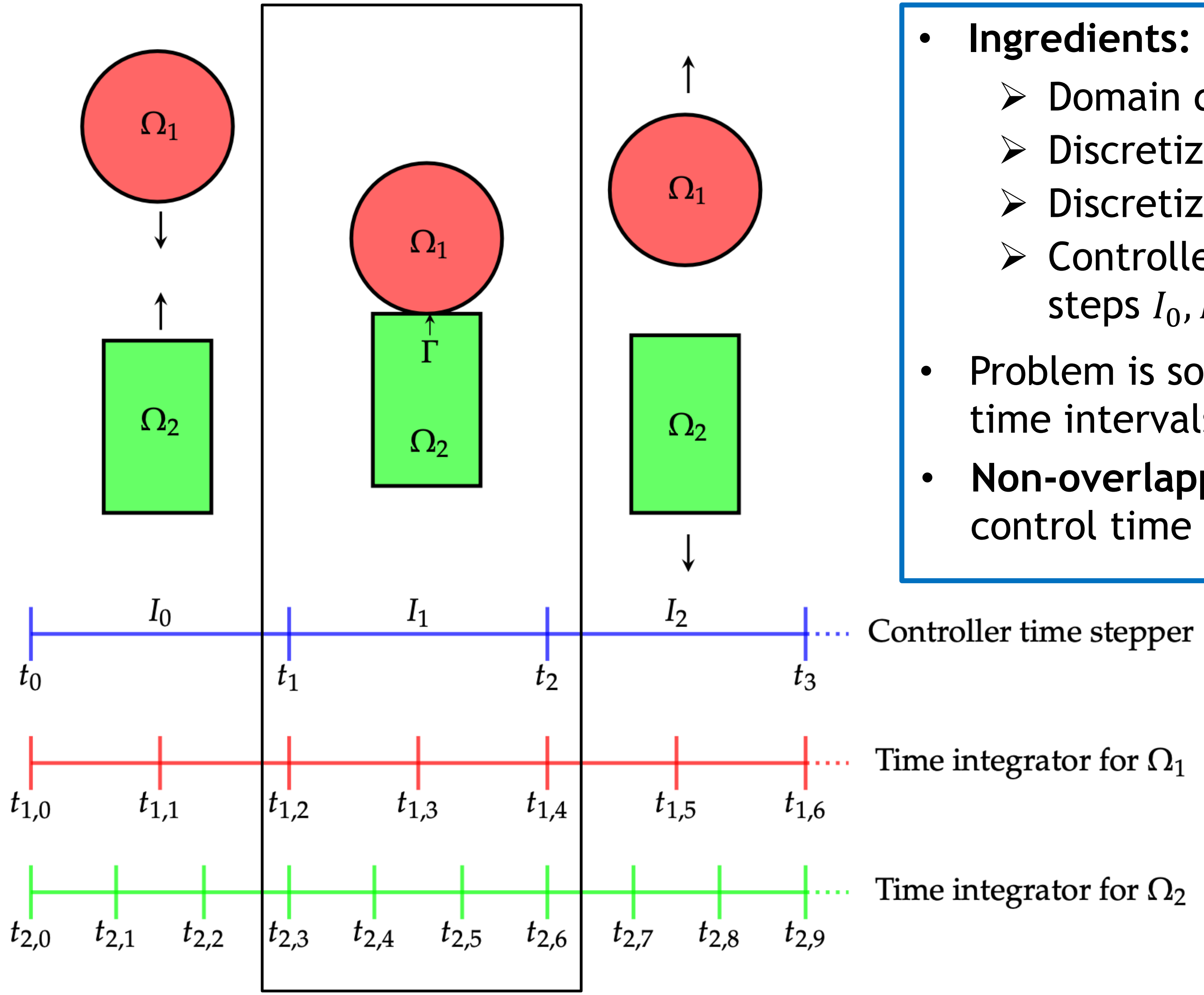

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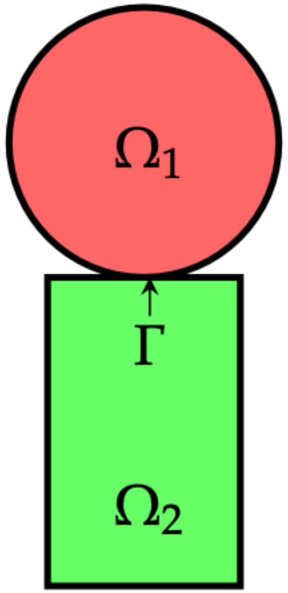
  - Controller time-stepper (blue): defines global time-steps $I_0, I_1, \ldots$ at which subdomains are synchronized
- Problem is solved **without any Schwarz iteration** in time intervals I_0 and I_2, as there is no contact.
- **Non-overlapping Schwarz** algorithm **only applied** in control time interval I_1, when **contact is detected**.

Contact Criteria

- **Overlap:** interpenetration of subdomains
- **Compression:** positive normal traction
- **Persistence:** was in contact previous step

Non-Overlapping Schwarz Contact Formulation

- **Key idea:** a contact problem can be viewed as **coupled problem** while 2+ bodies are in contact
  - ➢ **Alternating** Dirichlet-Neumann (traction) **Schwarz iteration** is applied once interpenetration has been detected, to correct the **interpenetration**.



$$\begin{cases} \mathrm{Div}\boldsymbol{P}^{(n)} + \rho_0 \boldsymbol{B} = \rho_0 \ddot{\boldsymbol{\varphi}}^{(n)}, & \text{in} \quad \Omega_1 \times I_k, \\ \boldsymbol{\varphi}^{(n)}(\boldsymbol{X}, t) = \boldsymbol{\chi}, & \text{on} \quad \partial_{\varphi}\Omega_1 \times I_k, \\ \boldsymbol{\varphi}^{(n)}(\boldsymbol{X}, t) = P_{\Omega_2 \to \Gamma}[\boldsymbol{\varphi}^{(n-1)}(\Omega_2, t_k)], & \text{on} \quad \Gamma \times I_k, \\ \boldsymbol{P}^{(n)}\boldsymbol{N} = \boldsymbol{T}, & \text{on} \quad [\partial_{\boldsymbol{T}}\Omega_1 \cup \Gamma] \times I_k, \end{cases}$$

$$\begin{cases} \mathrm{Div}\boldsymbol{P}^{(n)} + \rho_0 \boldsymbol{B} = \rho_0 \ddot{\boldsymbol{\varphi}}^{(n)}, & \text{in} \quad \Omega_2 \times I_k, \\ \boldsymbol{\varphi}^{(n)}(\boldsymbol{X}, t) = \boldsymbol{\chi}, & \text{on} \quad [\partial_{\varphi}\Omega_2 \cup \Gamma] \times I_k, \\ \boldsymbol{P}^{(n)}\boldsymbol{N} = \boldsymbol{T}, & \text{on} \quad \partial_{\boldsymbol{T}}\Omega_2 \times I_k, \\ \boldsymbol{P}^{(n)}\boldsymbol{N} = P_{\Omega_1 \to \Gamma}[\boldsymbol{T}^{(n)}(\Omega_1, t_k)], & \text{on} \quad \Gamma \times I_k, \end{cases}$$

There are no contact constraints!

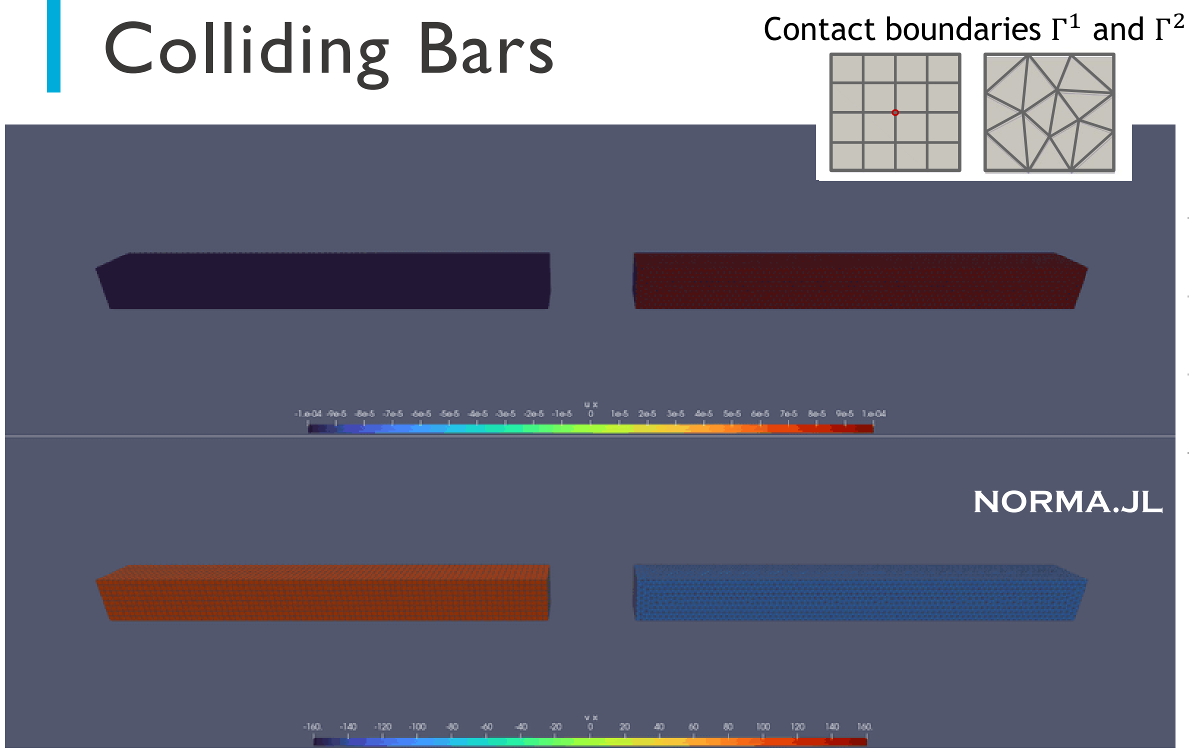
Contact constraints replaced with **BCs** applied **iteratively** at contact boundaries.

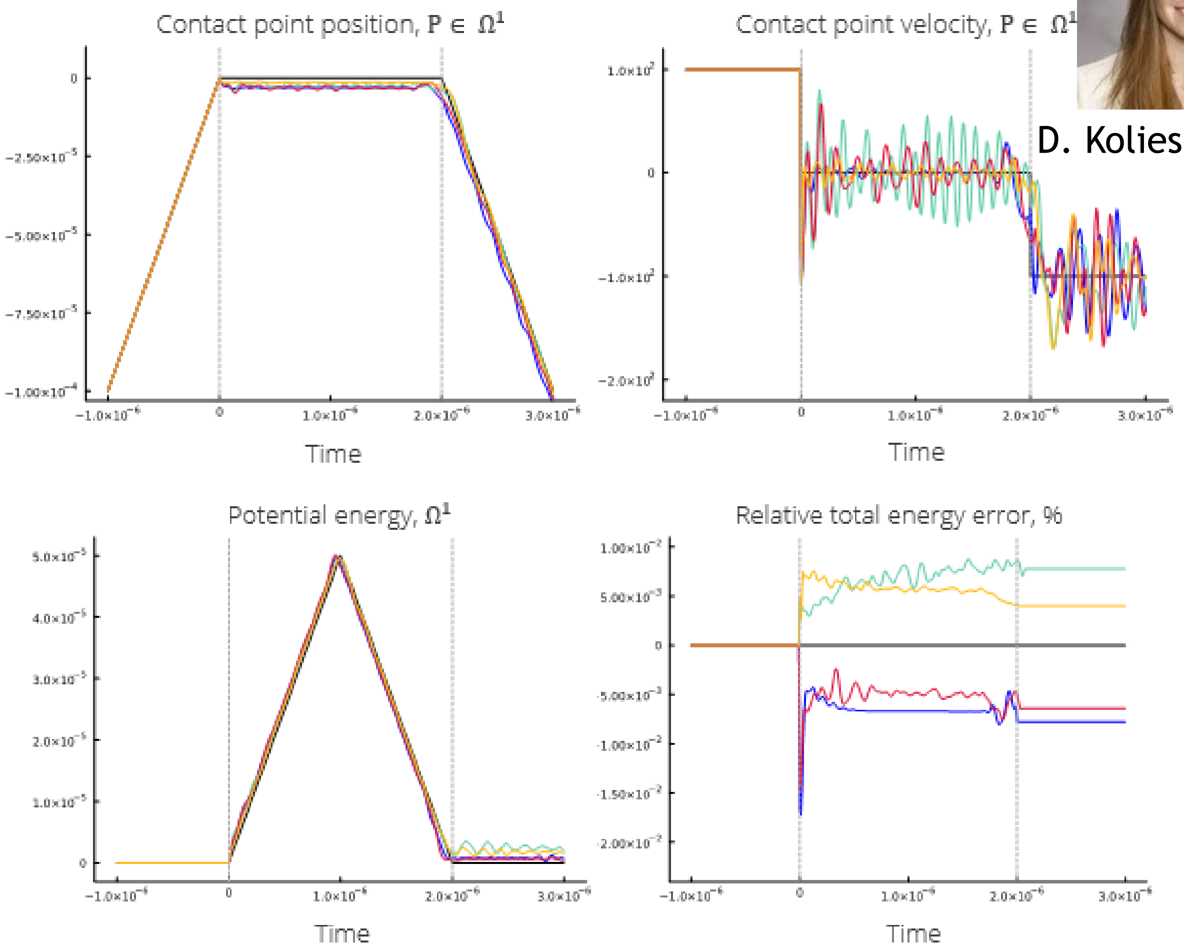
Outline

Insights, lessons learned, practical

1. Schwarz Alternating Method (SAM) for Coupling of Full Order Models (FOMs) in Solid Mechanics
   - Motivation & Background
   - Formulation
   - Numerical Examples
2. SAM for FOM-ROM* and ROM-ROM Coupling in Solid Mechanics
   - Motivation & Background
   - Formulation
   - Numerical Examples
3. **SAM as a Novel Contact Enforcement Met**
   - Motivation & Background
   - Formulation
   - **Numerical Examples**
4. Summary

Colliding Bars





Schwarz provides **more accurate predictions** than conventional methods and demonstrates **exceptional energy conservation** capabilities!

	Elements type		Mesh size		Number of nodes		Time step		Average number of Schwarz iterations
	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	
Imp-Imp Schwarz	HEX8	HEX8	$1/2 \cdot 10^{-4}$		189		$1 \cdot 10^{-8}$		7
Exp-Exp Schwarz	TETRA4	TETRA4	$1/2 \cdot 10^{-4}$		199		$1 \cdot 10^{-9}$		6
Imp-Exp Schwarz	HEX8	TETRA4	$1/2 \cdot 10^{-4}$		189	199	$1/2 \cdot 10^{-8}$	$1 \cdot 10^{-9}$	6
Exp-Imp Schwarz	HEX8	TETRA4	$1/4 \cdot 10^{-4}$	$1/3 \cdot 10^{-4}$	1025	745	$1 \cdot 10^{-9}$	$1/2 \cdot 10^{-8}$	8

Chatter can be mitigated via **"naïve" stabilization approach** which sets contact accelerations to 0 [Mota, Koliesnikova, **IT**, *et al.*, 2025].

References on SAM for Contact

- J. Hoy, **I. Tezaur**, A. Mota. "The Schwarz alternating method for multiscale contact mechanics". in *Computer Science Research Institute Summer Proceedings 2021*, J.D. Smith and E. Galvan, eds., Technical Report SAND2021-0653R, Sandia National Laboratories, 360-378, 2021.

- A. Mota, D. Koliesnikova, **I. Tezaur**, J. Hoy. "A Fundamentally New Coupled Approach to Contact Mechanics via the Dirichlet-Neumann Schwarz Alternating Method", *Int. J. Numer. Meth. Engng.*, 126(9) e70039, 2025.

I. Tezaur

A. Mota

D. Koliesnikova

B. Phung

J. Hoy

Outline

Insights, lessons learned, practical

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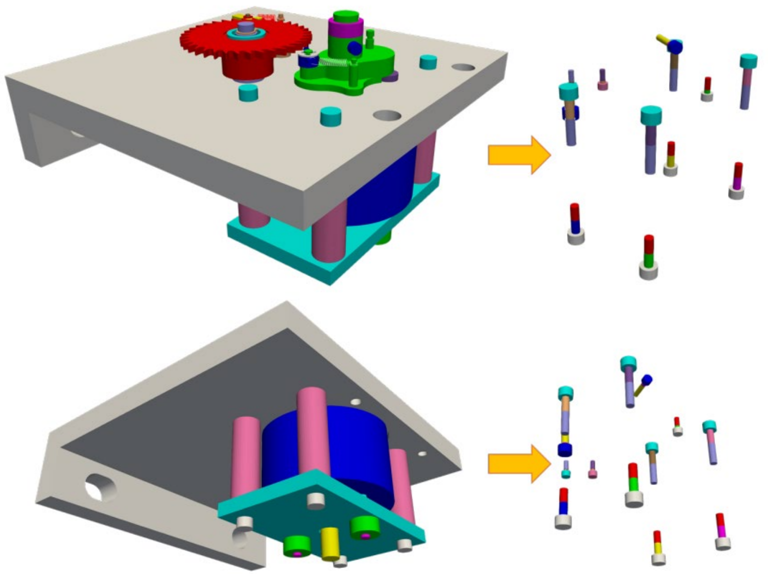
4. **Summary**

Summary

The **Schwarz alternating method** has been developed for concurrent multiscale coupling of **conventional** and **data-driven models,** and as a **novel contact enforcement** algorithm.

- ☺ 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 (including ROM/FOM)*** and ***time-integrators*** in different regions.
- ☺ ***Scalable***, ***fast***, ***robust*** on ***real*** engineering problems
- ☺ Coupling does not introduce ***nonphysical artifacts***.
- ☺ ***Theoretical*** convergence properties/guarantees.
- ☺ A ***promising alternative*** to conventional ***contact*** methods

Practical Takeaways Summary

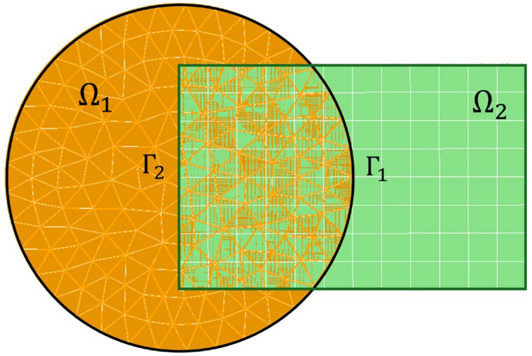


- *Meshing is no joke!*
- *Implementation is a big deal!*
  - ➢ Legacy production codes can be around for decades
- *Online speedups are not everything!*
  - ➢ "Fast is fine, but accuracy is everything." – Wyatt Earp
- *Know your target!*
  - ➢ Assess your methods in terms of QOIs relevant to your users/customers

- *Have pity on whoever is using your method!*
  - ➢ *Important considerations*: usability, robustness, minimal tuning knobs/parameters, etc.
- *There <u>is</u> room for new methods/innovation even in a mission-focused production setting!*

"We've made this elegantly simple app so complicated with features that no one knows how to use it."

Thank you! Questions?



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LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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Call For Papers: Special Issue on Controversies on the Usage of AI/ML for Science and Engineering

CiSE seeks submissions for this upcoming special issue.

Contact: Irina Tezaur
ikalash@sandia.gov

Due date: Jan. 21, 2026

Publication date: Summer-Fall 2026

Goal: Give authors the opportunity to present their perspectives on **potentially controversial topics** involving the **usage of AI/ML** in **science** and **engineering applications**.

Authors are encouraged to include ideas on how to resolve perceived controversies and/or address/mitigate the challenges/open questions these controversies relate to.

Anticipated contributions:

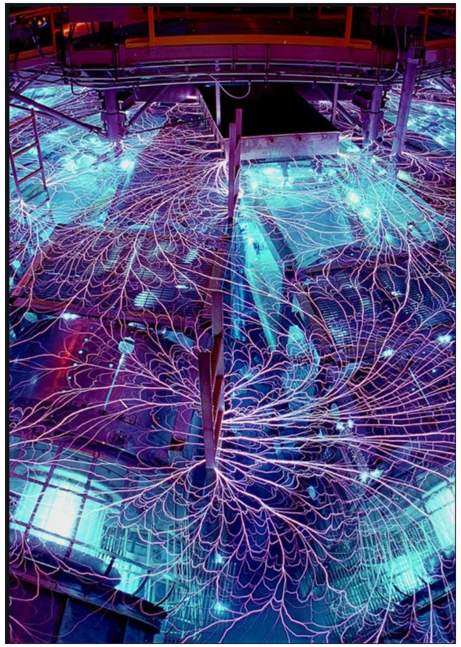
- **Research papers** describing new methods/frameworks in the context of this special issue's theme
- **Survey papers** evaluating/comparing existing methods
- Higher-level evidence-based **position papers**

About Sandia National Laboratories

Akin to

LNCC
Laboratório Nacional de Computação Científica

in Brazil



- Sandia is a **multi-mission** national lab aimed at advancing **U.S. national security**
- 1 of 3 U.S. Department of Energy's (**DOE's**) National Nuclear Security Administration (**NNSA**) R&D labs (along with **Lawrence Livermore** and **Los Alamos**)
- **Two main sites**: Albuquerque, NM and Livermore, CA

Theory: Overlapping SAM for Quasistatic Multiscale Coupling*

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 $\left\{\tilde{\varphi}^{(n)}\right\}$ 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 $\tilde{\varphi}^{(0)}$.*

* Mota, **IT,** *et al.*, 2017.

Theory: Overlapping SAM for Dynamic Multiscale Coupling*

- Like for quasistatics, dynamic alternating Schwarz method converges provided each single-domain problem is ***well-posed*** and ***overlap region*** is ***non-empty***, under some ***conditions*** on Δt.
- ***Well-posedness*** for the dynamic problem requires that action functional $S[\boldsymbol{\varphi}] := \int_I \int_\Omega L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) dV dt$ be ***strictly convex*** or ***strictly concave***, where $L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) := T(\dot{\boldsymbol{\varphi}}) + V(\boldsymbol{\varphi})$ is the Lagrangian.
  - ➢ This is studied by looking at its second variation $\delta^2 S[\boldsymbol{\varphi}_h]$
- We can show assuming a ***Newmark*** time-integration scheme that for the ***fully-discrete*** problem:

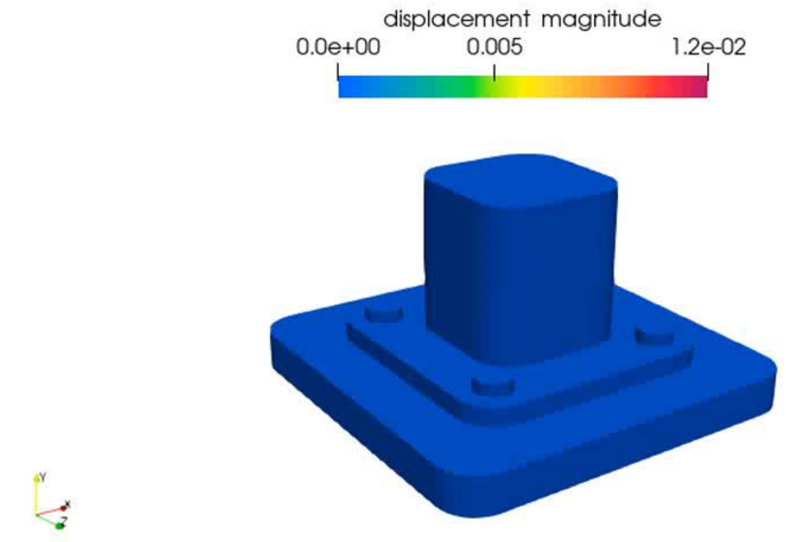
$$\delta^2 S[\boldsymbol{\varphi}_h] = \boldsymbol{x}^T \left[\frac{\gamma^2}{(\beta \Delta t)^2} \boldsymbol{M} - \boldsymbol{K} \right] \boldsymbol{x}$$

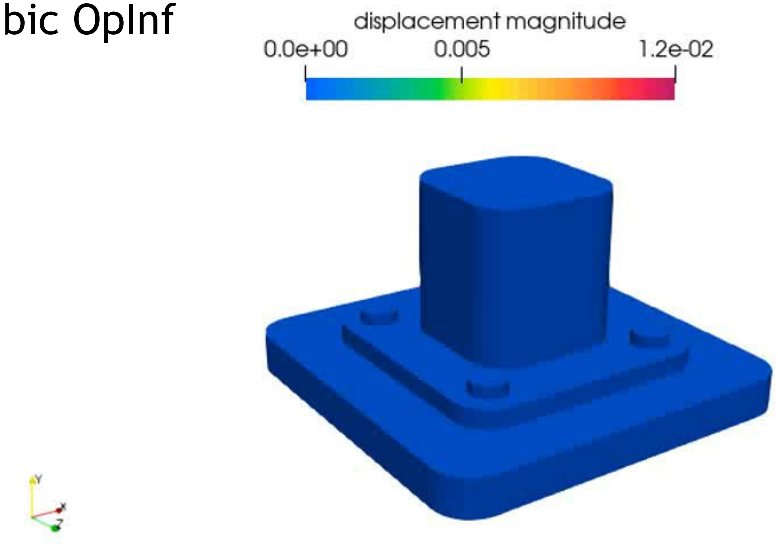
  - ➢ $\delta^2 S[\boldsymbol{\varphi}_h]$ can always be made positive by choosing a ***sufficiently small*** Δt
  - ➢ Numerical experiments reveal that Δt requirements for ***stability/accuracy*** typically lead to automatic satisfaction of this bound.

* Mota, **IT**, *et al.*, 2022.

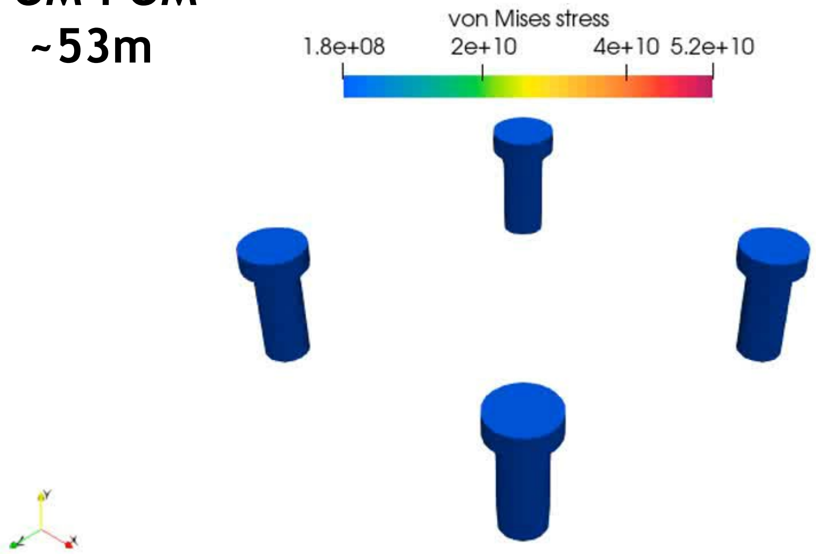
Bolted Joint (Overlapping SAM, Predictive): Animations

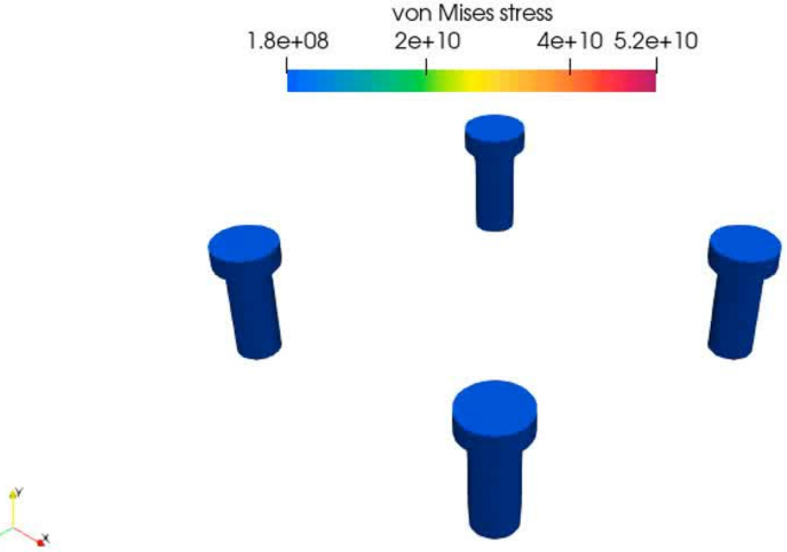
COpInf = Cubic OpInf





FOM-FOM
~53m





COpInf-COpInf
~8.5m

References on SAM for FOM-ROM and ROM-ROM Coupling (cont'd)

Schwarz Couplings Involving Intrusive Projection-Based ROMs:

- J. Barnett, **I. Tezaur**, A. Mota. "The Schwarz alternating method for the seamless coupling of nonlinear reduced order models and full order models", CSRI Summer Proceedings 2023, Sandia National Laboratories. https://arxiv.org/abs/2210.12551
- C. Wentland, F. Rizzi, J. Barnett, **I. Tezaur**. "The role of interface boundary conditions and sampling strategies for Schwarz-based coupling of projection-based reduced order models", *J. Comput. Appl. Math.*, 465 116584, 2025

Schwarz Couplings Involving Physics-Informed Neural Networks (PINNs):

- W. Snyder, **I. Tezaur**, C. Wentland. "Domain decomposition-based coupling of PINNs via the Schwarz alternating method", CSRI Summer Proceedings 2023, Sandia National Laboratories. https://arxiv.org/abs/2311.00224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E. Parish


C. Wentland


A. Gruber


C. Rodriguez

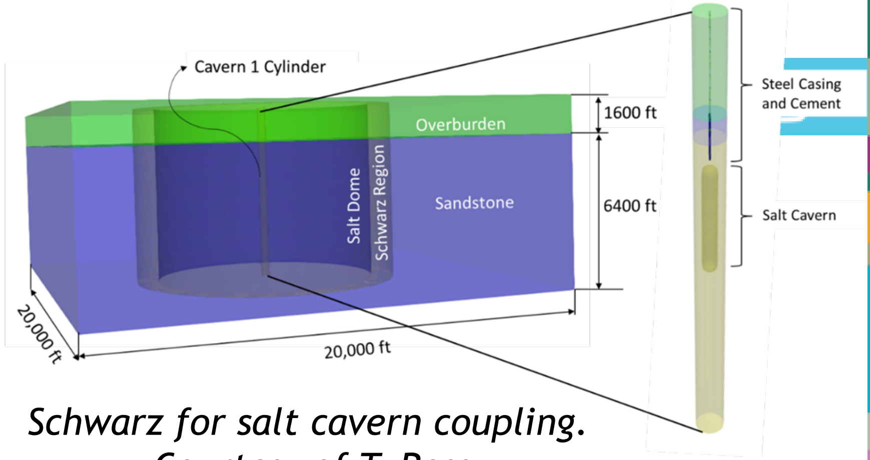

W. Snyder


G. Sambataro

Current Research Directions

Production Applications

- 4-way multiscale coupling in salt caverns for Strategic Petroleum Reserve (SPR)
- Schwarz coupling for J-integral around crack front on pressure vessel
- Multiscale coupling for stronglinks
- Schwarz multiphysics coupling for electronics package survivability



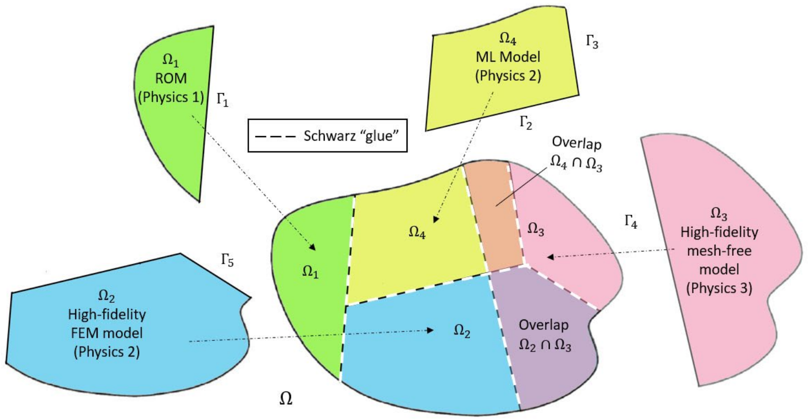
Schwarz for salt cavern coupling. Courtesy of T. Ross.

Performance Improvements

- Acceleration of Schwarz
- Asynchronous additive Schwarz on GPUs

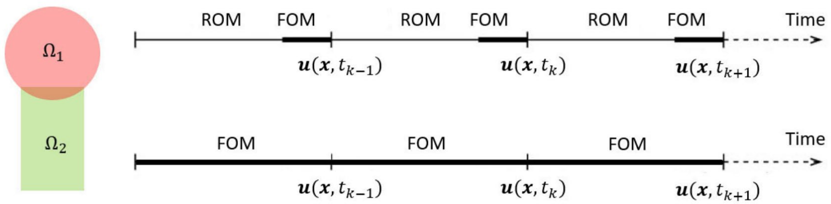
Automated & Adaptive Schwarz

- Automated optimization of meshes/DD with multiple constraints
- Automated criteria to determine appropriate use of less refined or reduced-order models w/o sacrificing accuracy

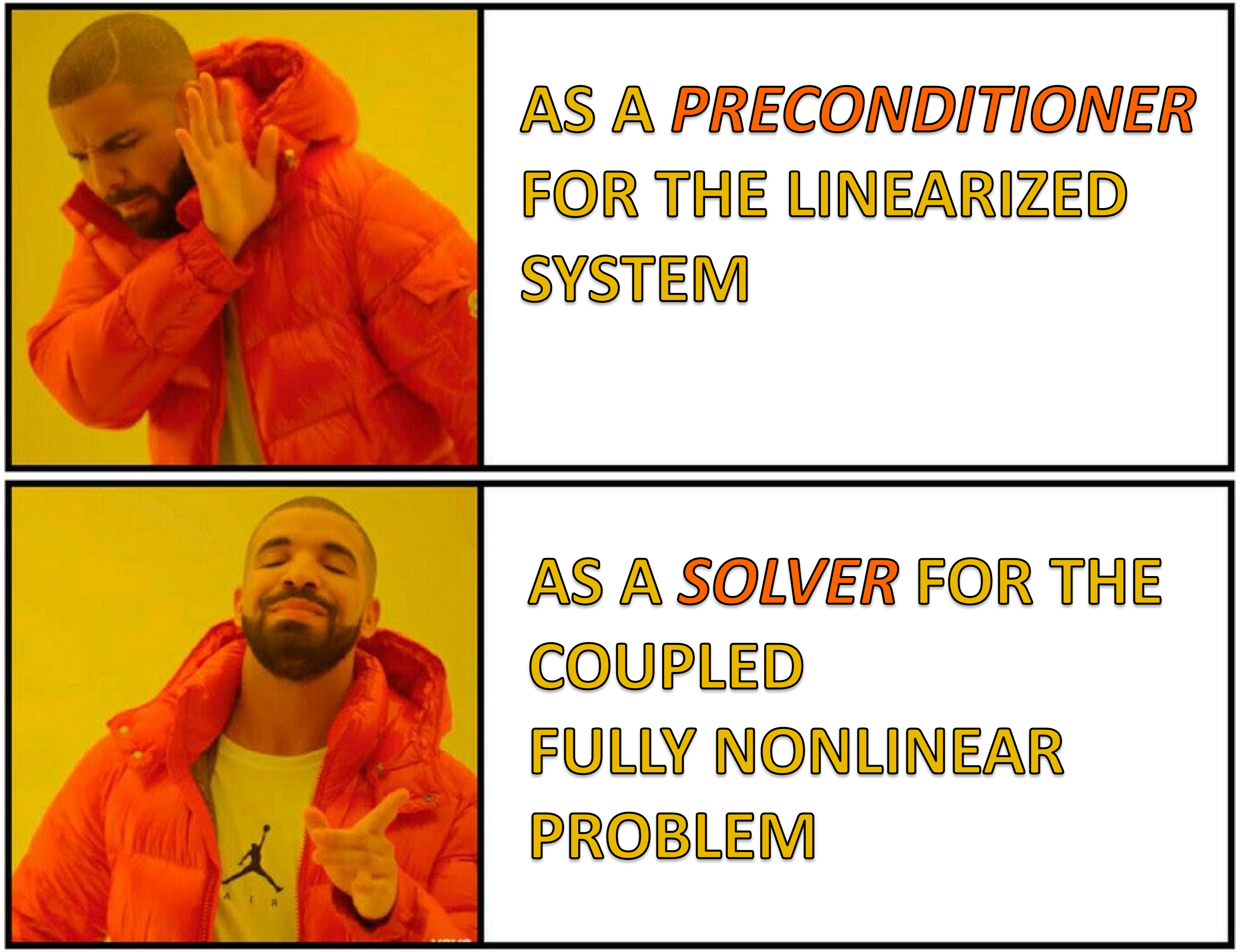


Schwarz for ROM/Data-Driven Model Coupling

- Non-overlapping Schwarz + OpInf
- Schwarz + Deep NN-based ROMs
- Schwarz + kernel-based ROMs
- Fully non-intrusive ROM-FOM coupling (w/ K. Willcox & N. Aretz, UT Austin)
- On-the-fly switching between ROMs and FOMs
- Implementation in SIERRA/SM



How We Use the Schwarz Alternating Method

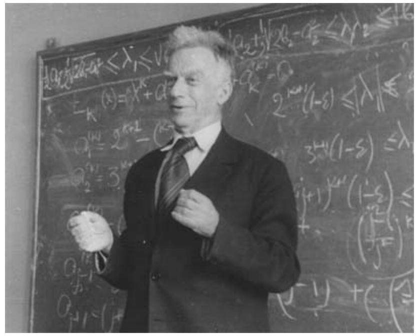


Theoretical Foundation

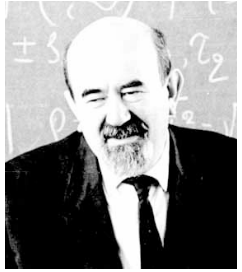
Using the Schwarz alternating as a ***discretization method*** for PDEs is natural idea with a sound ***theoretical foundation***.

- 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.
- P.-L. Lions (1988): studied convergence of Schwarz for ***nonlinear monotone elliptic problems*** using max principle.
- A. Mota, I. Tezaur, C. Alleman (2017): proved ***convergence*** of the alternating Schwarz method for ***finite deformation quasi-static nonlinear PDEs*** (with energy functional $\boldsymbol{\Phi}[\boldsymbol{\varphi}]$) with a ***geometric convergence rate***.

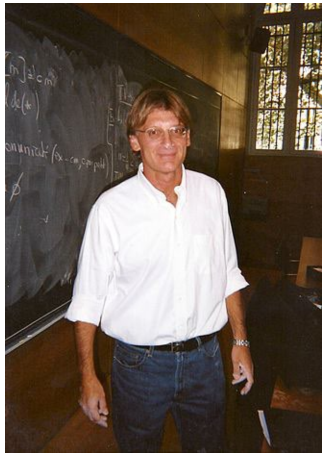
$$\boldsymbol{\Phi}[\boldsymbol{\varphi}] = \int_B A(\boldsymbol{F},\boldsymbol{Z})\,dV - \int_B \boldsymbol{B}\cdot\boldsymbol{\varphi}\,dV$$
$$\nabla\cdot\boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



S.L. Sobolev (1908 – 1989)



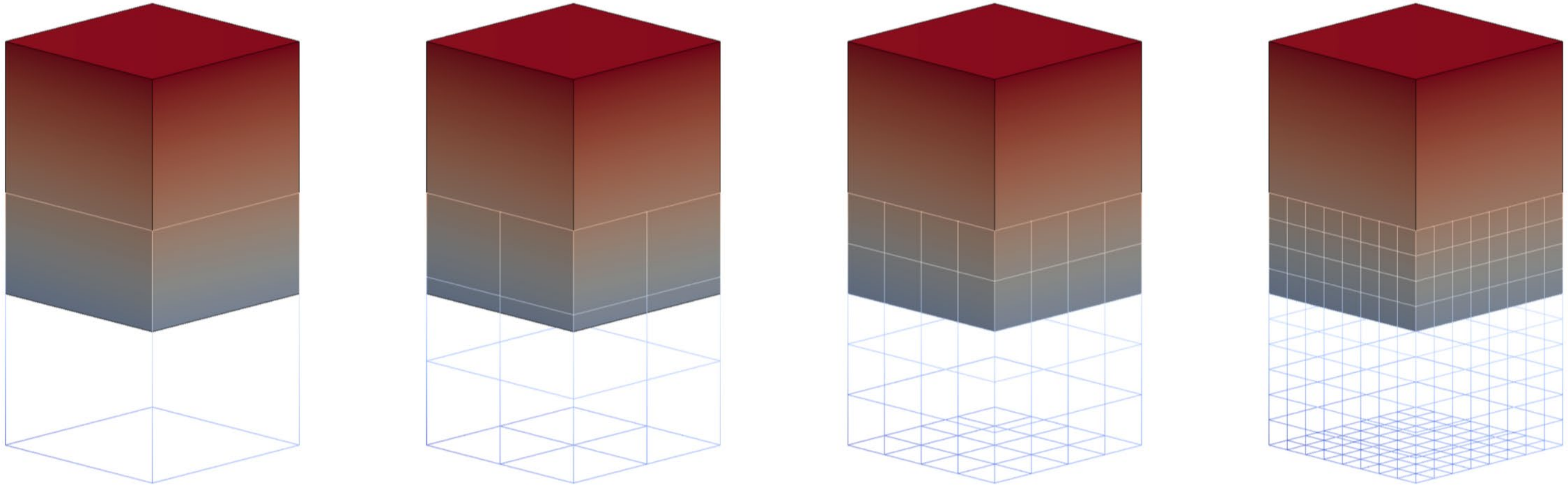
S.G. Mikhlin (1908 – 1990)



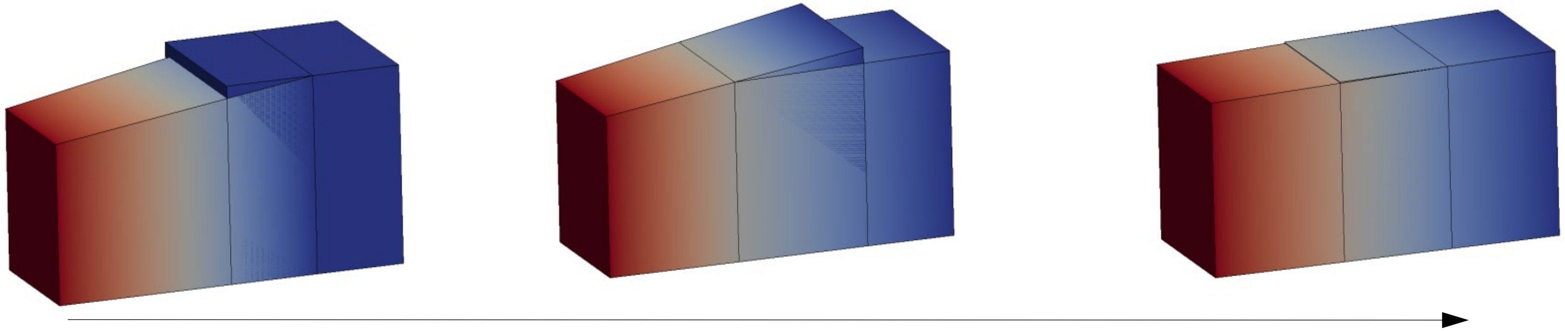
P.- L. Lions (1956-)

A. Mota, I. Tezaur, C. Alleman

Cuboid Problem



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



Schwarz Iteration

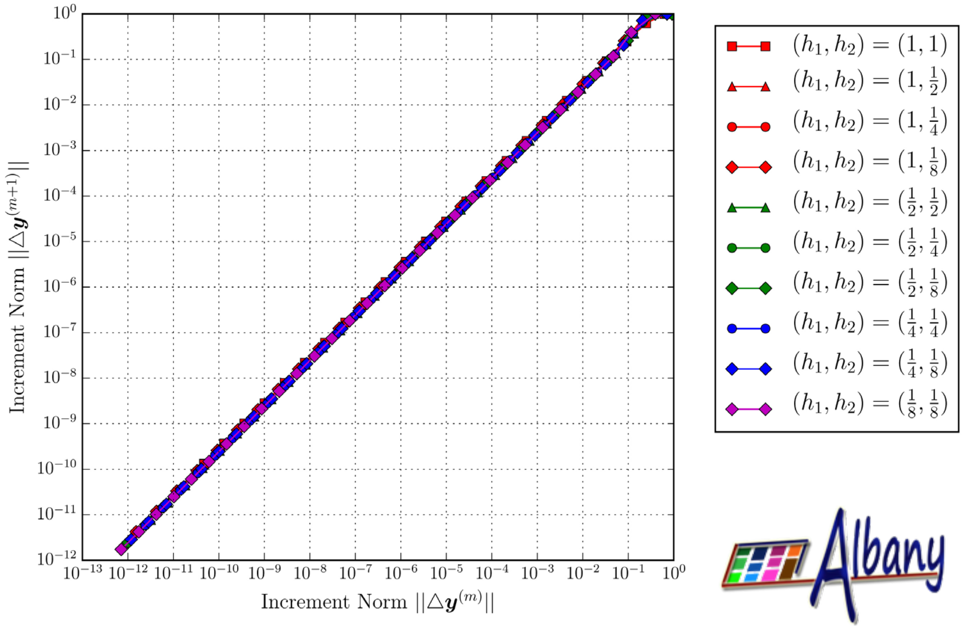
Cuboid Problem: Convergence and Accuracy

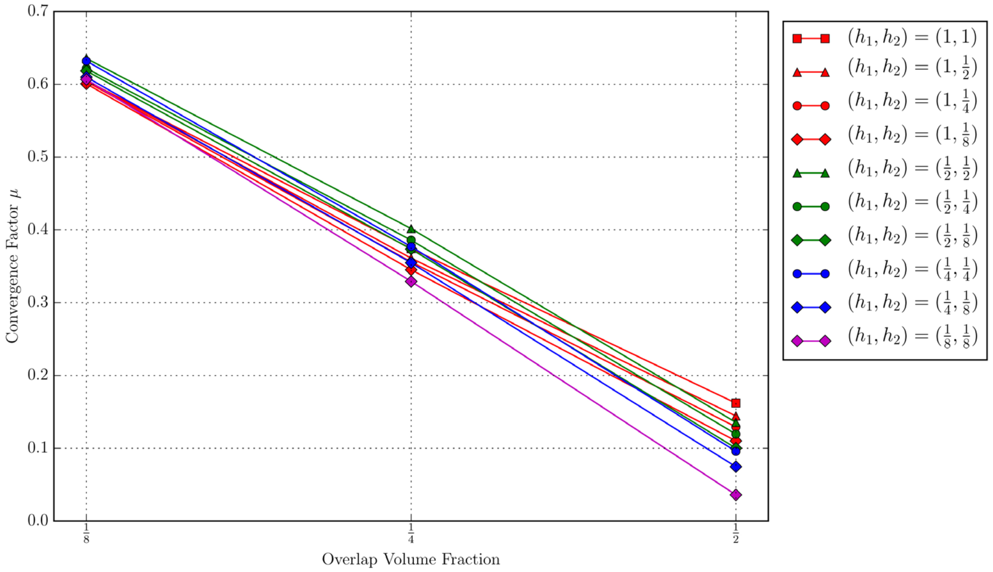
- **Top right:** convergence of the cuboid problem for ***different mesh sizes*** and ***fixed overlap volume fraction***. The Schwarz alternating method converges ***linearly***.
- **Bottom right:** convergence factor μ as a function of overlap volume and different mesh. There is ***faster linear convergence***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

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

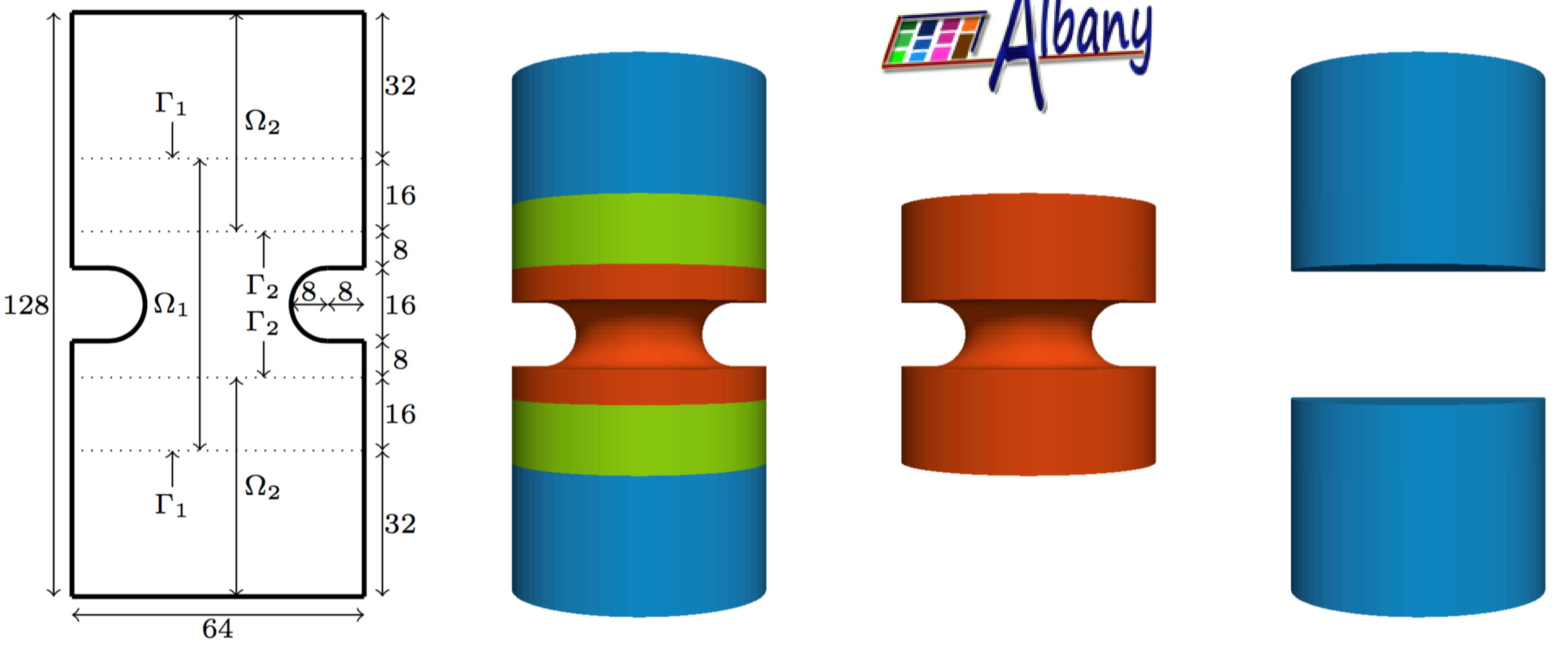
- **Below:** ***relative errors*** in displacement and stress w.r.t. single-domain reference solution. Errors are on the order of ***machine precision***.

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





Notched Cylinder



(a) Schematic **(b)** Entire Domain Ω **(c)** Fine Region Ω_1 **(d)** Coarse Region Ω_2

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

Notched Cylinder: Coupling Different Materials

The Schwarz method is capable of coupling regions with ***different material models***.

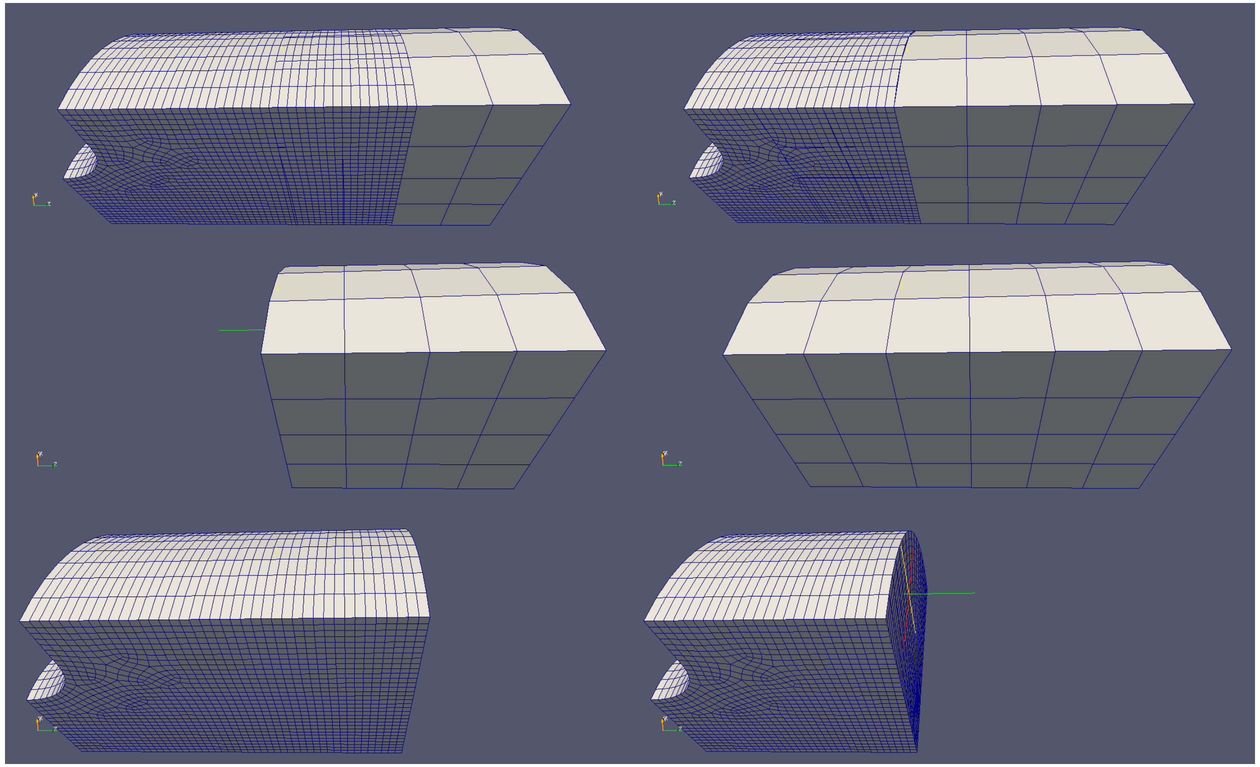
- Notched cylinder subjected to tensile load with an ***elastic*** and ***J2 elasto-plastic*** regions.
- ***Coarse*** region is ***elastic*** and ***fine*** region is ***elasto-plastic***.
- The ***overlap region*** in the first mesh is nearer the notch, where plastic behavior is expected.

Overlap far from notch. Overlap near notch.

Coupled regions

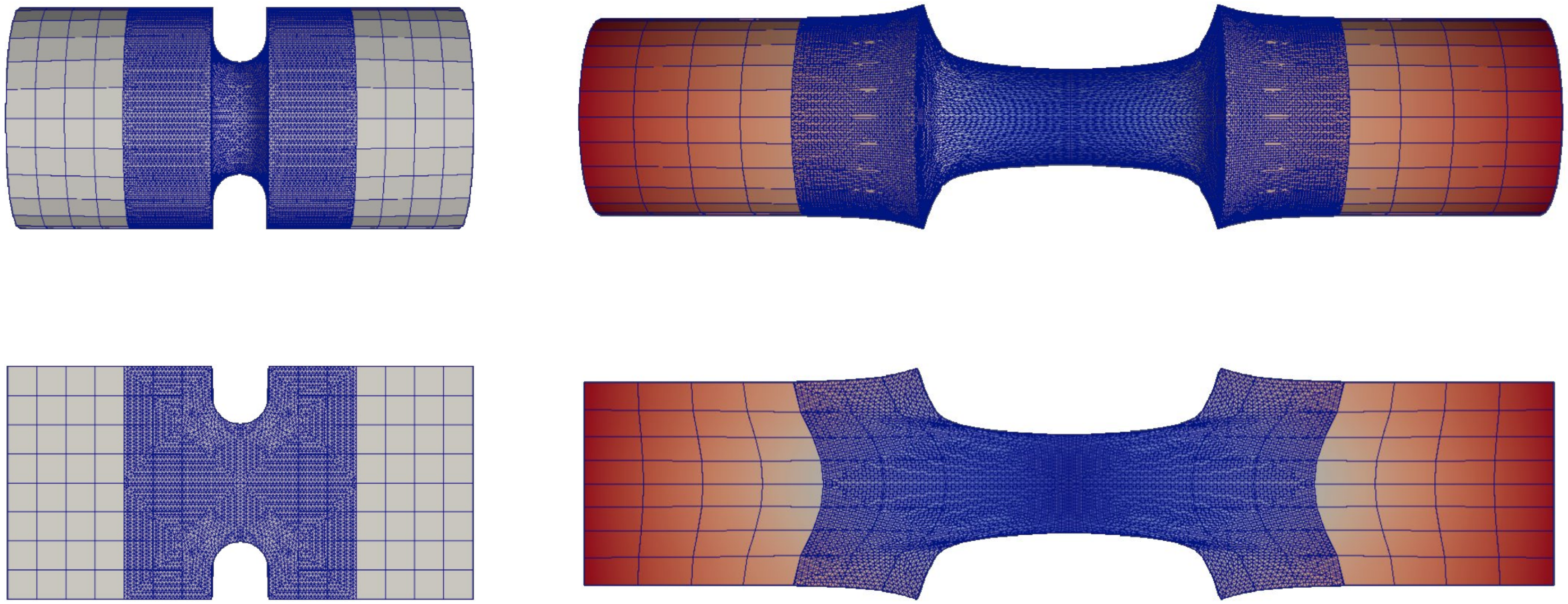
Coarse, elastic region

Fine, elasto-plastic region

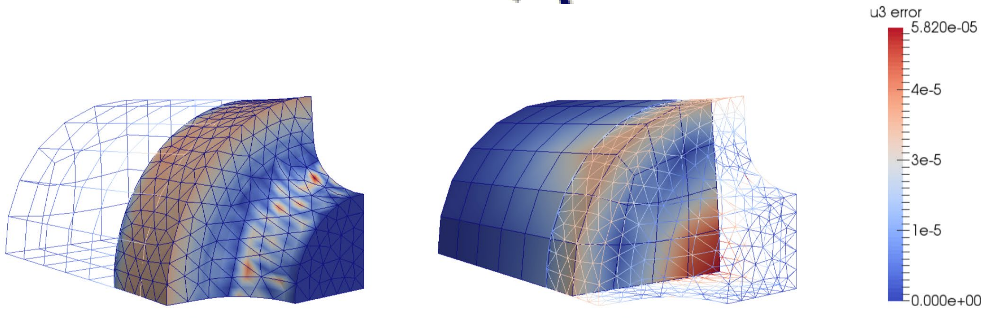


Notched Cylinder: TET - HEX Coupling

- 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



(a) Ω_1 **(b)** Ω_2

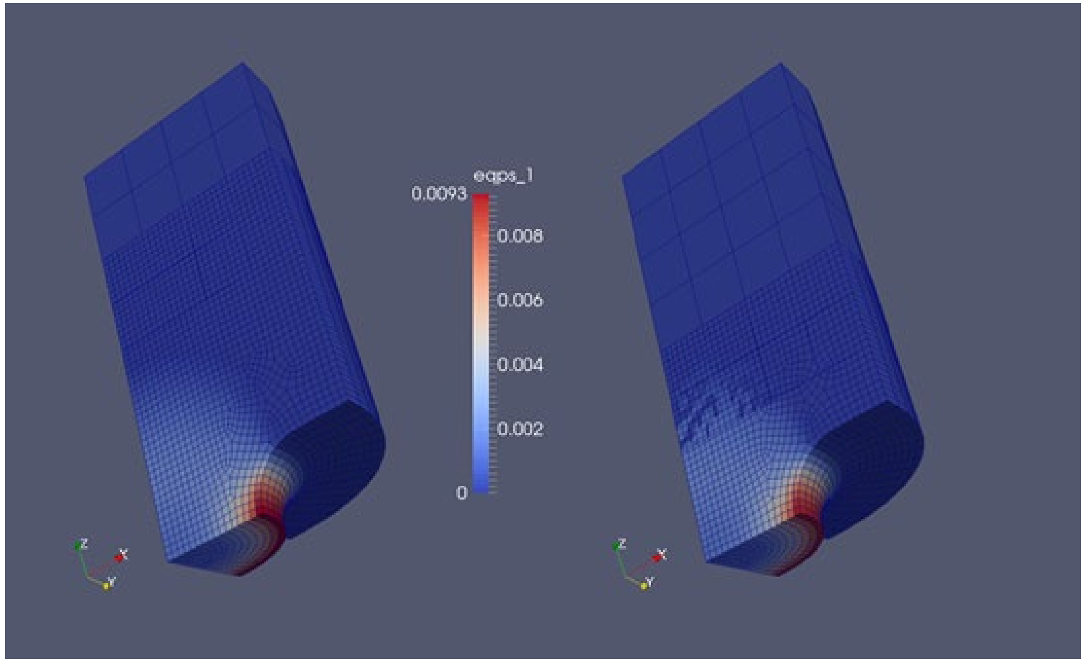
Absolute residual tolerance	u_3 relative error Ω_1	u_3 relative error Ω_2
1.0×10^{-14}	9.27×10^{-3}	3.70×10^{-3}

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

Notched Cylinder: Coupling Different Materials

Need to be careful to do domain decomposition so that material models are ***consistent*** in overlap region.

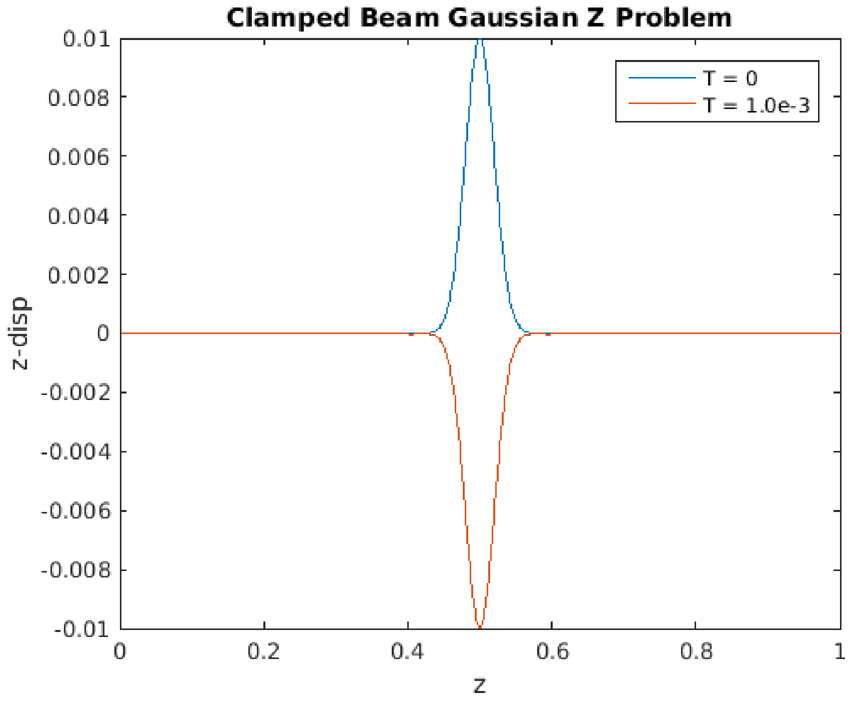
- When the ***overlap*** region is ***far from the notch***, no plastic deformation exists in it: the coarse and fine regions predict the ***same behavior***.
- When the ***overlap*** region is ***near the notch***, plastic deformation spills onto it and the two models predict different behavior, affecting convergence ***adversely***.



Overlap far from notch. Overlap near notch.

Elastic Wave Propagation

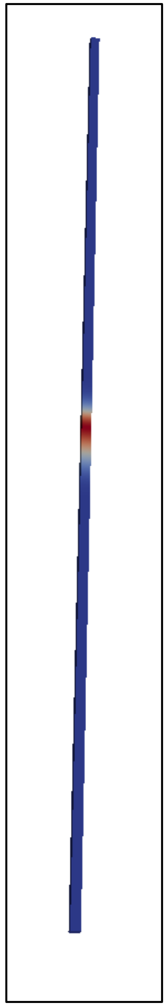
- Linear elastic ***clamped beam*** with Gaussian initial condition for the z-displacement.
- Simple problem with analytical exact solution but very ***stringent test*** for discretization methods.
- Test Schwarz with ***2 subdomains***: $\Omega_0 = (0,0.001) \times (0,0.001) \times (0,0.75), \Omega_1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



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

Time-discretizations: Newmark (implicit, explicit).

Meshes: HEX, TET

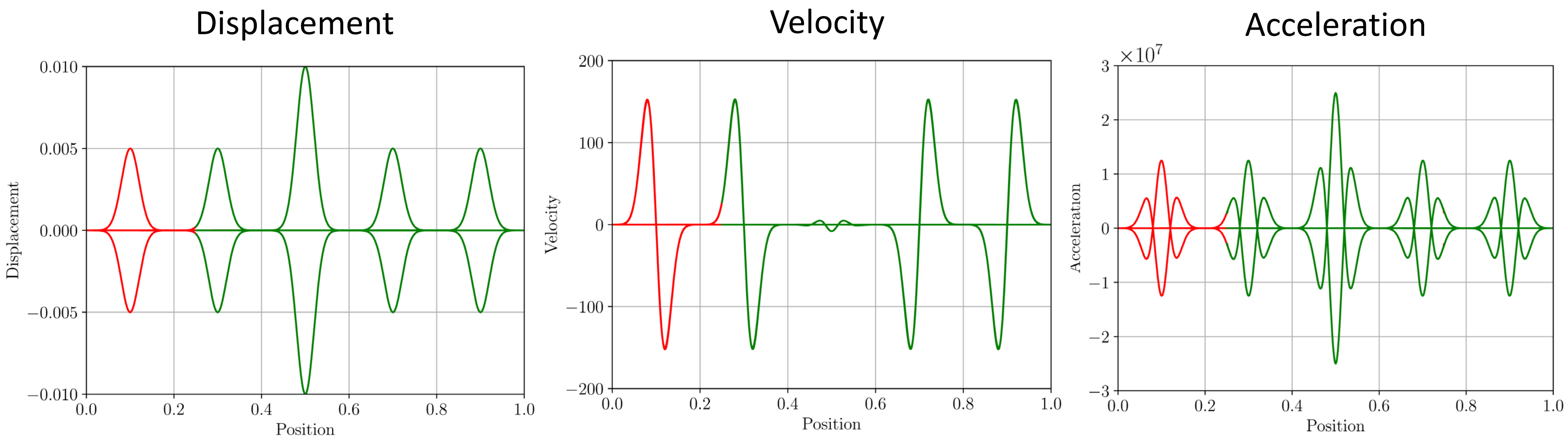


Elastic Wave: Different Integrators, Same Δts

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

	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 Δts

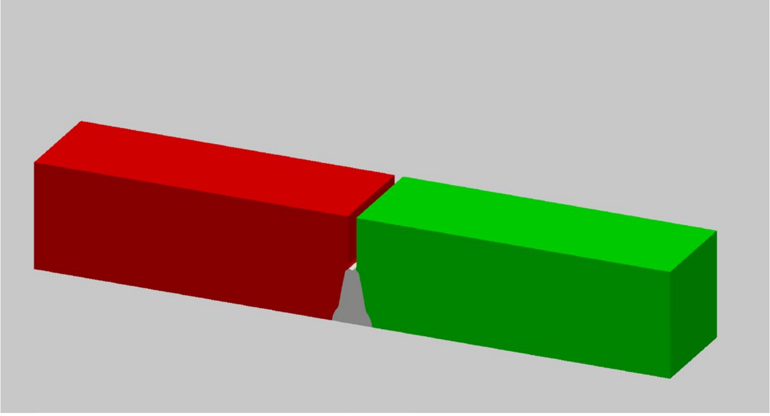


Figures above: Plots of displacement, velocity and acceleration for the elastic wave propagation problem using different time integrators (implicit and explicit) and different time steps (1e-2s and 2e-7s) for each subdomain, superimposed over the analytic single domain solution.

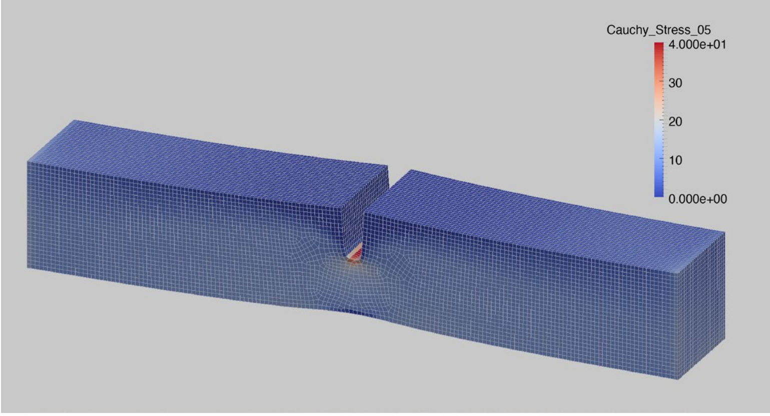
The analytic solution is ***indistinguishable*** from Schwarz solutions (hidden behind the solutions for Ω_0 (red) and Ω_1 (green))!

Laser Weld (Albany/LCM)

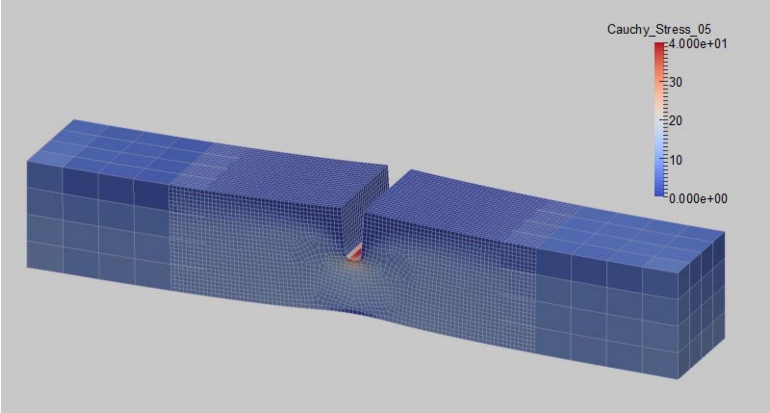
Laser weld specimen



Single domain discretization

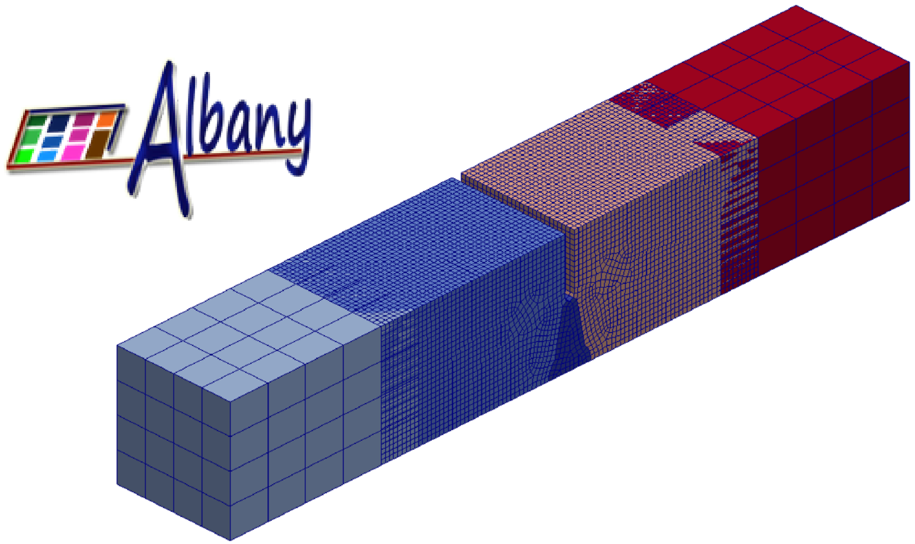


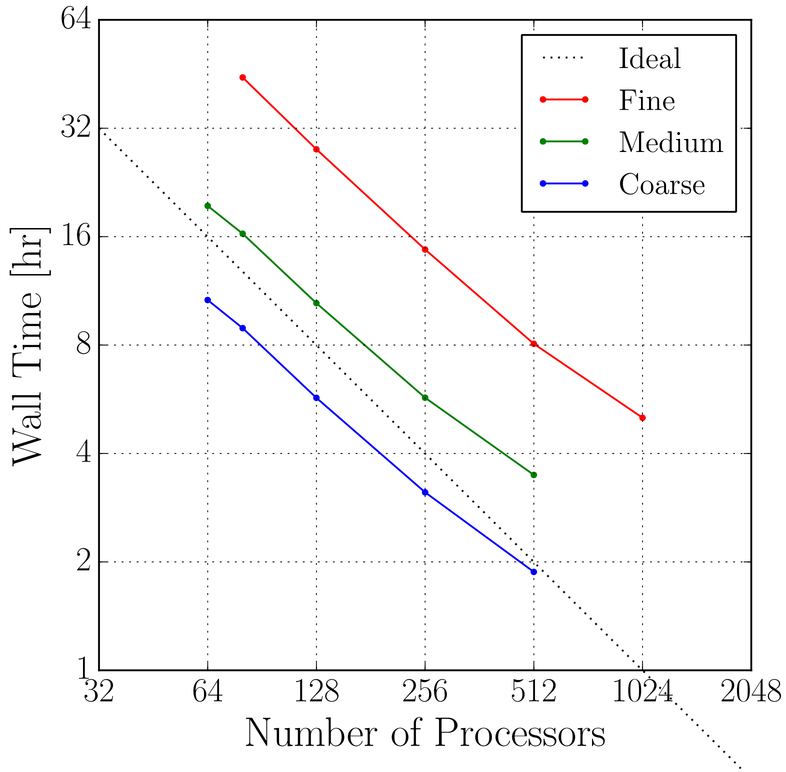
Coupled Schwarz discretization
(50% reduction in model size)



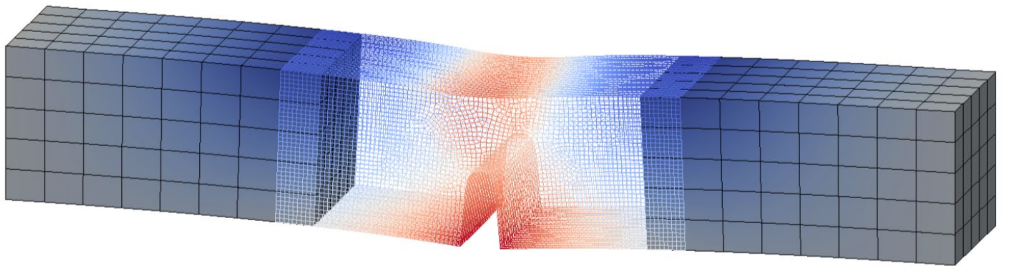
- Problem of ***practical scale***.
- ***Isotropic elasticity*** and J_2 ***plasticity*** with linear isotropic hardening.
- ***Identical parameters*** for weld and base materials for proof of concept, to become independent models.

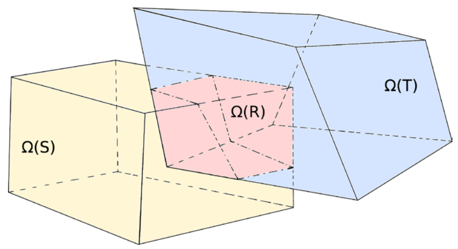
Laser Weld (Albany/LCM): Strong Scalability of Parallel Schwarz with DTK





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



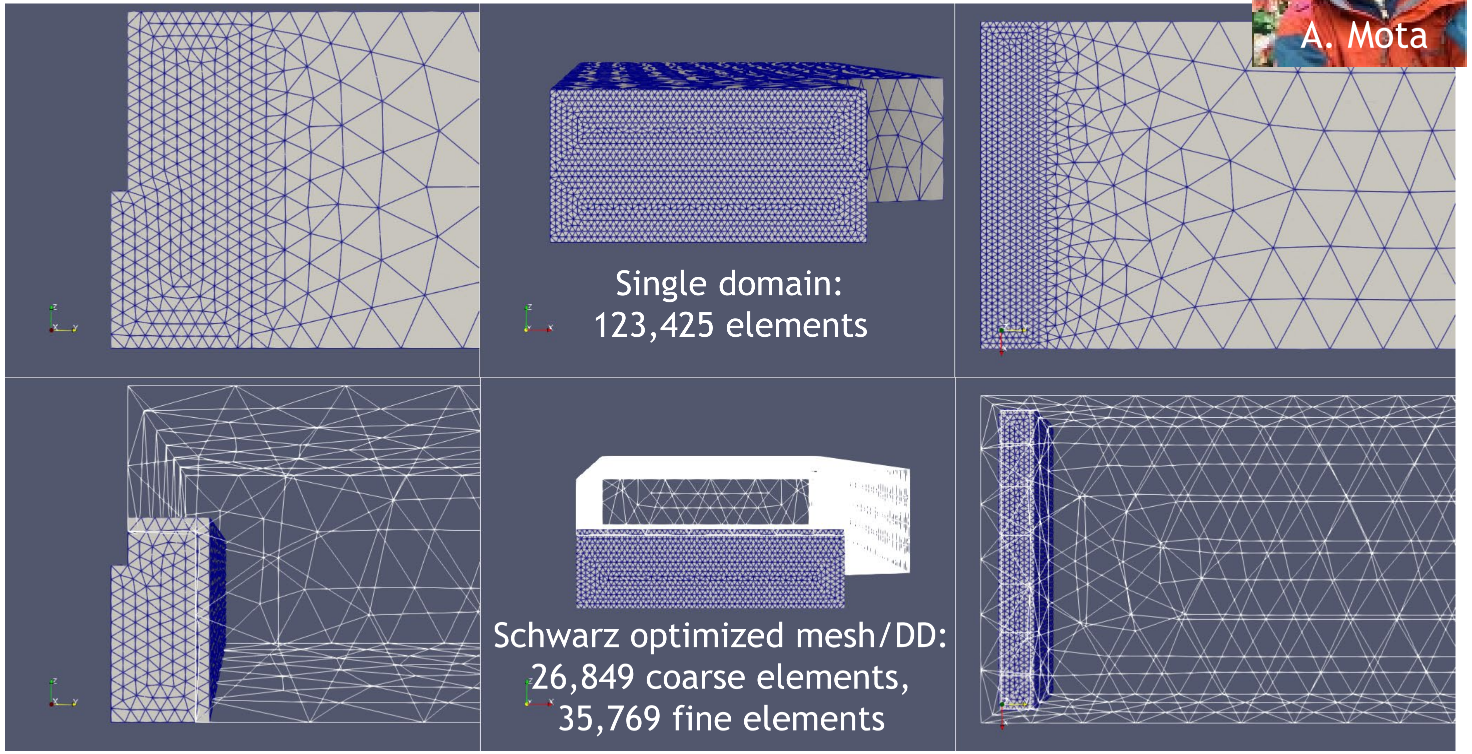


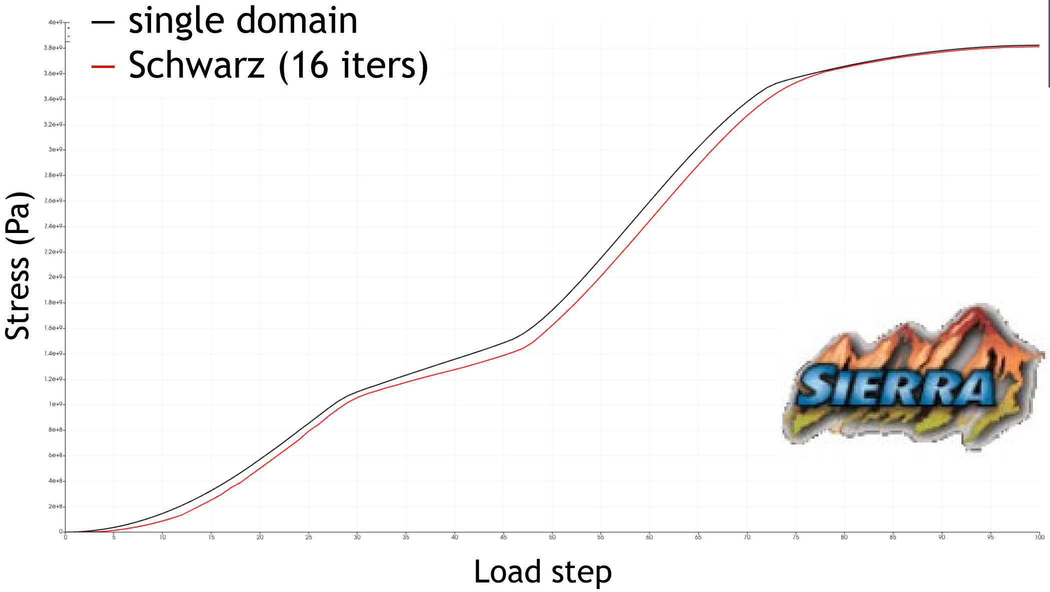
Data Transfer Kit (DTK)

Laser Weld: Improving Performance via Mesh/DD Design

- **Production** problem in SIERRA/SM with plasticity
- **Overlapping** Schwarz with **naïve DD/meshing** takes ~**3**× longer to run than single Ω solve

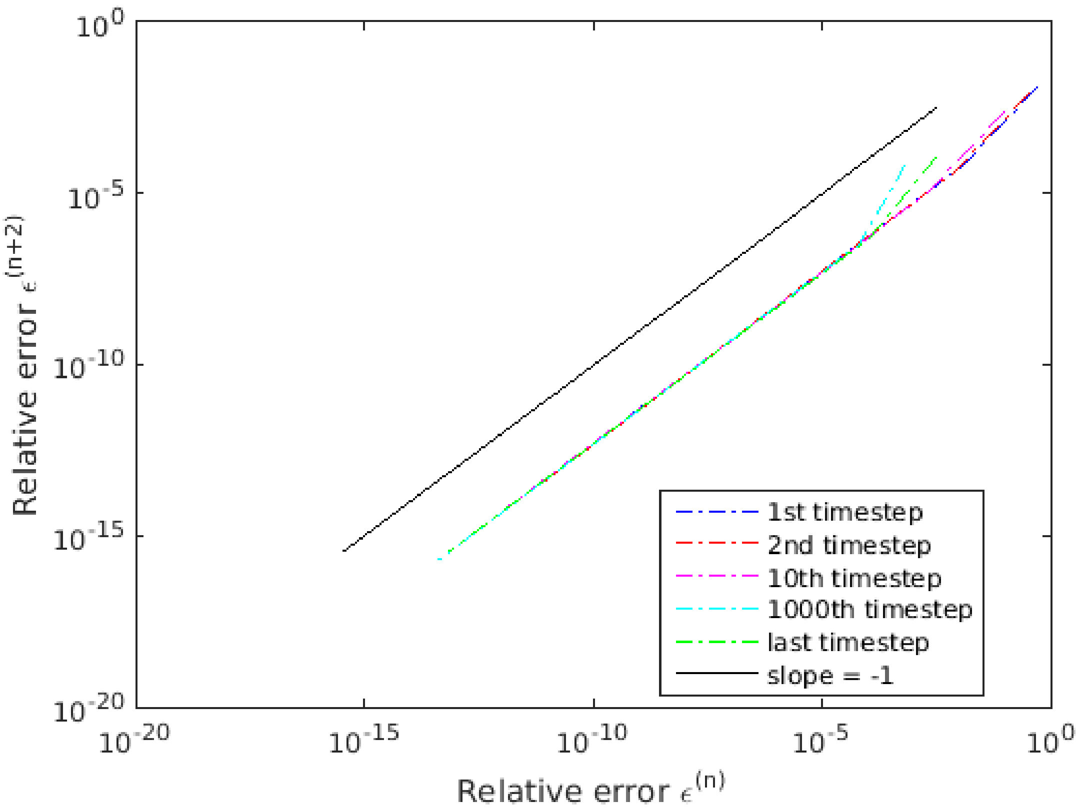
Schwarz performance can be **improved by** ~**3**× while maintaining the **same accuracy** by **optimizing** the **mesh design**





Simulation Type	Wall Time 64 procs
Single domain	3 hr 17 min
Overlapping SAM (16 iters, optimized DD and mesh design)	3 hr 37 min

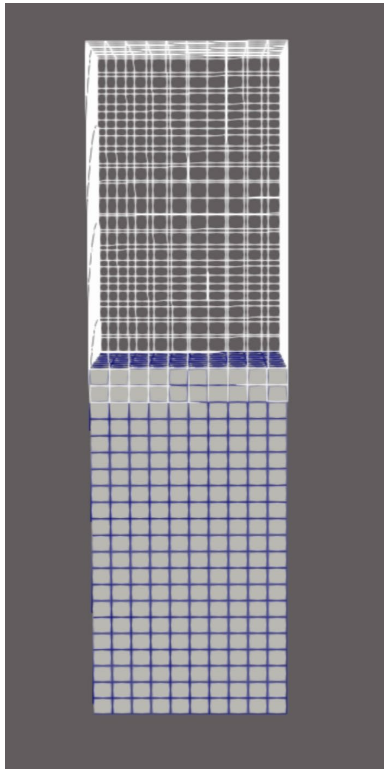
Bolted Joint Problem: Convergence Rate (Multiplicative Schwarz)



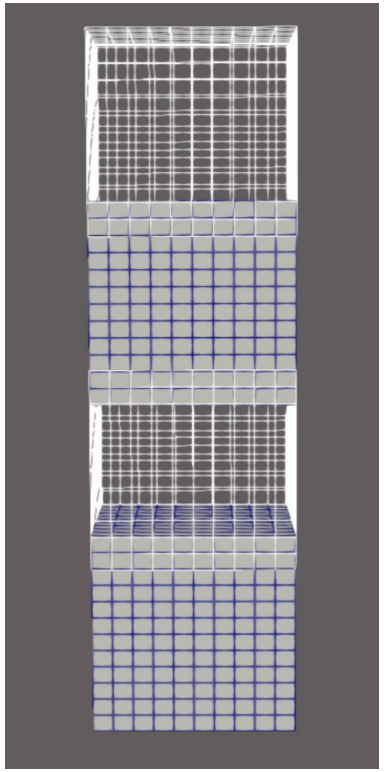
Linear convergence rate is observed for ***dynamic*** Schwarz algorithm, as expected from the theory.

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

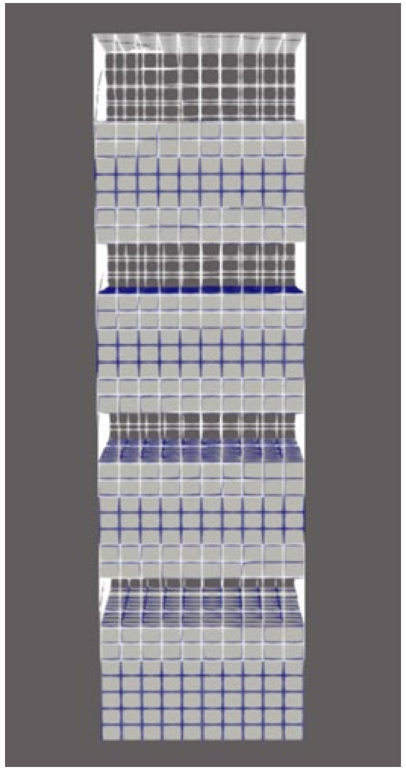
Scaling with Respect to the Number of Subdomains



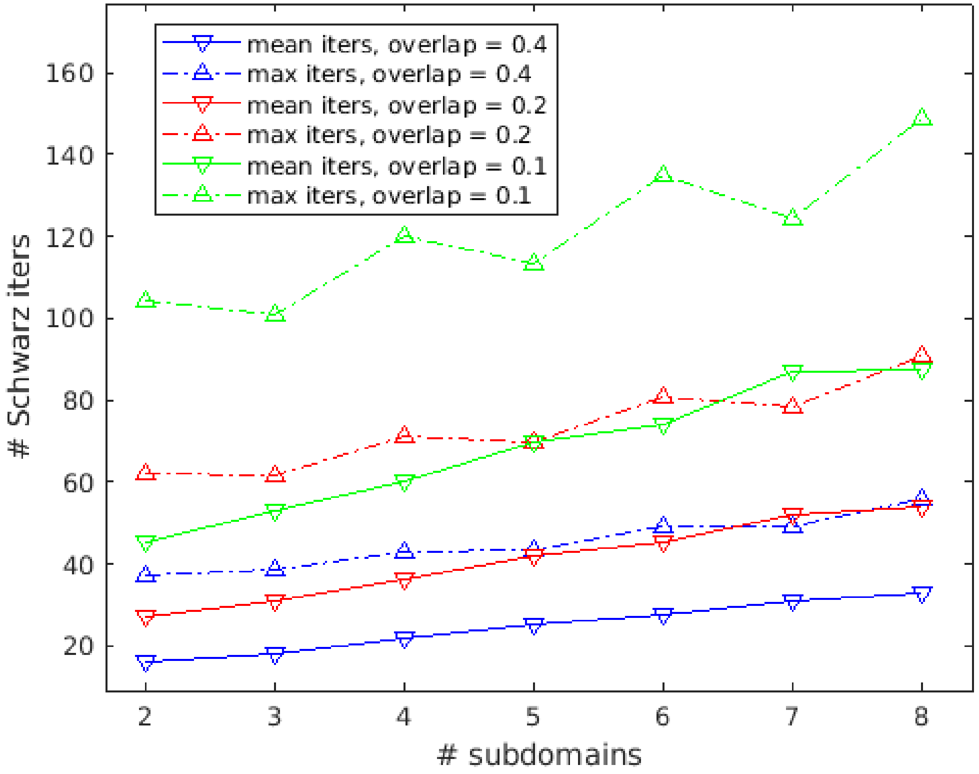
2 subdomains



4 subdomains



8 subdomains

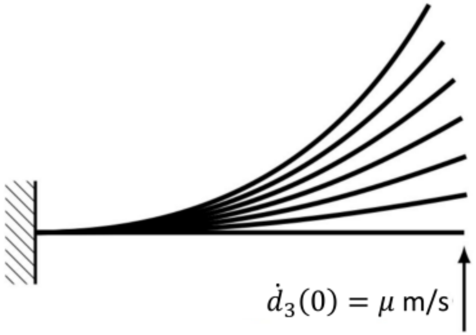


- Overlapping SAM scaling study from 2 to 8 subdomains
- Linear elastic cuboid problem, pulled from top at rate of $0.5 - 0.5\cos(\pi t)$
- Overlap size varied: 0.4, 0.2 (above) and 0.1
- Same mesh resolution of 0.1 in all subdomains
- Linear convergence observed w.r.t. # subdomains

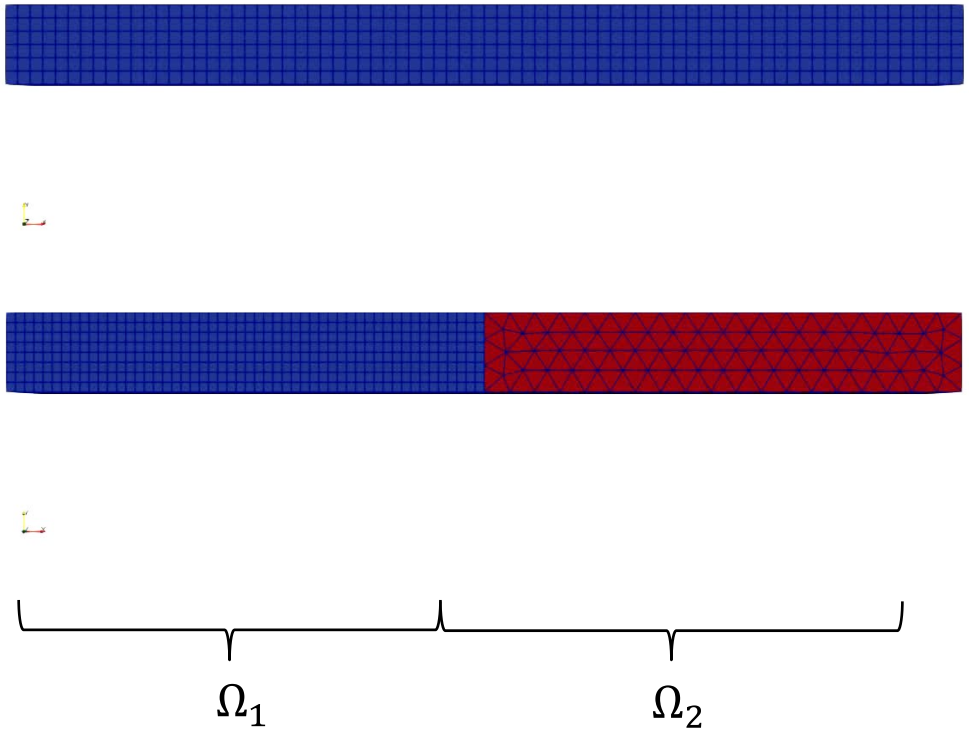
Generally, we do not target cases with >5-6 subdomains

Beam Bending (Non-Overlapping SAM)

M. Merewether



- Linear elastic 3D beam initialized with given ***velocity μ*** at right nodeset.
- ***Non-overlapping*** domain decomposition into ***two subdomains*** (bottom right) discretized using ***non-conformal HEX meshes***.
- Coupling via ***relaxed Dirichlet-Neumann Schwarz*** in SIERRA/SM.
- On average, took ***10-15 Schwarz iterations*** to achieve relative tolerance of 1e-7 with relaxation parameter $\theta \in [0.3, 0.5]$.
- SAM solution ***indistinguishable*** from single domain solution (right)



Non-overlapping Schwarz

Schwarz Extensions to FOM-ROM and ROM-ROM Couplings

Choice of domain decomposition

- **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

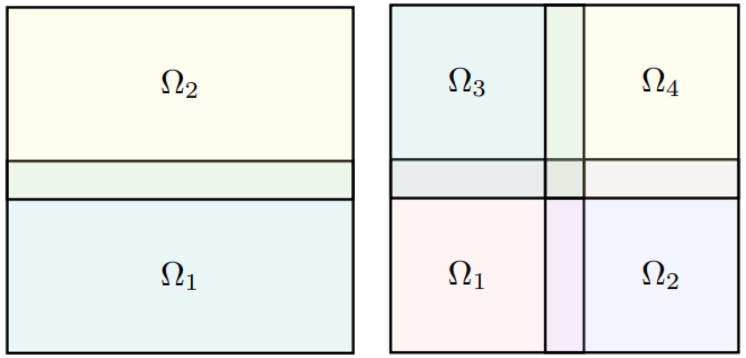
Overlapping SAM-based Coupling for Non-Intrusive OpInf ROMs

Offline stage:

- Create **DD** of Ω into d **overlapping subdomains** Ω_i
- Perform a SAM-coupled **all-FOM simulation** on $\cup_i \Omega_i$
- Compute **POD basis** $\boldsymbol{\Phi}_i$ on each Ω_i
- Assume a **functional form** for your ROM in Ω_i, informed by the functional form of the corresponding FOM
  - ➢ ***Key question****: how to impose Schwarz BCs in OpInf ROMs?*
    - ❖ *Boundary transmission enters through* ***learned source term*** $\widehat{\boldsymbol{B}}_i \boldsymbol{g}_i$ *added to OpInf ROM dynamical system*
    - ❖ ***Further reduction*** *achieved by expanding* $\boldsymbol{g}_i$ in its own POD basis $\boldsymbol{\Phi}_i^g$ and approximating $\widehat{\boldsymbol{B}}_i \boldsymbol{g}_i \approx \widehat{\boldsymbol{B}}_i \widehat{\boldsymbol{g}}_i = \widetilde{\boldsymbol{B}}_i \boldsymbol{g}_i$ where $\widehat{\boldsymbol{g}}_i = \boldsymbol{\Phi}_i^g \boldsymbol{g}_i$
- Compute OpInf operators $\widehat{\boldsymbol{A}}_i, \widehat{\boldsymbol{H}}_i$ and $\widetilde{\boldsymbol{B}}_i$ in each subdomain Ω_i by solving regularized OpInf LS **minimization problem**

Online stage:

- Apply **Schwarz iteration procedure**, with Schwarz BC transfer via pre-learned boundary contributions $\widetilde{\boldsymbol{B}}_i \boldsymbol{g}_i$



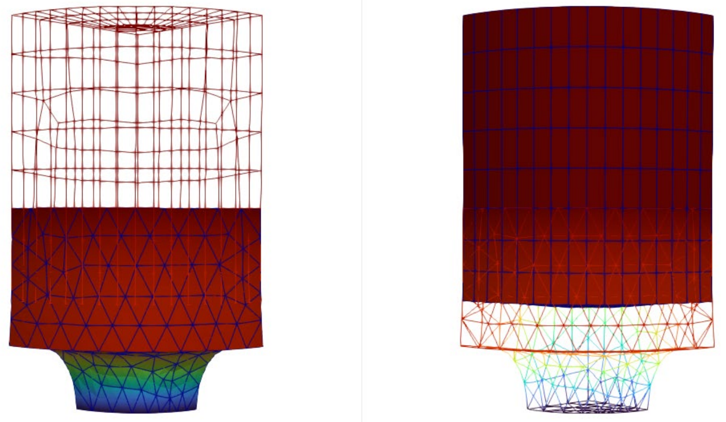
OpInf ROM + Schwarz BCs in Ω_i:

$$\dot{\widehat{\boldsymbol{q}}}_i + \widehat{\boldsymbol{A}}_i \widehat{\boldsymbol{q}}_i + \widehat{\boldsymbol{H}}_i(\widehat{\boldsymbol{q}}_i \otimes \widehat{\boldsymbol{q}}_i) + \underbrace{\widetilde{\boldsymbol{B}}_i \boldsymbol{g}_i}_{\text{Schwarz Dirichlet BC term}} = \boldsymbol{0}$$

Motivated by implementation of **Dirichlet BCs** in **FEM**

[Farcas et al., 2023] coupling formulation is ***similar*** *but solves each subdomain problem* ***once*** *rather than iterating to convergence.*

3D Linear Elastic Notched Cylinder Problem



- Geometry is ***linear elastic notched cylinder*** pulled from top ***dynamically*** to time $T_{max} = 1.5$ at rate of $0.0064t$ with $\Delta t = 0.005$
- Demonstration of SAM's ability to ***couple disparate meshes***, ***element types*** and ***models***: TET10 + FOM (notched region) and HEX8 + Linear OpInf with $M = 30$ modes (top region)
- ***Linear OpInf*** trained on 301 snapshots in time
- ***Reproductive*** problem for now

Key result*:** **regularization parameter** γ influences **accuracy** & **convergence**. Coupled models are remarkably **accurate**! Schwarz is ***not introducing **coupling error/artifacts**.

	Mean/max # Schwarz iters	Max z-disp rel error Ω_1	Max z-disp rel error Ω_2
FOM-FOM	5.83/9	–	–
FOM-OpInf ($\gamma = 1 \times 10^{-6}$)	5.09/8	2.9e-3	4.2e-3
FOM-OpInf ($\gamma = 1 \times 10^{-7}$)	5.48/9	3.8e-4	4.3e-4
FOM-OpInf ($\gamma = 1 \times 10^{-8}$)	5.54/9	1.3e-4	2.2e-4
FOM-OpInf ($\gamma = 1 \times 10^{-9}$)	5.52/9	3.1e-5	3.6e-5

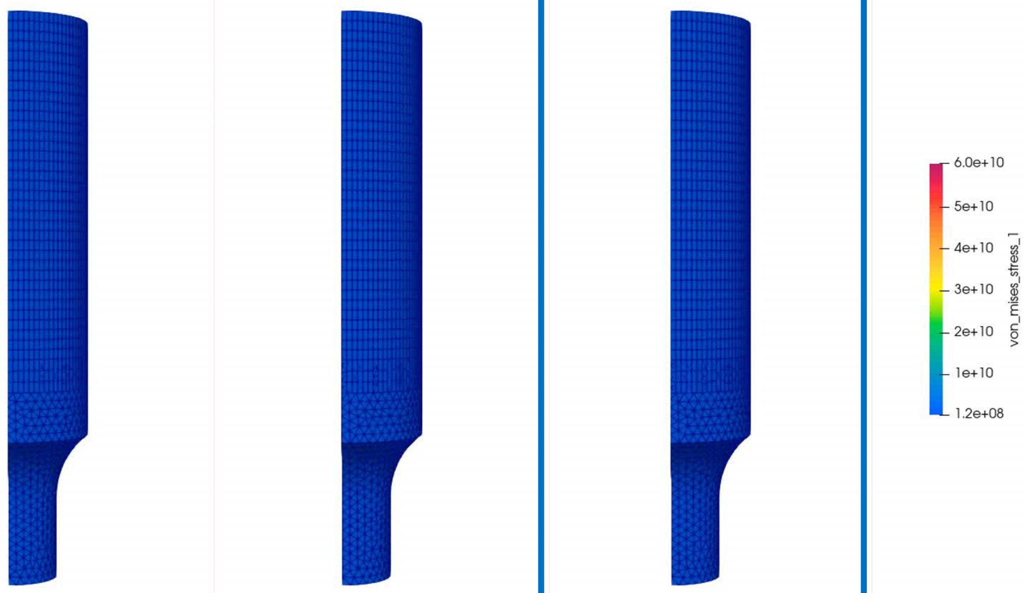
FOM-FOM FOM-OpInf

Movies above: z-displacement solutions for FOM-FOM and FOM-OpInf ($M = 30$, $\gamma = 1 \times 10^{-6}$)

Tension Specimen (Overlapping SAM)

QOpInf = Quadratic OpInf

- **Hyperelastic** variant of previous problem (Neohookean material model)
- **TET10 - HEX overlapping** coupling with **implicit Newmark** with **same** $\boldsymbol{\Delta t}$
- **QOpInf** models with M=2 POD modes, capturing 99.9999% snapshot energy
- All results are **predictive** w.r.t. DBC applied at top of holder



FOM-FOM | FOM-QOpInf Full Schwarz | FOM-QOpInf 1 iteration

		FOM-FOM	FOM-QOpInf	QOpInf-QOpInf
Ω_1 rel errs	displacement	–	3.44e-4	5.73e-4
	velocity	–	1.72e-2	1.83e-2
	σ_{vm} stress	–	3.41e-4	8.53e-4
Ω_2 rel errs	displacement	–	2.50e-4	4.41e-4
	velocity	–	1.86e-2	1.96e-2
	σ_{vm} stress	–	2.40e-3	6.00e-3
CPU time	–	8h 19m 29.5s	1h 21m 25.9s	4m 42.1s
Mean/max # Schwarz iters	–	32.0/32	7.03/8	7.74/8

- Relative errors of $\boldsymbol{O}$**(1e-4)-**$\boldsymbol{O}$**(1e-3)** are achieved for the displacement and von Mises stress (σ_{vm})

Impressive **6.13**× and **106**× **speedups** are achieved via **FOM-QOpInf** and **QOpInf-QOpInf** couplings, respectively!

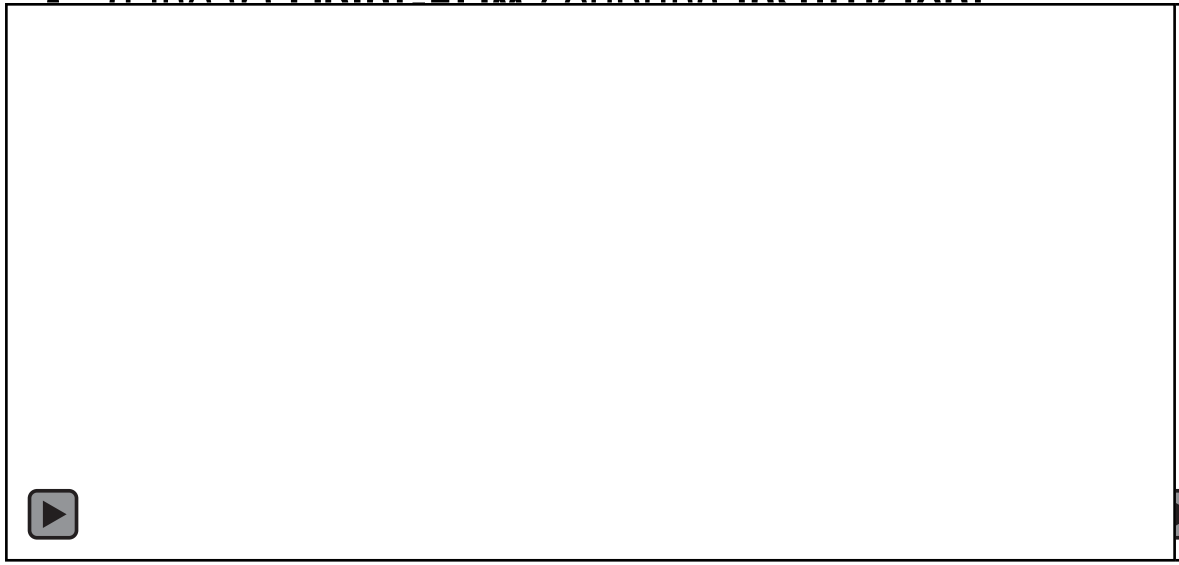
- Method of [Farcas *et al.*, 2023] (1 Schwarz iteration) gives **incorrect solution.**

NORMA.JL

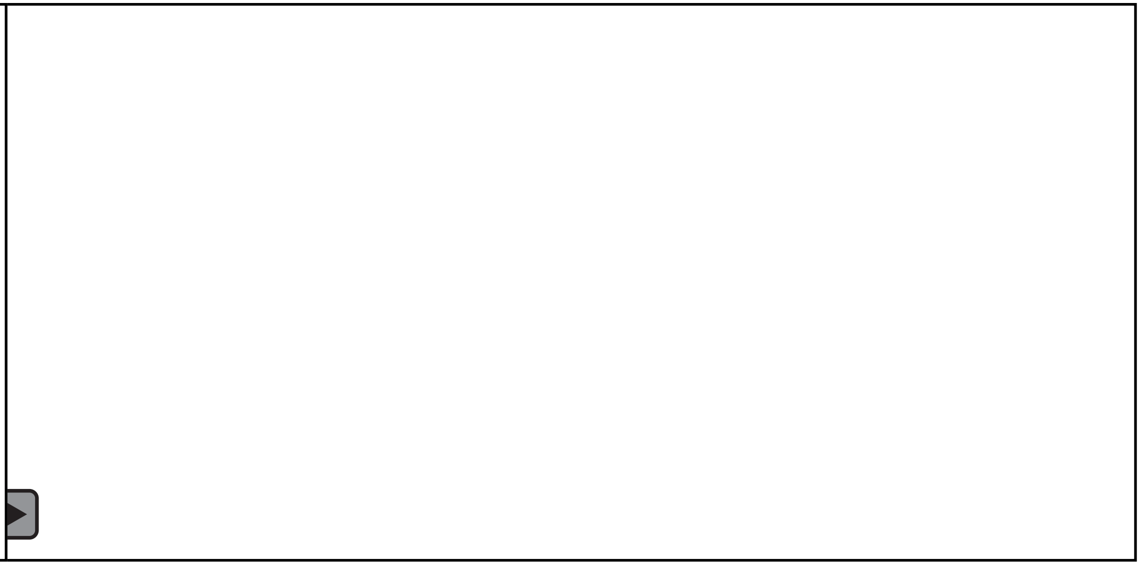
Torsion (Overlapping SAM)

- **Neohookean** material model
- **TET4 - HEX8 overlapping** coupling with **implicit-explicit Newmark** having **different Δt**
- **QOpInf-FOM** coupled models with M=27 and M=30 POD modes, capturing 99.9999% snapshot energy
- **Prediction** w.r.t. **initial velocity** (rotation speed/direction)
- (Linear) **OpInf-FOM** coupling **insufficient**

		FOM-FOM	QOpInf-FOM reproductive	QOpInf-FOM predictive
Ω_1 rel errs	displacement	–	2.67e-3	4.32e-2
	velocity	–	3.56e-2	1.49e-1
Ω_2 rel errs	displacement	–	1.13e-3	2.44e-2
	velocity	–	1.12e-2	9.52e-2
CPU time	–	39m 11.8s	1m 40.2s	1m 39.5s
Mean/max # Schwarz iters	–	3.0/3	2.0/2	2.0/2



OpInf = Linear OpInf



QOpInf = Quadratic OpInf

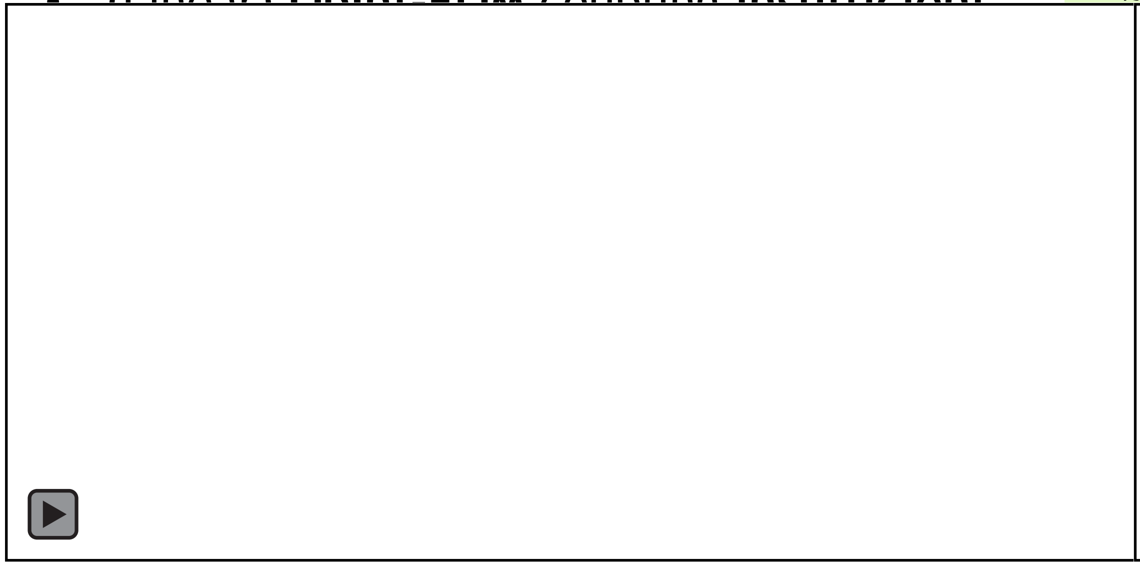
Torsion (Overlapping SAM)

- **Neohookean** material model
- **TET4 - HEX8 overlapping** coupling with **implicit-explicit Newmark** having **different Δt**
- **QOpInf-FOM** coupled models with M=27 and M=30 POD modes, capturing 99.9999% snapshot energy
- **Prediction** w.r.t. **initial velocity** (rotation speed/direction)
- (Linear) **OpInf-FOM** coupling **insufficient**

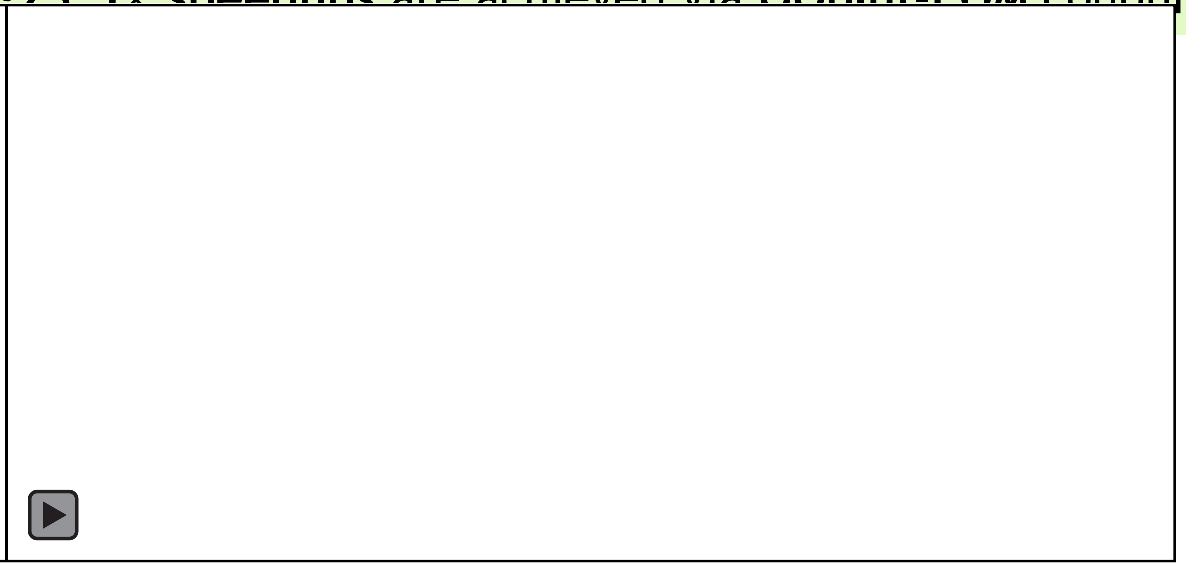
		FOM-FOM	QOpInf-FOM reproductive	QOpInf-FOM predictive
Ω_1 rel errs	displacement	–	2.67e-3	4.32e-2
	velocity	–	3.56e-2	1.49e-1
Ω_2 rel errs	displacement	–	1.13e-3	2.44e-2
	velocity	–	1.12e-2	9.52e-2
CPU time	–	39m 11.8s	1m 40.2s	1m 39.5s
Mean/max # Schwarz iters	–	3.0/3	2.0/2	2.0/2

Relative errors are of $\mathcal{O}$**(1e-3)**-$\mathcal{O}$**(1e-2)** for displacement and velocity!

~**23.5× speedups** are achieved via **QOpInf-FOM** couplings



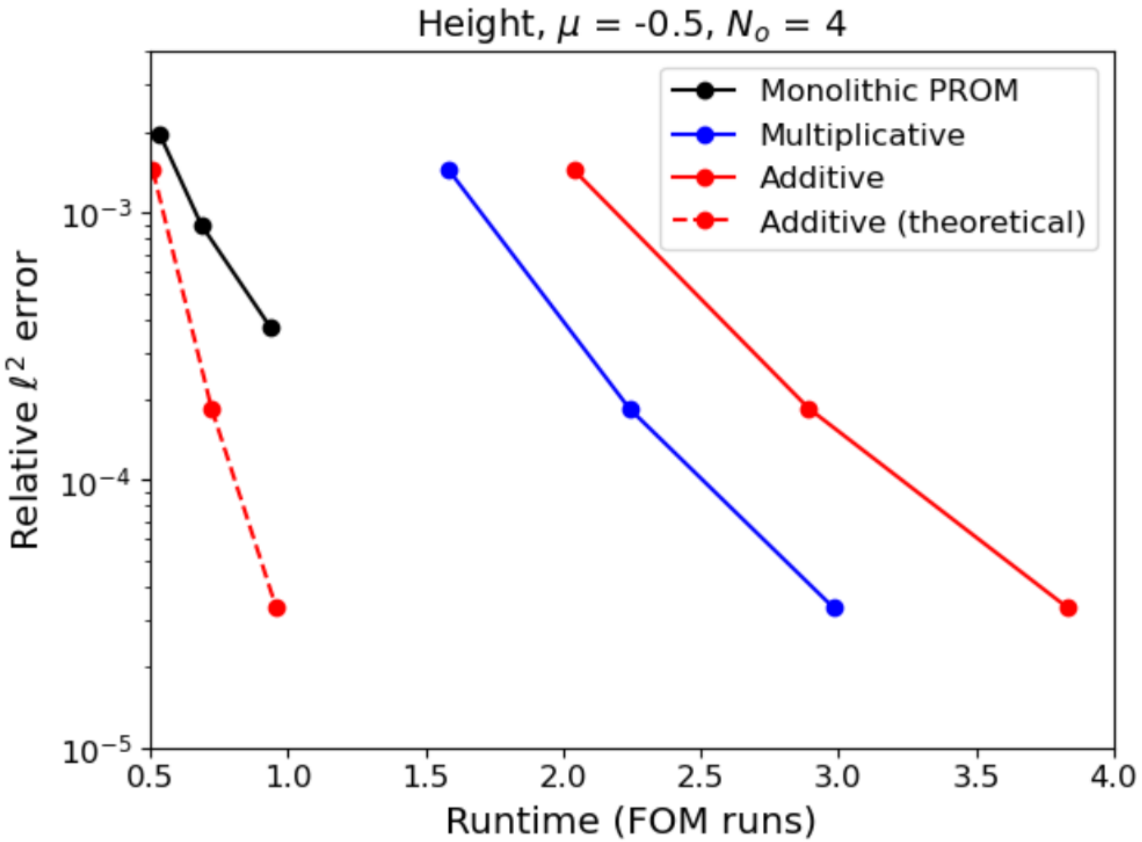
OpInf = Linear OpInf



QOpInf = Quadratic OpInf

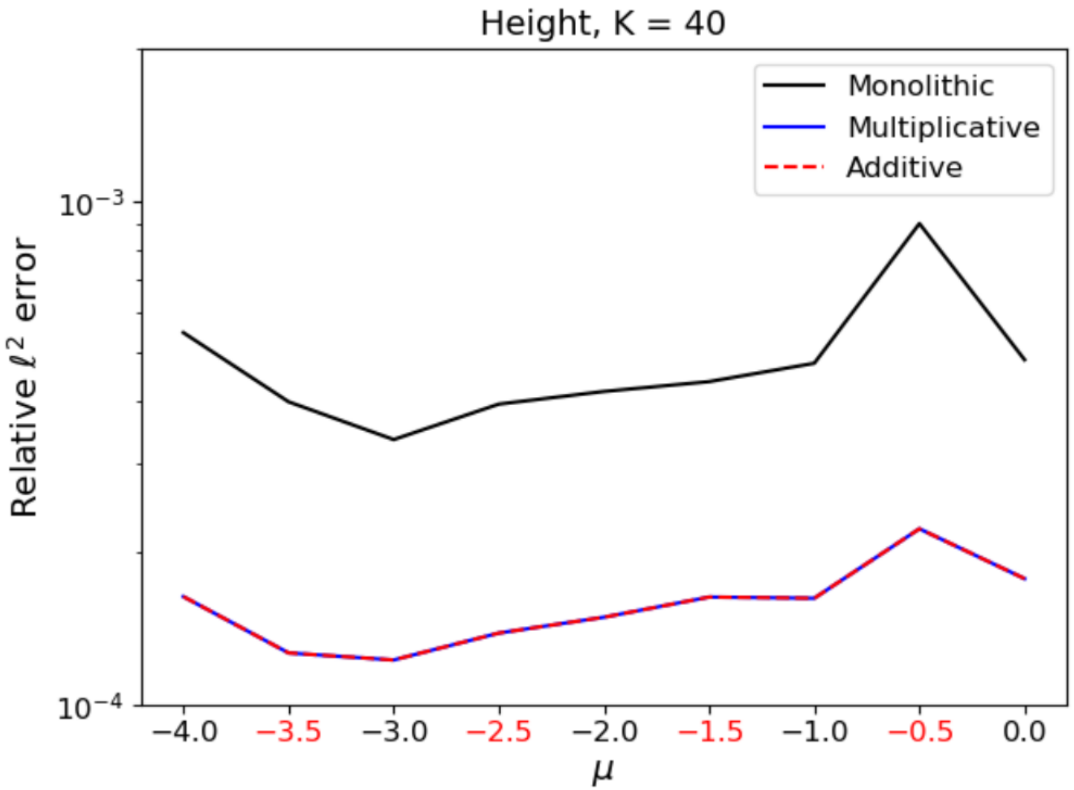
2D SWE: Takeaways

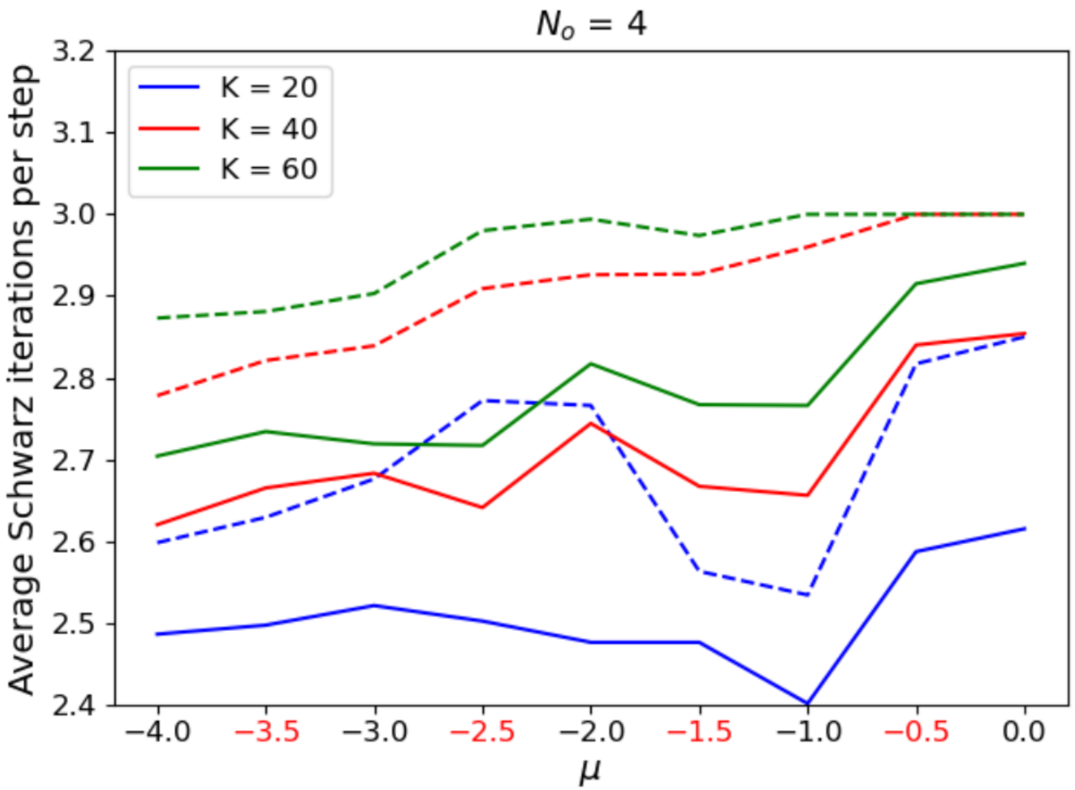
- Resolving overlap region discrepancy is critical
- Additive Schwarz exacerbates PROM dimension costs
- Available parallel cost savings
- Unexpected overlap error requires further investigation



2D SWE: PROMs, additive Schwarz

- Additive does not affect accuracy, converging to same result
- As expected, additive incurs additional Schwarz iterations
- Increased PROM dimension also degrades convergence

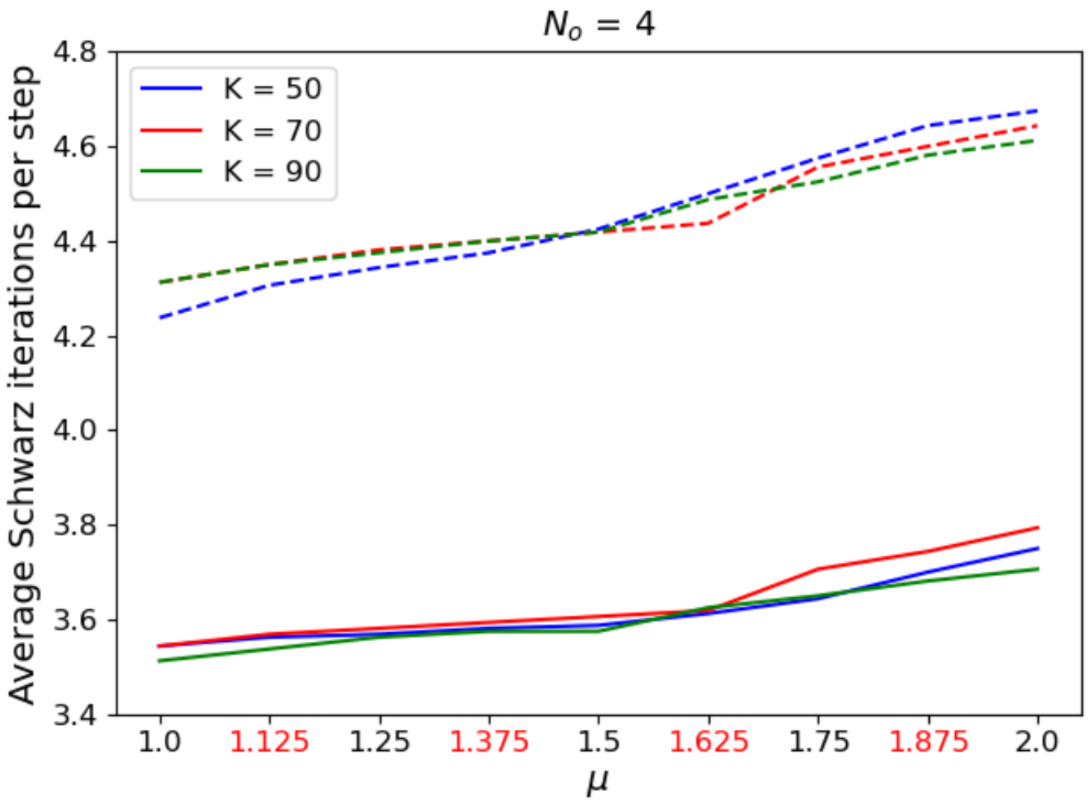


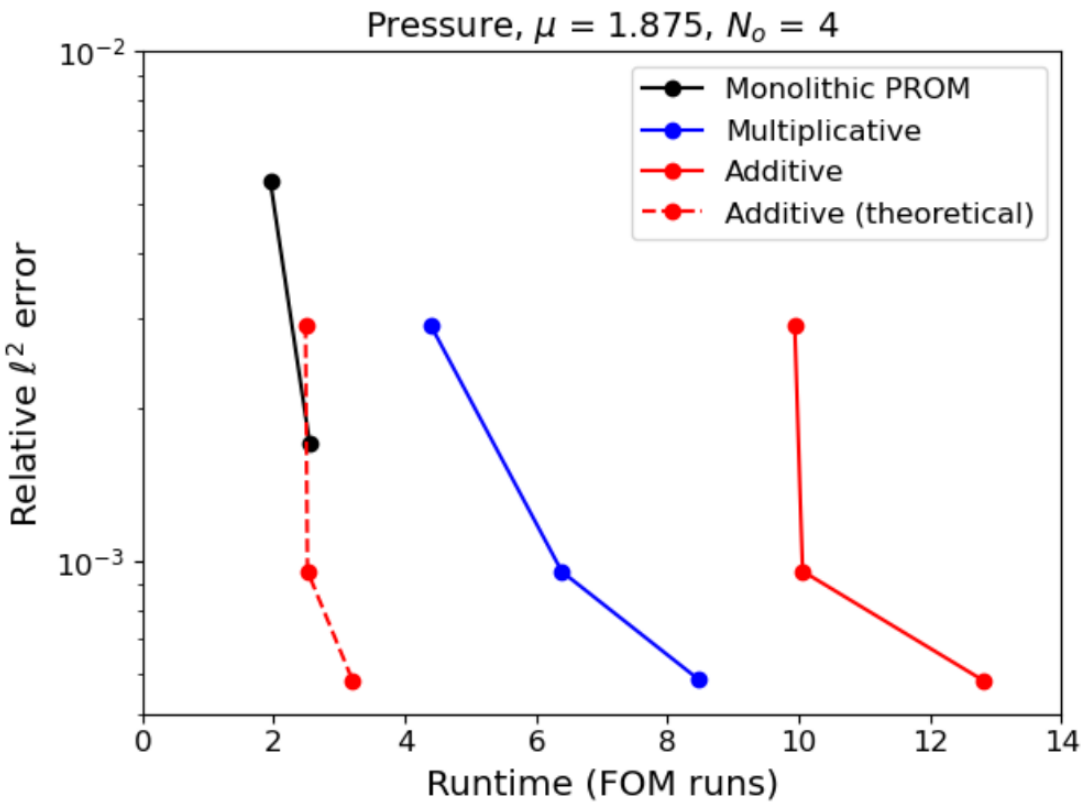


Solid: multiplicative, Dashed: additive

2D Euler: Schwarz PROMs

- PROM dimension has **less** effect on convergence, additive has **more**
- True cost savings unachievable without hyper-reduction





Solid: multiplicative, Dashed: additive

Schwarz for everyone

4-way multiscale coupling in salt caverns for SPR

Tonya Ross (8912)

Schwarz coupling for J-integral around crack front on pressure vessel

Dallin Morris (8752), Jay Foulk (8363)

Multiscale coupling for stronglinks

Rob Flicek (1556), Kiri Welsh (1556)

Schwarz multiscale coupling for electronics package survivability

Damon Burnett (7627), Christie Crandall (8752)

Automated optimization of DD with multiple constraints

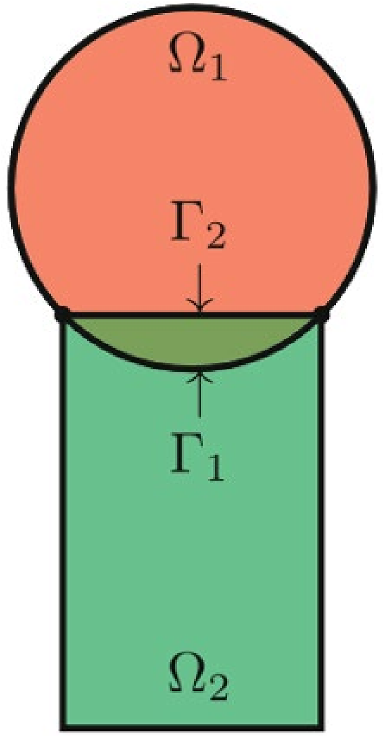
Chris Wentland (8734)

Schwarz contact and Anderson acceleration

Brian Phung (8752)

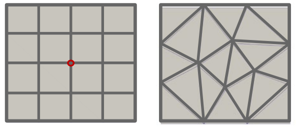
Asynchronous Schwarz for GPU decomposition

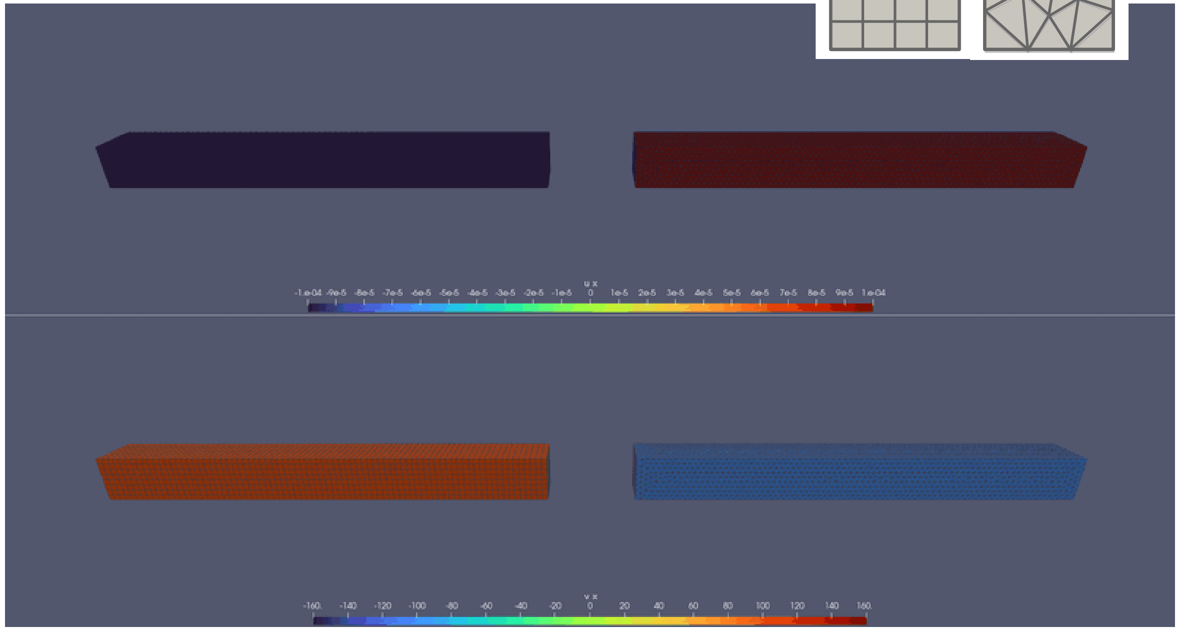
Erik Boman (1465), Craig Hamel (1558)

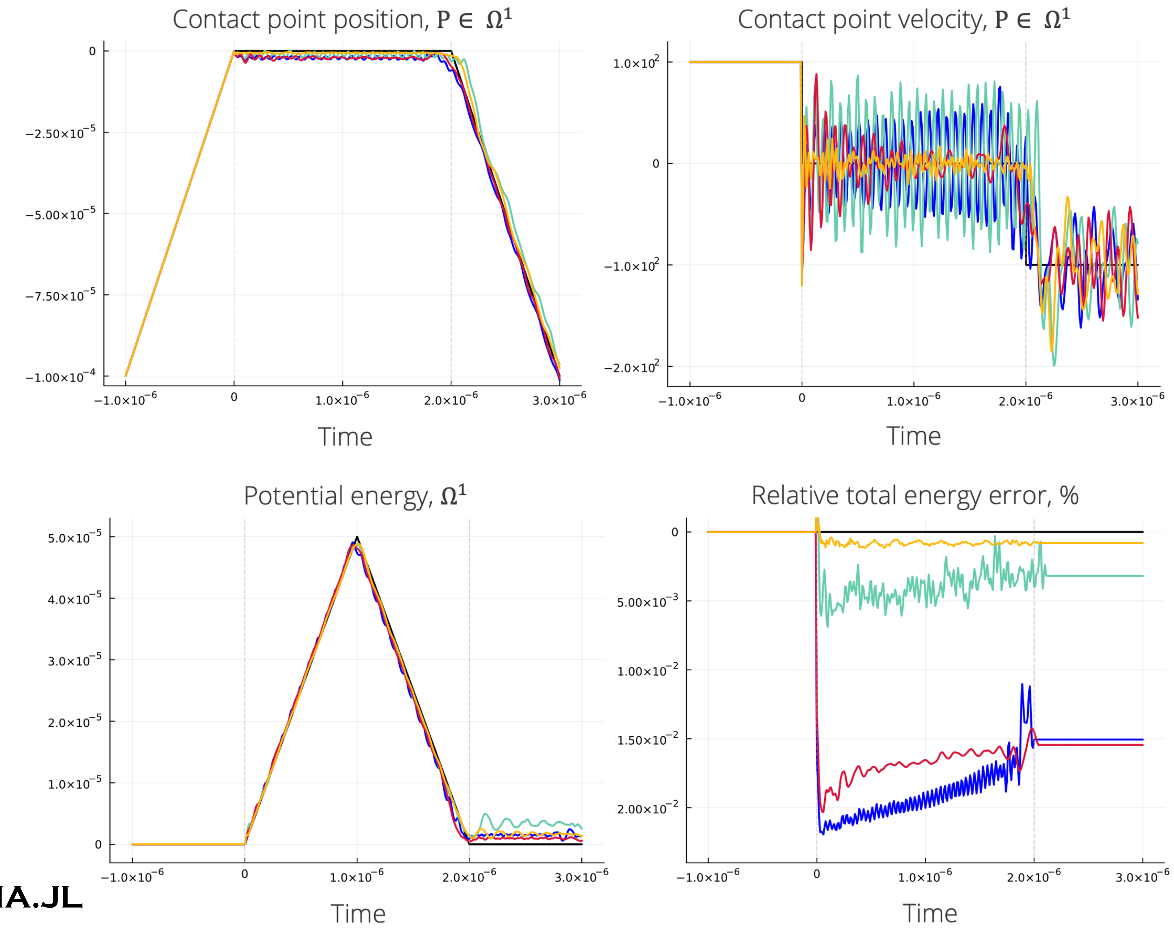


Colliding Bars

Contact boundaries Γ^1 and Γ^2







Schwarz provides **more accurate predictions** than conventional methods and demonstrates **exceptional energy conservation** capabilities!

NORMA.JL

	Elements type		Mesh size		Number of nodes		Time step		Average number of Schwarz iterations
	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	Ω^1	Ω^2	
Imp-Imp Schwarz	HEX8	HEX8	$1/2 \cdot 10^{-4}$		189		$1 \cdot 10^{-8}$		7
Exp-Exp Schwarz	TETRA4	TETRA4	$1/2 \cdot 10^{-4}$		199		$1 \cdot 10^{-9}$		6
Imp-Exp Schwarz	HEX8	TETRA4	$1/2 \cdot 10^{-4}$		189	199	$1/2 \cdot 10^{-8}$	$1 \cdot 10^{-9}$	6
Exp-Imp Schwarz	HEX8	TETRA4	$1/4 \cdot 10^{-4}$	$1/3 \cdot 10^{-4}$	1025	745	$1 \cdot 10^{-9}$	$1/2 \cdot 10^{-8}$	8