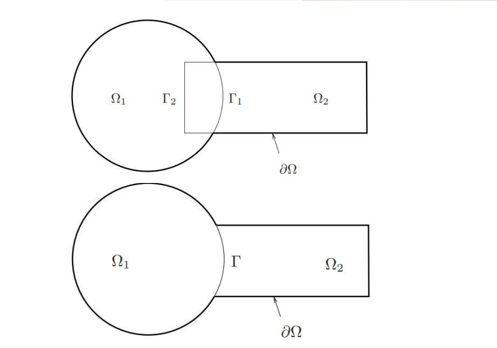
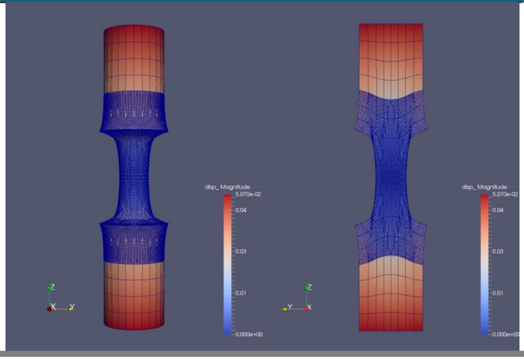
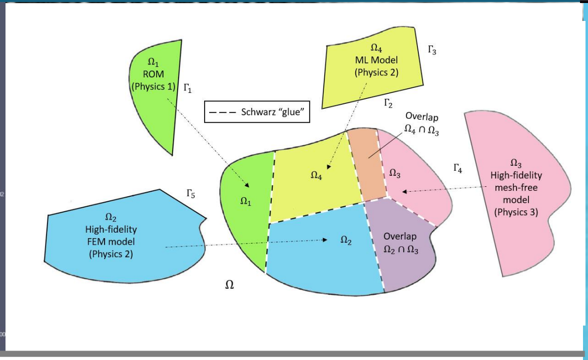
Accelerating mod/sim workflows through hybrid domain decomposition-based models and the Schwarz alternating method







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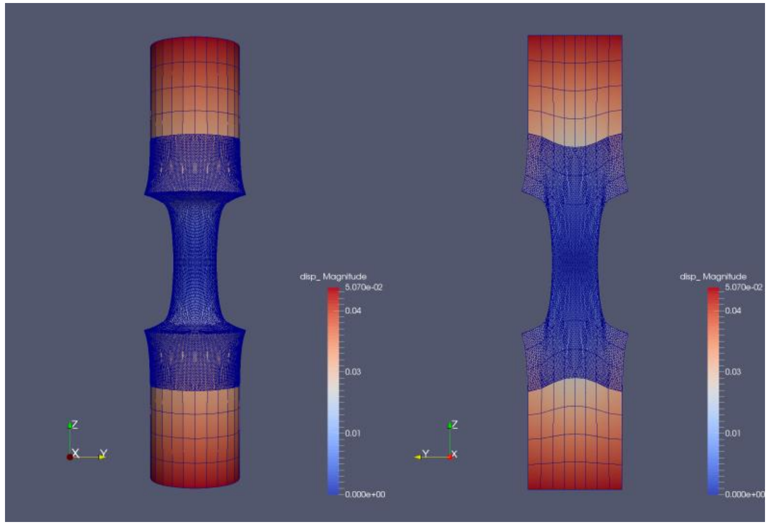
Outline



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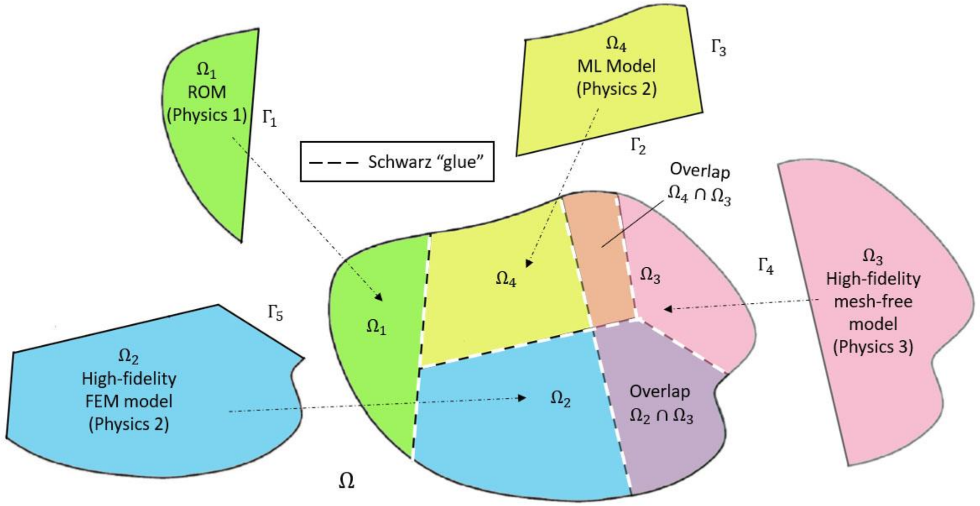
    - Numerical Examples
3. Summary and Future Work



* Projection-based Reduced Order Model

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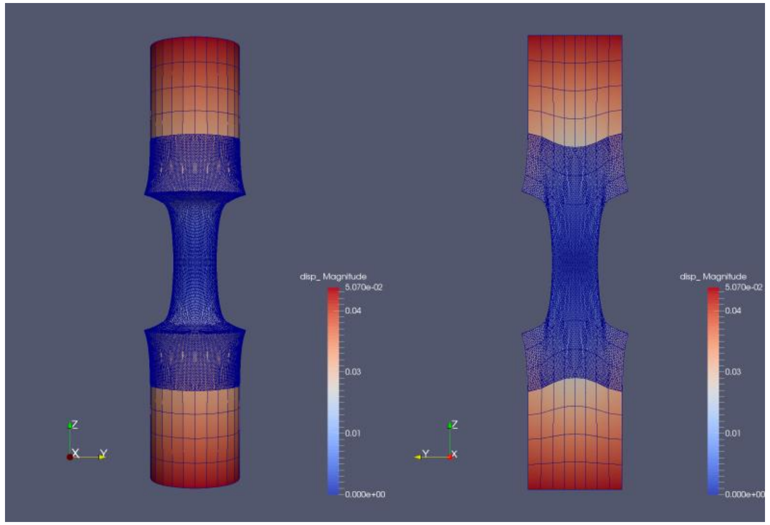

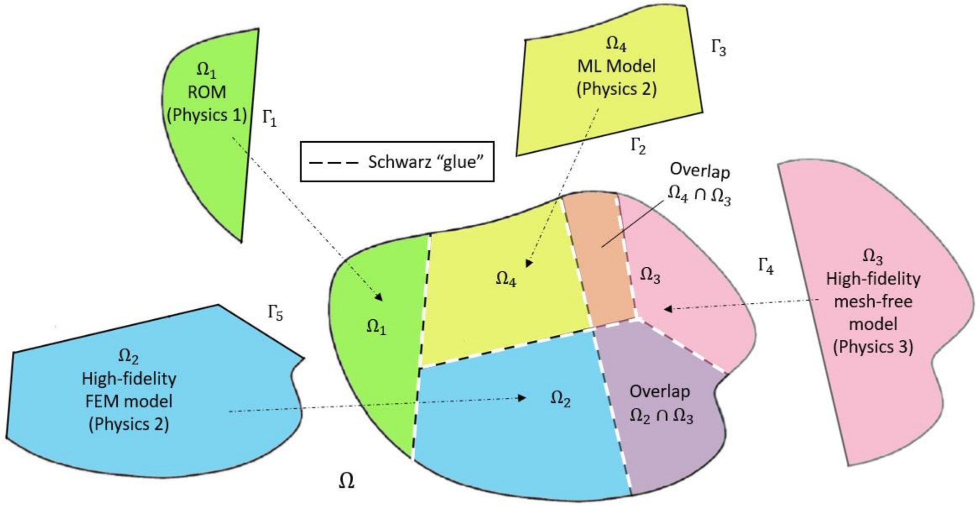

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Motivation for Coupling in Solid Mechanics

Concurrent multiscale coupling for predicting failure

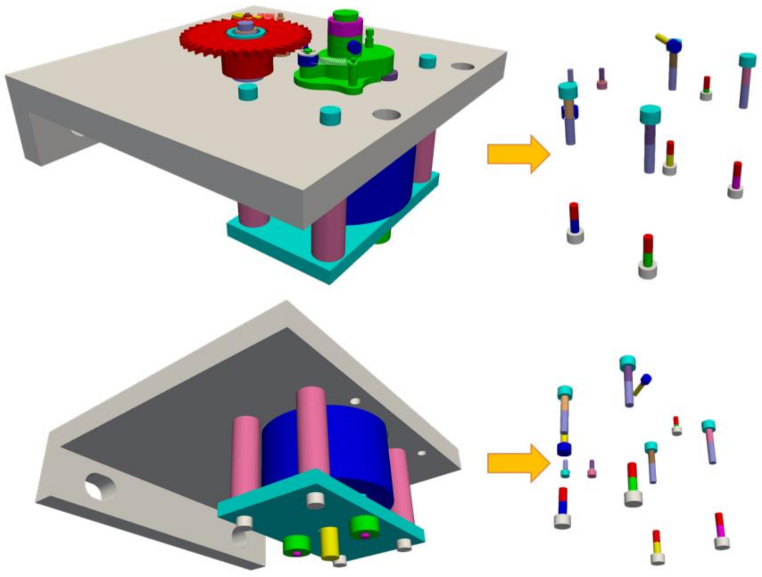
- ***Large scale*** structural ***failure*** frequently originates from ***small scale*** phenomena such as defects, microcracks, inhomogeneities and more, which grow quickly in unstable manner
- Failure occurs due to ***tightly coupled interaction*** between small scale (stress concentrations, material instabilities, cracks, etc.) and large scale (vibration, impact, high loads and other perturbations)
- ***Concurrent multiscale methods*** are ***essential*** for understanding and prediction of behavior of engineering systems when a ***small scale failure*** determines the performance of the entire system

Simplification of mesh generation

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

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

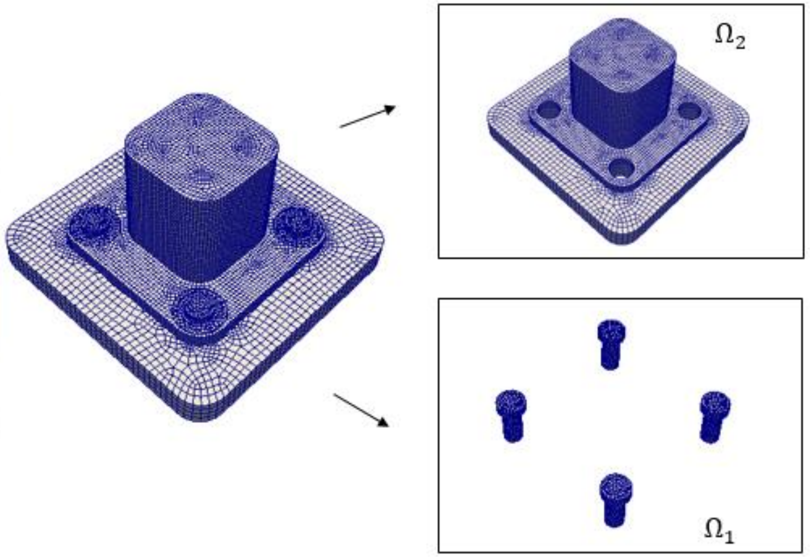
Roof failure of Boeing 737 aircraft due to fatigue cracks. From *imechanica.org*



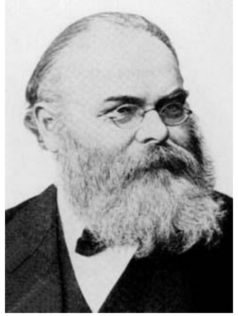
Schematic of difficult-to-mesh ratcheting mechanism with multiple threaded fasteners. From Parish *et al.*, 2024.

Requirements for Multiscale Coupling Method

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



Schwarz Alternating Method for Domain Decomposition



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

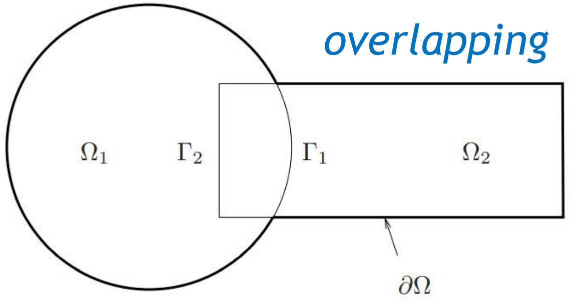
Initialize:

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

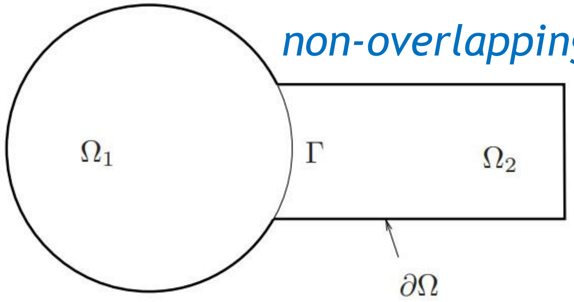
Iterate until convergence:

- Solve PDE by any method on Ω_2 w/ transmission BCs on Γ_2 based on values just obtained for Ω_1.
- Solve PDE by any method on Ω_1 w/ transmission BCs on Γ_1 based on values just obtained for Ω_2.

overlapping



non-overlapping



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

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

How We Use the Schwarz Alternating Method

AS A *PRECONDITIONER* FOR THE LINEARIZED SYSTEM

AS A *SOLVER* FOR THE COUPLED FULLY NONLINEAR PROBLEM

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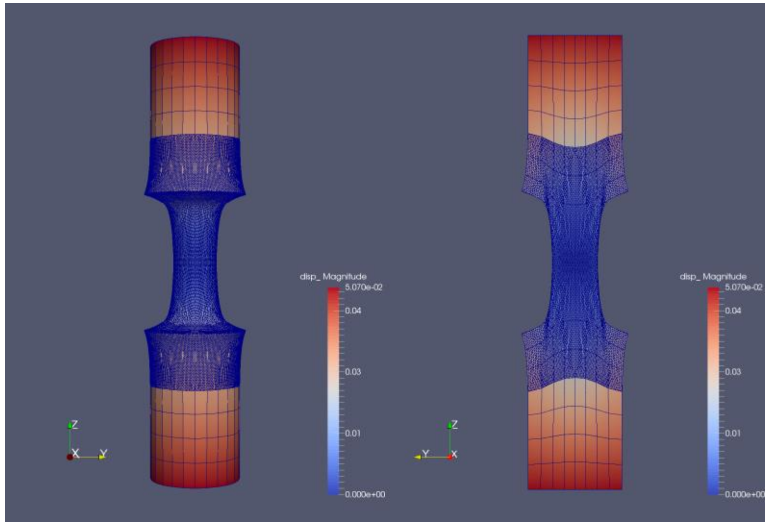

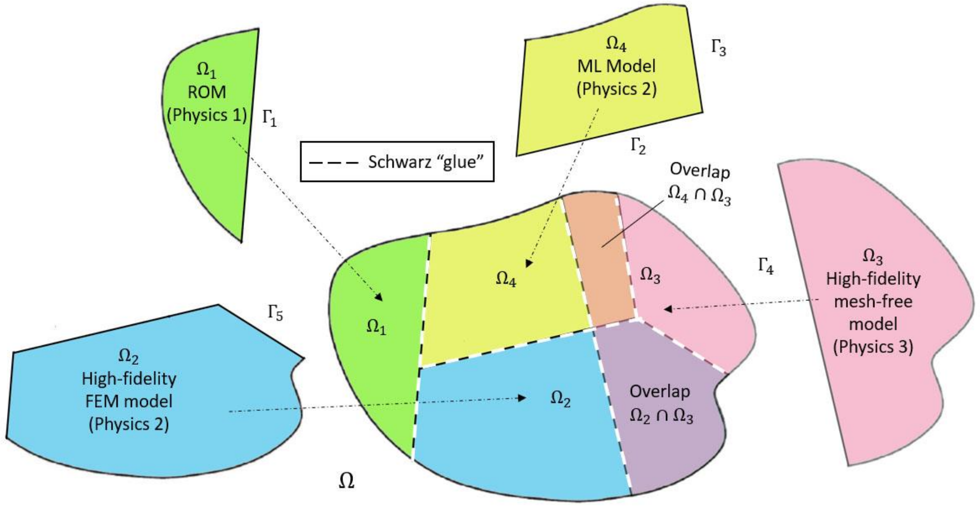

* Projection-based Reduced Order Model

Quasistatic Solid Mechanics Formulation

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

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

  - $A(\boldsymbol{F}, \boldsymbol{Z})$: 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 $i = 1, \dots, n$
  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}

Spatial Coupling via (Multiplicative) Alternating Schwarz

Overlapping Domain Decomposition

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

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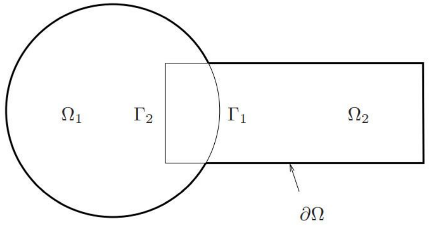


Model PDE:

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

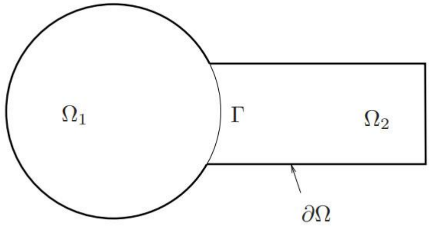
- Dirichlet-Dirichlet transmission BCs [Schwarz, 1870; Lions, 1988]

Non-overlapping Domain Decomposition

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

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

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



- 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)

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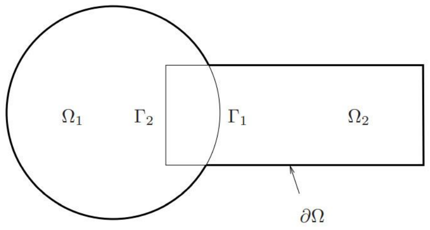

Model PDE:

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

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

Part 1 of talk

Non-overlapping Domain Decomposition

Part 2 of talk

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

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Additional Parallelism via Additive Schwarz

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Multiplicative Overlapping Schwarz

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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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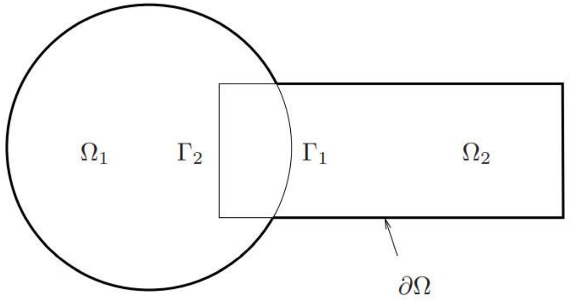

- **Multiplicative Schwarz:** solves subdomain problems **sequentially** (in serial)
- **Additive Schwarz:** advance subdomains in **parallel**, communicate boundary condition data later
  - Typically requires a few more **Schwarz iterations**, but does not degrade **accuracy**
  - **Parallelism** helps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

Additional Parallelism via Additive Schwarz

Part 1 of talk

Multiplicative Overlapping Schwarz

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Part 2 of talk

Additive Overlapping Schwarz

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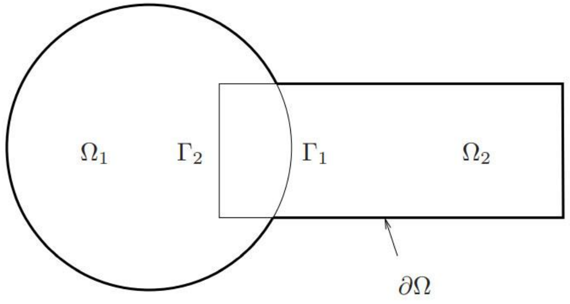

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Overlapping Schwarz Coupling in Quasistatics

outer quasistatic loop

$\varphi^{(0)} \leftarrow \mathrm{id}_{\boldsymbol{X}}$ in Ω_2 $\quad\triangleright$ initialize to zero displacement or a better guess in Ω_2

$n \leftarrow 1$

repeat $\quad\triangleright$ Schwarz loop

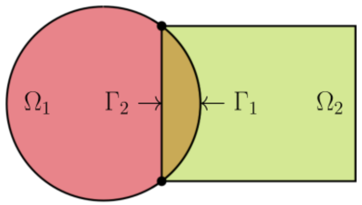
$\quad \varphi^{(n)} \leftarrow \chi$ on $\partial_\varphi \Omega_i$ $\quad\triangleright$ Dirichlet BC for Ω_i

$\quad \varphi^{(n)} \leftarrow P_{\Omega_j \to \Gamma_i}[\varphi^{(n-1)}]$ on Γ_i $\quad\triangleright$ Schwarz BC for Ω_i

$\quad \varphi^{(n)} \leftarrow \arg\min\limits_{\varphi \in S_i} \Phi_i[\varphi]$ in Ω_i $\quad\triangleright$ solve in Ω_i

$\quad n \leftarrow n + 1$

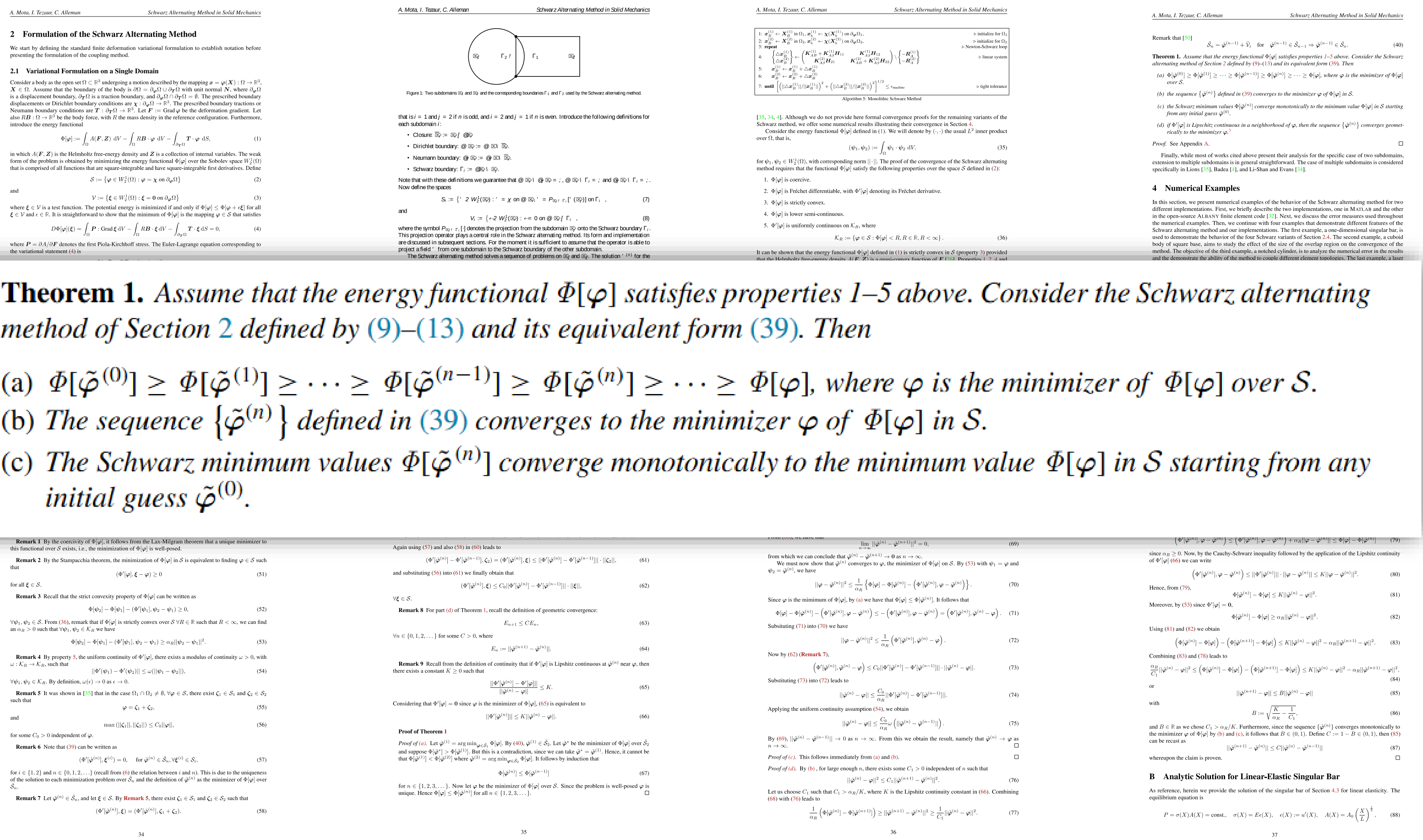
until converged



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.

Convergence Proof*



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

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

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

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

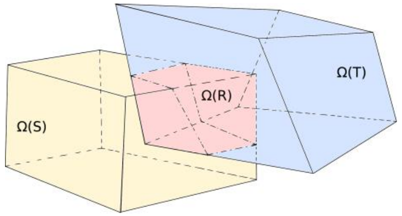
Albany-LCM[1]

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

Sierra/Solid Mechanics (Sierra/SM)

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

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



Data Transfer Kit (DTK)

[1]https://github.com/sandialabs/LCM.git. [2]http://github.com/trilinos/Trilinos.git. [3]https://github.com/ORNL-CEES/DataTransferKit.

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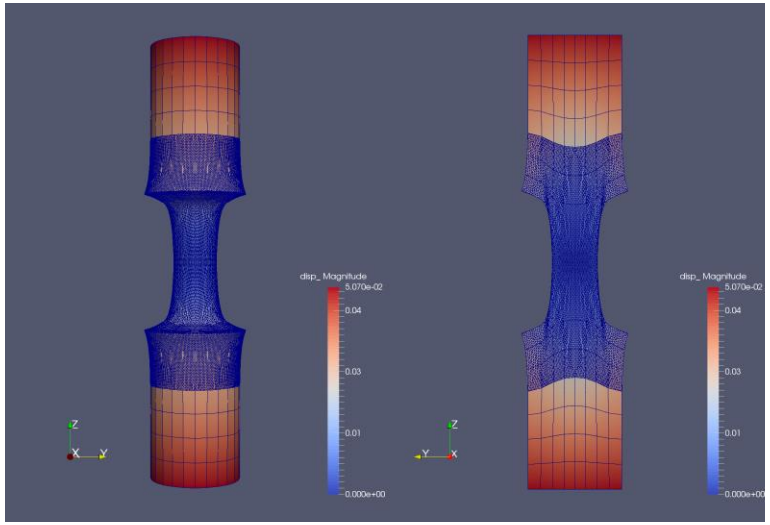
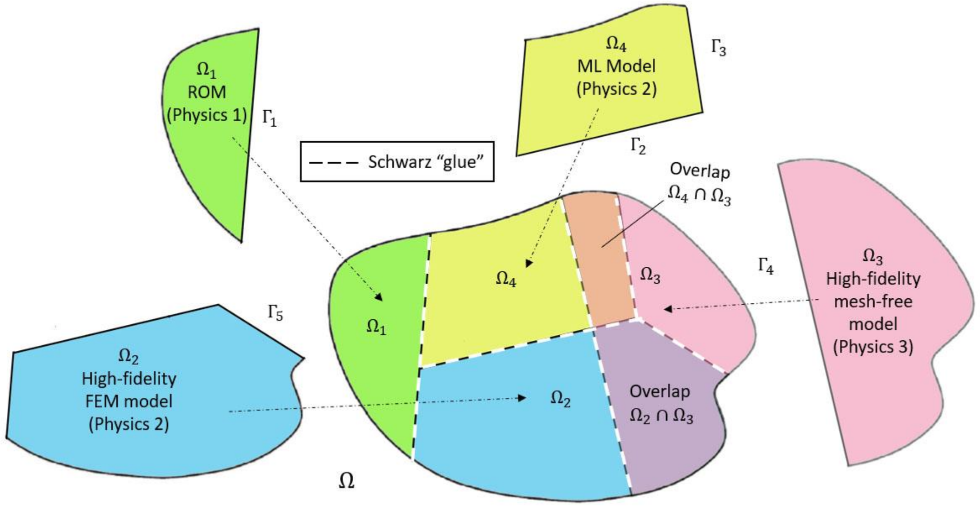
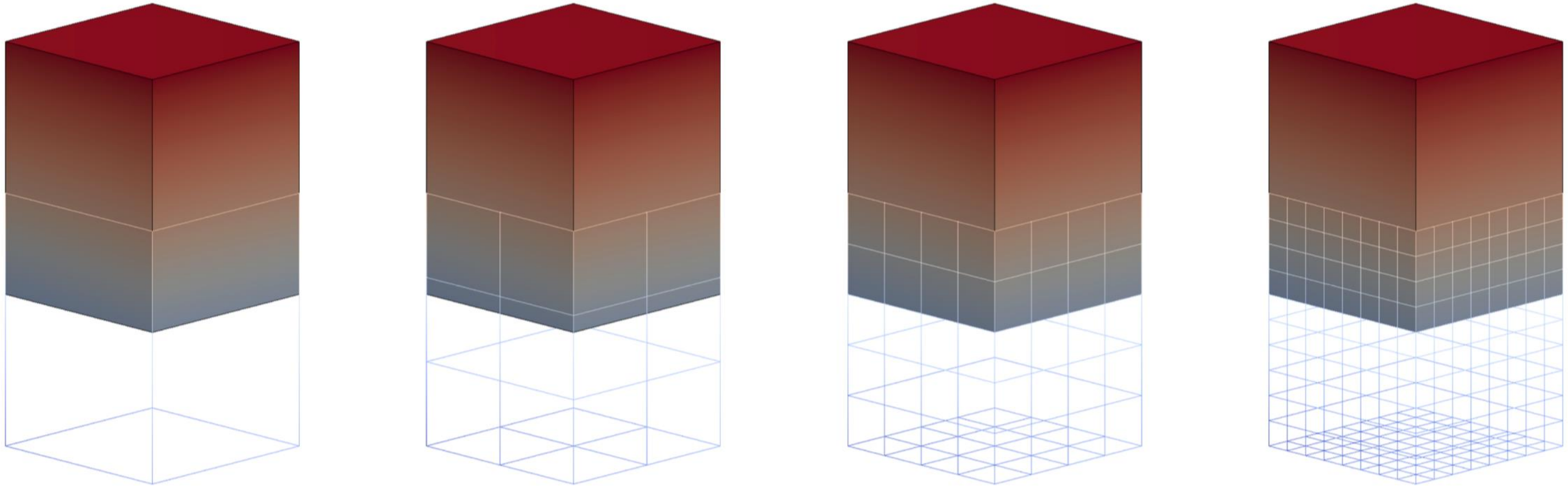


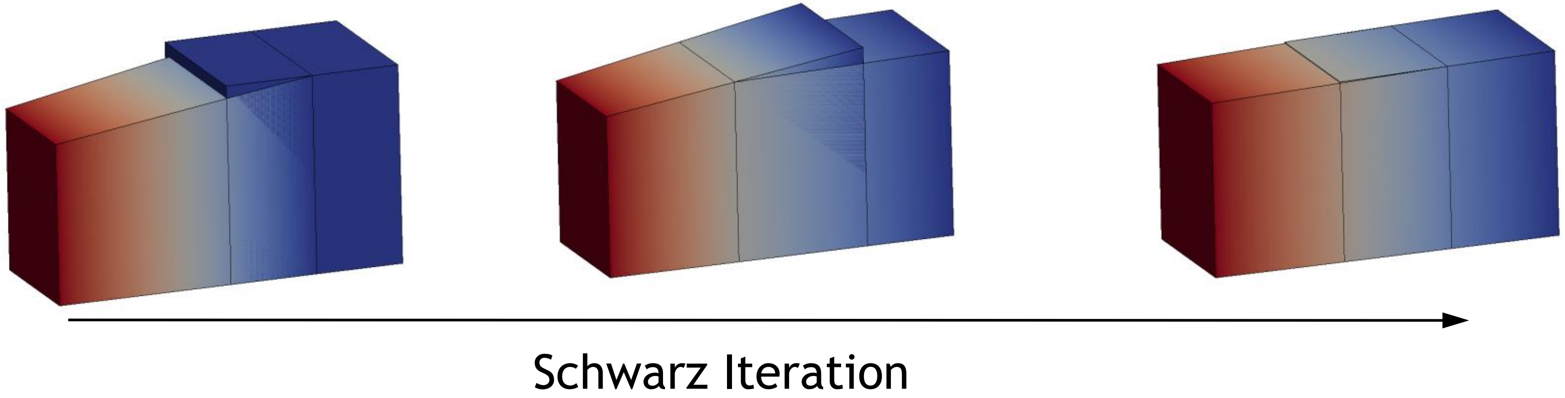


* Projection-based Reduced Order Model

Cuboid Problem



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



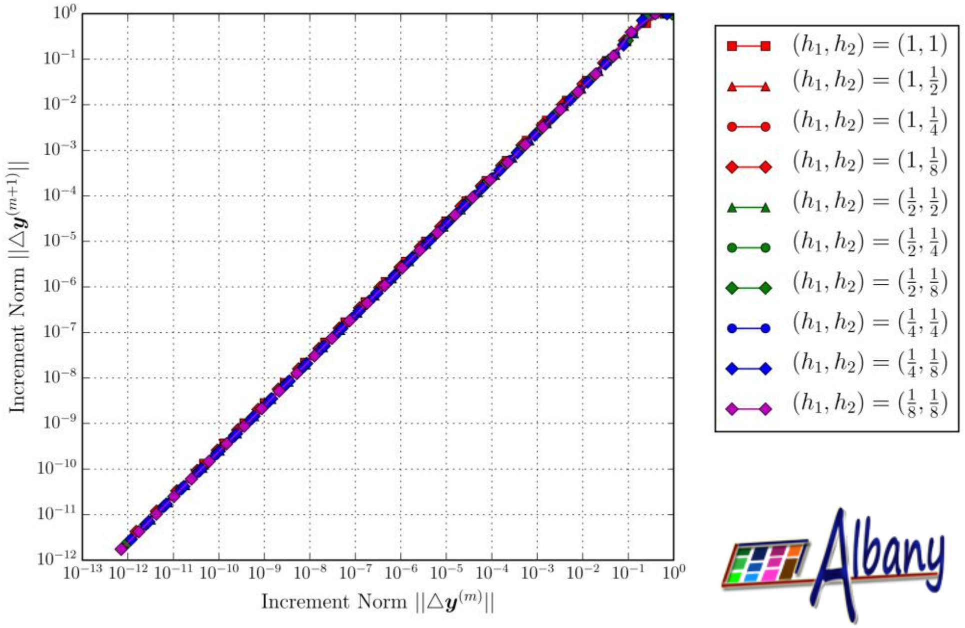
Cuboid Problem: Convergence and Accuracy

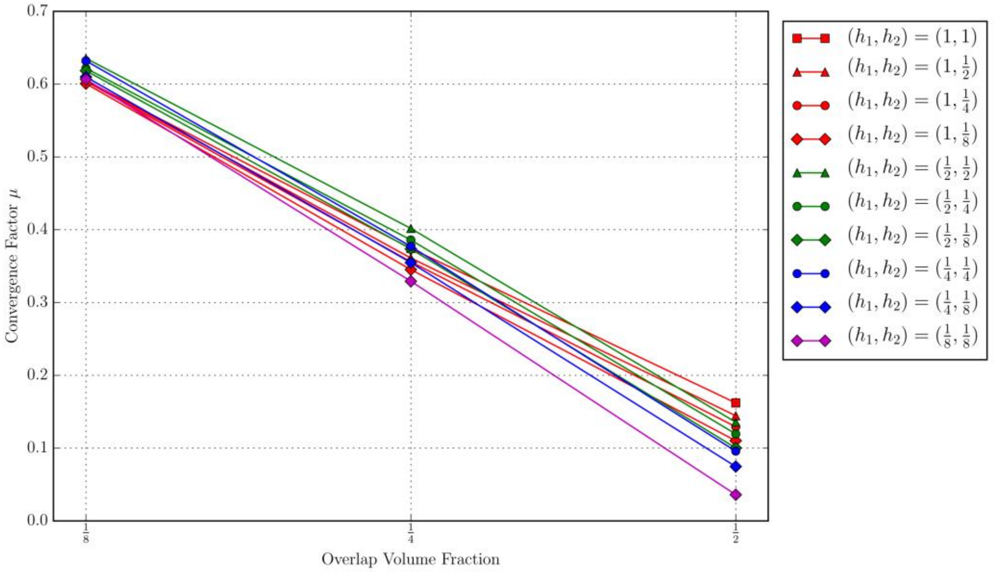
- **Top right:** convergence of the cuboid problem for ***different mesh sizes*** and ***fixed overlap volume fraction***. The Schwarz alternating method converges ***linearly***.
- **Bottom right:** convergence factor μ as a function of overlap volume and different mesh. There is ***faster linear convergence***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

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

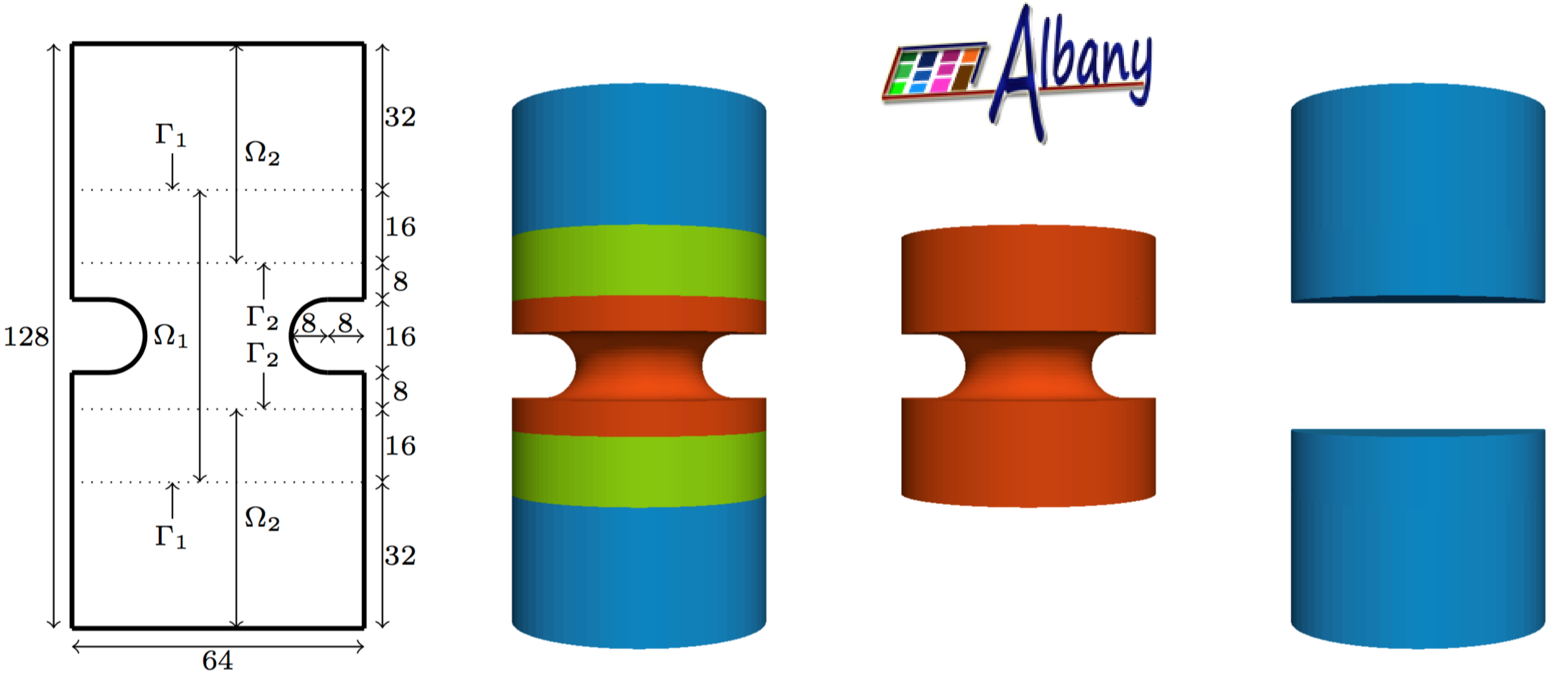
- **Below:** ***relative errors*** in displacement and stress w.r.t. single-domain reference solution. Errors are on the order of ***machine precision***.

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

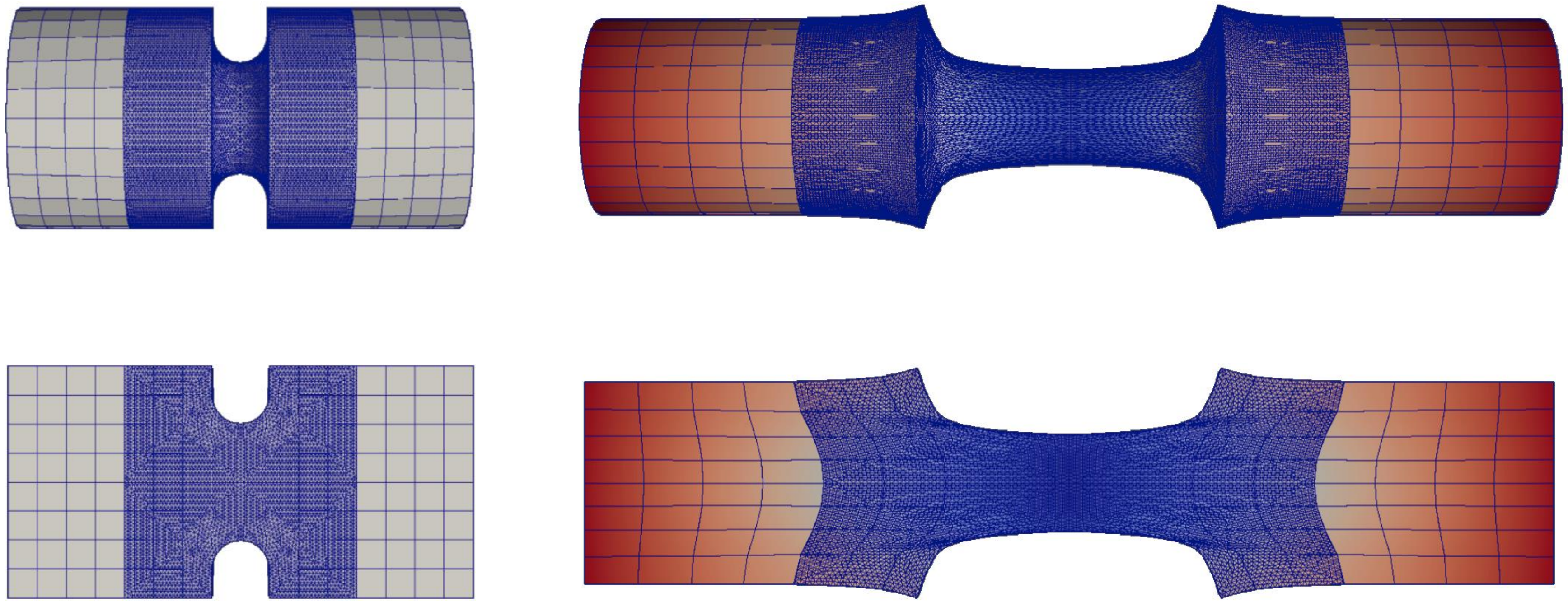


(a) Schematic **(b)** Entire Domain Ω **(c)** Fine Region Ω_1 **(d)** Coarse Region Ω_2

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

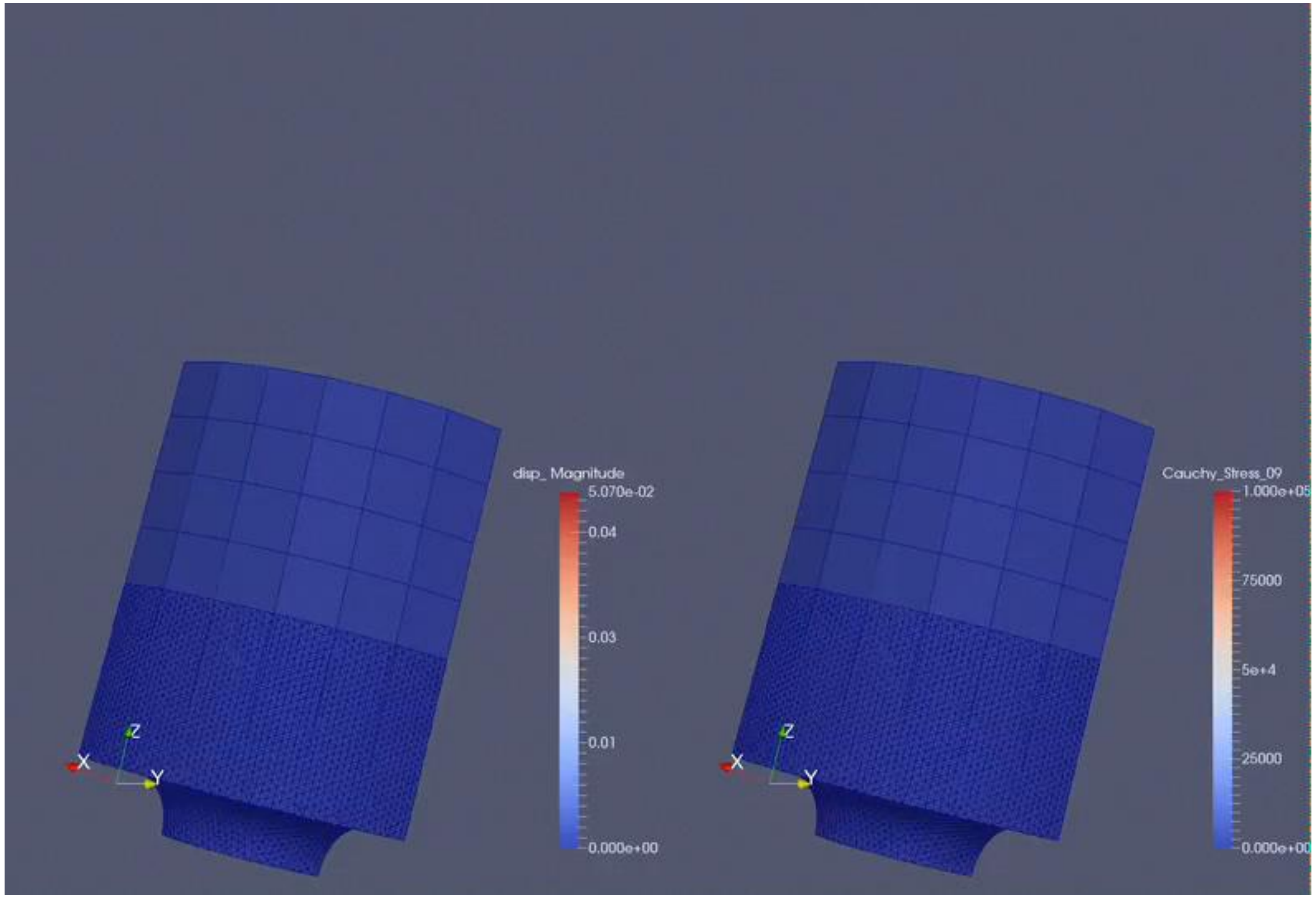
Notched Cylinder: TET - HEX Coupling

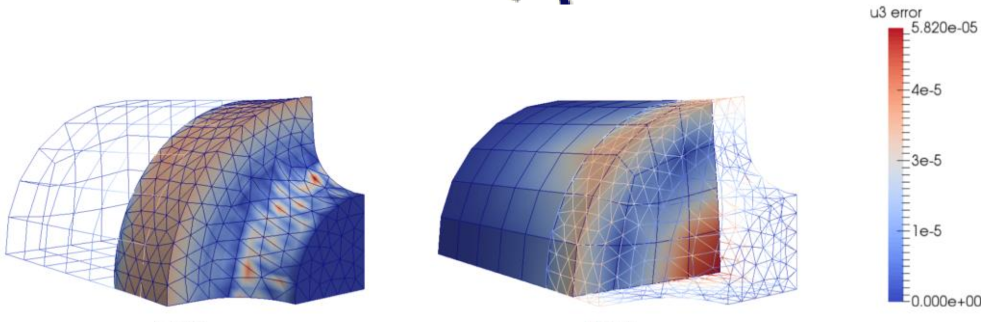
- The Schwarz alternating method is capable of coupling ***different mesh topologies***.
- The notched region, where stress concentrations are expected, is ***finely*** meshed with ***tetrahedral*** elements.
- The top and bottom regions, presumably of less interest, are meshed with ***coarser hexahedral***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



Albany

Notched Cylinder: TET - HEX Coupling





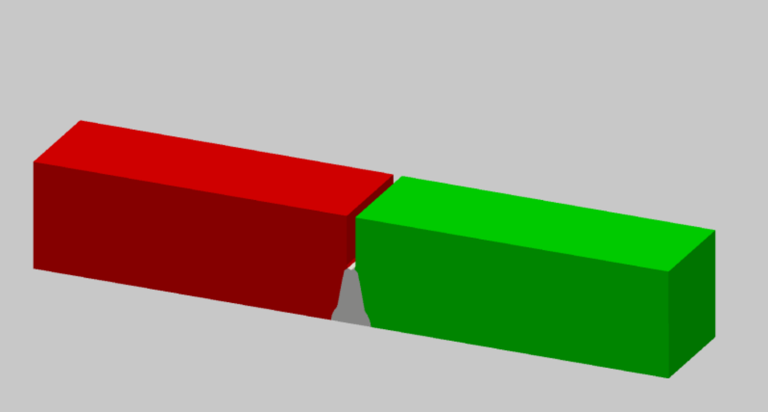
(a) Ω_1 (b) Ω_2

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

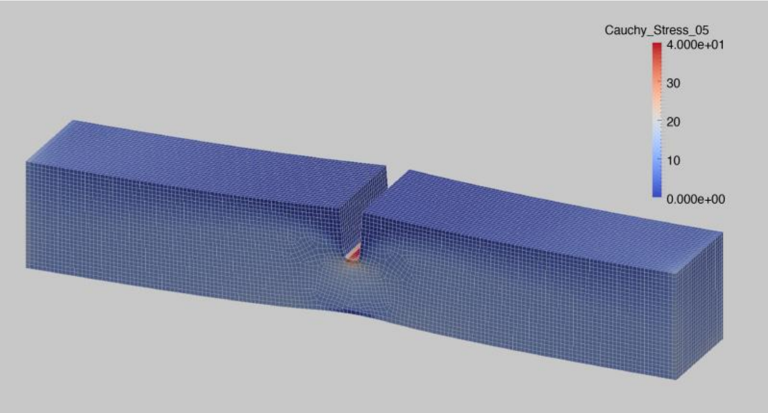
- Relative errors in displacement w.r.t. single-domain reference solution are dominated by ***geometric*** (rather than coupling) ***error***.

Laser Weld (Albany/LCM)

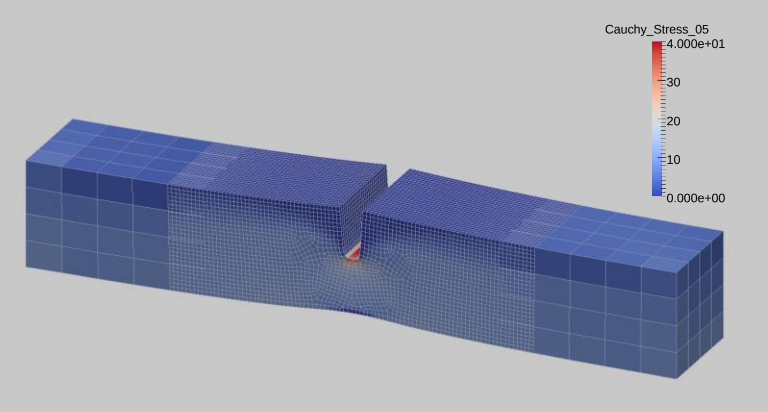
Laser weld specimen



Single domain discretization

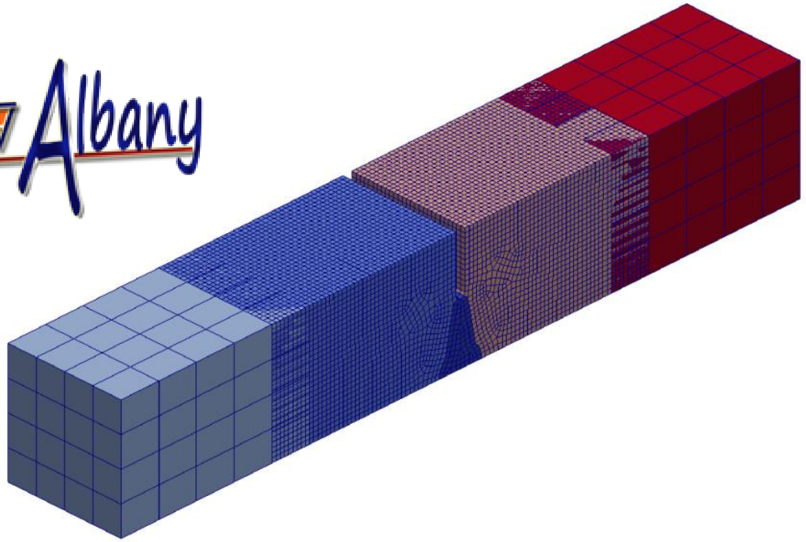


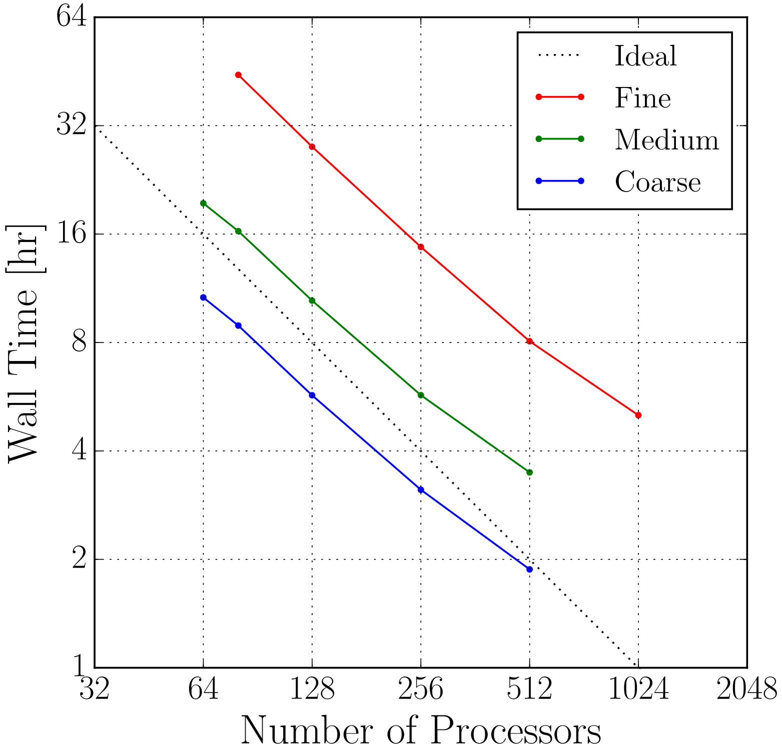
Coupled Schwarz discretization
(50% reduction in model size)



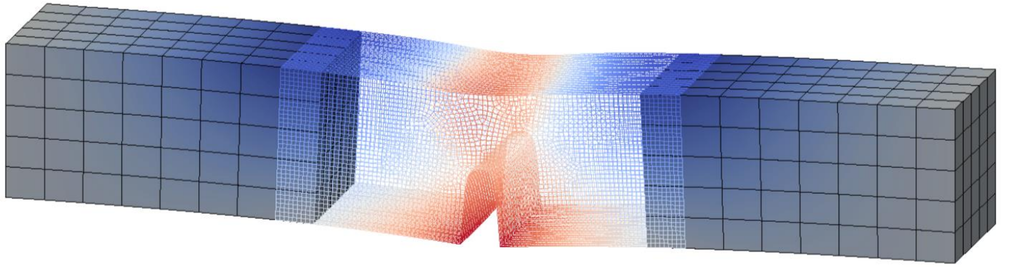
- Problem of ***practical scale***.
- ***Isotropic elasticity*** and ***J_2 plasticity*** with linear isotropic hardening.
- ***Identical parameters*** for weld and base materials for proof of concept, to become independent models.

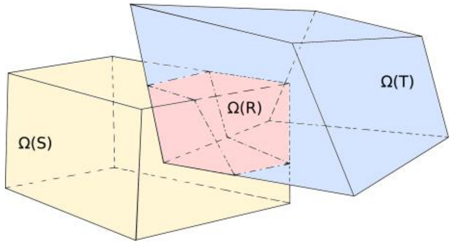
Laser Weld (Albany/LCM): Strong Scalability of Parallel Schwarz with DTK





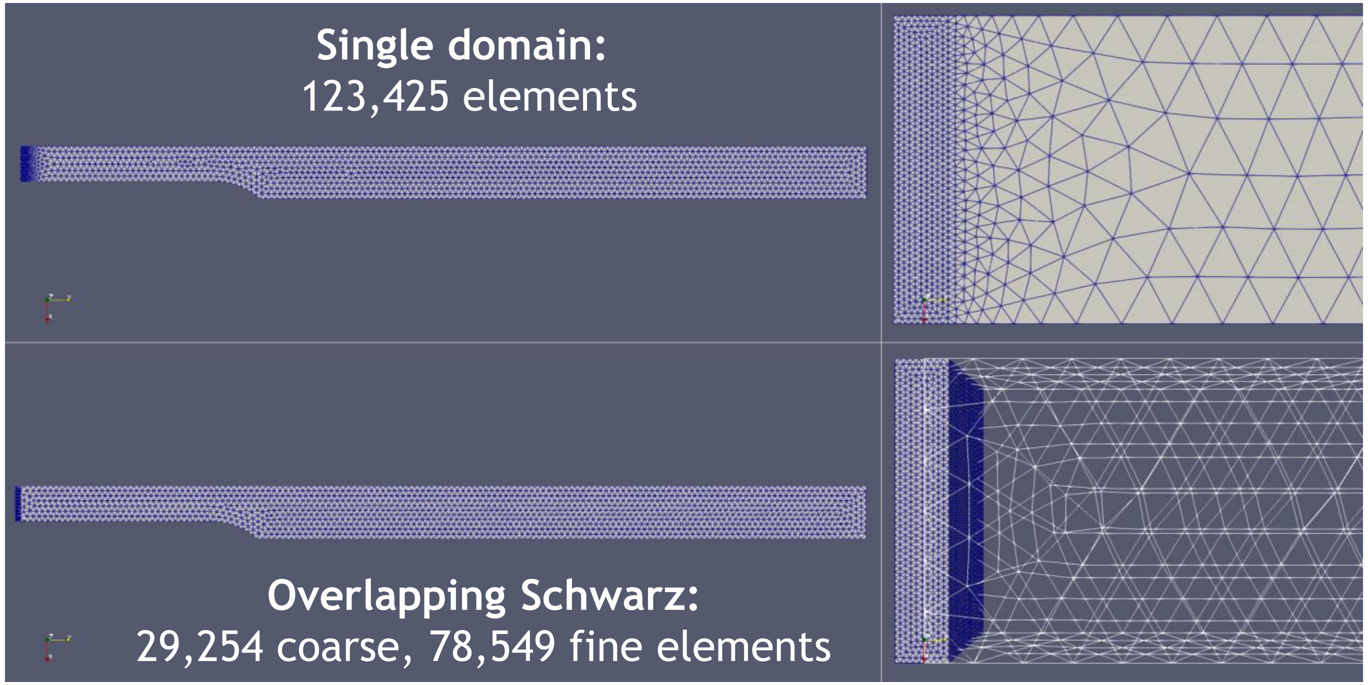
- ***Near-ideal linear speedup*** (64-1024 cores).

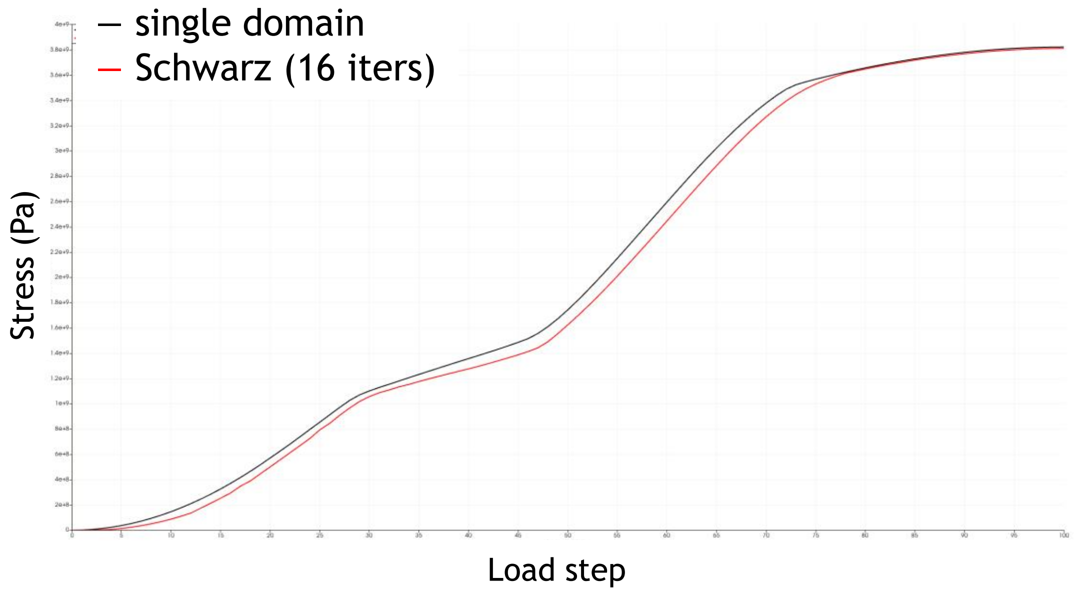




Data Transfer Kit (DTK)

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



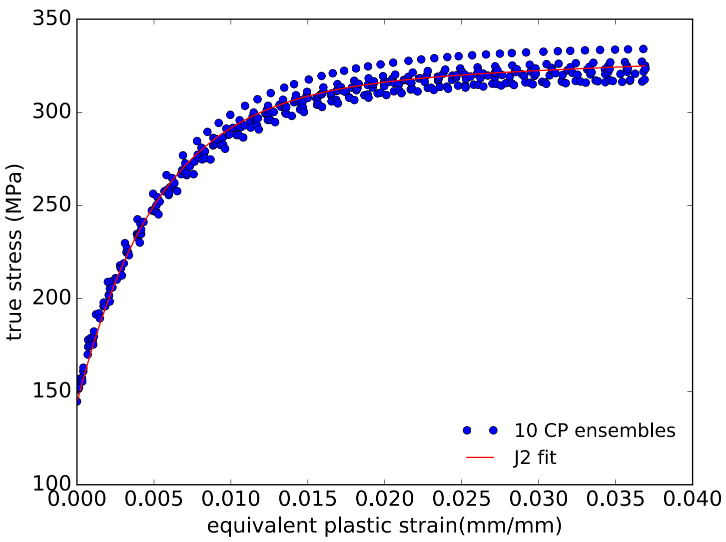


- The domains for Schwarz coupling are **meshed independently**
- This provides the ability to try **different meshing schemes** for each subdomain
- **No need** to **re-mesh** entire domain
- Schwarz gives **accurate prediction** of stress states if tight enough Schwarz tolerance is used
    - ➢ **Tight Schwarz tolerance** needed due **to large disparity** between **element sizes**
- For now, Schwarz is **slower** on this problem, but we are optimizing this

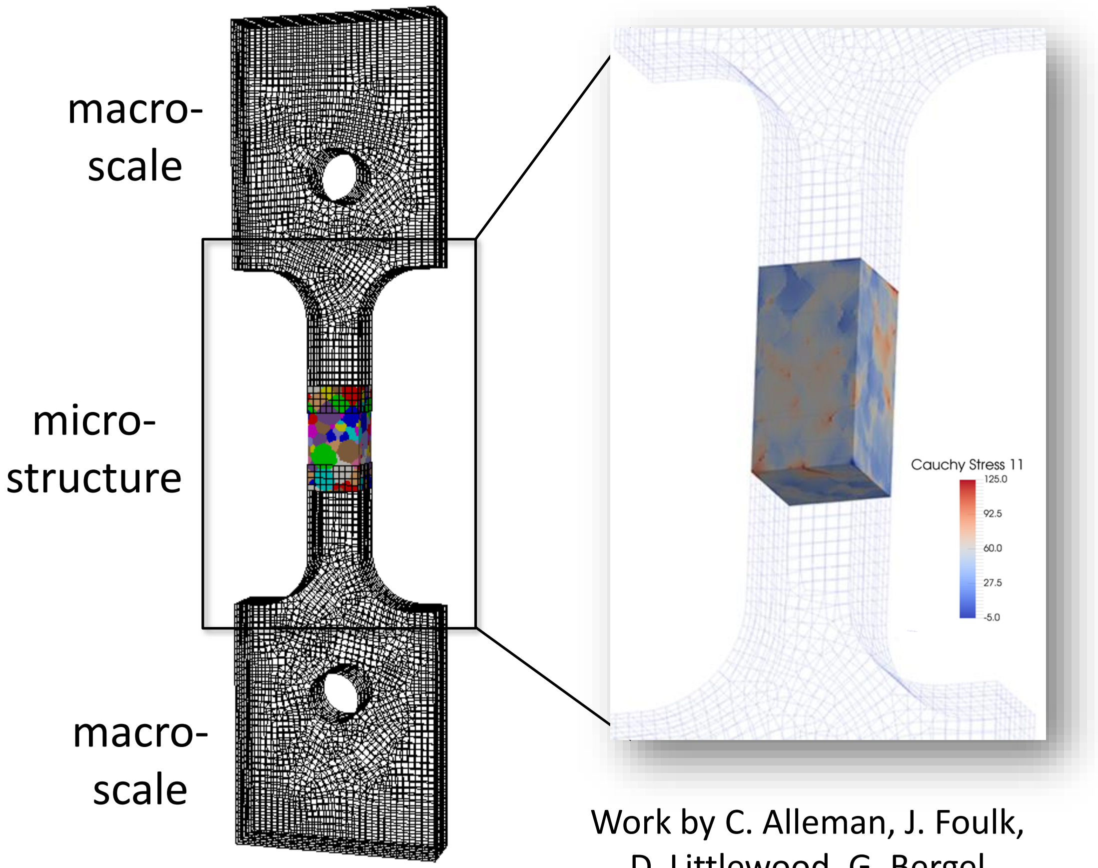
Tensile Bar

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

- ***Microstructure*** embedded in ASTM tensile geometry (right).
- Fix microstructure, investigate ***ensemble*** of uniaxial loads.
- Fit flow curves with a ***macroscale*** J_2 plasticity model (below).



Goal: *study strain localization in microstructure.*



Work by C. Alleman, J. Foulk, D. Littlewood, G. Bergel

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   - Quasistatic Formulation
     - ➢ Numerical Examples
   - **Extension to Dynamics**
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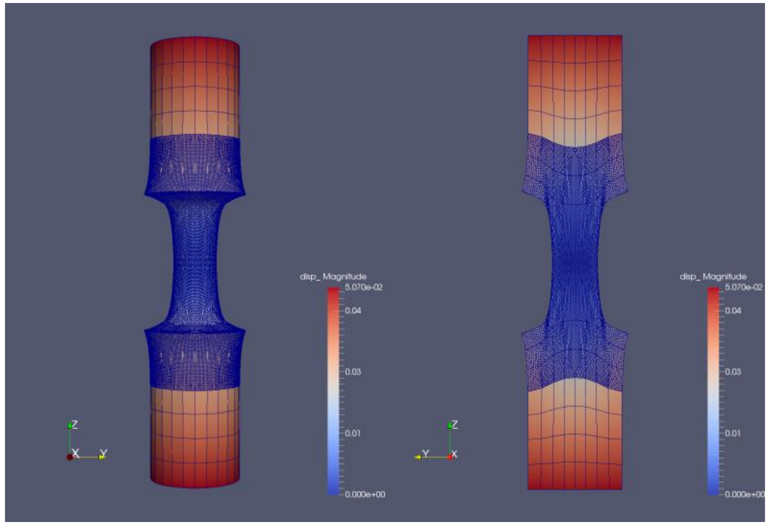
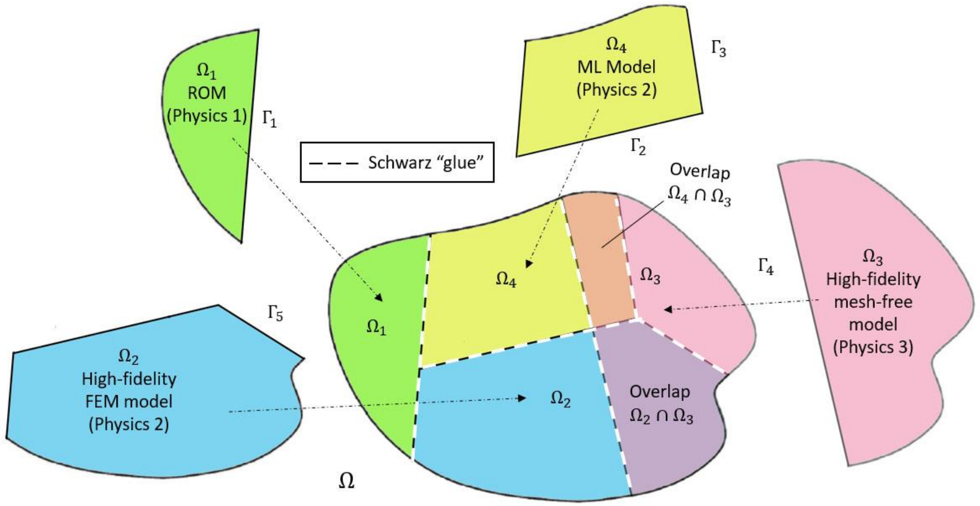




* Projection-based Reduced Order Model

Solid Dynamics Formulation

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

- Potential energy: $V(\boldsymbol{\varphi}) \coloneqq \displaystyle\int_{\Omega} A(\boldsymbol{F}, \boldsymbol{Z}) dV - \int_{\Omega} \rho \boldsymbol{B} \cdot \boldsymbol{\varphi} \, dV$

- Lagrangian: $L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) \coloneqq T(\dot{\boldsymbol{\varphi}}) - V(\boldsymbol{\varphi})$

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

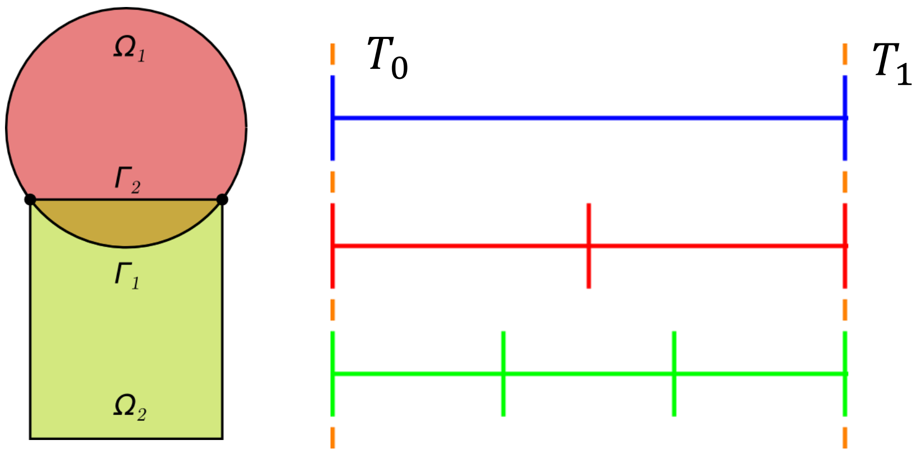
- Euler-Lagrange equations:

$$\begin{cases} \operatorname{Div} \boldsymbol{P} + \rho \boldsymbol{B} = \rho \ddot{\boldsymbol{\varphi}}, & \text{in } \Omega \times I \\ \boldsymbol{\varphi}(\boldsymbol{X}, t_0) = \boldsymbol{x}_0, & \text{in } \Omega \\ \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t_0) = \boldsymbol{v}_0, & \text{in } \Omega \\ \boldsymbol{\varphi}(\boldsymbol{X}, t) = \boldsymbol{\chi}, & \text{on } \partial\Omega \times I \end{cases}$$

- Semi-discrete problem following FEM discretization in space:

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

Time-Advancement Within the Schwarz Framework



Controller time stepper

Time integrator for Ω_1

Time integrator for Ω_2

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

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

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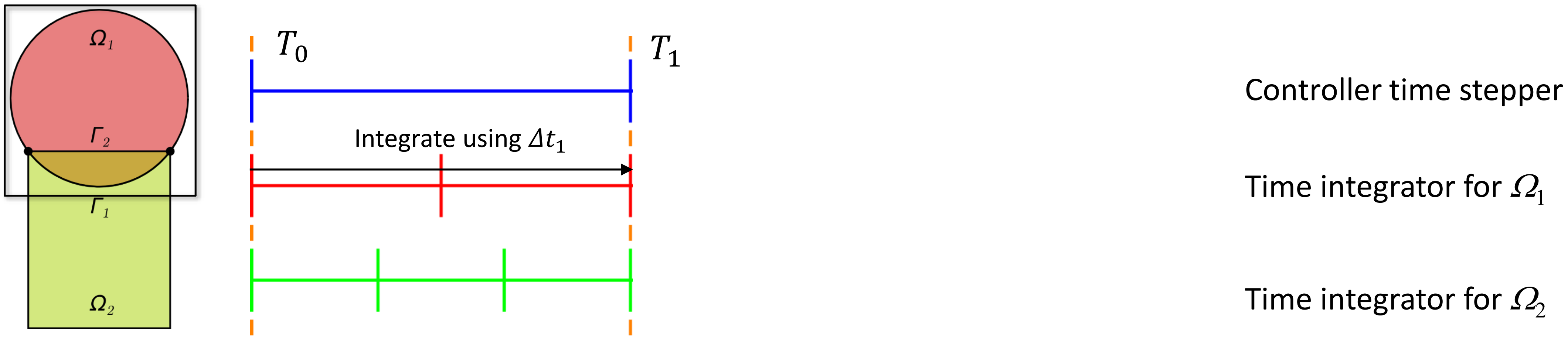

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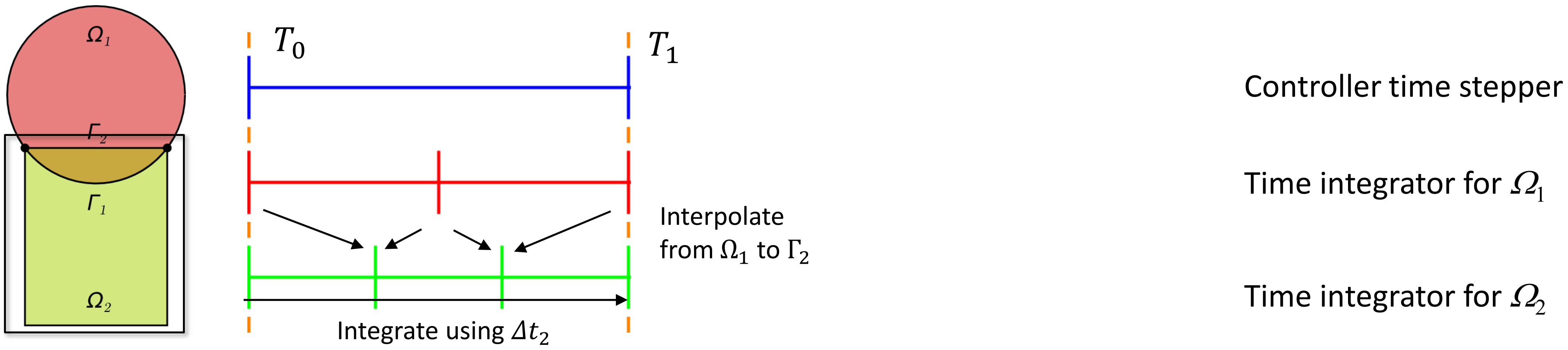

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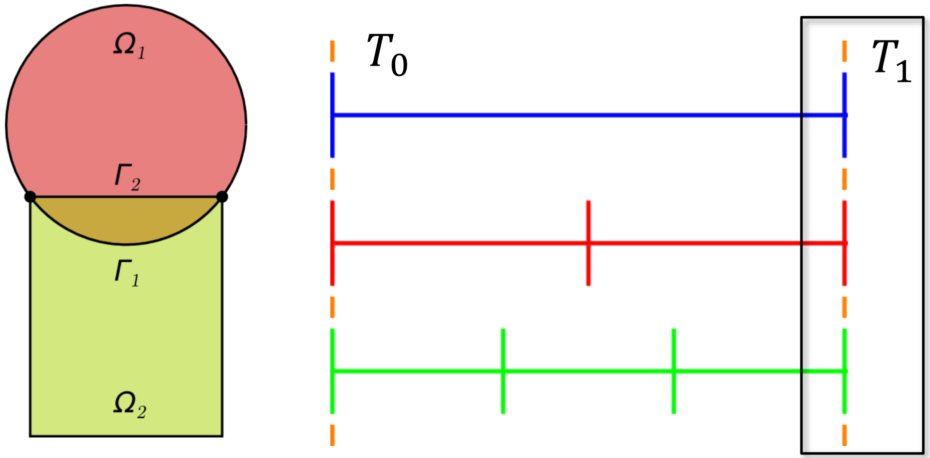

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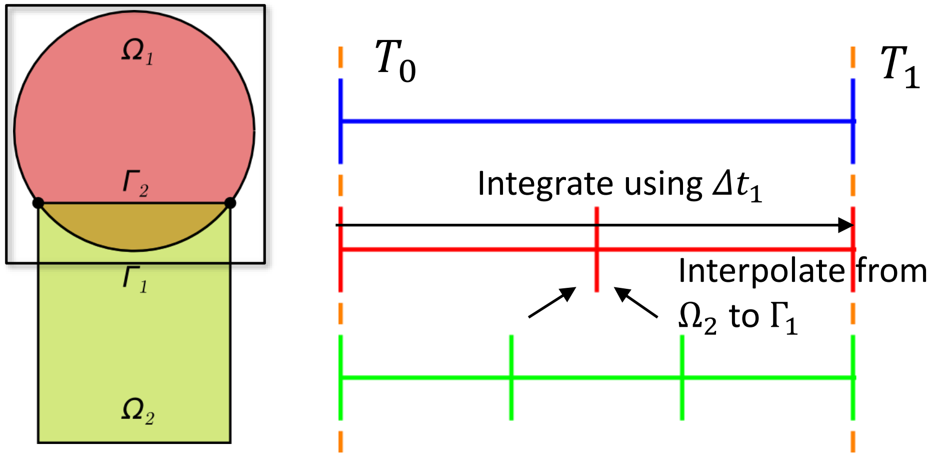

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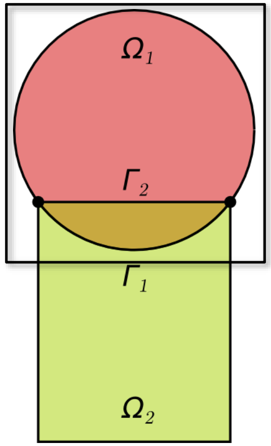

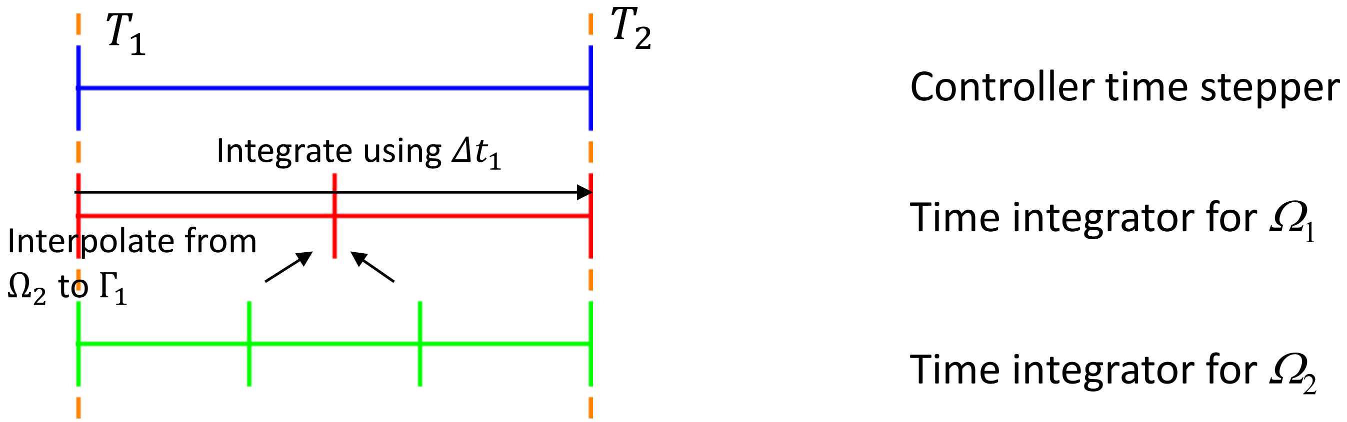

Can use ***different integrators*** with ***different time steps*** within each domain!

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

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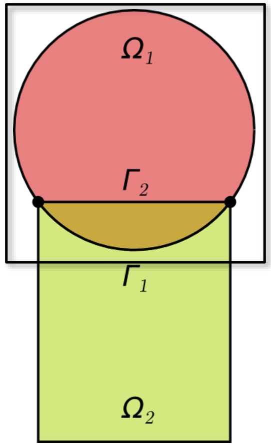

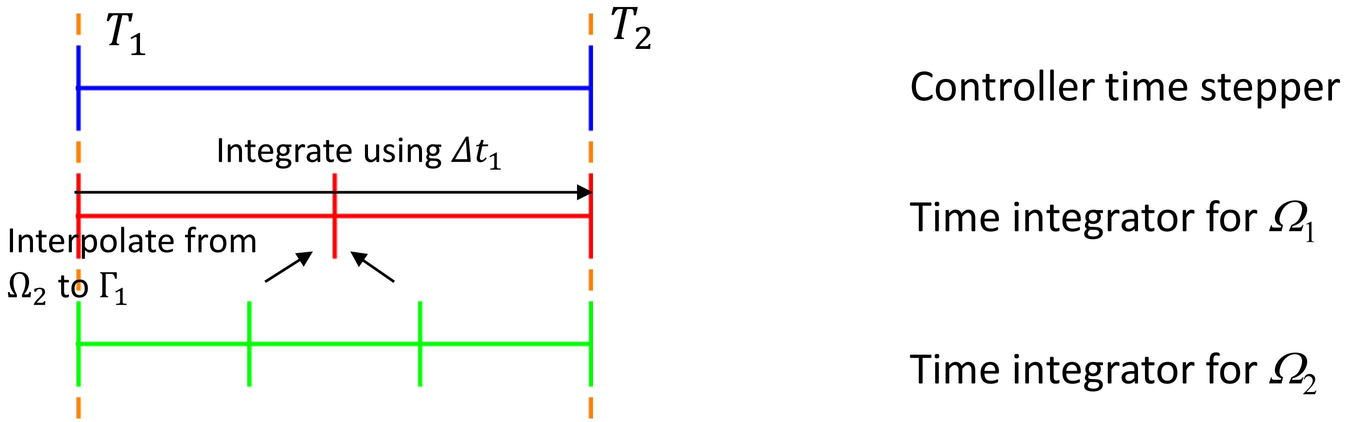

Time-stepping procedure is **equivalent** to doing Schwarz on **space-time domain** [Mota *et al*. 2022].

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Schwarz Alternating Method for Dynamic Multiscale Coupling: Theory

- 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.

*A. Mota, **I. Tezaur**, G. Phlipot. "The Schwarz alternating method for dynamic solid mechanics", *IJNME*, 2022.

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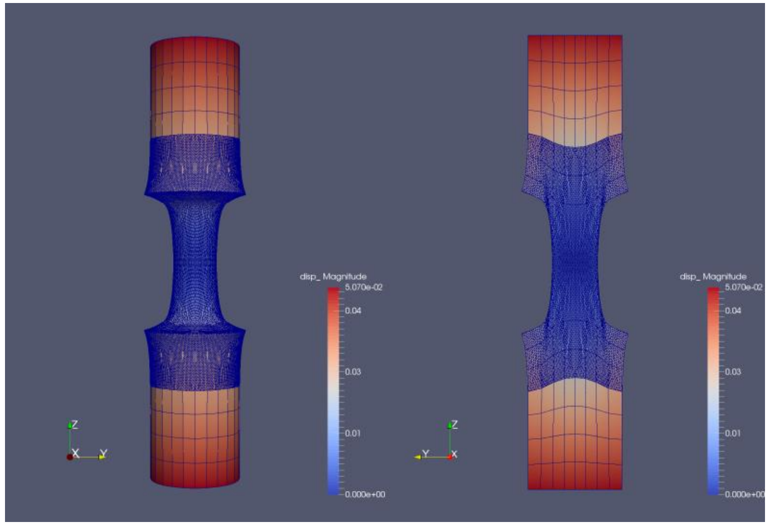
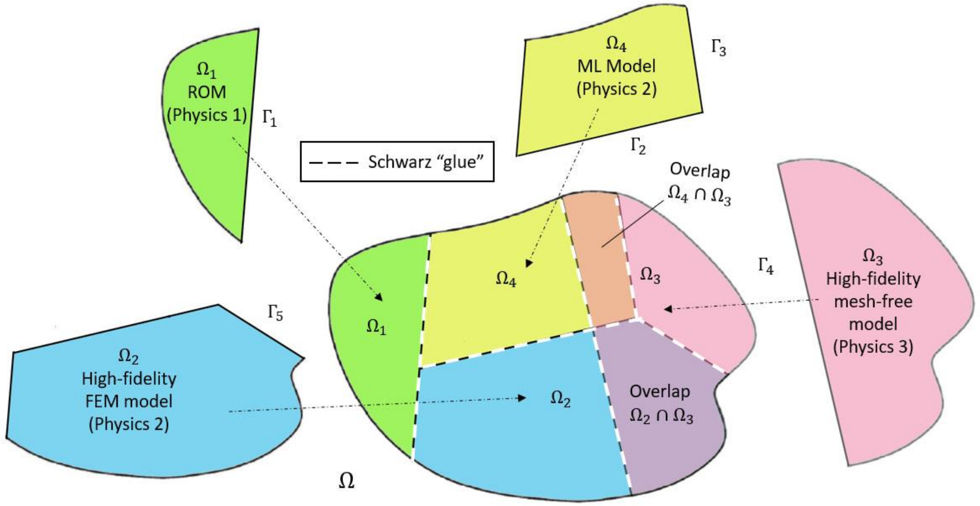
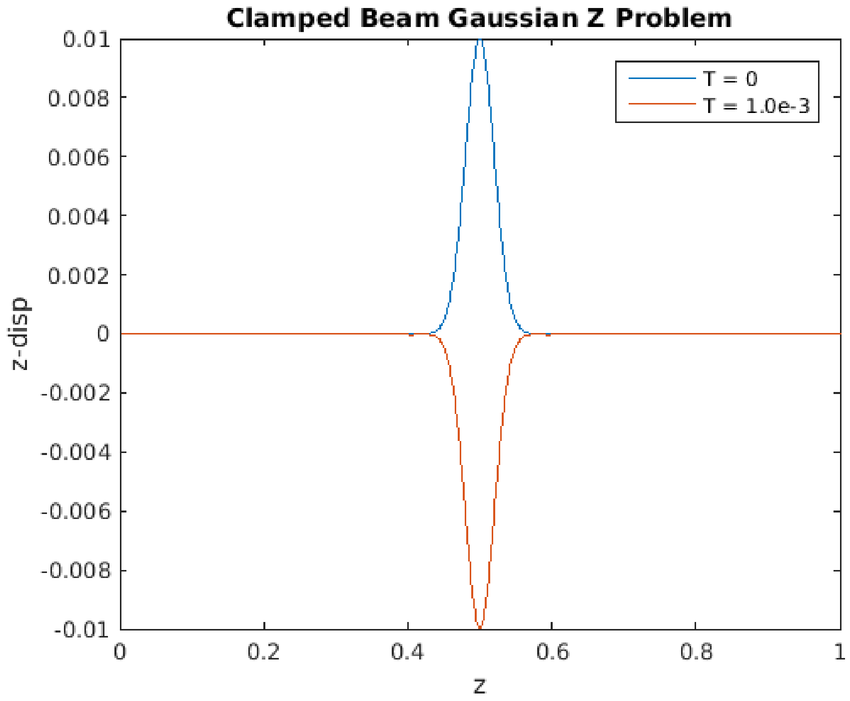




* Projection-based Reduced Order Model

Elastic Wave Propagation

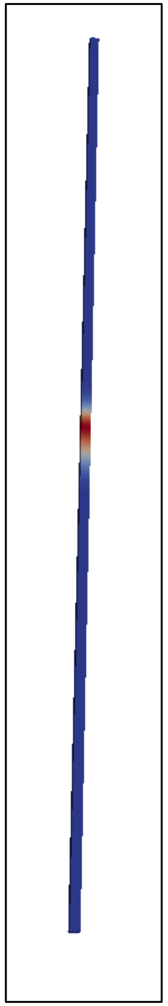
- Linear elastic ***clamped beam*** with Gaussian initial condition for the z-displacement.
- Simple problem with analytical exact solution but very ***stringent test*** for discretization methods.
- Test Schwarz with ***2 subdomains***: $\Omega_0 = (0{,}0.001) \times (0{,}0.001) \times (0{,}0.75), \Omega_1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



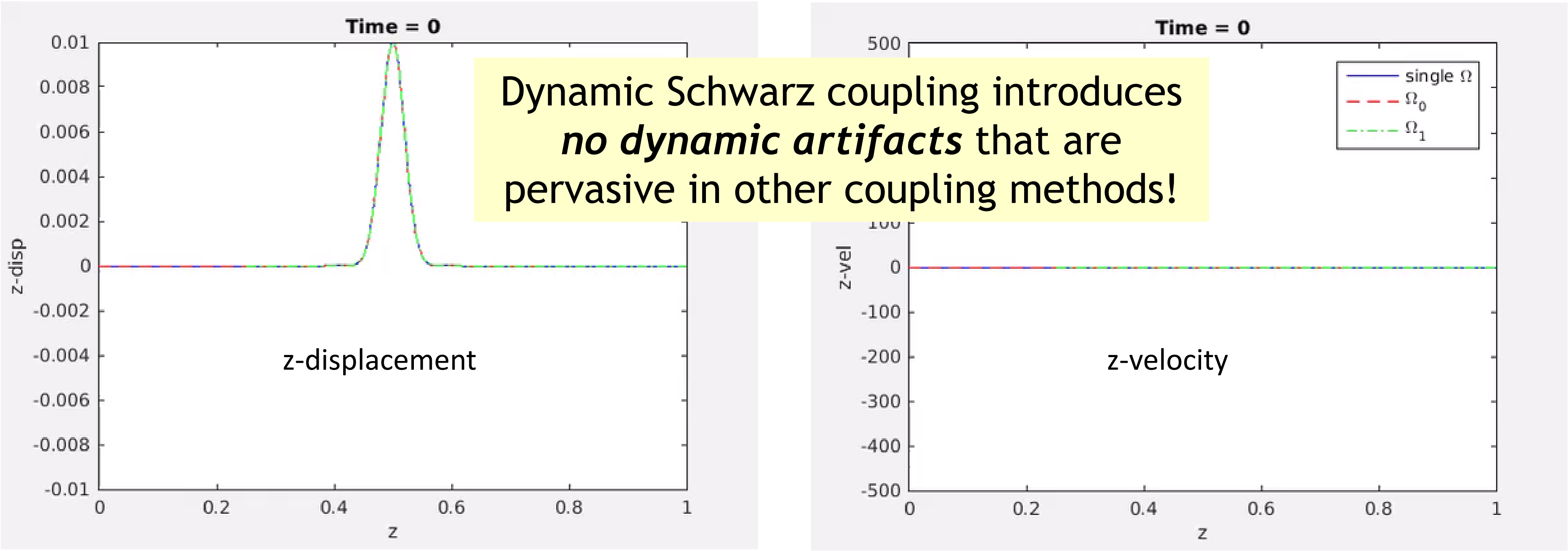
Left: Initial condition (blue) and final solution (red). Wave profile is negative of initial profile at time T = 1.0e-3.

Time-discretizations: Newmark (implicit, explicit).

Meshes: HEX, TET



Elastic Wave: Different Integrators, Same Δts

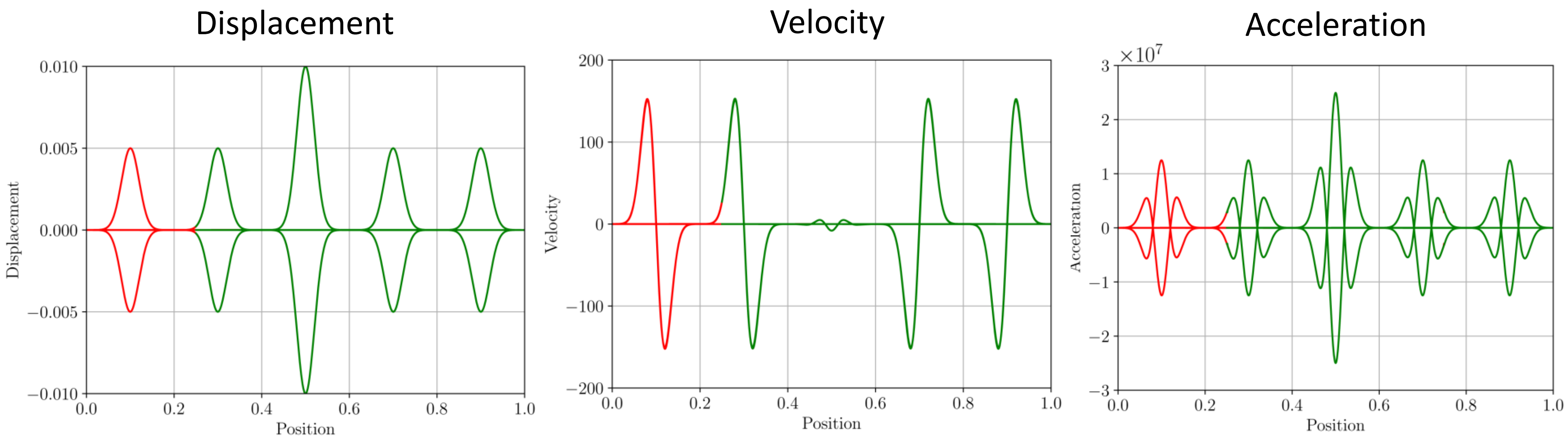


Dynamic Schwarz coupling introduces ***no dynamic artifacts*** that are pervasive in other coupling methods!

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

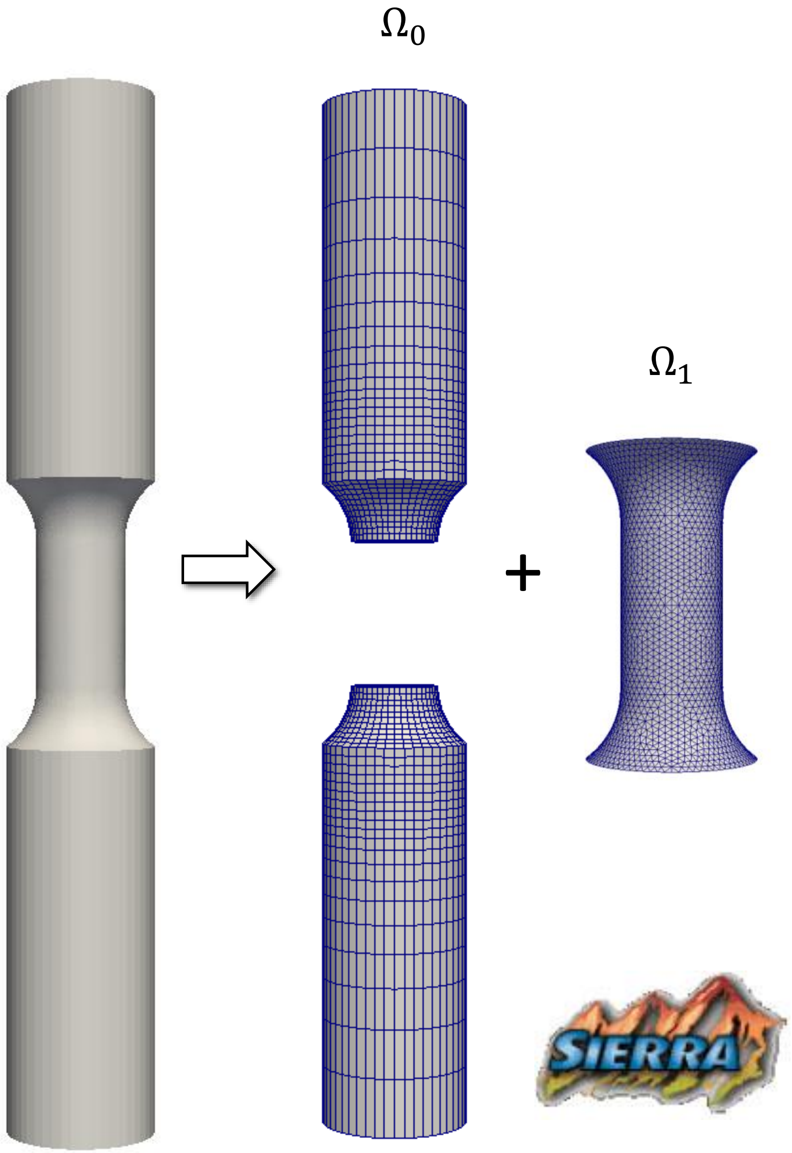


Figures above: Plots of displacement, velocity and acceleration for the elastic wave propagation problem using different time integrators (implicit and explicit) and different time steps (1e-2s and 2e-7s) for each subdomain, superimposed over the analytic single domain solution.

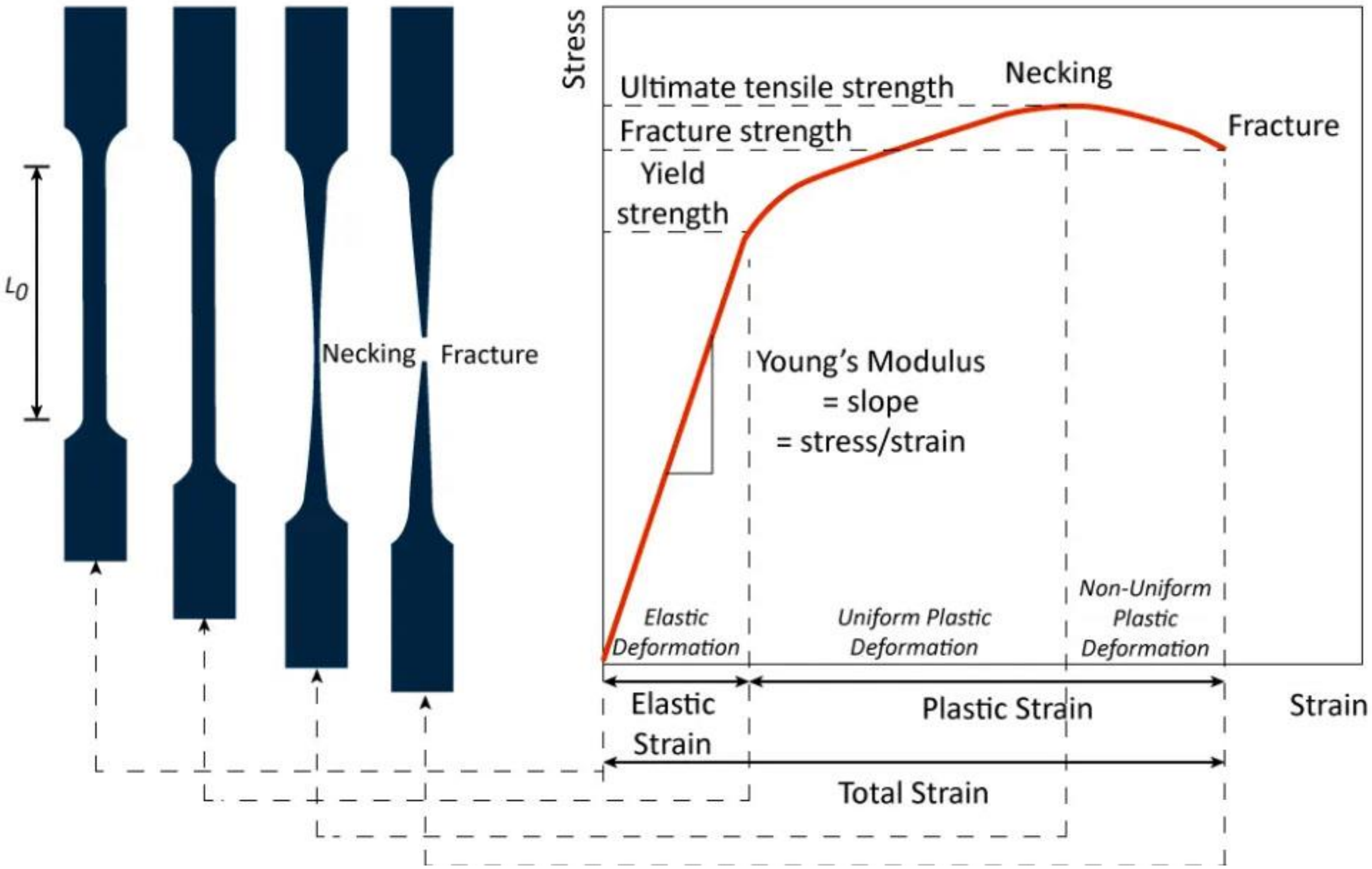
The analytic solution is ***indistinguishable*** from Schwarz solutions (hidden behind the solutions for Ω_0 (red) and Ω_1 (green))!

Tension Specimen

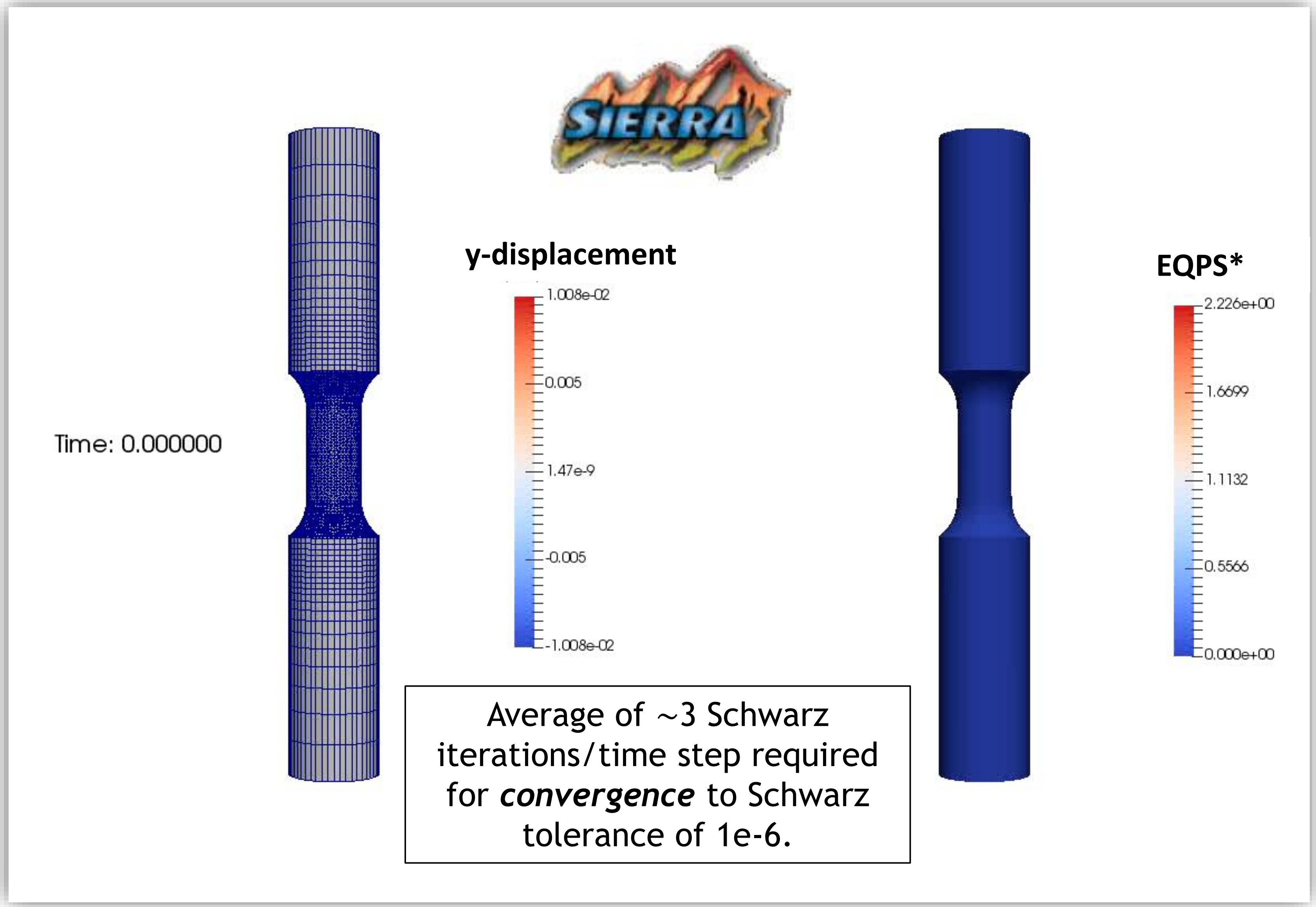
- Uniaxial aluminum cylindrical tensile specimen with ***inelastic J_2 material model***.
- Domain decomposition into ***two subdomains*** (right): Ω_0 = ends, Ω_1 = gauge.
- ***Nonconformal HEX + composite TET10*** coupling via Schwarz.
- ***Implicit*** Newmark time-integration with ***adaptive time-stepping*** algorithm employed in both subdomains.
- Slight ***imperfection*** introduced at center of gauge to force ***necking*** upon pulling in vertical direction.



Tension Specimen: Expected Result



Tension Specimen: Displacement & EQPS*

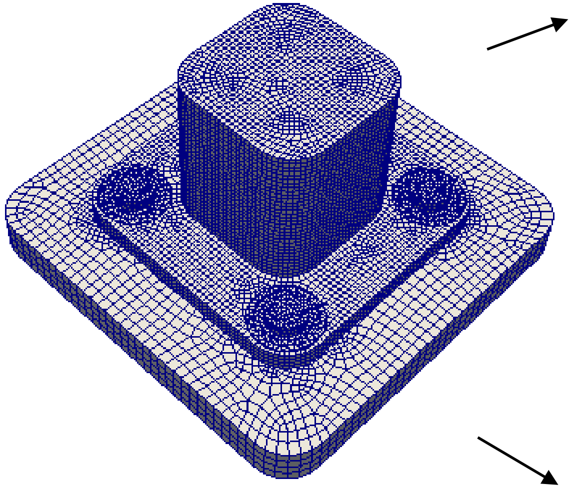


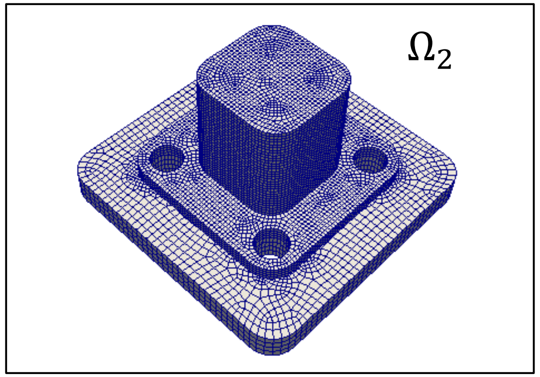
*EQPS = Equivalent Plastic Strain

Bolted Joint Problem

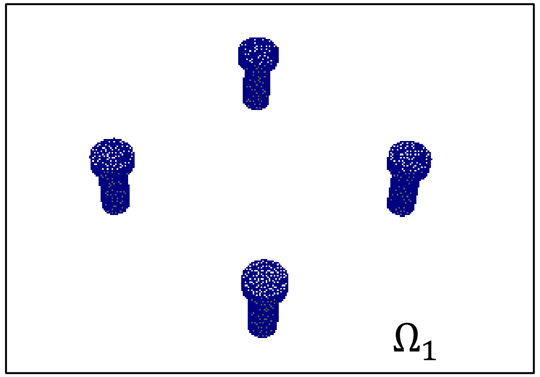
Problem of ***practical scale***.

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



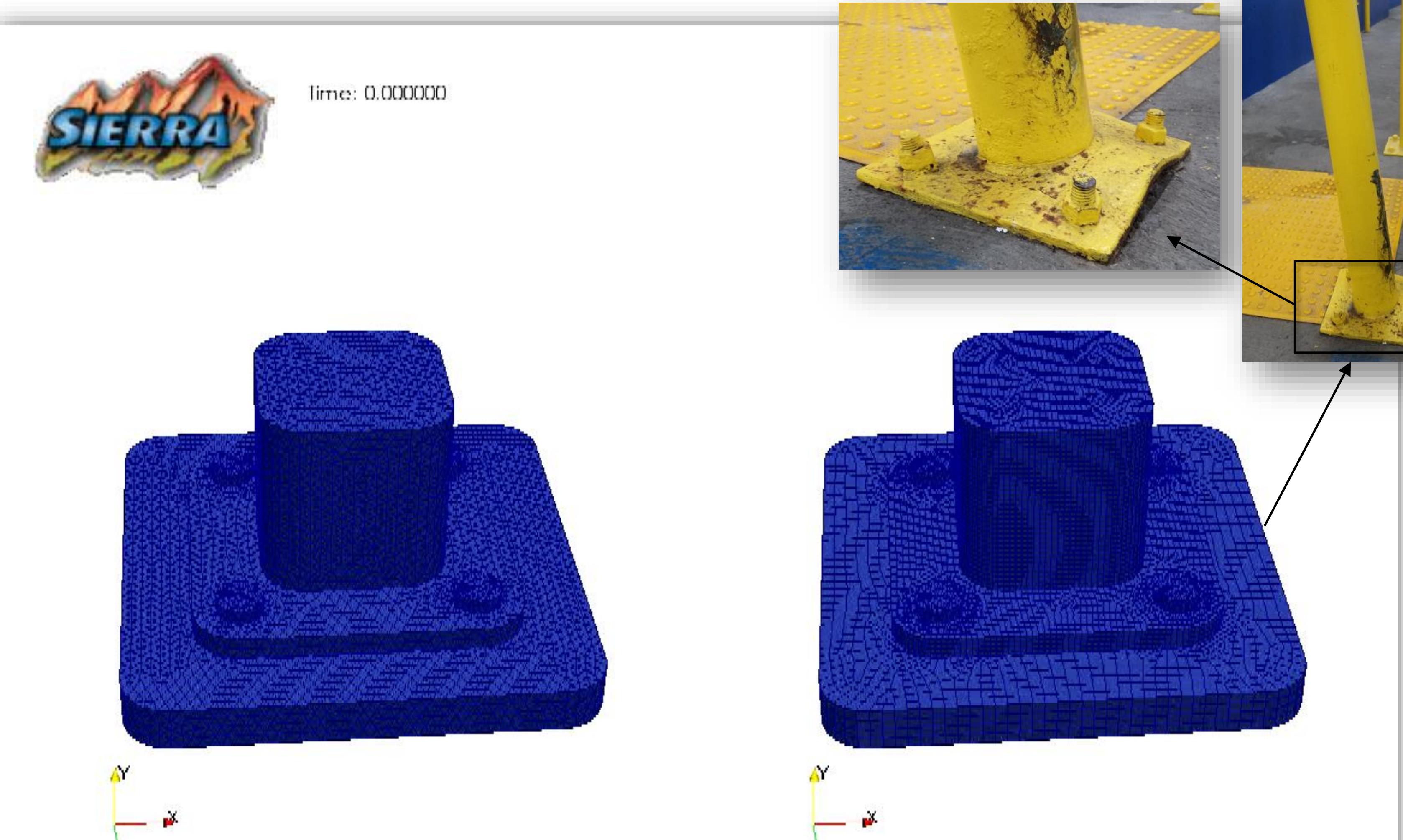


- BC: x-disp = 0.02 at T = 1.0e-3 on top of parts.
- Run until T = 5.0e-4 w/ dt = 1e-5 + implicit Newmark with analytic mass matrix for composite tet 10s.



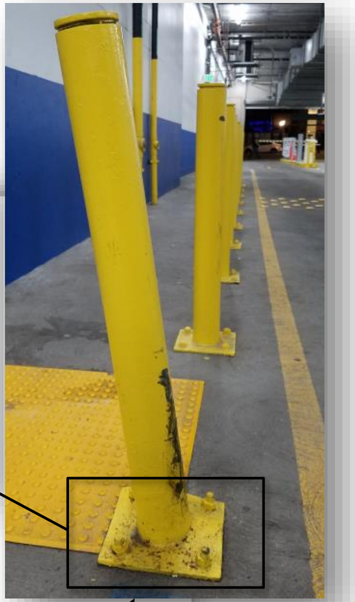
- Ω_1 = bolts (Composite TET10), Ω_2 = parts (HEX).
- ***Inelastic J_2 material model*** in both subdomains.
  - Ω_1: steel
  - Ω_2: steel component, aluminum (bottom) plate

Bolted Joint Problem: Displacement

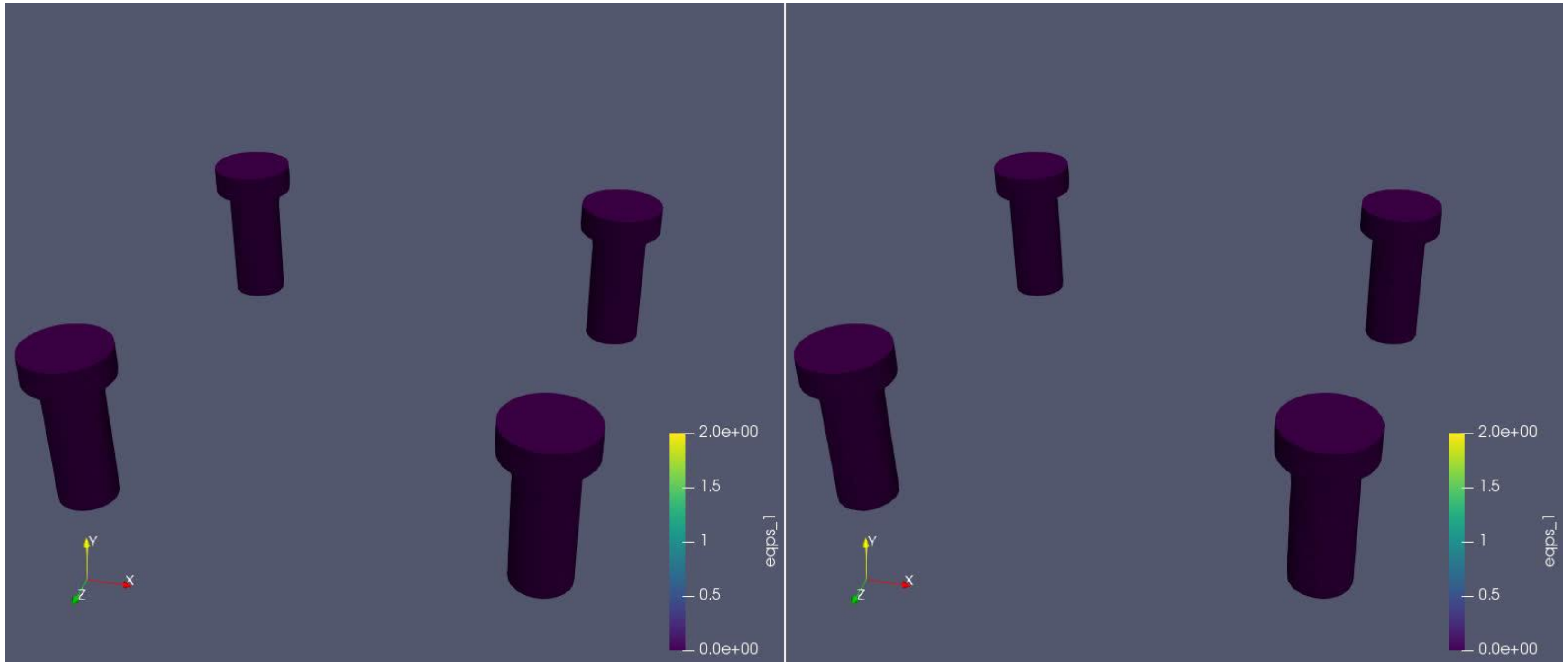


Single Ω

Schwarz



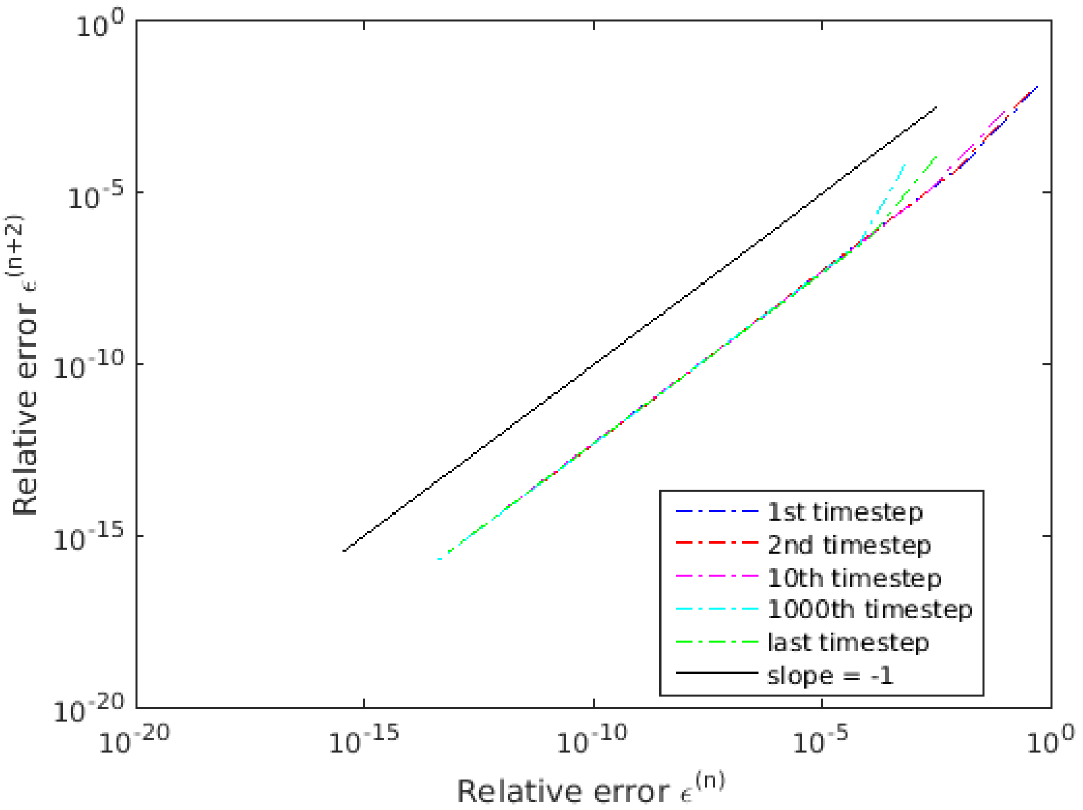
Bolted Joint Problem: Equivalent Plastic Strain (EQPS)



Single Ω

Schwarz

Bolted Joint Problem: Convergence Rate



Linear convergence rate is observed for ***dynamic*** Schwarz algorithm, as for the quasistatic Schwarz algorithm.

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

Bolted Joint Problem: Performance

	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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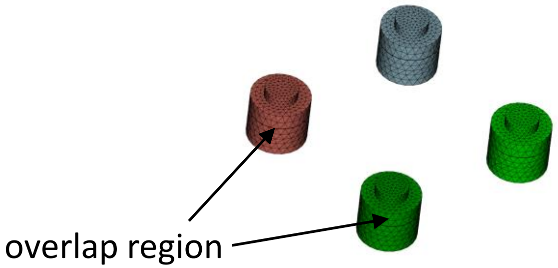
    - ➢ Even if the method is more computationally expensive for some resolutions, it may be preferred for its ability to ***rapidly change*** and ***evaluate*** a ***variety*** of ***engineering designs*** (our typical use case).
- Dynamic Schwarz converges in between ***2-4 Schwarz iterations*** per time-step despite the ***overlap*** region being ***very small*** for this problem.



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Outline

1. Schwarz Alternating Method for Coupling of Full Order Models (FOMs) in Solid Mechanics
   - Motivation & Background
   - Quasistatic Formulation
     - ➢ Numerical Examples
   - Extension to Dynamics
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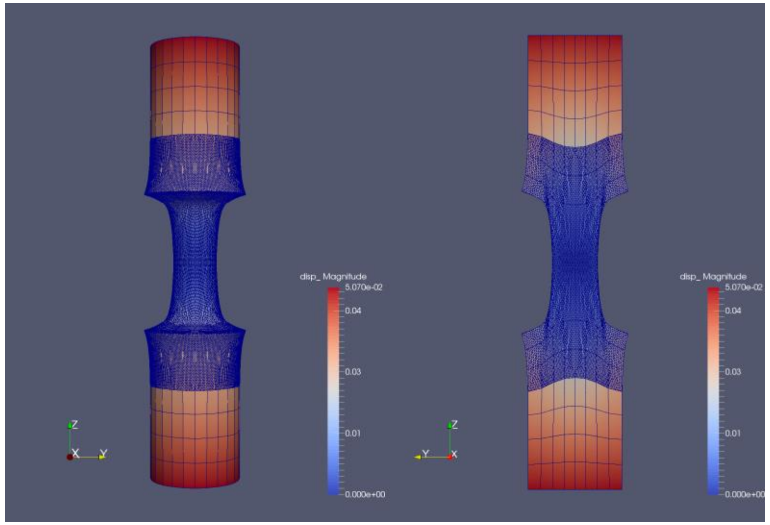
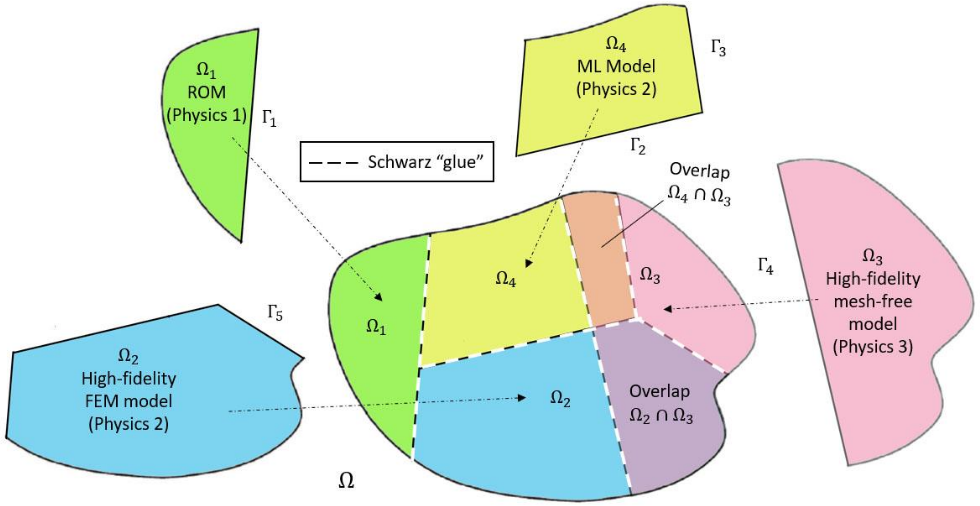
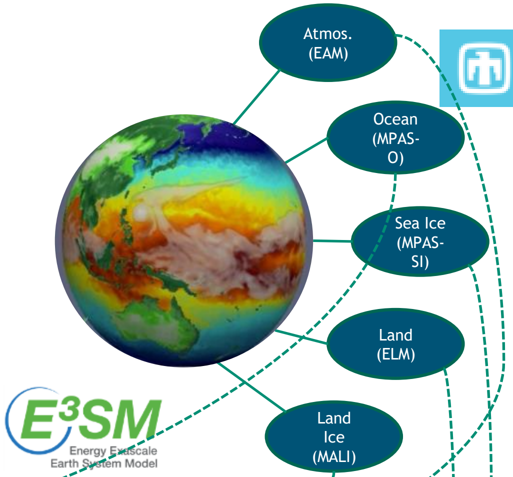




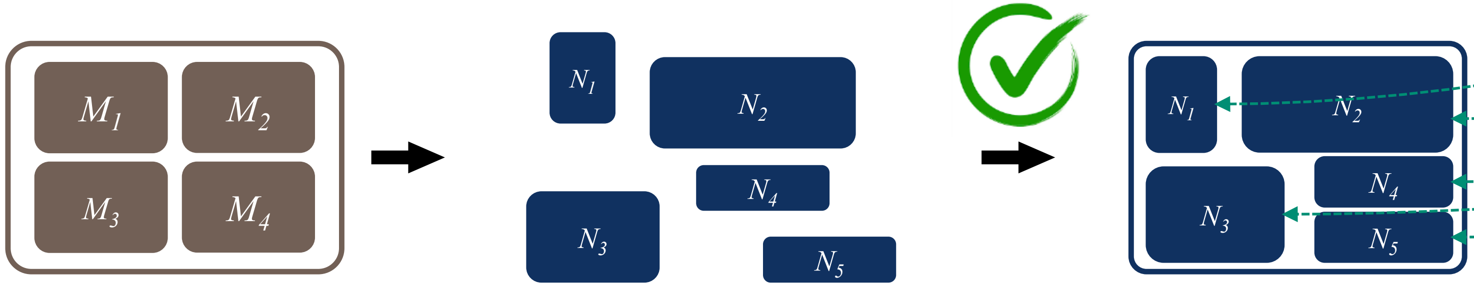
* Projection-based Reduced Order Model

Motivation for ROM-ROM/ROM-FOM Couplings



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

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



Complex System Model

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

Traditional Methods

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

Coupled Numerical Model

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

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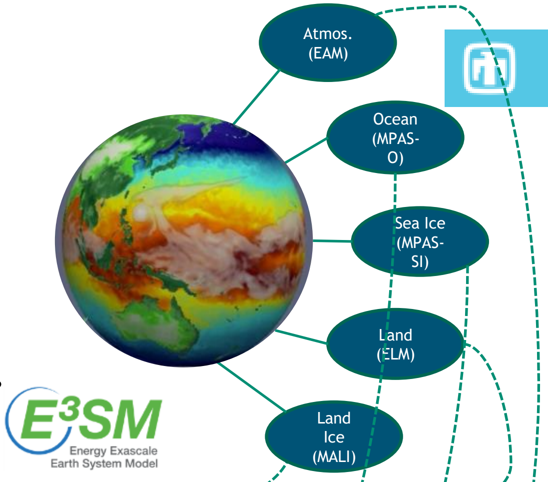

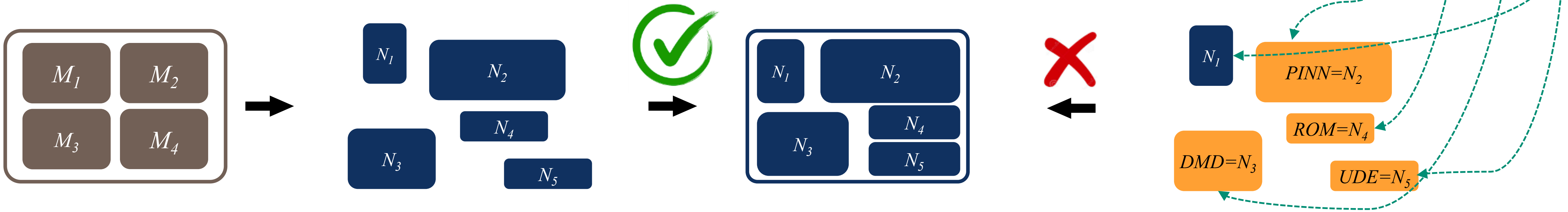

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Traditional + Data-Driven Methods

- PINNs
- Neural ODEs
- Projection-based ROMs, …

- There is currently a big push to integrate **data-driven methods** into modeling & simulation toolchains.

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

Flexible Heterogeneous Numerical Methods (fHNM) Project

Principal research objective:

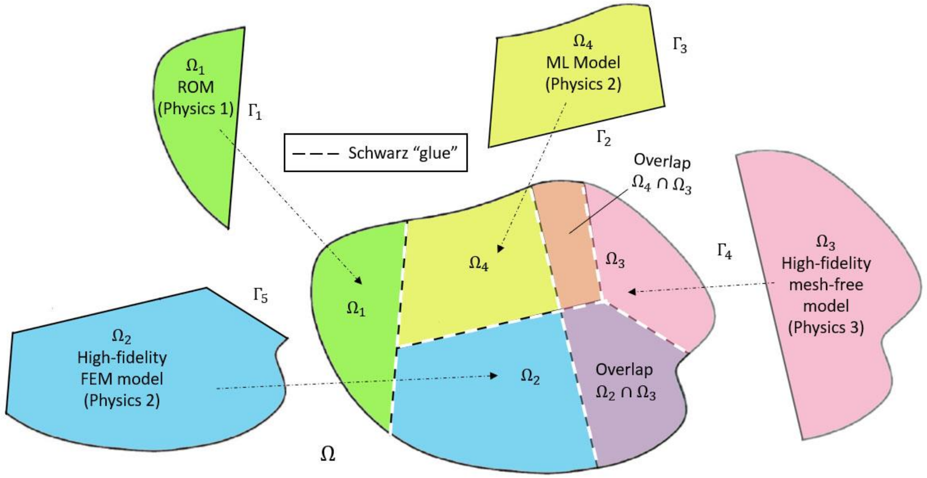
- **Discover mathematical principles** guiding the assembly of **standard** and **data-driven** numerical models in stable, accurate and physically consistent ways.

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

- **"Mix-and-match" standard** and **data-driven models** from three-classes
  - *Class A*: projection-based reduced order models (ROMs) ***This talk.***
  - *Class B*: machine-learned models, i.e., Physics-Informed Neural Networks (PINNs)
  - *Class C*: flow map approximation models, i.e., dynamic model decomposition (DMD) models
- Ensure **well-posedness & physical consistency** of resulting **heterogeneous models.**
- **Solve** such heterogeneous models efficiently.

Three coupling methods:

- Alternating Schwarz-based coupling ***This talk.***
- Optimization-based coupling
- Coupling via generalized mortar methods

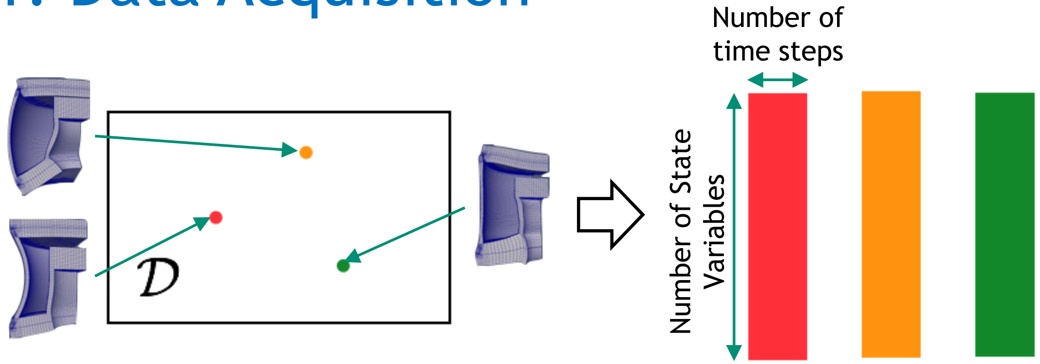


Projection-Based Model Order Reduction via the POD/LSPG* Method

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

*Least-Squares Petrov-Galerkin

1. Data Acquisition

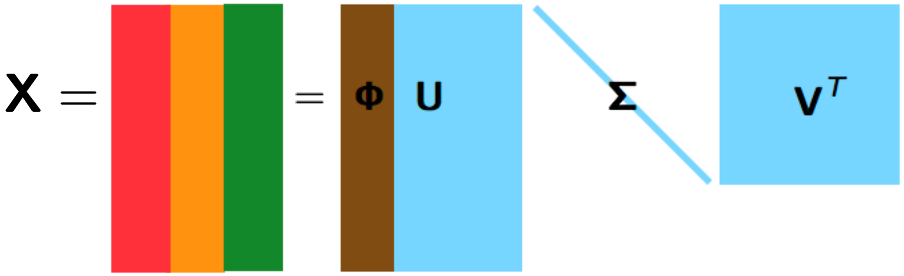


Solve ODE at different design points

Save solution data

2. Learning of Reduced Basis

Proper Orthogonal Decomposition (POD):



ROM = projection-based Reduced Order Model

3. Projection-Based Reduction

Discretize FOM in time

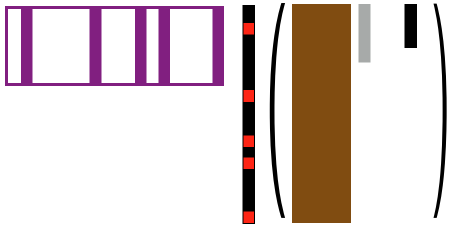
$$\dot{\boldsymbol{q}} = \boldsymbol{f}(\boldsymbol{q}, t; \boldsymbol{\mu})$$
$$\Downarrow$$
$$\boldsymbol{r}^n(\boldsymbol{q}^n; \boldsymbol{\mu}) = \boldsymbol{0}, \; n = 1, \dots, T$$

Reduce the number of unknowns

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

Apply hyper-reduction and minimize residual

$$\text{minimize}_{\hat{\boldsymbol{v}}} \; || \;\; \boldsymbol{A} \;\; \boldsymbol{r}^{\boldsymbol{n}}(\boldsymbol{\Phi}\hat{\boldsymbol{v}}; \boldsymbol{\mu}) ||_2$$



Hyper-reduction/sample mesh

HROM = Hyper-reduced ROM

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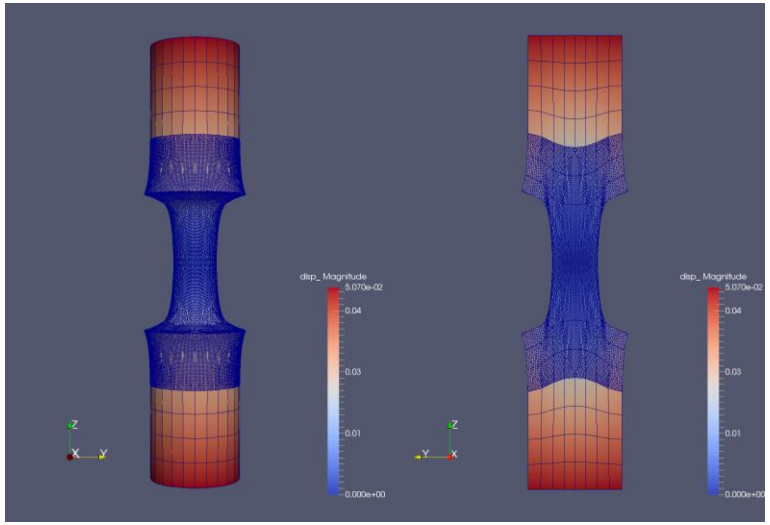

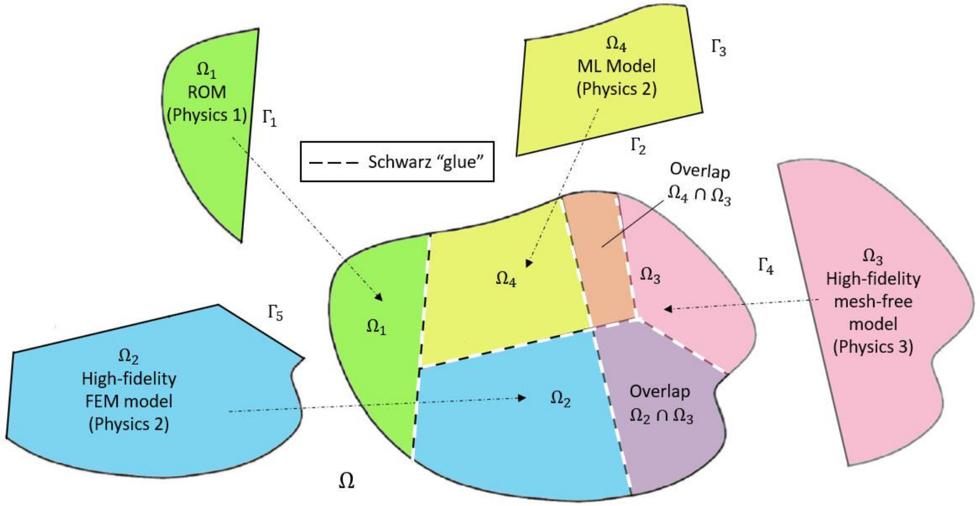

* Projection-based Reduced Order Model

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

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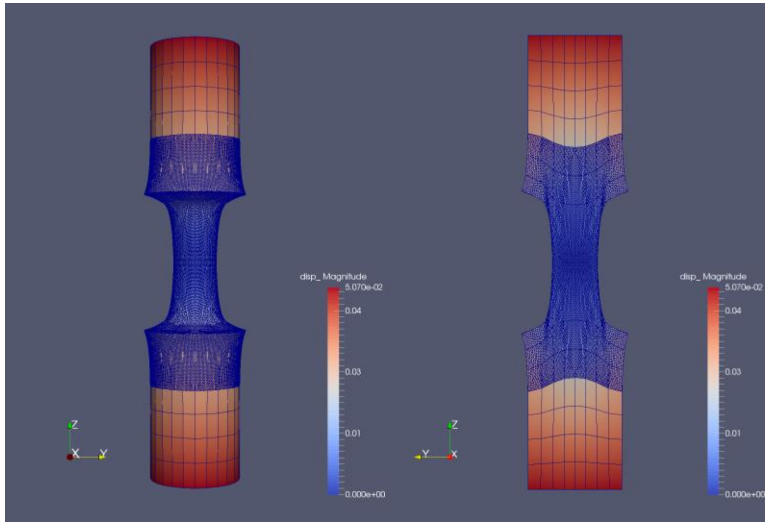
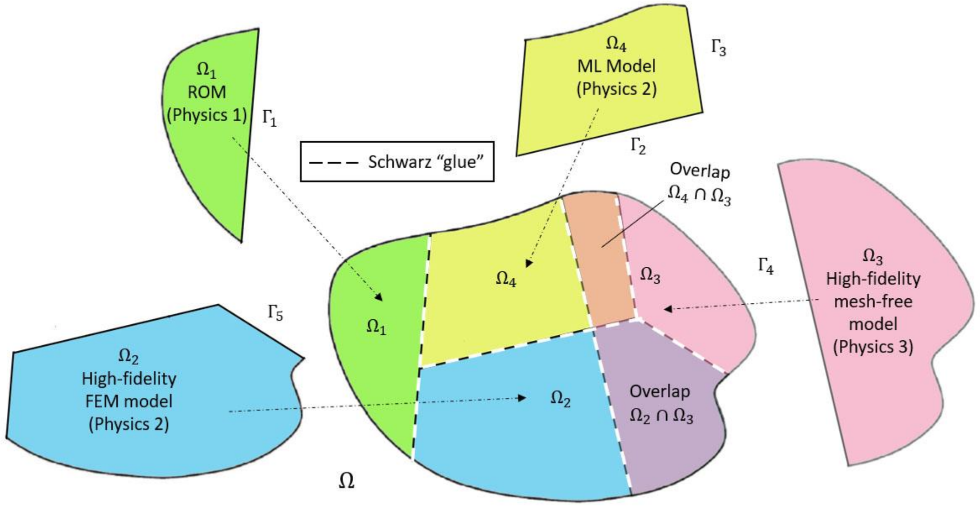




* Projection-based Reduced Order Model

2D Inviscid Burgers Equation

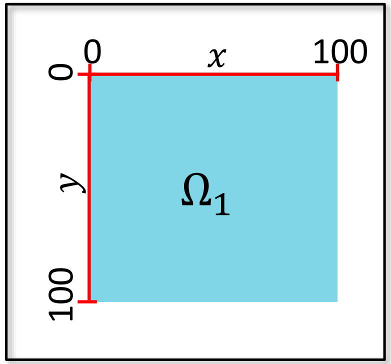
Popular analog for fluid problems where **shocks** are possible, and particularly **difficult** for conventional projection-based ROMs

$$\frac{\partial u}{\partial t} + \frac{1}{2}\left(\frac{\partial (u^2)}{\partial x} + \frac{\partial (uv)}{\partial y}\right) = 0.02 \exp(\mu_2 x)$$

$$\frac{\partial v}{\partial t} + \frac{1}{2}\left(\frac{\partial (vu)}{\partial x} + \frac{\partial (v^2)}{\partial y}\right) = 0$$

$$u(0, y, t; \boldsymbol{\mu}) = \mu_1$$

$$u(x, y, 0) = v(x, y, 0) = 1$$



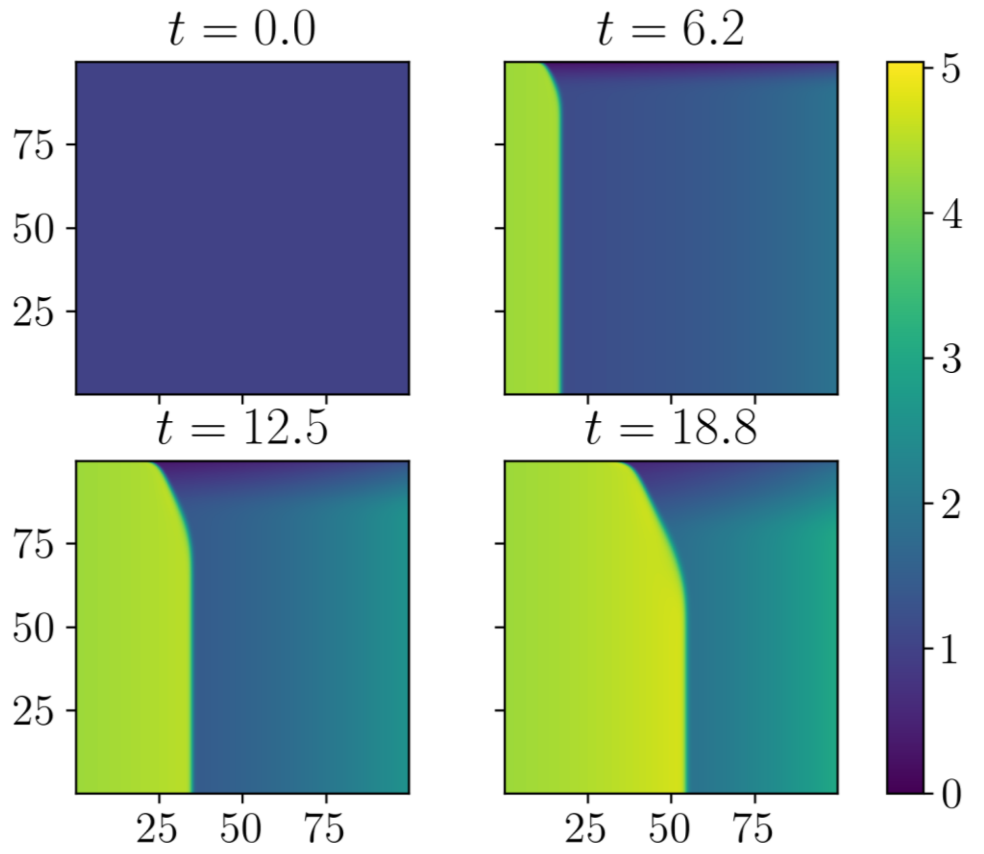


Figure above: solution of u component at various times

Problem setup:

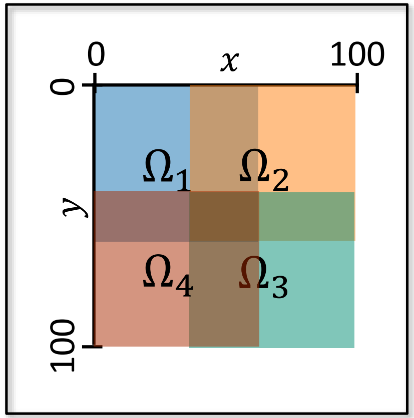
- $\Omega = (0,100)^2$, $t \in [0, 25]$
- Two **parameters** $\boldsymbol{\mu} = (\mu_1, \mu_2)$. **Training:** uniform sampling of $= [4.25, 5.50] \times [0.015, 0.03]$ by a 3×3 grid. **Testing:** query unsampled point $\boldsymbol{\mu} = [4.75, 0.02]$

FOM discretization:

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

Schwarz Coupling Details

Choice of domain decomposition



- **Overlapping** DD of Ω into **4 subdomains** coupled via **multiplicative Schwarz**
- Solution in Ω_1 is **most difficult** to capture by ROM

Snapshot collection and reduced basis construction

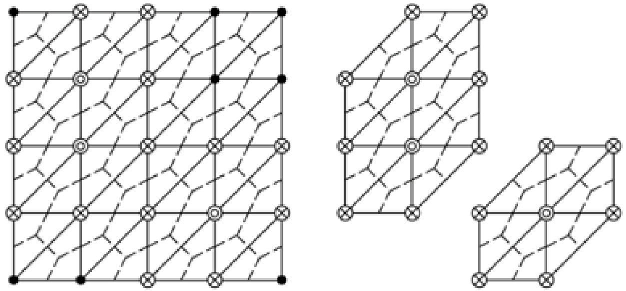
- **Single-domain FOM** on Ω used to generate snapshots/POD modes

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

- BCs imposed **strongly** using Method 1 of [Gunzburger *et al.*, 2007] at indices i_{Dir}

$$\boldsymbol{q}(t) \approx \bar{\boldsymbol{q}} + \boldsymbol{\Phi}\hat{\boldsymbol{q}}(t)$$

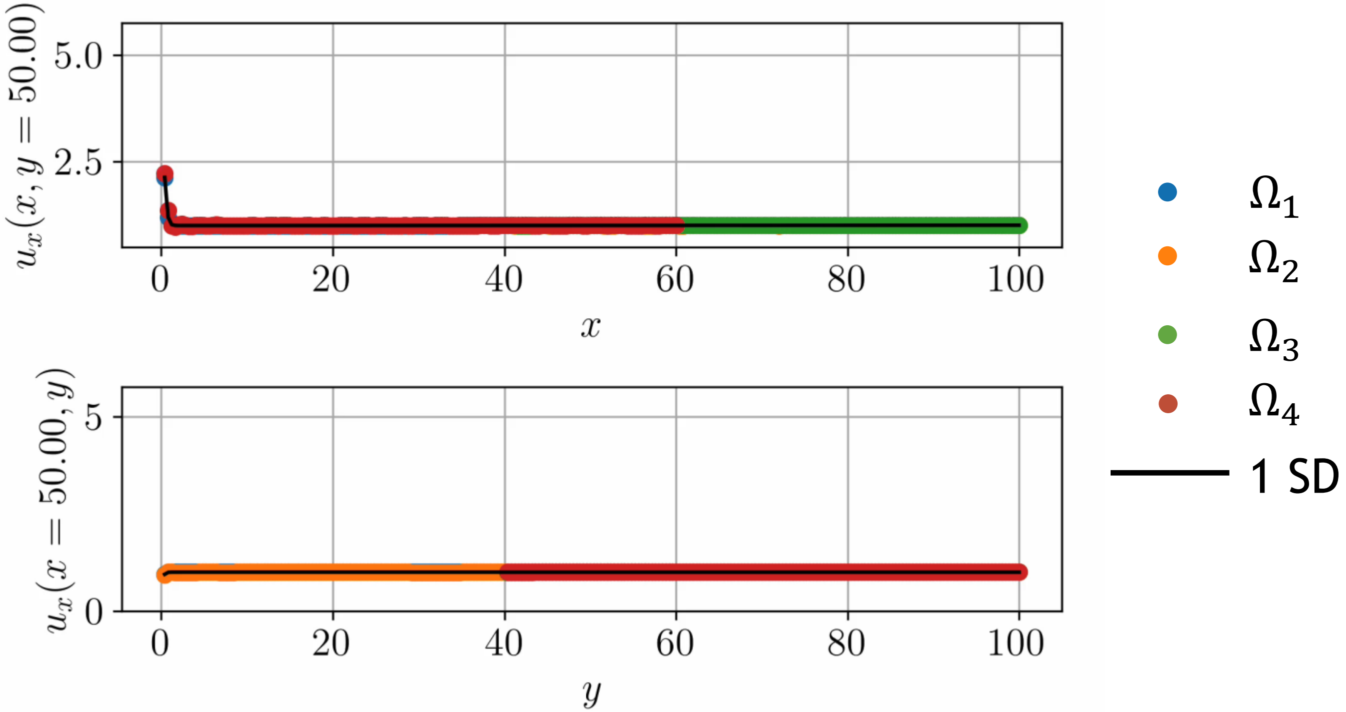
  - POD modes made to satisfy homogeneous DBCs: $\boldsymbol{\Phi}(\boldsymbol{i}_{\mathrm{Dir}}, :) = \mathbf{0}$
  - BCs imposed by modifying $\bar{\boldsymbol{q}}$: $\bar{\boldsymbol{q}}(\boldsymbol{i}_{\mathrm{Dir}}) \leftarrow \boldsymbol{\chi}_{\boldsymbol{q}}$



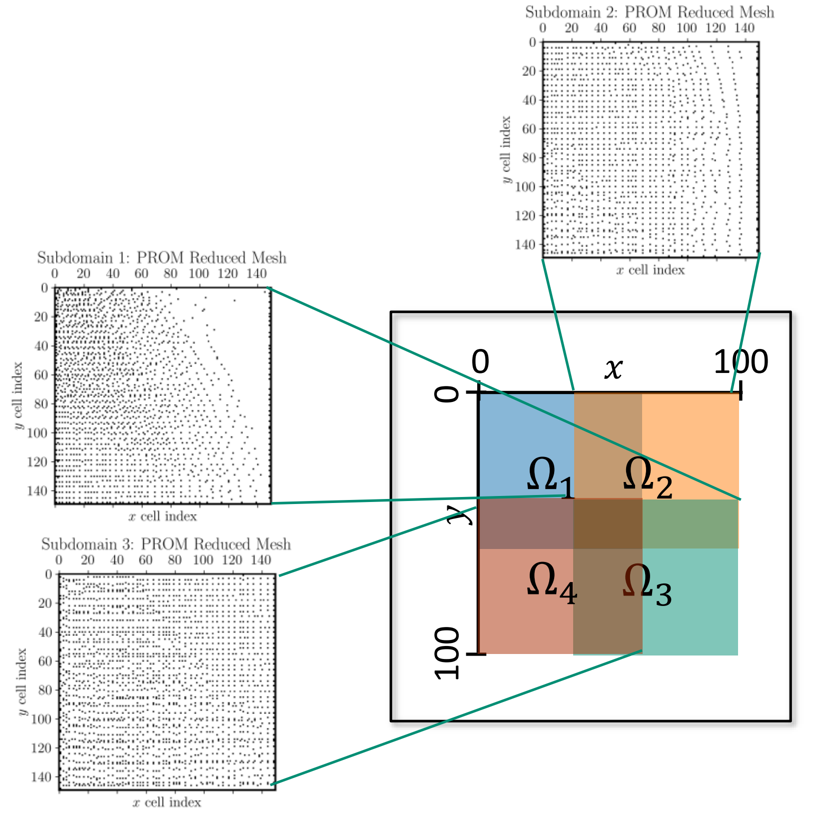
Choice of hyper-reduction

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

FOM-HROM-HROM-HROM Coupling



Subdomains	99% SV Energy		
	M	MSE (%)	CPU time (s)
Ω_1	–	0.0	95
Ω_2	120	0.26	26
Ω_3	60	0.43	17
Ω_4	66	0.34	21
Total			159



- **FOM** in Ω_1 as this is **"hardest" subdomain** for ROM
- **HROMs** in Ω_2, Ω_3, Ω_4 capture **99% snapshot energy**
- Method converges in **3 Schwarz iterations** per controller time-step
- **Errors $O(0.1\%)$** with 0 error in Ω_1
- **2.26× speedup** achieved over all-FOM coupling

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

2D Shallow Water Equations (SWE)

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

$$\frac{\partial h}{\partial t} + \frac{\partial (hu)}{\partial x} + \frac{\partial (hv)}{\partial y} = 0$$

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

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

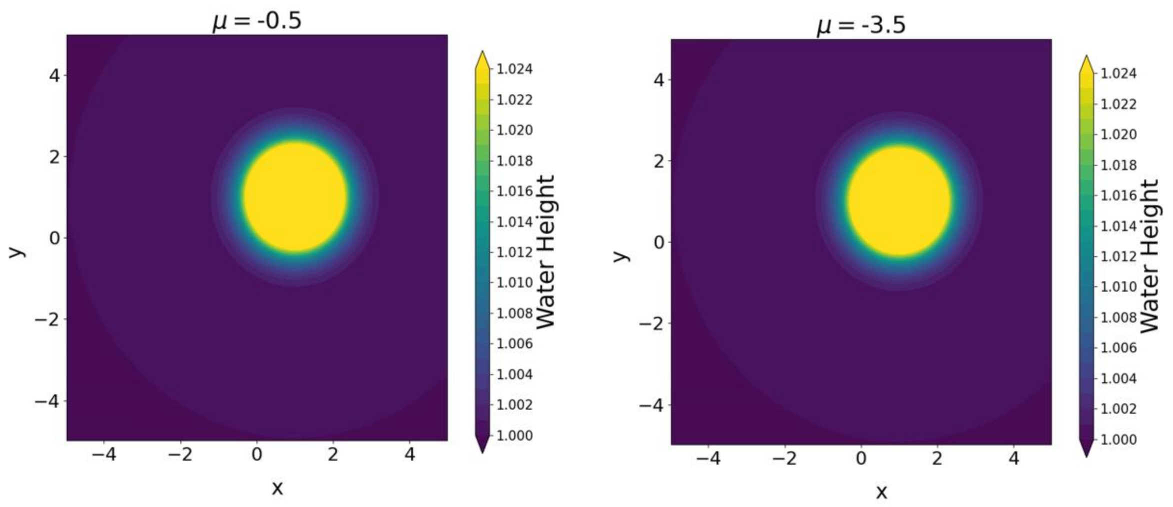


Figure above: FOM solutions to SWE for $\mu = -0.5$ (left) and $\mu = -3.5$ (right).

Problem setup:

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

FOM discretization:

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

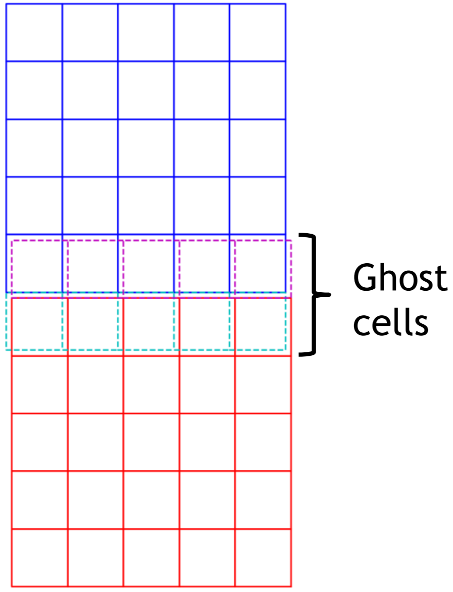
Schwarz Coupling Details

Green: different from Burgers' problem

Choice of domain decomposition

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

Figure right: non-overlapping DD w/ ghost cells creating overlap



Snapshot collection and reduced basis construction

- **Single-domain FOM** on Ω used to generate snapshots/POD modes

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

- BCs are imposed approximately by fictitious ghost cell states
  - ➢ Implementing Neumann and Robin BCs is **challenging**
- Ghost cells introduce some overlap even with non-overlapping DD
  - ➢ $\Rightarrow$ Dirichlet-Dirichlet non-overlapping Schwarz is stable/convergent!

Choice of hyper-reduction

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

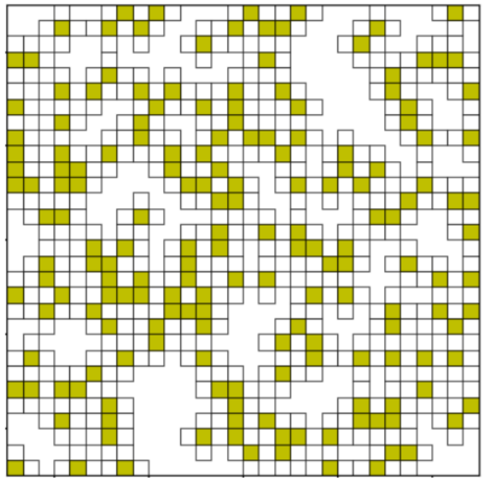
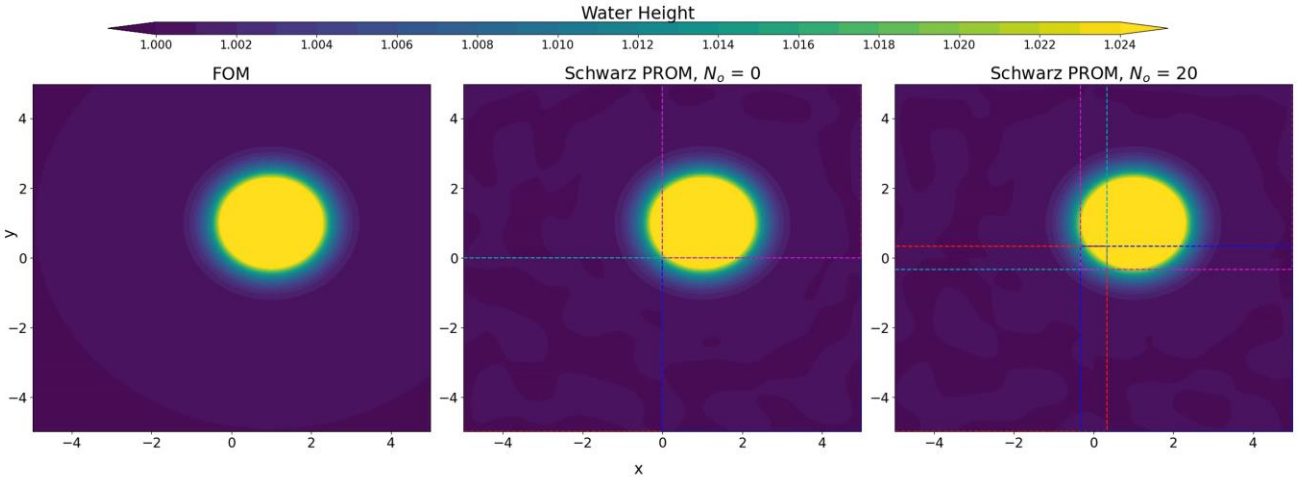


Figure above: sample mesh (yellow) and stencil (white) cells

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

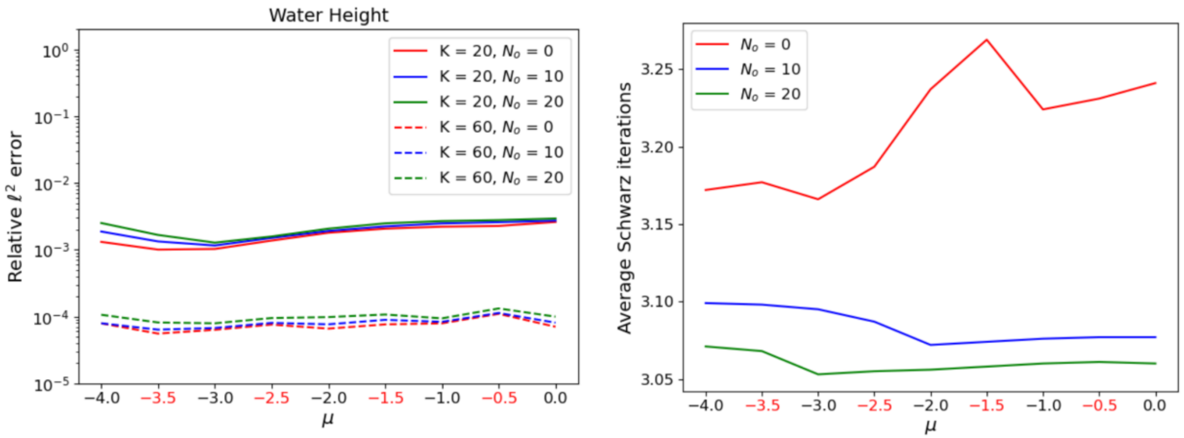
Schwarz All-ROM Domain Overlap Study

Study of **Schwarz convergence** for **all-ROM coupling** as a function of $\boldsymbol{N_o}$ **:= cell width of overlap region** (not including ghost cells).



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

- Dirichlet-Dirichlet coupling with **no-overlap** ($N_o = 0$) performs well with **no convergence issues** (movie, left) and **errors comparable** to Dirichlet-Dirichlet coupling with overlap (figure below, left)



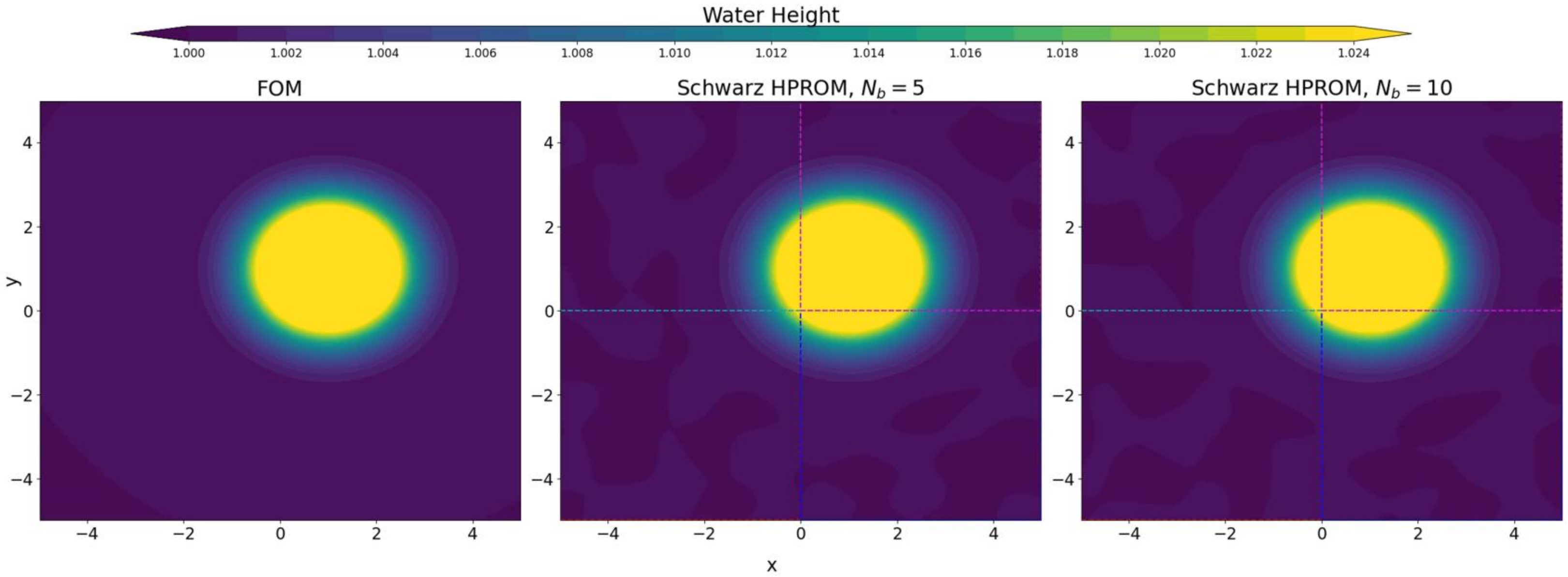
Figures above: relative error and average # Schwarz iterations as a function of μ and N_o. Black μ: training, red μ: testing.

- **Schwarz iterations** decrease (very roughly) with $N_o^{0.25}$ (figure, right) whereas evaluating $\boldsymbol{r}(\boldsymbol{q})$ scales with N_o^2
  - ➢ $\Rightarrow$ there is no reason not to do **non-overlapping coupling** for this problem

Schwarz Boundary Sampling for All-HROM Coupling

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

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



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

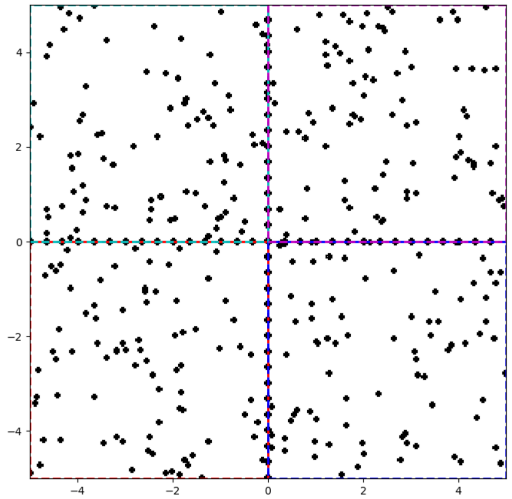
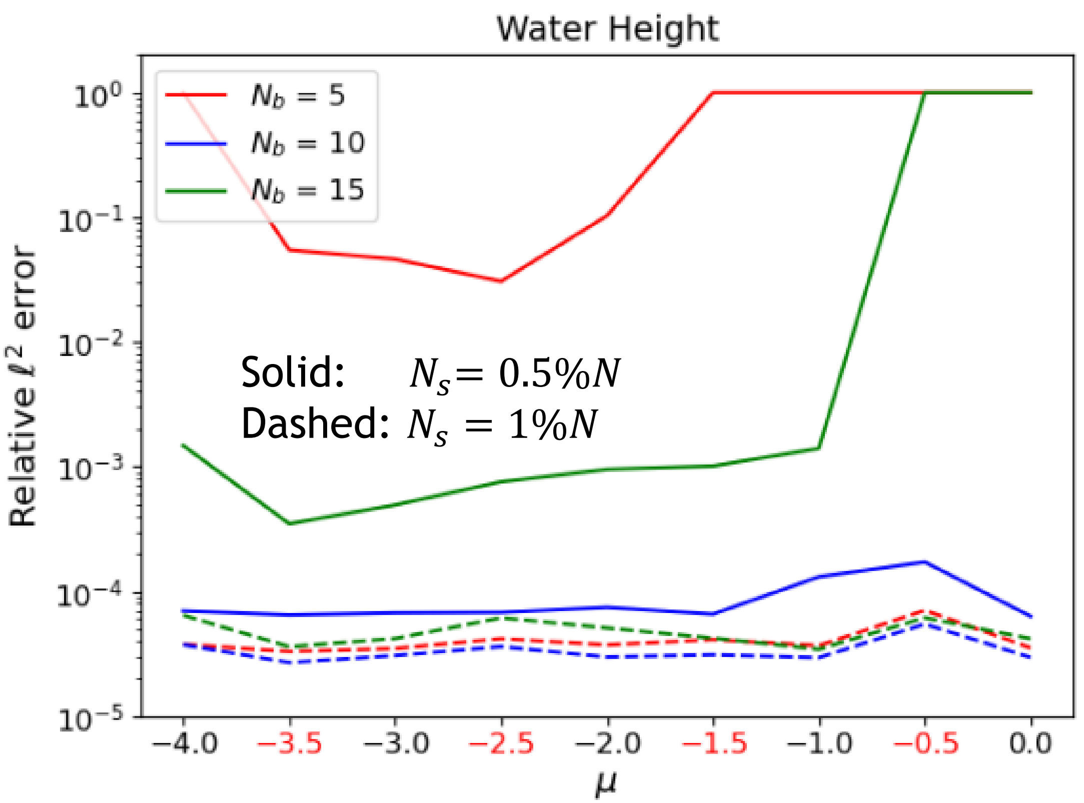
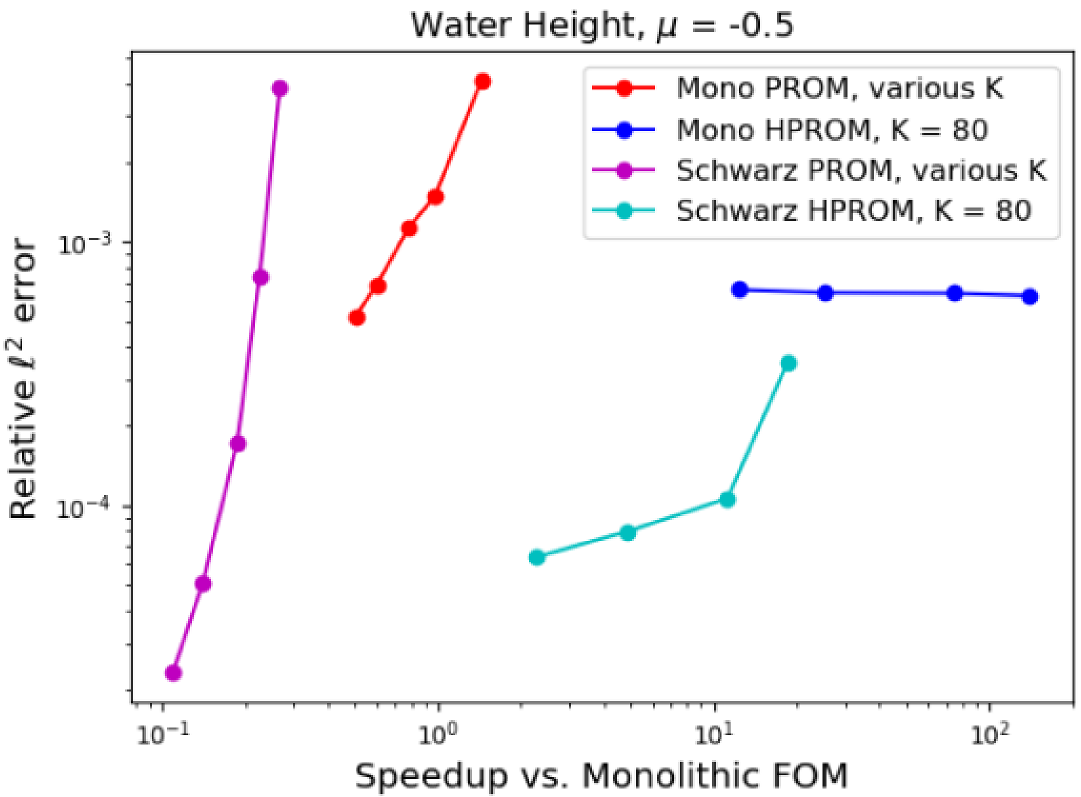


Figure above: example sample mesh with sampling rate $N_b = 10\%$

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

Coupled HROM Performance



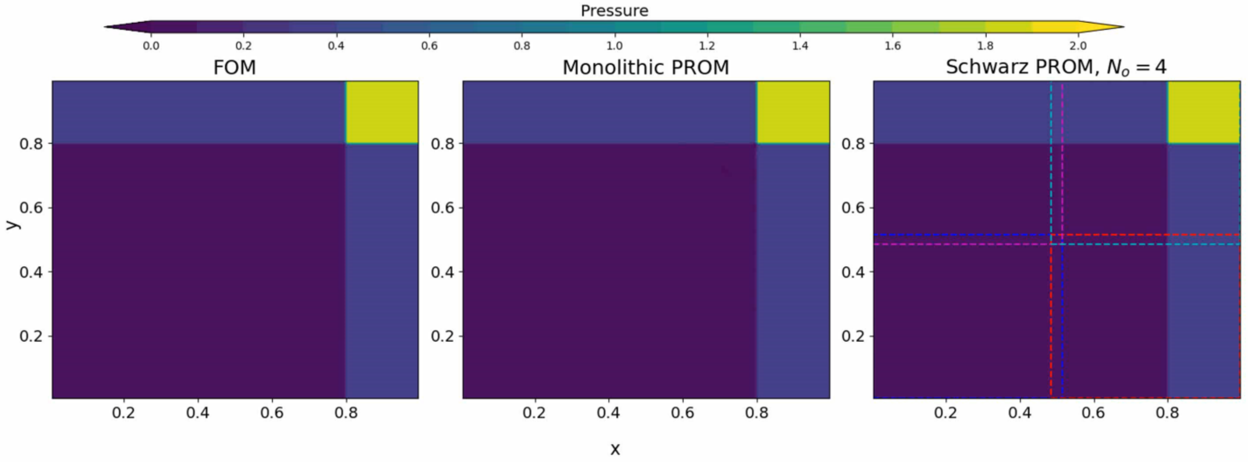


- For a fixed ROM dimension, Schwarz delivers **lower error** and **comparable cost!**
- There are noticeable **cost savings** relative to **monolithic FOM**!
- Accuracy similar for **predictive** μ (red) and **non-predictive** μ (black) cases.

Teaser: 2D Euler Equations Riemann Problem

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

$$p=(\gamma-1)\left(\rho E-\frac{1}{2}\rho(u^2+v^2)\right)$$



Problem setup:

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

Preliminary results:

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

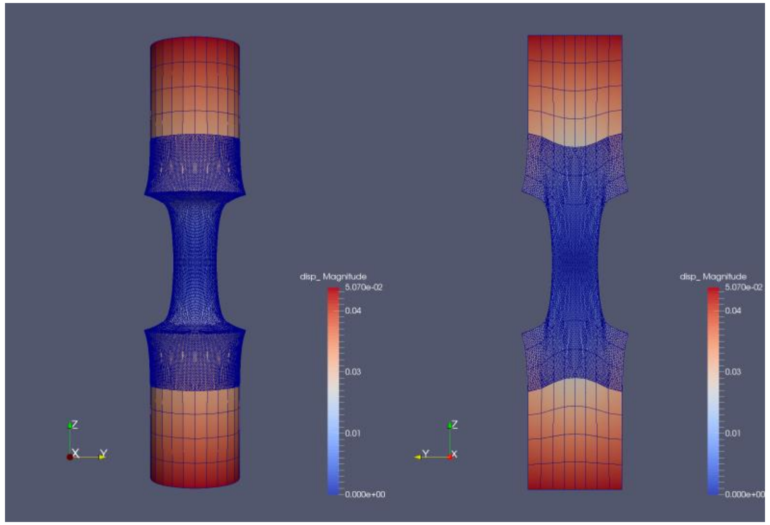
FOM discretization:

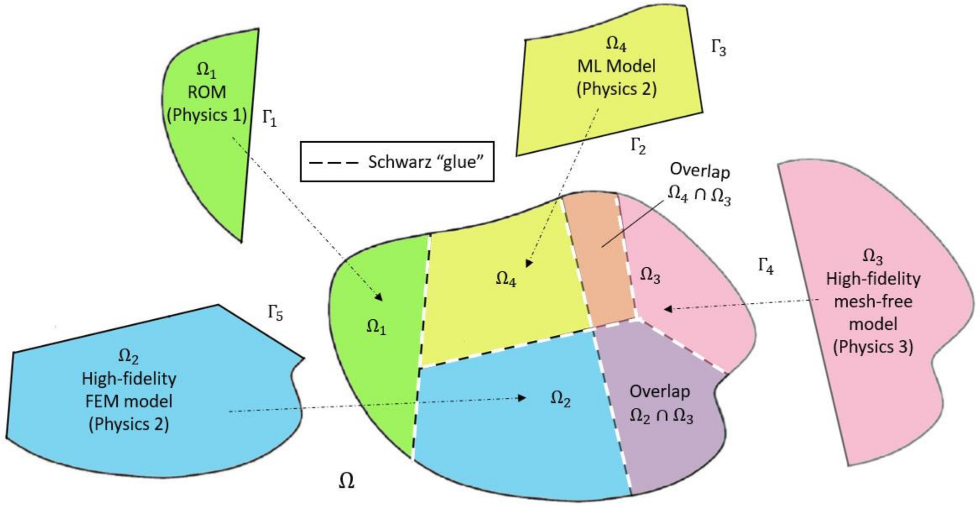
- Spatial discretization given by a first-order **cell-centered finite volume** discretization with $N=300$ or $N=N=100$ elements in each dimension
- Implicit first order temporal discretization: **backward Euler** with fixed $\Delta t=0.005$
- Implemented in **Pressio-demoapps** (https://github.com/Pressio/pressio-demoapps)

*Schulz-Rinne, 1993.

Outline

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





* Projection-based Reduced Order Model

Summary

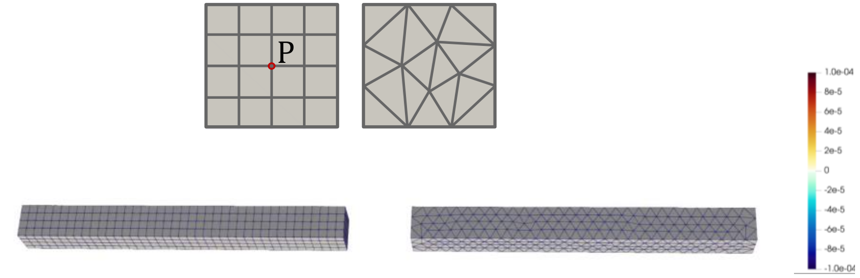
The **Schwarz alternating method** has been developed for concurrent multi-scale coupling of **conventional** and **data-driven models.**

- ☺ 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.

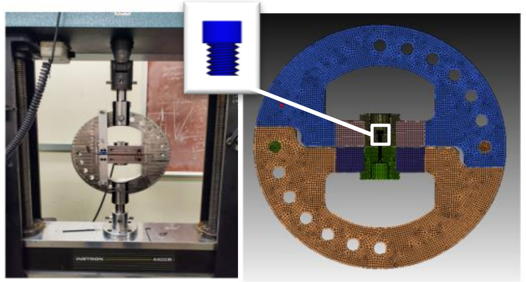
Ongoing & Future Work

- Development fundamentally new approach for simulating multi-scale **mechanical contact** using the Dirichlet-Neumann **Schwarz alternating method**
  - ➢ **Contact constraints** are replaced with **boundary conditions** applied **iteratively** at contact boundaries
- Implementation of **non-overlapping** Schwarz in Sierra/SM
- Working with **analysts** to **apply** Schwarz to problems of interest to Sandia **missions**
  - ➢ **Laser welds**
  - ➢ **Fastener** modeling for joints
  - ➢ Salt caverns for **oil storage**
- **Rigorous analysis** of why Dirichlet-Dirichlet BC “work” when employing non-overlapping Schwarz with discretizations that employ ghost cells
- Extension to coupling of **non-intrusive ROMs** (dynamic mode decomposition, operator inference, neural networks)
- Development of **automated criteria** to determine appropriate use of less refined or reduced-order models w/o sacrificing accuracy, enabling **real-time transitions** between different model fidelities

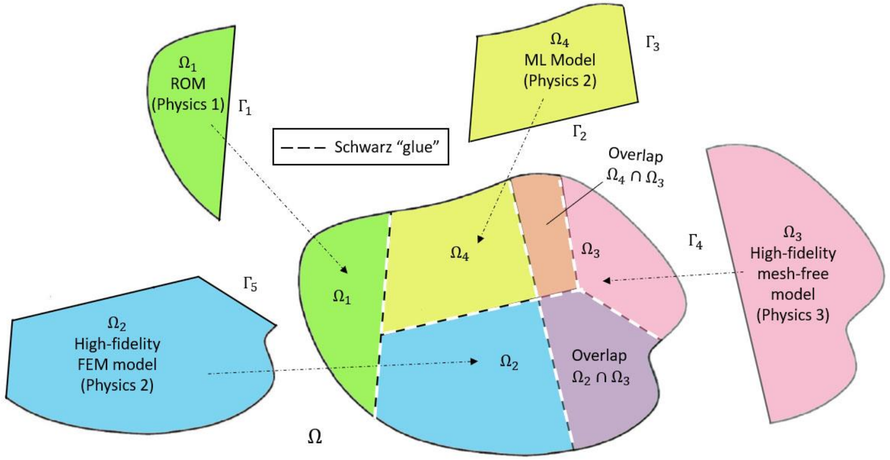
Contact boundaries Γ^1 and Γ^2

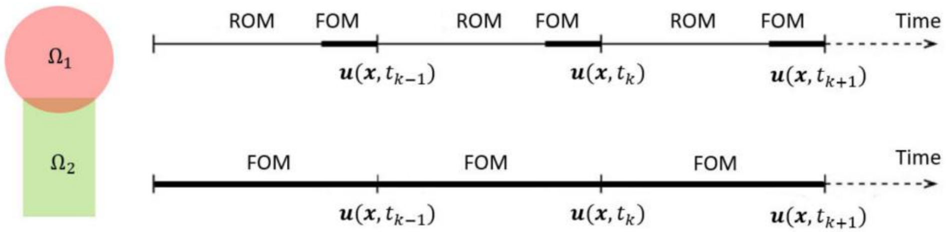


Impact of two 3D beams having different meshes with Schwarz contact method. From [Mota et al., 2023].



From Murugesan *et al.*, 2020.





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Sandia National Laboratories

Coleman Alleman

Greg Phlipot

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

References

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

[2] A. Mota, **I. Tezaur**, G. Phlipot. "The Schwarz Alternating Method for Dynamic Solid Mechanics", *Comput. Meth. Appl. Mech. Engng.* 121 (21) (2022) 5036-5071.

[3] J. Barnett, **I. Tezaur**, A. Mota. "The Schwarz alternating method for the seamless coupling of nonlinear reduced order models and full order models", ArXiv pre-print, 2022. https://arxiv.org/abs/2210.12551

[4] W. Snyder, **I. Tezaur**, C. Wentland. "Domain decomposition-based coupling of physics-informed neural networks via the Schwarz alternating method", ArXiv pre-print, 2023. https://arxiv.org/abs/2311.00224

[5] A. Mota, D. Koliesnikova, **I. Tezaur**. "A Fundamentally New Coupled Approach to Contact Mechanics via the Dirichlet-Neumann Schwarz Alternating Method", ArXiv pre-print, 2023. https://arxiv.org/abs/2311.05643

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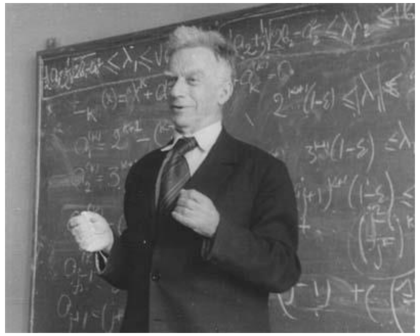
Start of Backup Slides

Theoretical Foundation

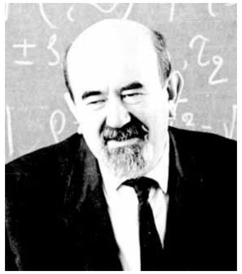
Using the Schwarz alternating as a ***discretization method*** for PDEs is natural idea with a sound ***theoretical foundation***.

- 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***.

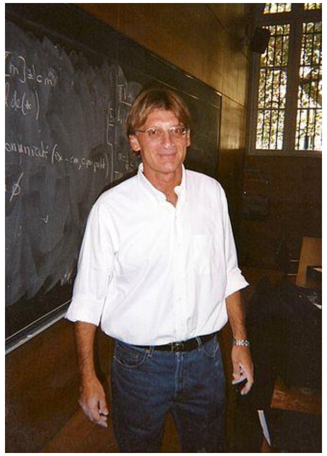
$$\boldsymbol{\Phi}[\boldsymbol{\varphi}] = \int_B A(\boldsymbol{F}, \boldsymbol{Z})\, dV - \int_B \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV$$
$$\nabla \cdot \boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



S.L. Sobolev (1908 – 1989)



S.G. Mikhlin (1908 – 1990)



P.- L. Lions (1956-)

A. Mota, I. Tezaur, C. Alleman

Notched Cylinder: Coupling Different Materials

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

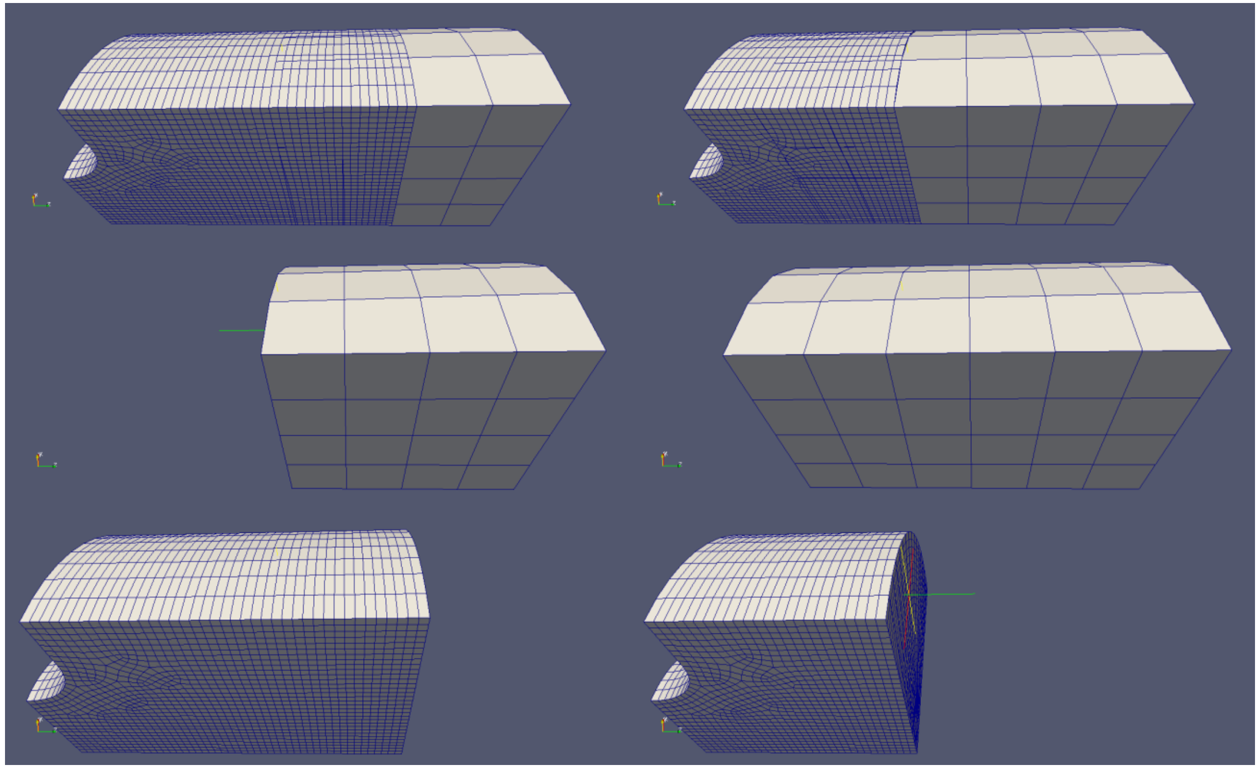
- Notched cylinder subjected to tensile load with an ***elastic*** and ***J2 elasto-plastic*** regions.
- ***Coarse*** region is ***elastic*** and ***fine*** region is ***elasto-plastic***.
- The ***overlap region*** in the first mesh is nearer the notch, where plastic behavior is expected.

Overlap far from notch. Overlap near notch.

Coupled regions

Coarse, elastic region

Fine, elasto-plastic region

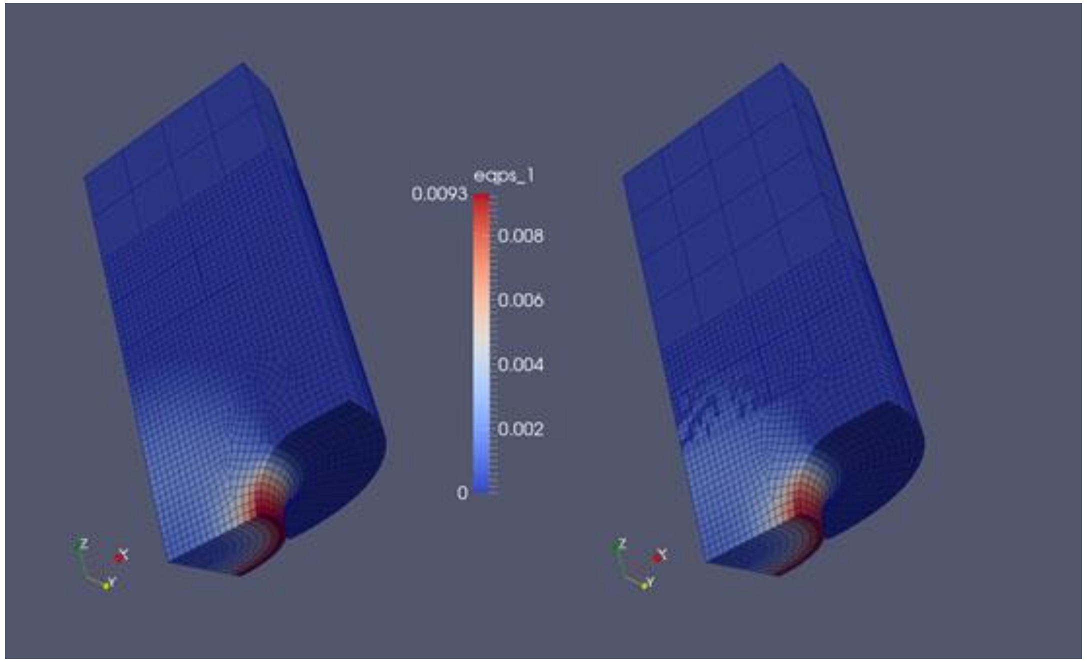


Notched Cylinder: Coupling Different Materials

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

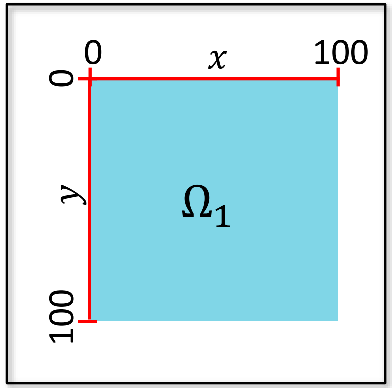
- When the ***overlap*** region is ***far from the notch***, no plastic deformation exists in it: the coarse and fine regions predict the ***same behavior***.
- When the ***overlap*** region is ***near the notch***, plastic deformation spills onto it and the two models predict different behavior, affecting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

Albany



Overlap far from notch. Overlap near notch.

Single Domain Predictive ROM



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

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

* Numbers in table are w/o hyper-reduction

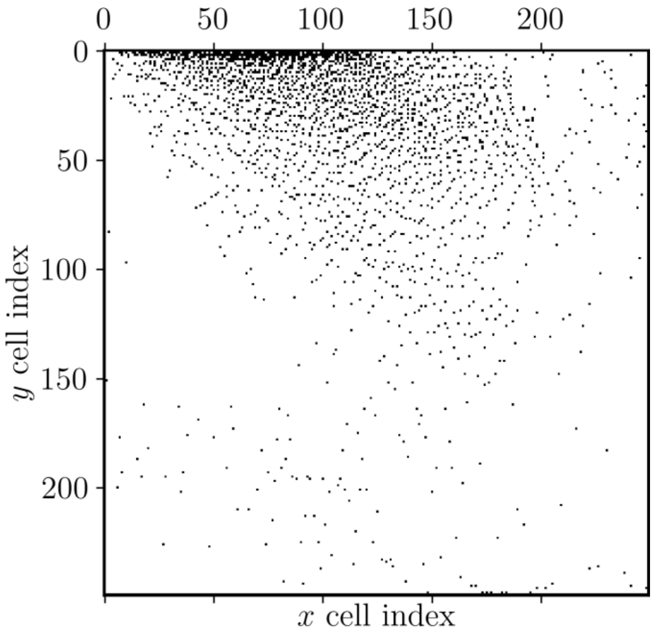


Figure above: Reduced mesh of single domain HROM

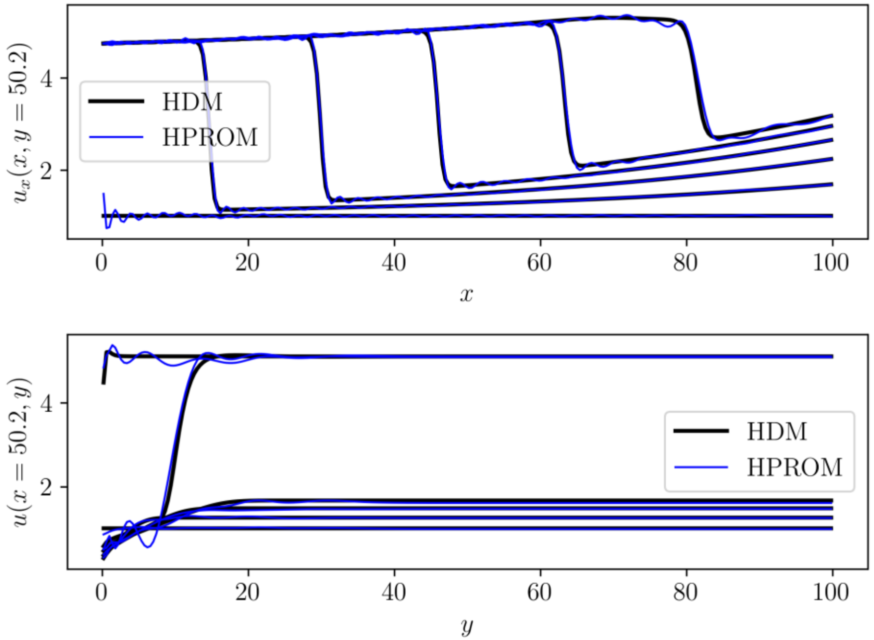
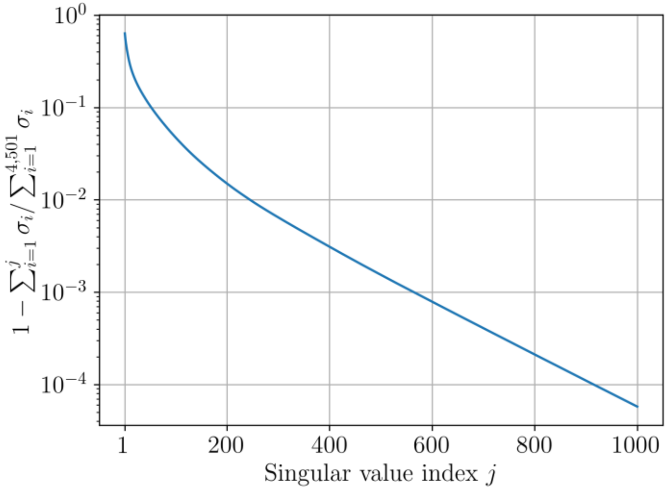
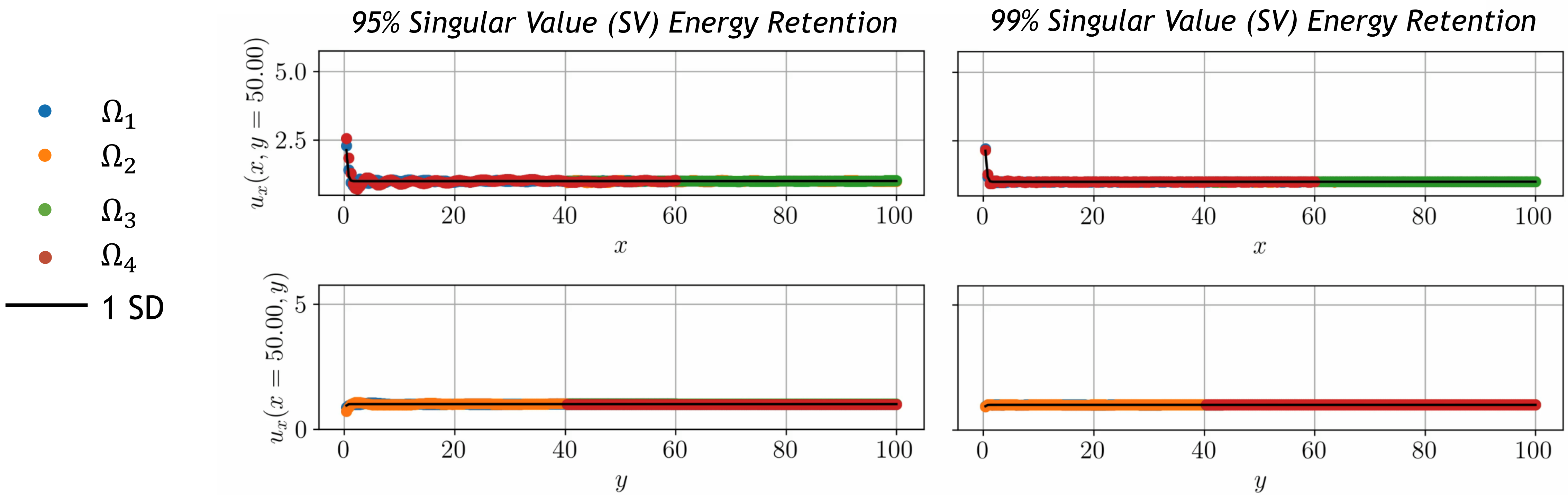


Figure above: HROM and FOM results at various time steps

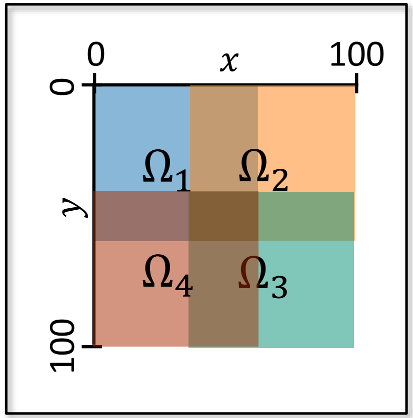


All-ROM Coupling



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

Subdomains	95% SV Energy			99% SV Energy		
	M	MSE (%)	CPU time (s)	M	MSE (%)	CPU time (s)
Ω_1	57	1.1	85	146	0.18	295
Ω_2	44	1.2	56	120	0.18	216
Ω_3	24	1.4	43	60	0.16	89
Ω_4	32	1.9	61	66	0.25	100
Total			245			**700**



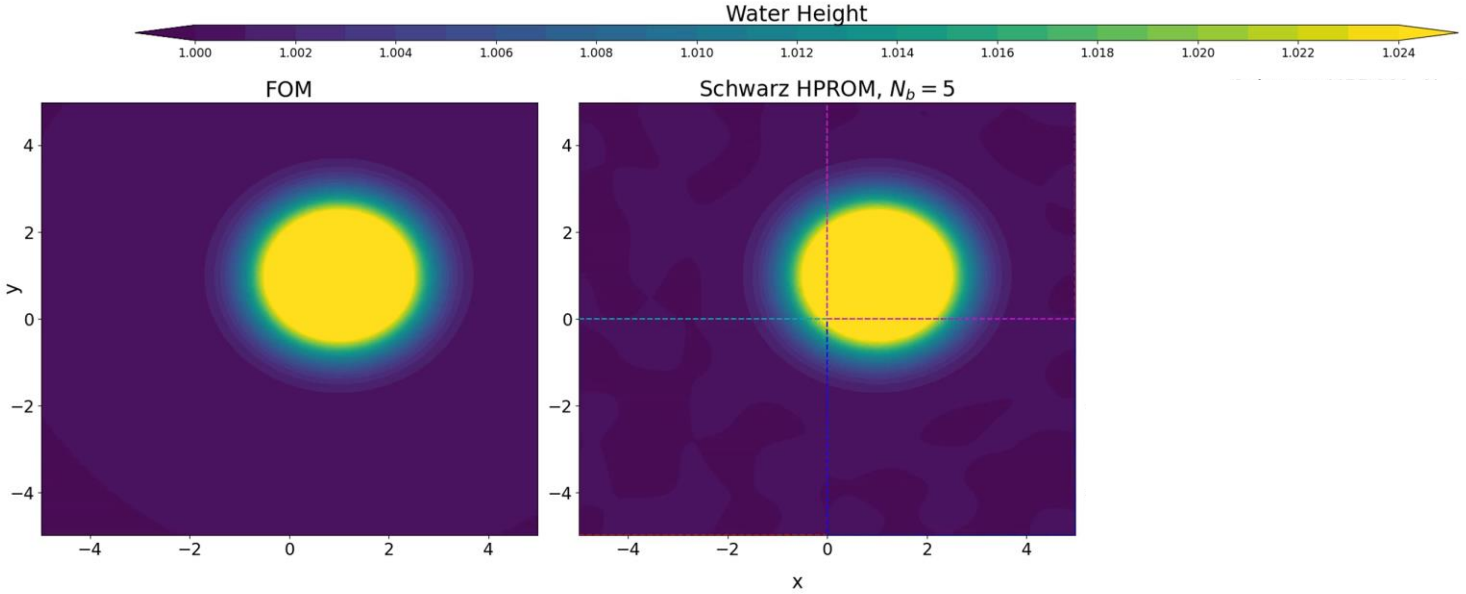
Schwarz Boundary Sampling for All-HROM Coupling

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

Schwarz Boundary Sampling for All-HROM Coupling

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

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



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

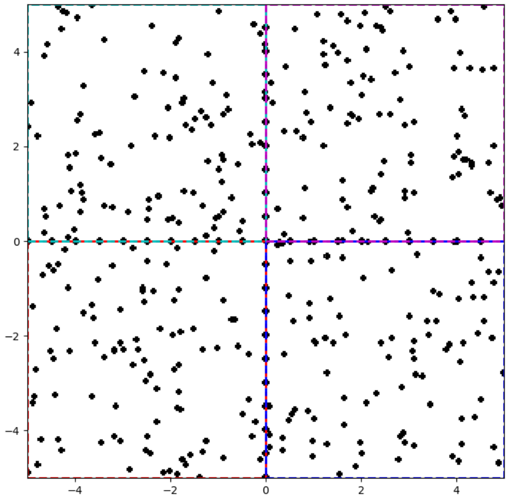


Figure above: example sample mesh with sampling rate $N_b = 5\%$.

Schwarz Boundary Sampling for All-HROM Coupling

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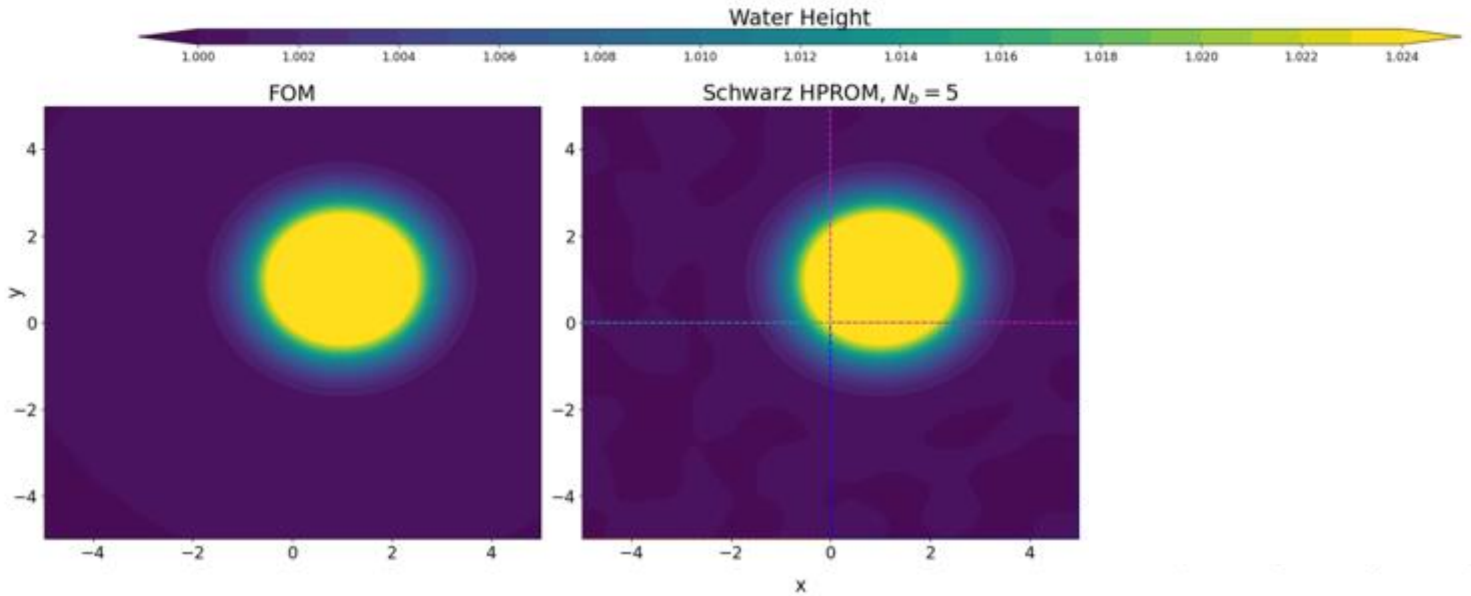

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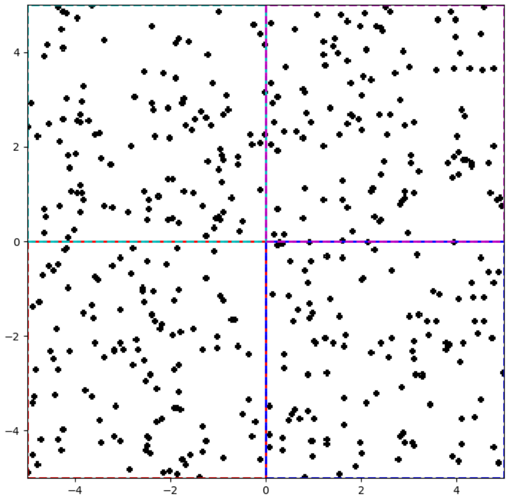


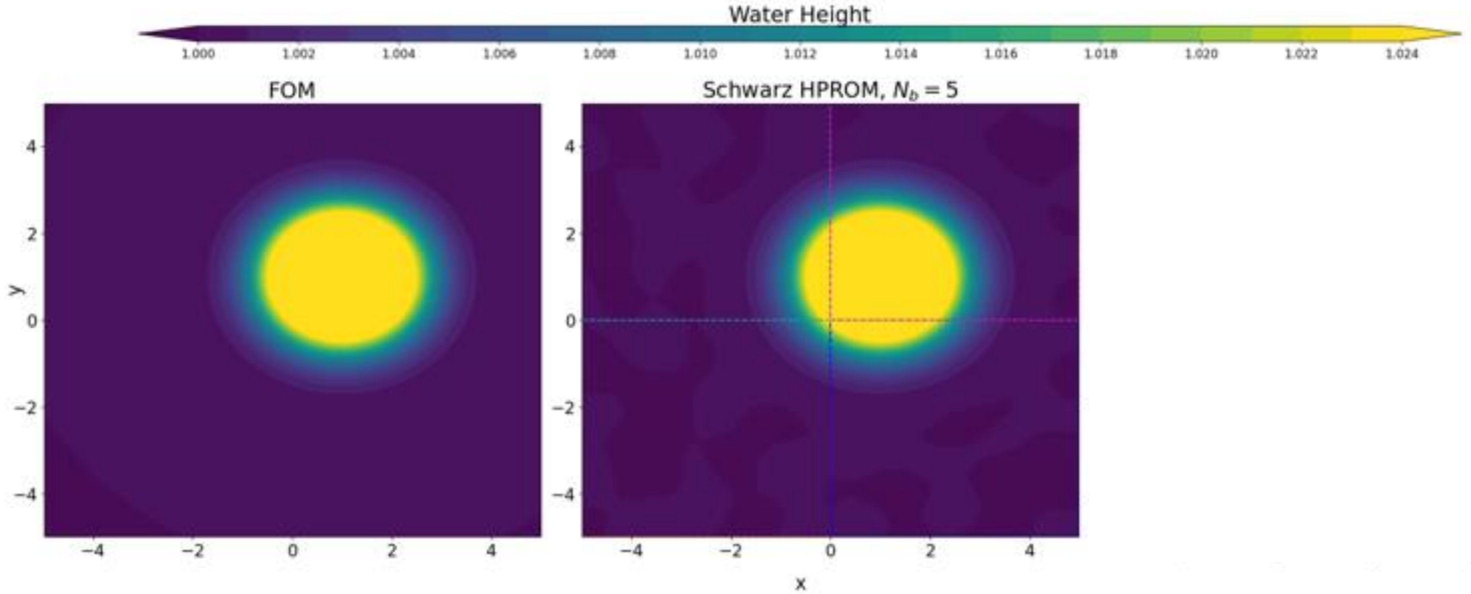
Figure above: example sample mesh with sampling rate $N_b = 0$.

- Including **too many Schwarz boundary points** (N_b) in sample mesh given **fixed budget** of N_s sample mesh points may lead to **too few sample mesh points** in **interior**

Schwarz Boundary Sampling for All-HROM Coupling

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

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



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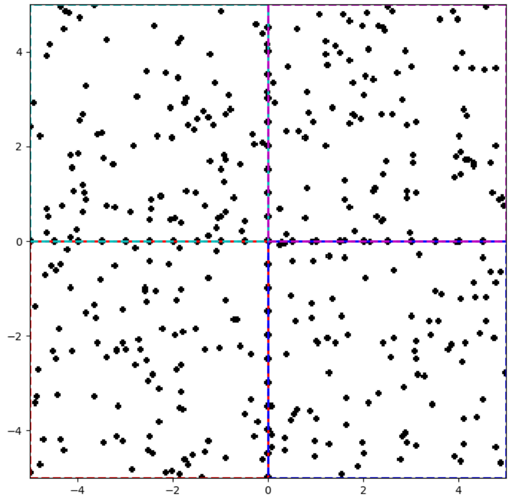

Figure above: example sample mesh with sampling rate $N_b = 5\%$.

- Including **too many Schwarz boundary points** (N_b) in sample mesh given **fixed budget** of N_s sample mesh points may lead to **too few sample mesh points** in **interior**

Schwarz Boundary Sampling for All-HROM Coupling

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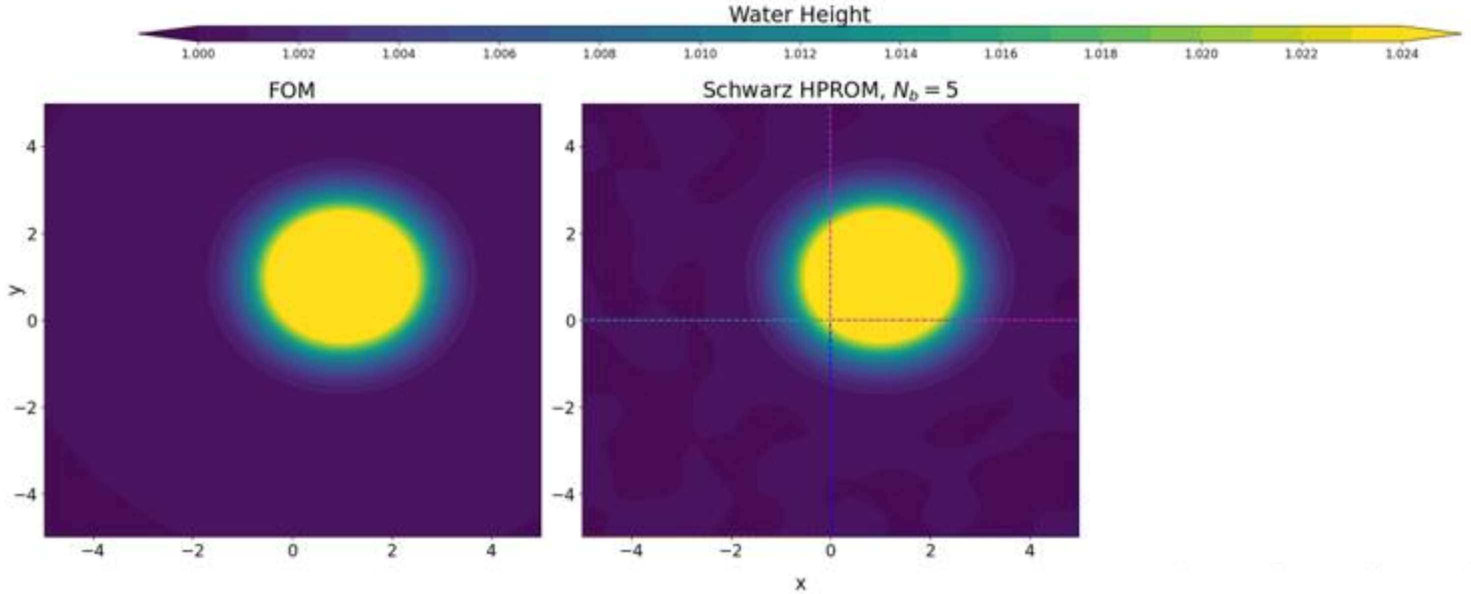

Movie above: FOM (left) and all HROM with $N_b = 5\%$ (right).
ROMs have $K = 100$ modes and $N_s = 0.5\% N$ sample mesh points.

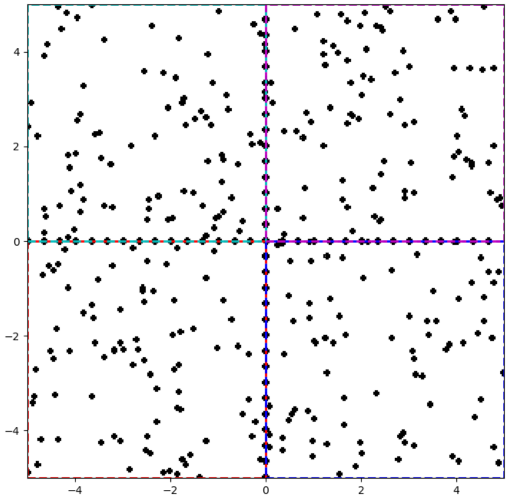

Figure above: example sample mesh with sampling rate $N_b = 10\%$.

- Including **too many Schwarz boundary points** (N_b) in sample mesh given **fixed budget** of N_s sample mesh points may lead to **too few sample mesh points** in **interior**

Schwarz Boundary Sampling for All-HROM Coupling

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

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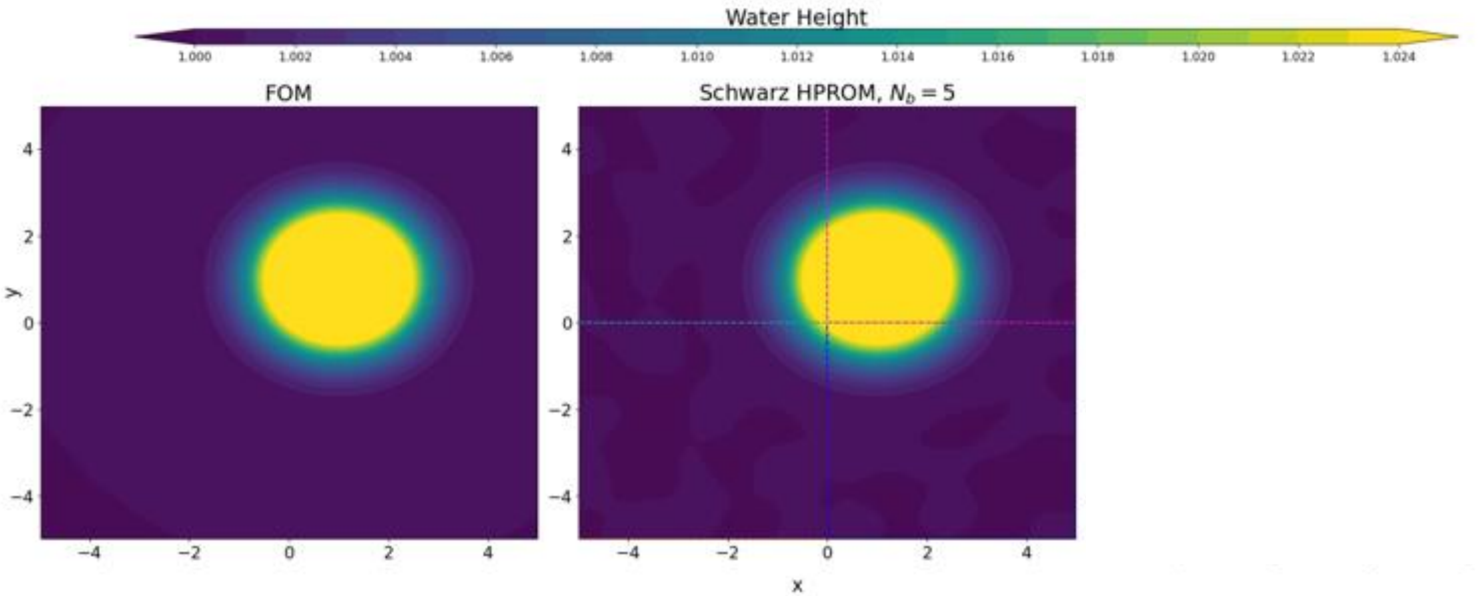

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ROMs have $K = 100$ modes and $N_s = 0.5\% N$ sample mesh points.

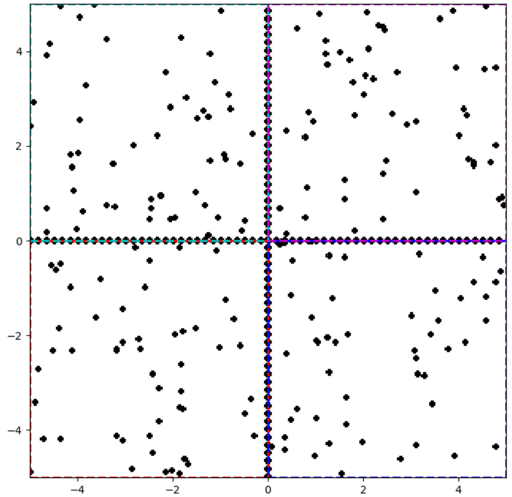


Figure above: example sample mesh with sampling rate $N_b = 15\%$.

- Including **too many Schwarz boundary points** (N_b) in sample mesh given **fixed budget** of N_s sample mesh points may lead to **too few sample mesh points** in **interior**

Model Problem 3: 2D Euler Equations Riemann Problem

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

$$p = (\gamma - 1)\left(\rho E - \frac{1}{2}\rho(u^2+v^2)\right)$$

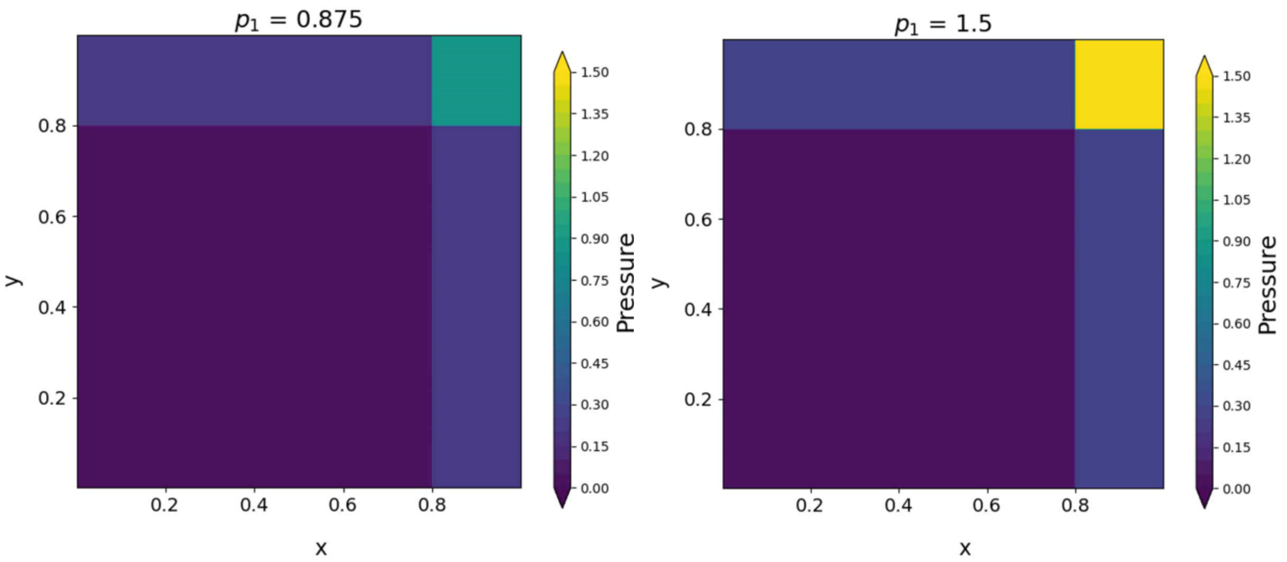


Figure above: FOM solutions to Euler Riemann problem for $p_1 = 0.875$ (left) and $p_1 = 1.5$ (right).

Preliminary results (WIP)

Problem setup:

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

FOM discretization:

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

*Schulz-Rinne, 1993.

Schwarz Coupling Details

Choice of domain decomposition

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

Snapshot collection and reduced basis construction

- **Single-domain FOM** on Ω used to generate snapshots/POD modes

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

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

Choice of hyper-reduction

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

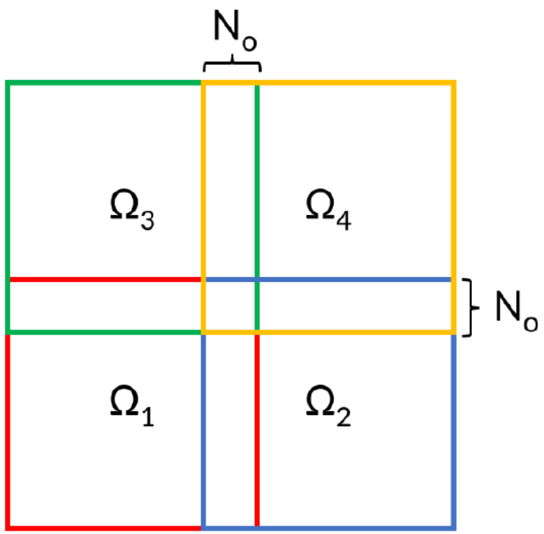


Figure above: DD of Ω into 4 subdomains

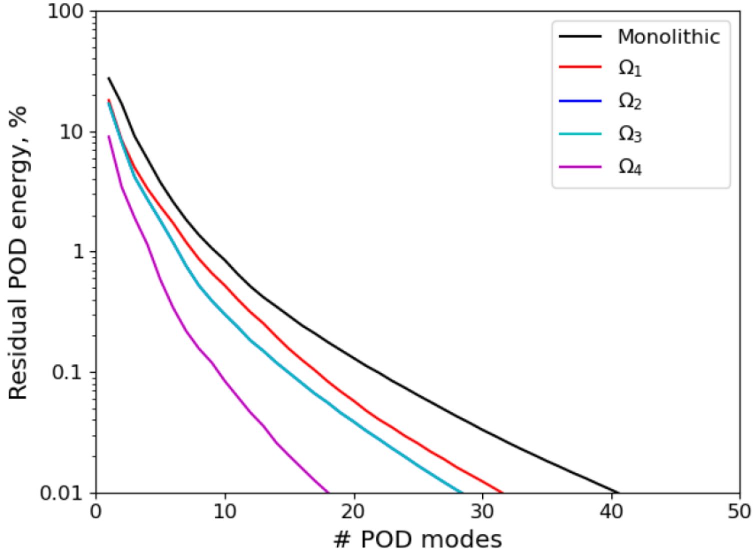
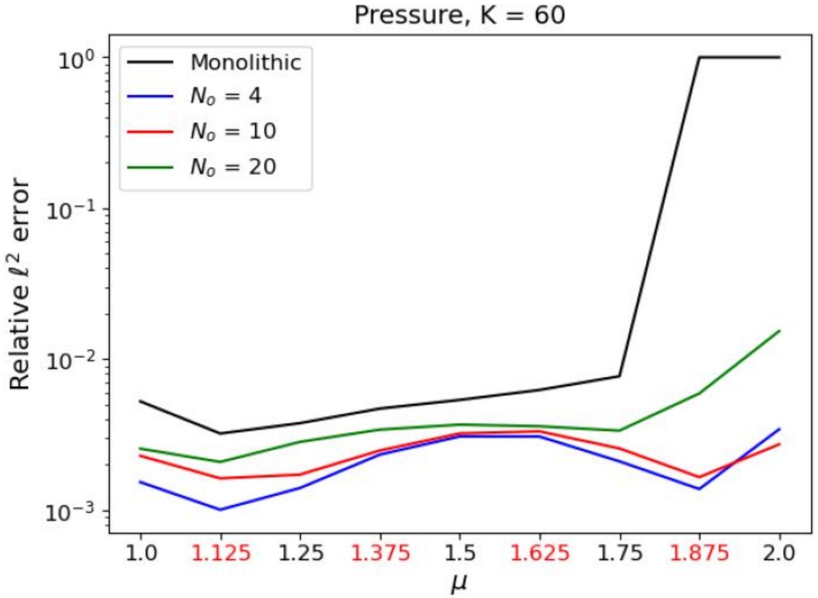


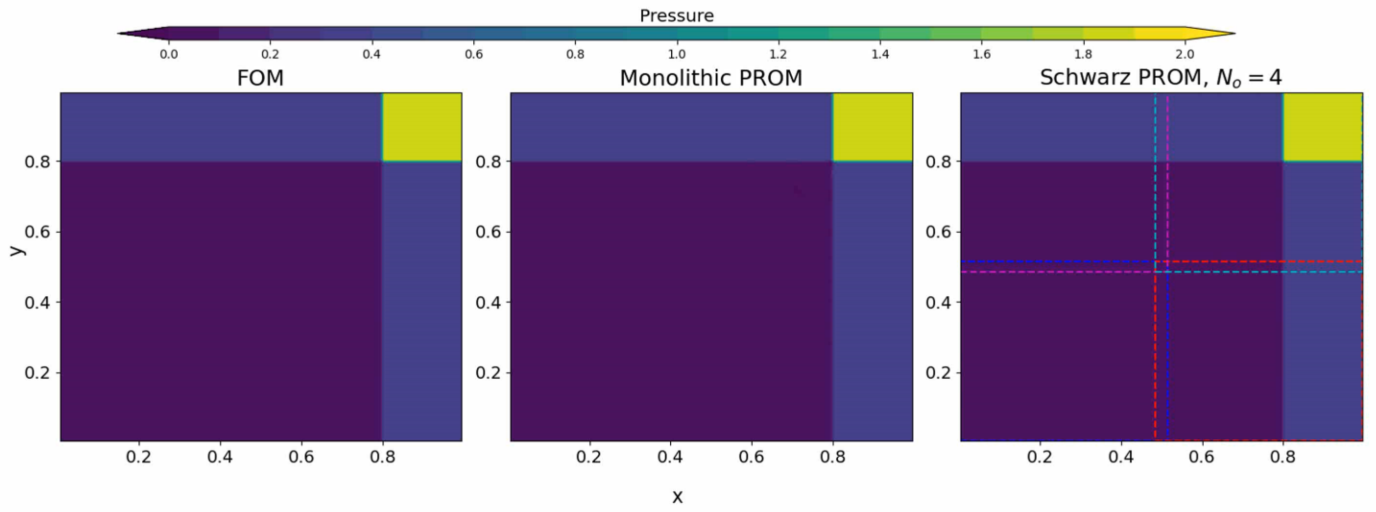
Figure above: Slow decay of POD energy for Euler problem

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

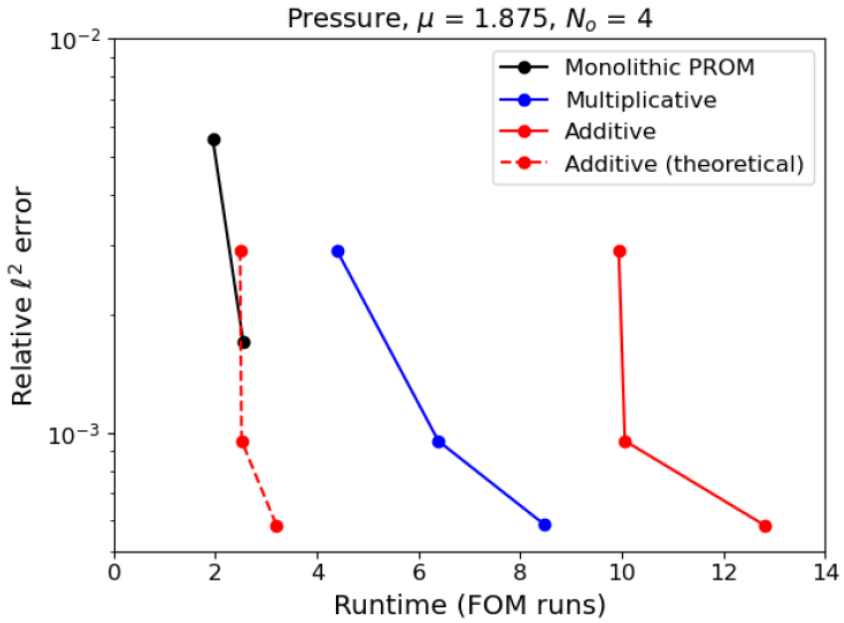
Model Problem 3: All-ROM Coupling + Overlapping Schwarz

- For smaller basis sizes and larger p_1, monolithic ROM is **unstable** whereas **Schwarz ROM** gives **accurate solution**!
- Increased **overlap** degrades accuracy (top right)
- Shock transmission **error** significantly **increases** with **overlap**
- $\sim$4.4 **average # Schwarz iterations** with additive Schwarz vs. $\sim$3.6 for multiplicative Schwarz
- With **additive Schwarz**, can achieve **lower error** than monolithic ROM for **same CPU time** (bottom right)



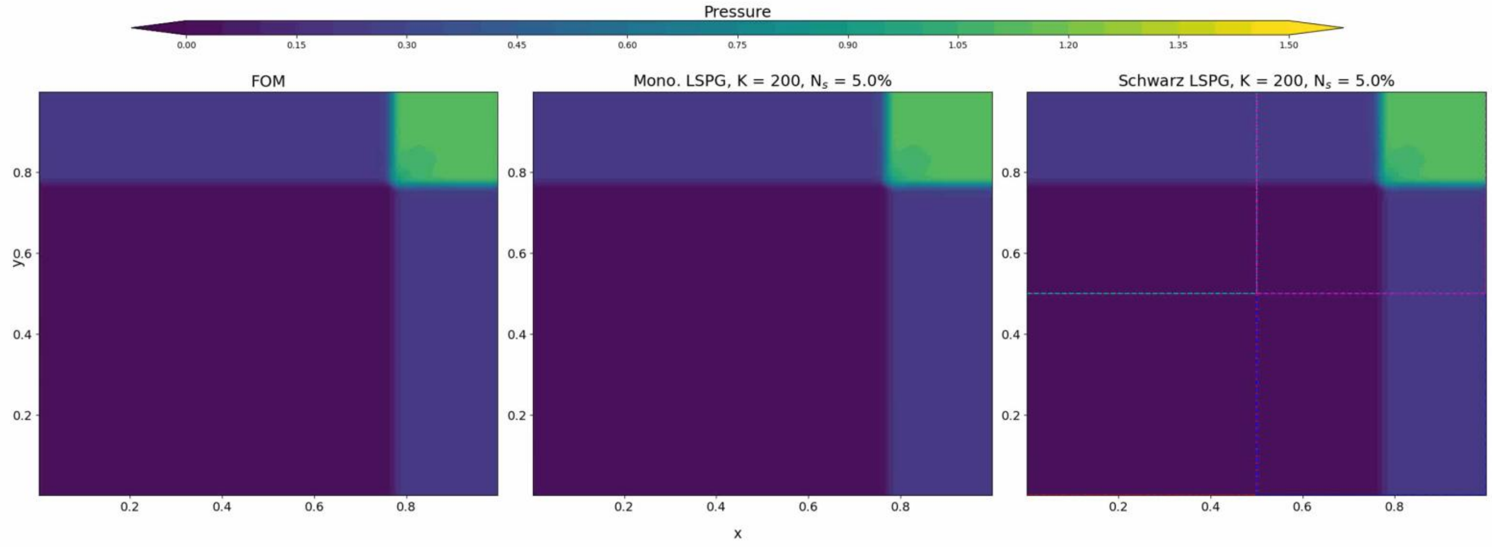


Movie above: FOM (left), $K = 50$ monolithic ROM (middle), and $K = 50$ overlapping Schwarz ROM with $N_o = 4$ (left) for $p_1 = 1.875$.



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

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



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

Preliminary results (WIP)

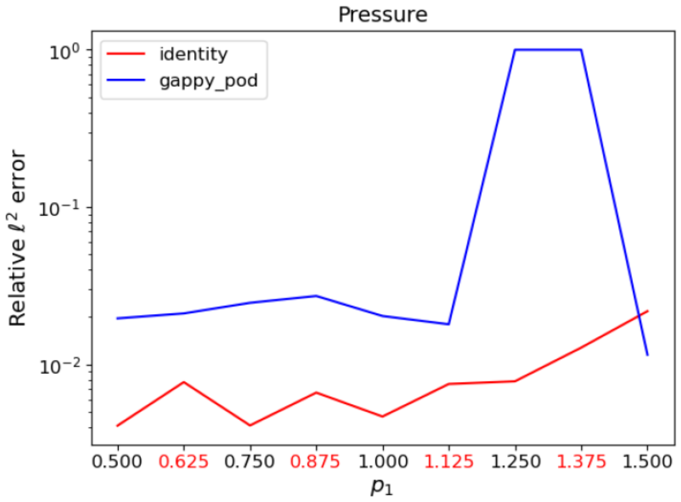


Figure above: collocation and gappy POD relative errors for K=200, 1% sampling rate.

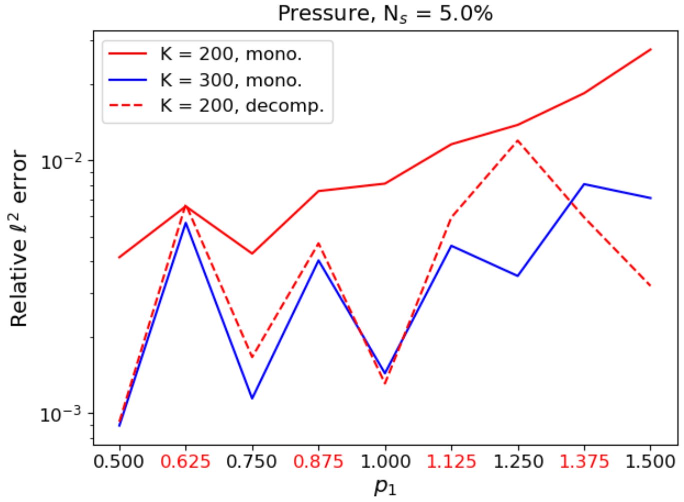


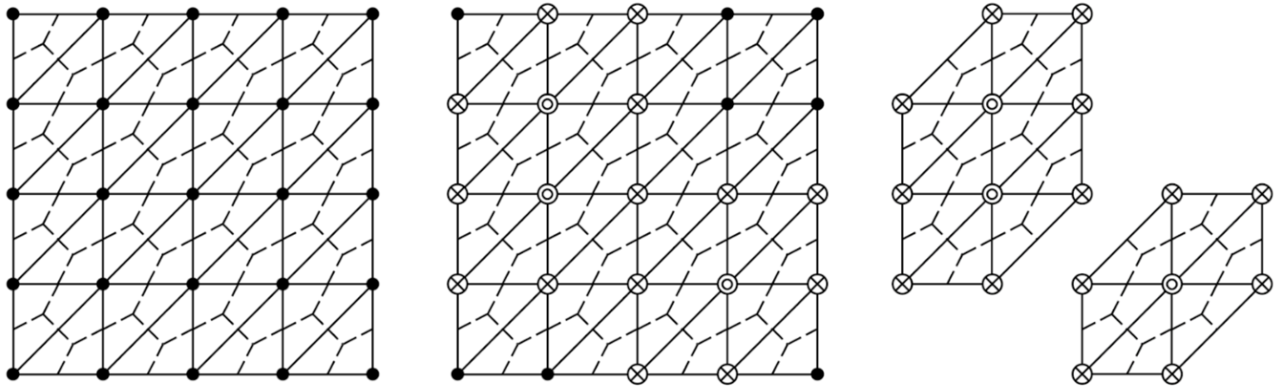
Figure above: monolithic vs. decomposed HROM errors with 5% sampling rate no overlap.

Energy-Conserving Sampling and Weighting (ECSW)

- **Project-then-approximate** paradigm (as opposed to approximate-then-project)

$$
\begin{aligned}
r_k(q_k, t) &= W^T r(\tilde{u}, t) \\
&= \sum_{e \in \mathcal{E}} W^T L_e^T r_e(L_{e^+} \tilde{u}, t)
\end{aligned}
$$

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



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

ECSW: Generating the Reduced Mesh and Weights

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

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

- We can then form the **system**

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

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

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

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