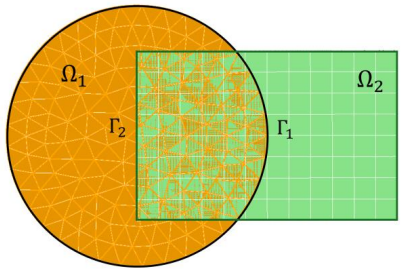
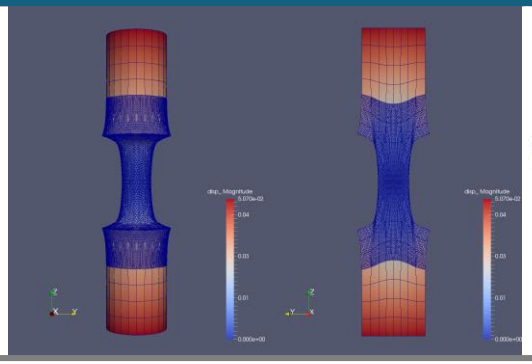
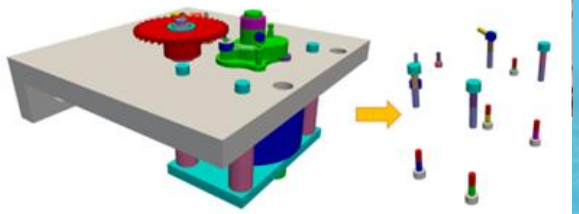
Accelerating analyst workflows via alternating Schwarz-based coupling and (non-intrusive Operator Inference-based) model order reduction







I. Tezaur[1], E. Parish[1], A. Gruber[1], I. Moore[1,2], C. Wentland[1], C. Rodriguez[3], A. Mota[1]

[1]Sandia National Laboratories, USA. [2]Virginia Tech, USA.
[3]Columbia University, USA

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   - Motivation
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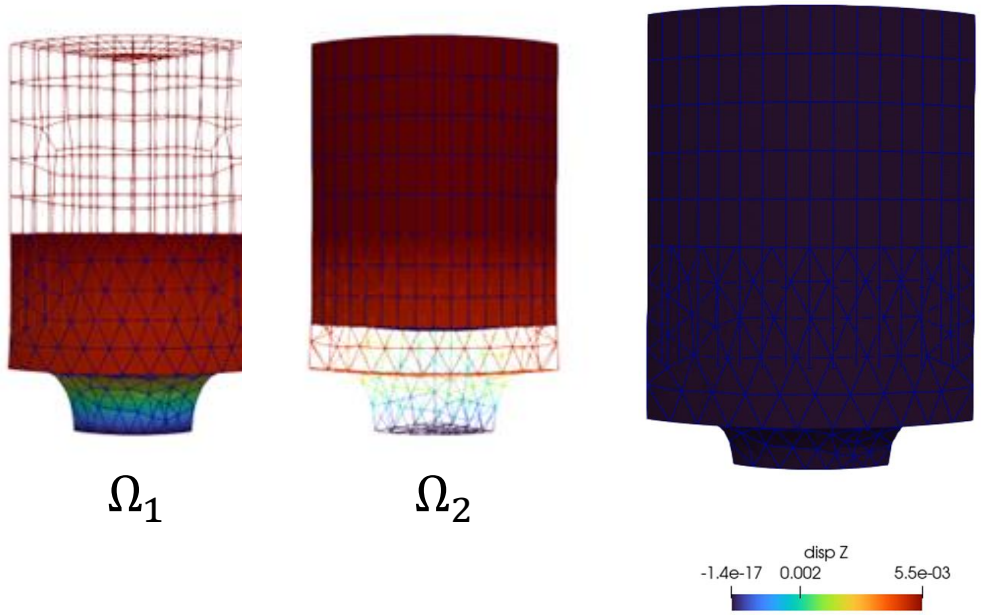

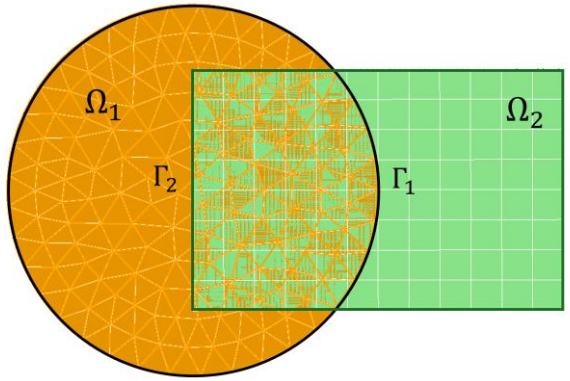

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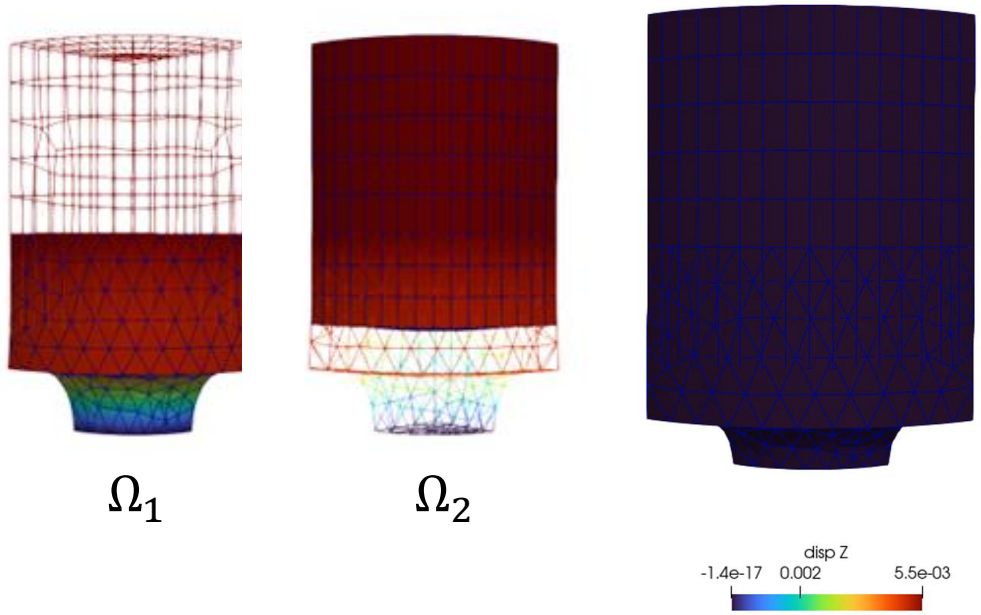
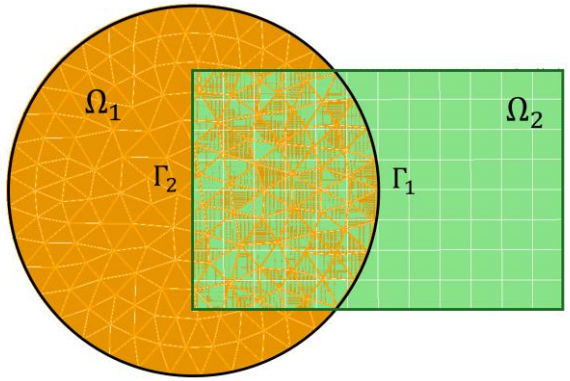
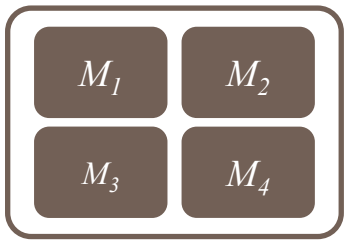
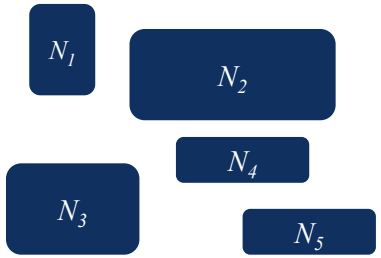


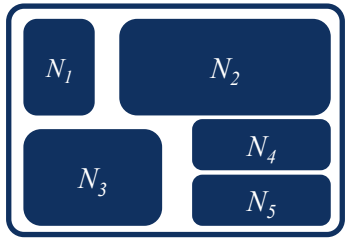


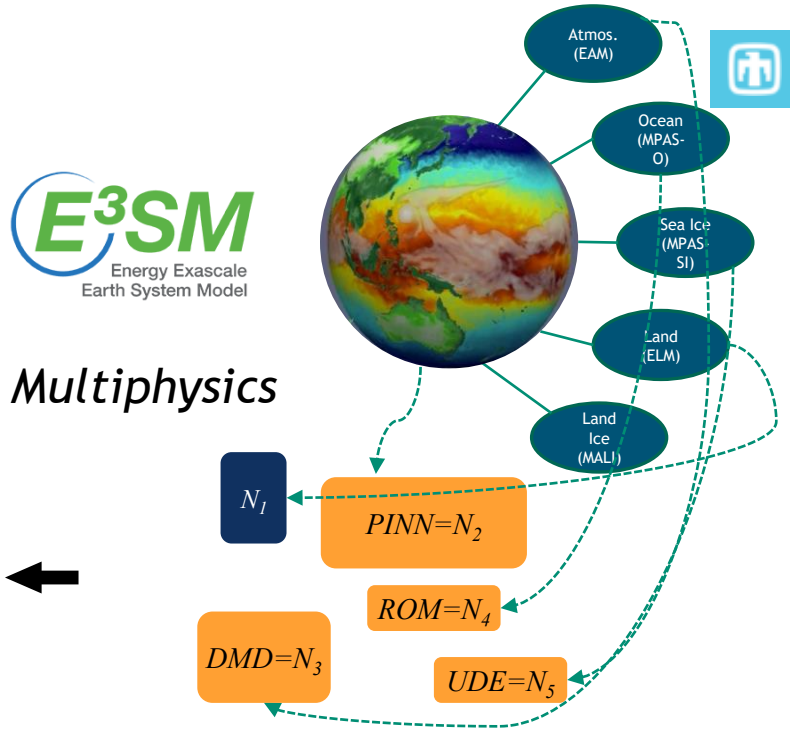
Motivation: Multiscale & Multiphysics Coupling for Predictive Digital Twins

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









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
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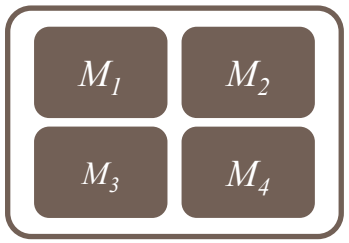

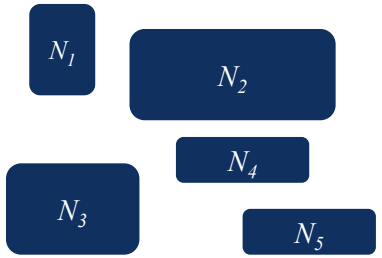

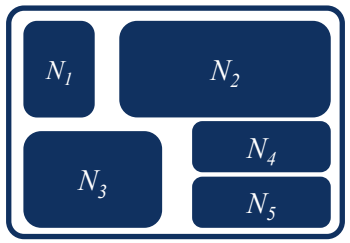

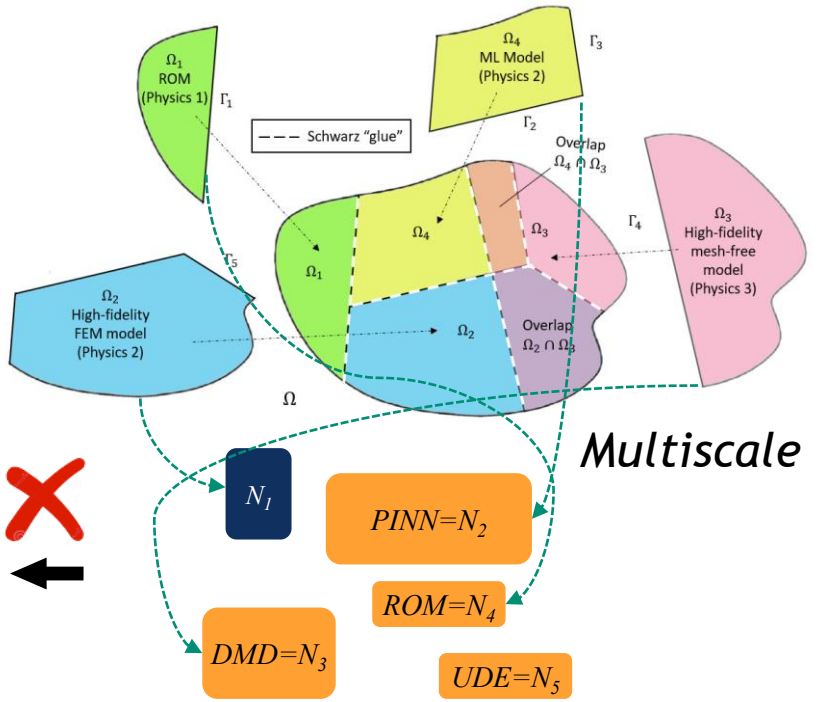

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  - Existing coupling methods for high-fidelity models **may not work** out-of-the-box when including **data-driven models**
  - **ROMs** can suffer from **lack of robustness**, **stability** and **accuracy**, and **cannot** be **easily refined** to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

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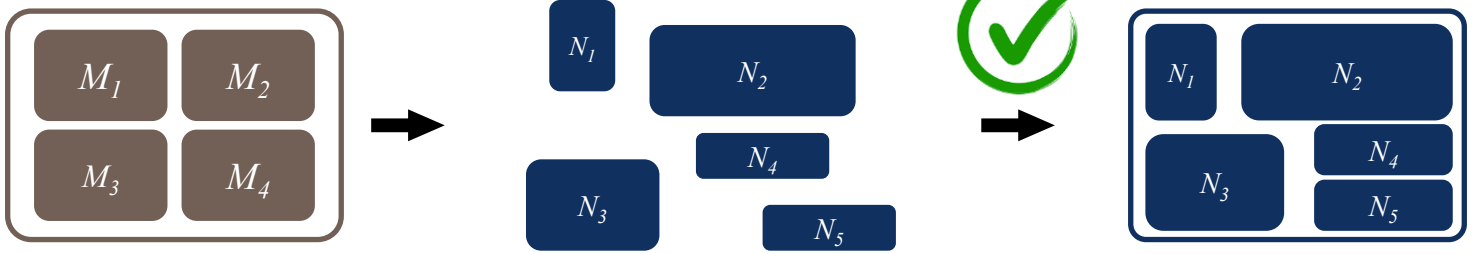

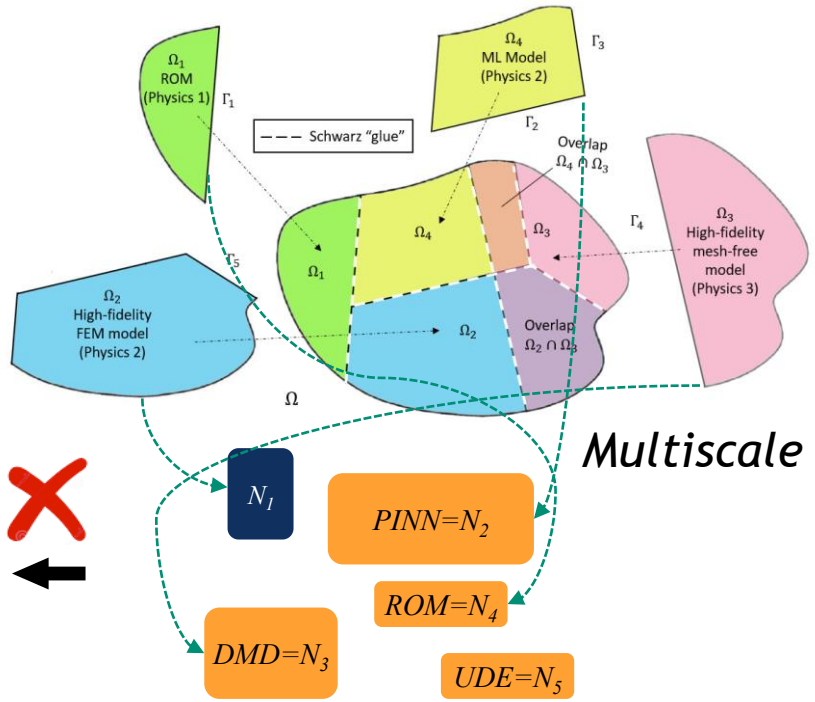

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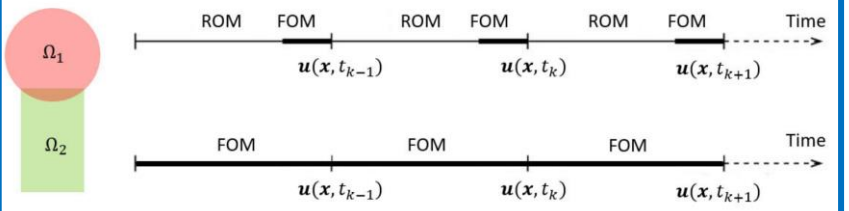
Proposed solution: domain decomposition- (DD-) based coupling via SAM & (soon) online model switching



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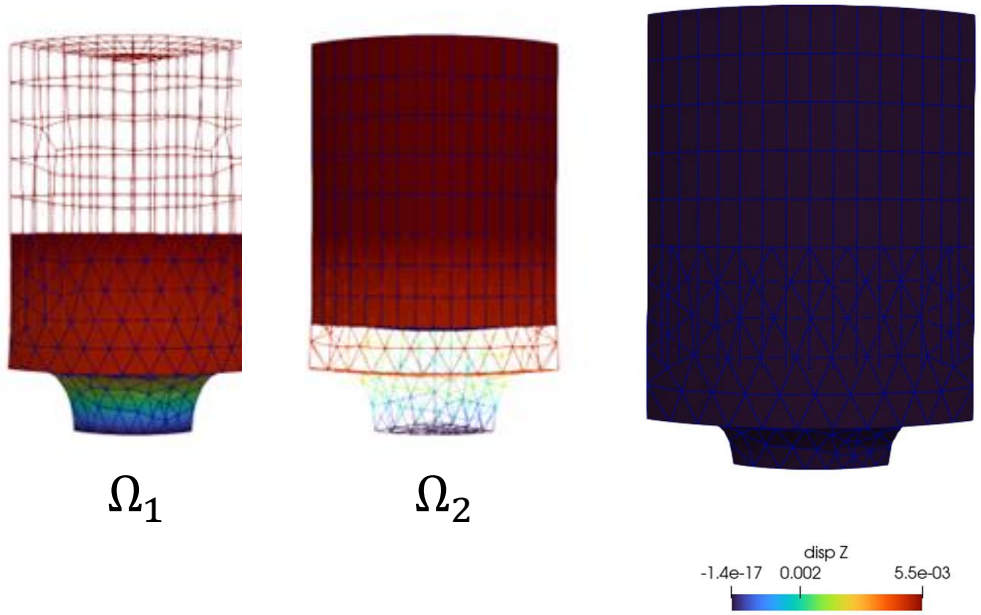
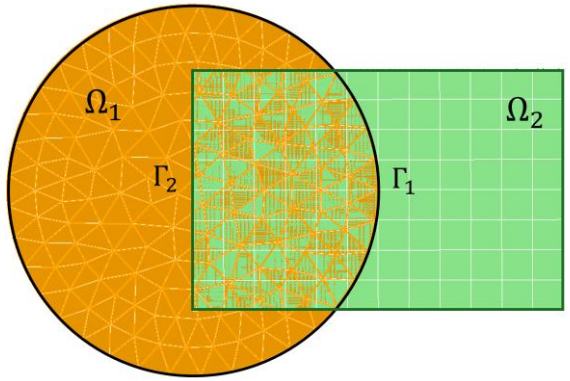
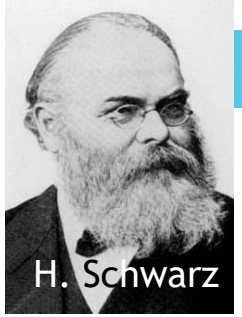




Schwarz Alternating Method (SAM)



- 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.

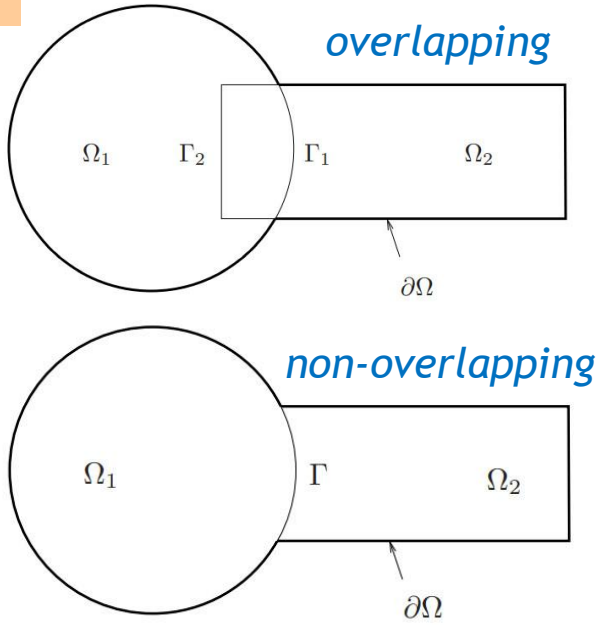
Basic Schwarz Algorithm

Initialize:

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

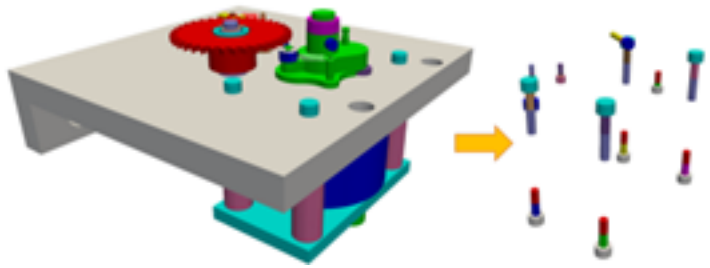
Iterate until convergence:

- 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.



- SAM most commonly used as a ***preconditioner*** for linear solvers.

Idea behind this work: using SAM as a ***discretization/ coupling method*** for solving multiscale PDEs.



Original driving application: *simplifying meshing in solid mechanics.*

- Enables coupling* of subdomains with ***different non-conformal meshes***, ***element types***, ***levels of refinement***, ***time-steppers***, ***solvers*** *and* ***models***

*Mota *et al.*, 2017; Mota *et al.*, 2022.

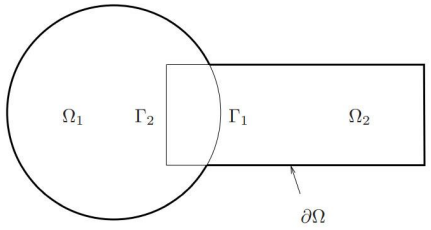
DD-based Coupling via SAM

Overlapping Domain Decomposition

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

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

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



Model PDE:

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

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

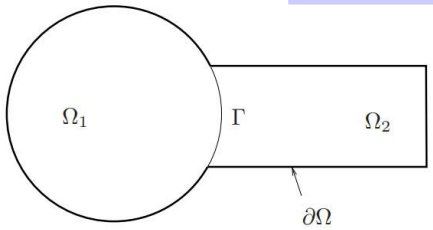
Non-overlapping Domain Decomposition

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

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

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

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



- Relevant for multi-material and multiphysics 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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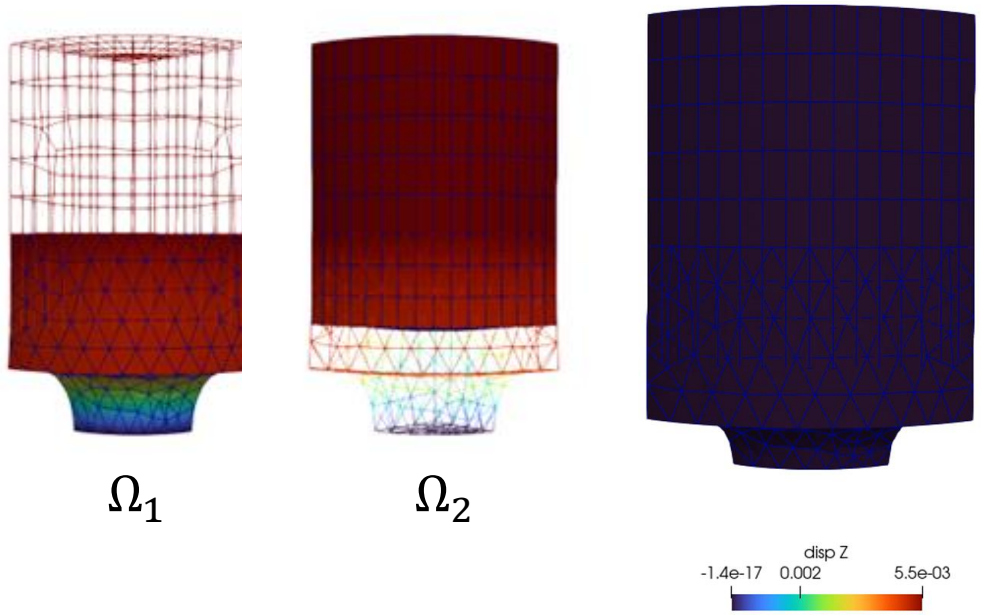
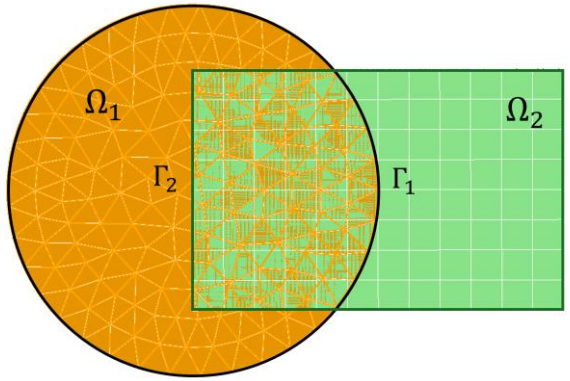
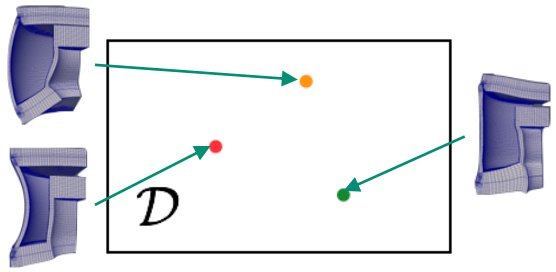




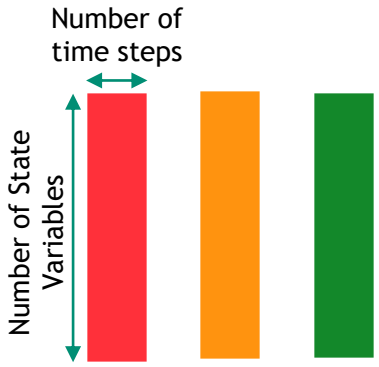
Projection-Based Model Order Reduction via the POD/Galerkin Method

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



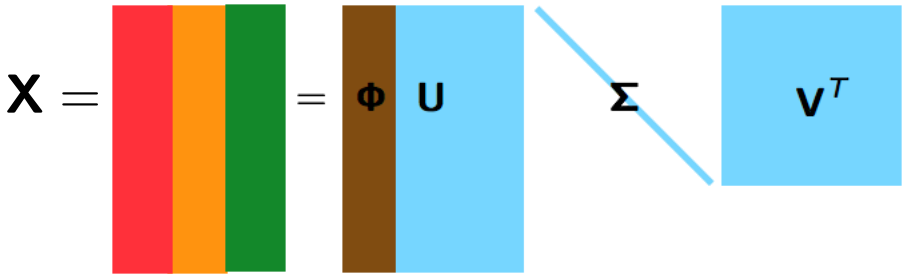
Solve ODE at different design points



Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



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

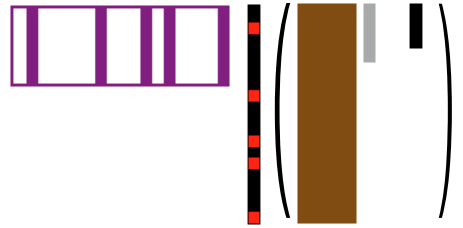
$$\boldsymbol{\Phi}^T\boldsymbol{M}\boldsymbol{\Phi}\frac{d^2\hat{\boldsymbol{u}}}{dt^2} + \boldsymbol{\Phi}^T\boldsymbol{f}_{\text{int}}(\boldsymbol{\Phi}\hat{\boldsymbol{u}}) = \boldsymbol{\Phi}^T\boldsymbol{f}_{\text{ext}}$$

***Disadvantage:** intrusive!*

Hyper-reduce nonlinear terms

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

Hyper-reduction/sample mesh



ROM = projection-based Reduced Order Model

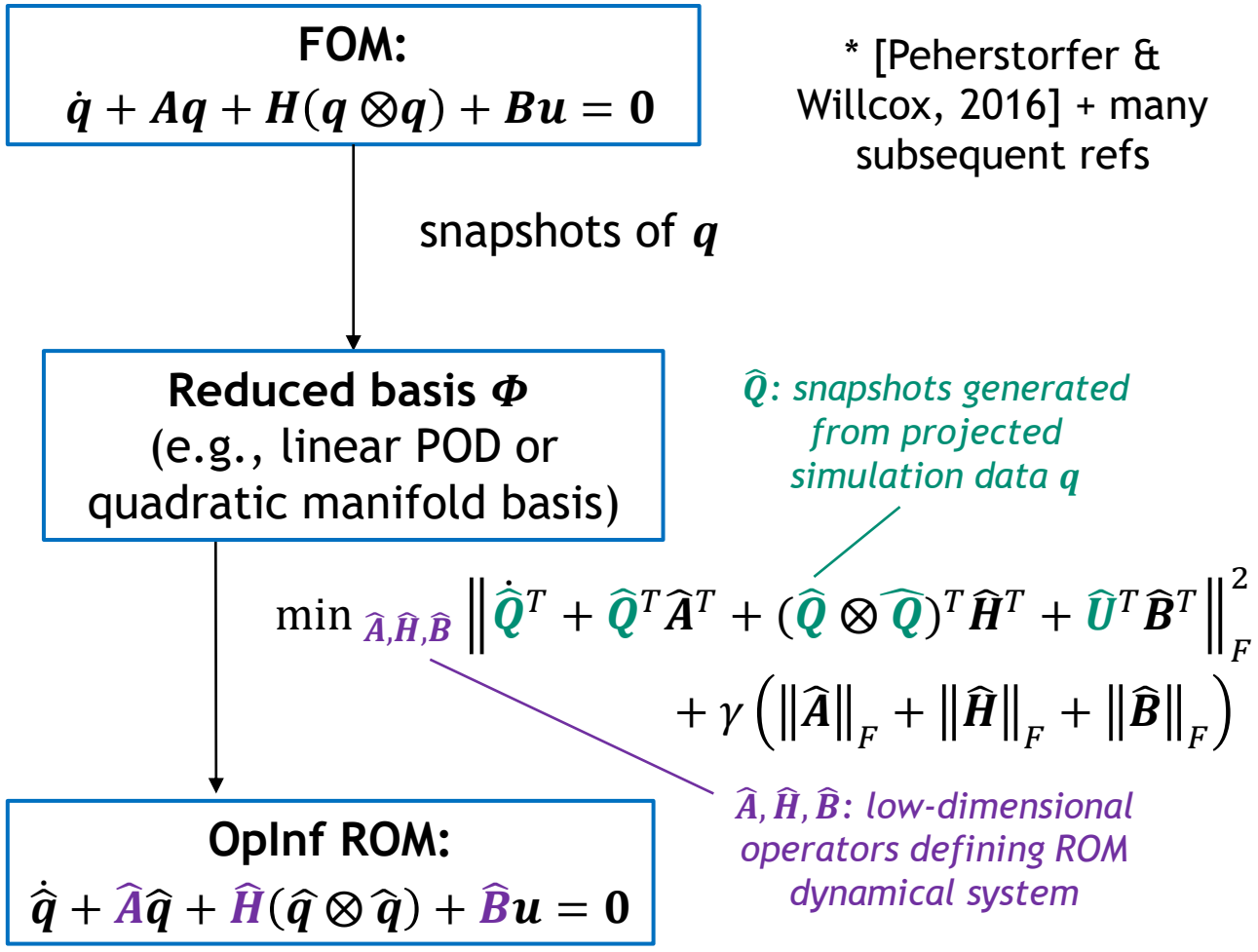
HROM = Hyper-reduced ROM

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



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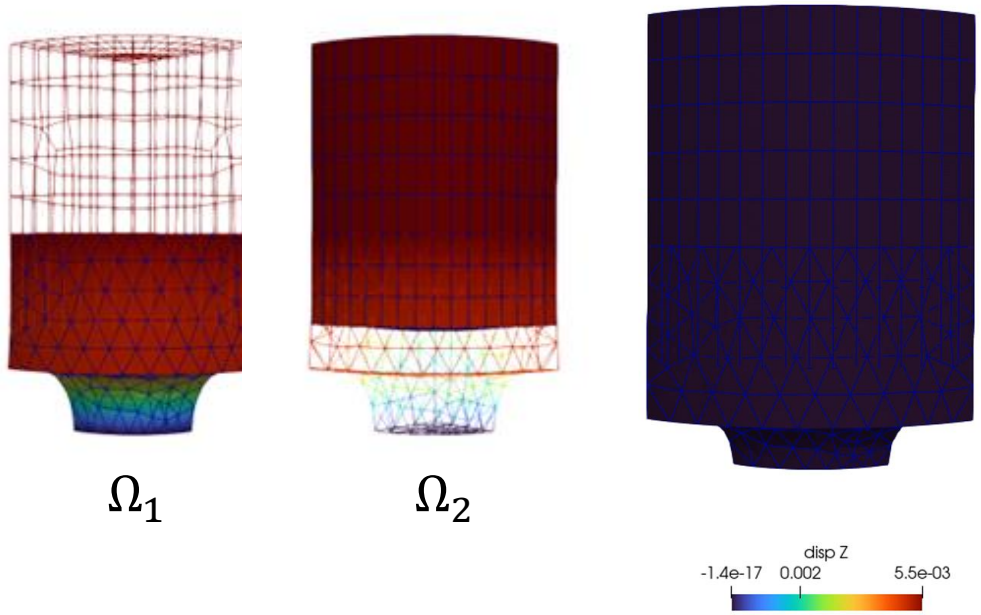

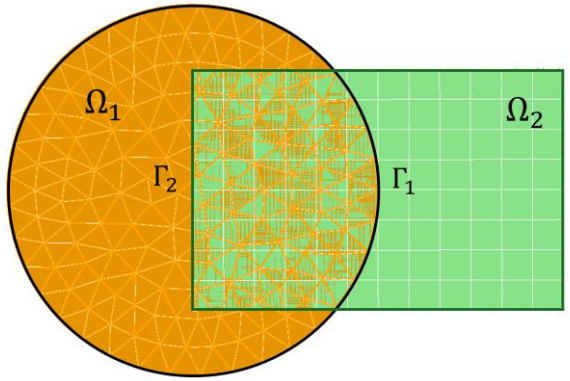

Overlapping SAM-based Coupling for Non-Intrusive OpInf ROMs

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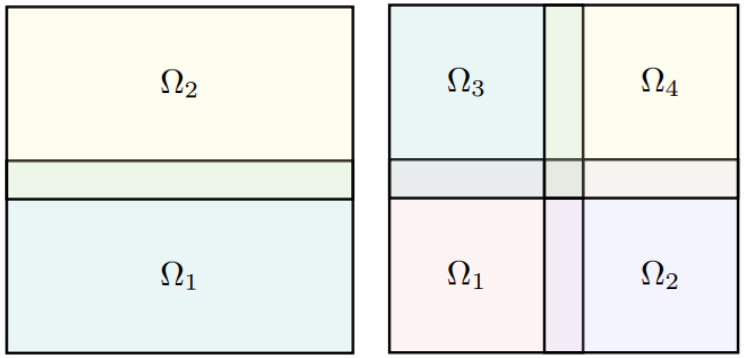

OpInf ROM in Ω_i:

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

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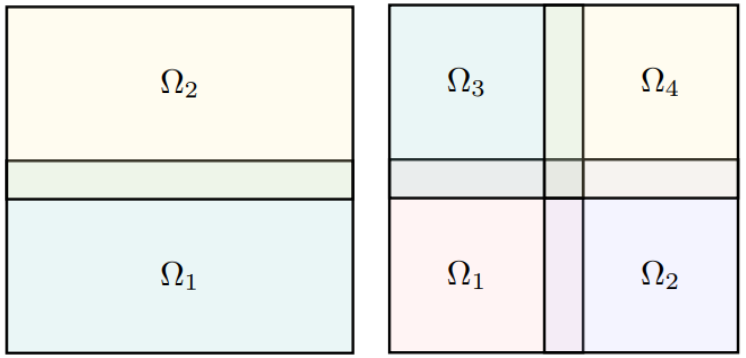

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Motivated by implementation of **Dirichlet BCs** in **FEM**

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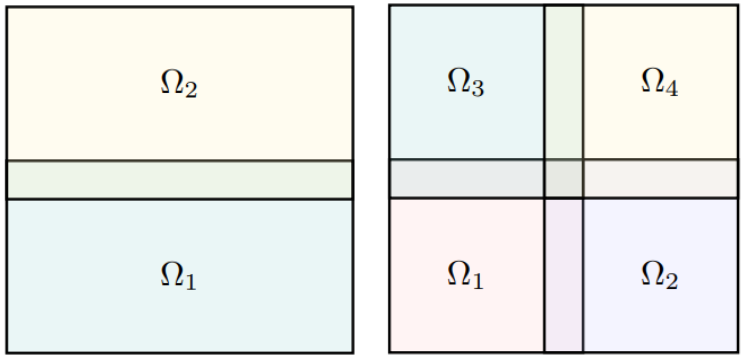

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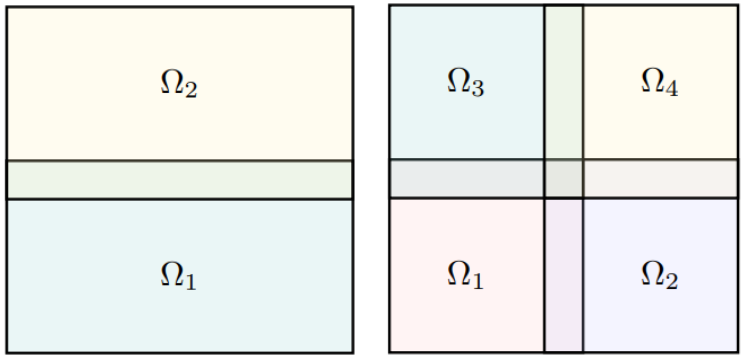

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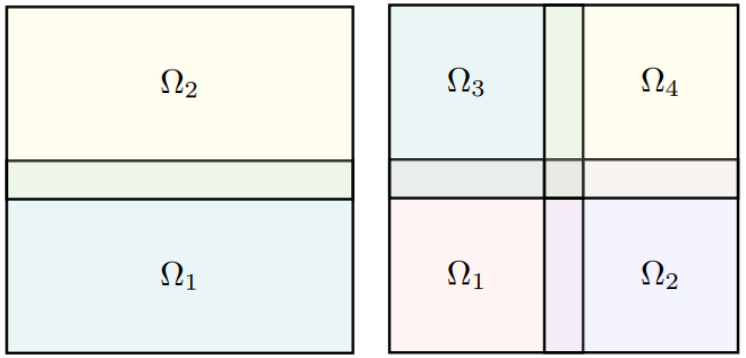

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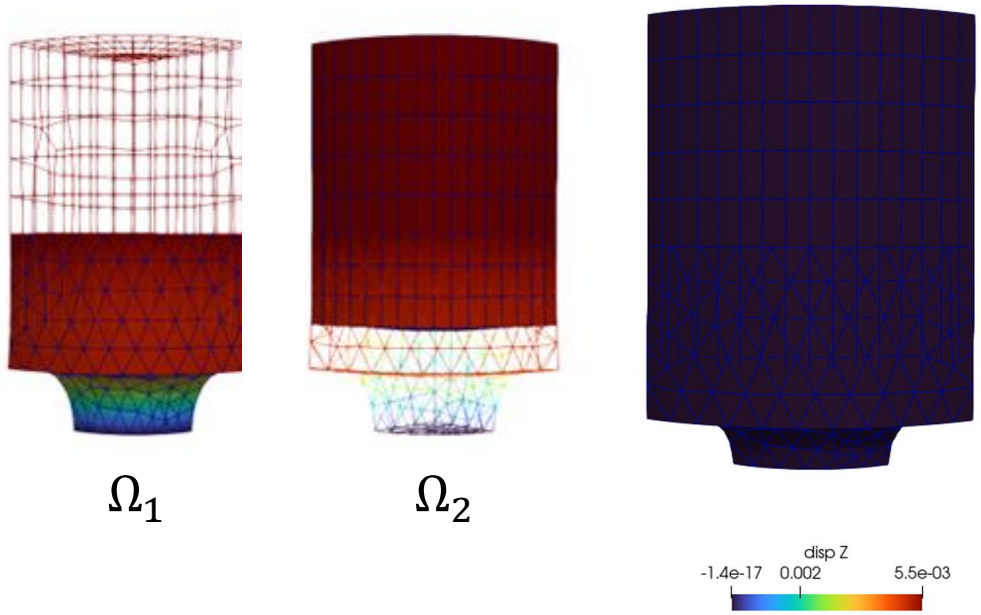
Motivated by implementation of **Dirichlet BCs** in **FEM**

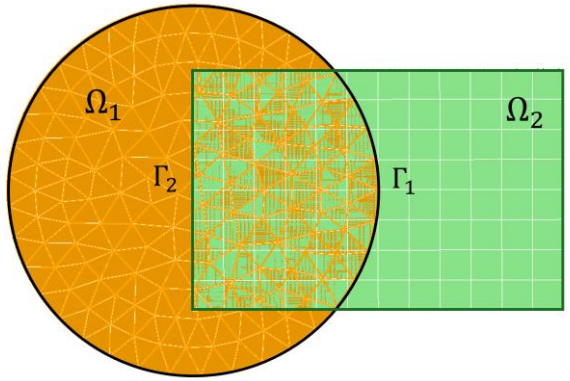
Online stage:

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

Outline

1. Preliminaries
   - Motivation
   - The Schwarz Alternating Method (SAM) for Multi-Scale Coupling
   - Non-Intrusive Operator Inference (OpInf)
2. **Overlapping SAM for OpInf Reduced Order Model (ROM) Coupling**
   - Methodology
   - **Numerical Examples**
3. Non-overlapping SAM for OpInf ROM Coupling
   - Methodology
   - Numerical Example
4. Summary
5. Ongoing & Future Work





Tension Specimen (Overlapping SAM, Predictive)

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Ω_2 rel errs	displacement	–	2.50e-4	4.41e-4
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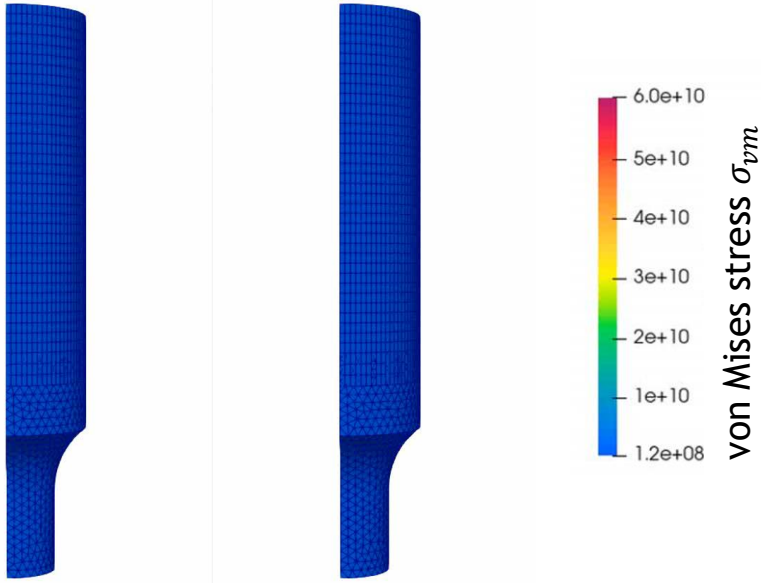

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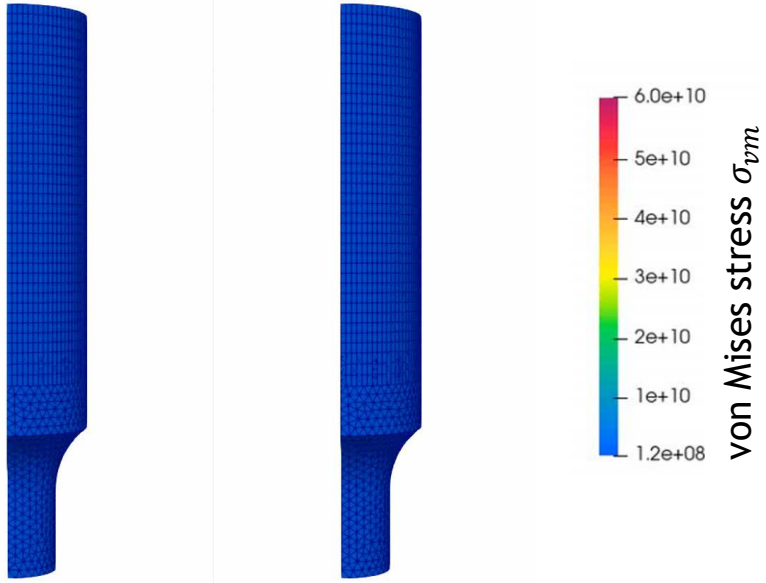

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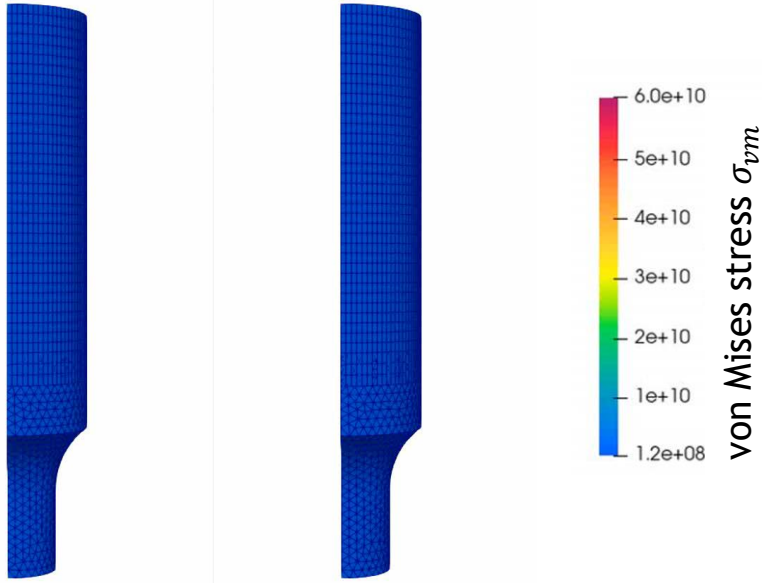

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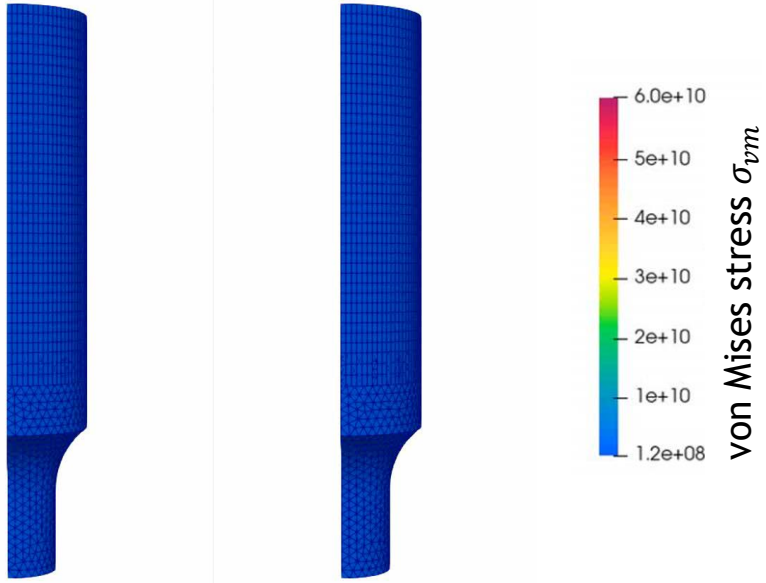

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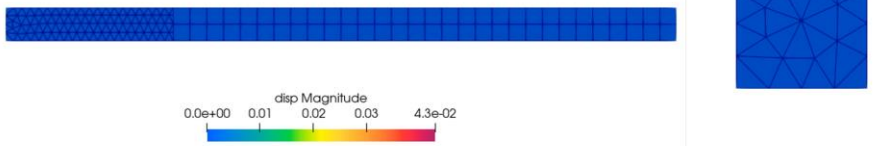

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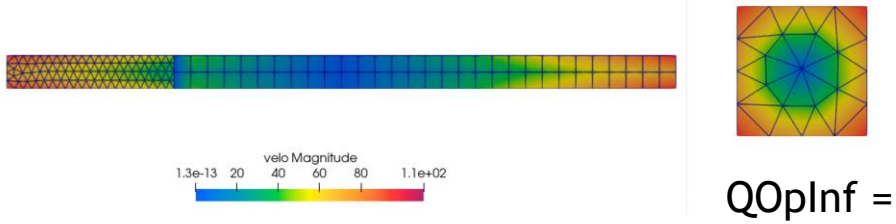

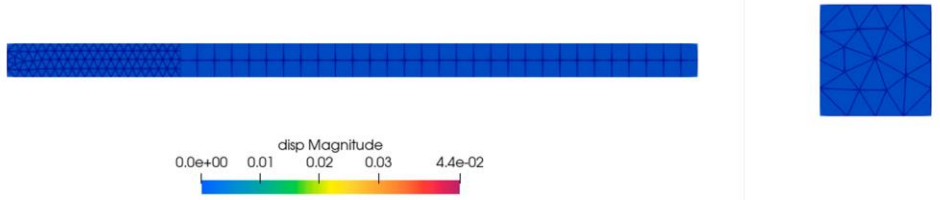

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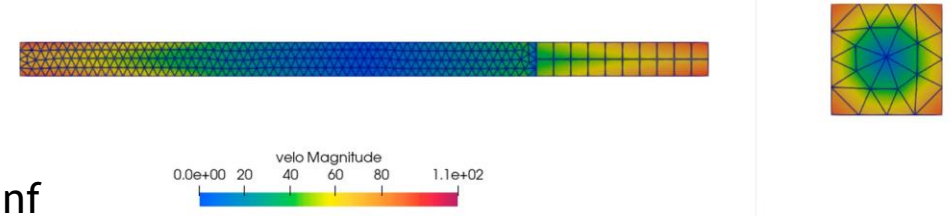

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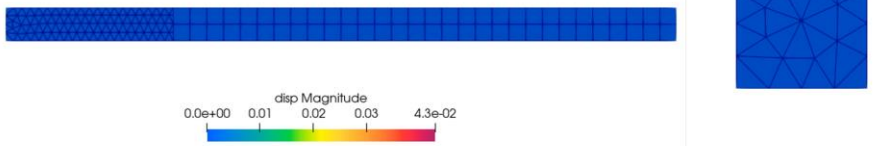

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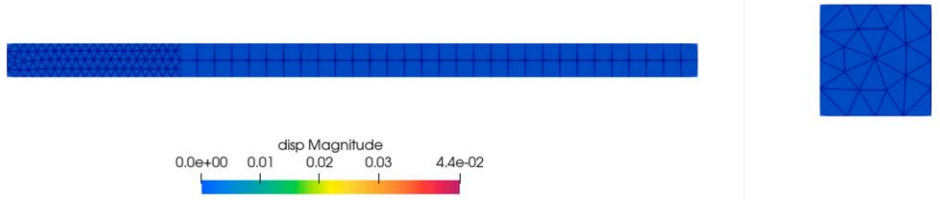

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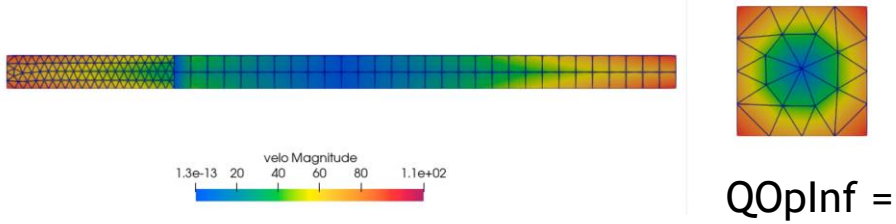

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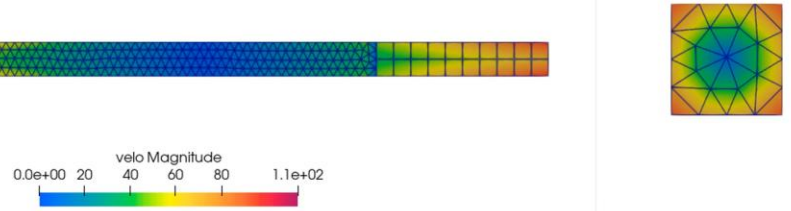

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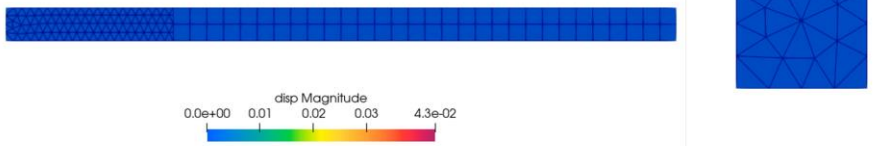
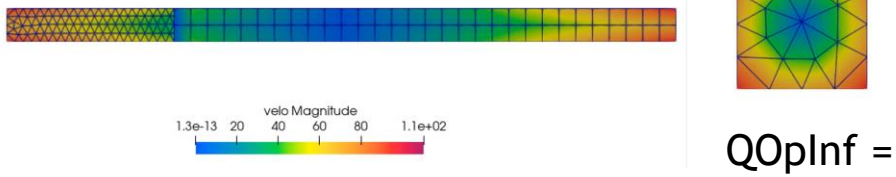
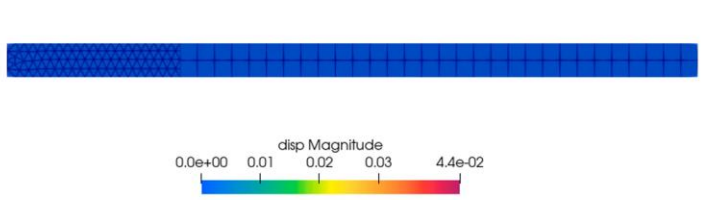
~**23.5× speedups** are achieved via **QOpInf-FOM** couplings

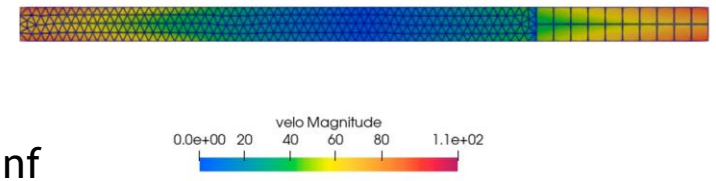


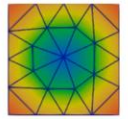
FOM-FOM



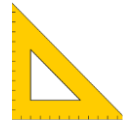


QOpInf-FOM





QOpInf = Quadratic OpInf



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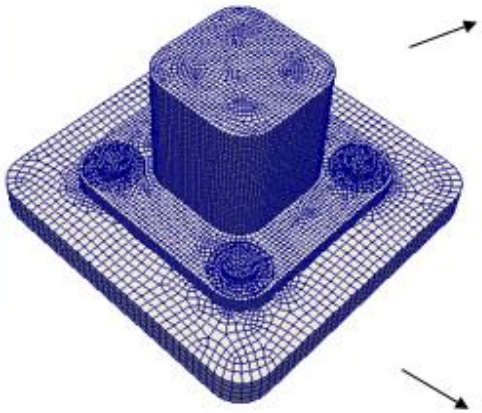
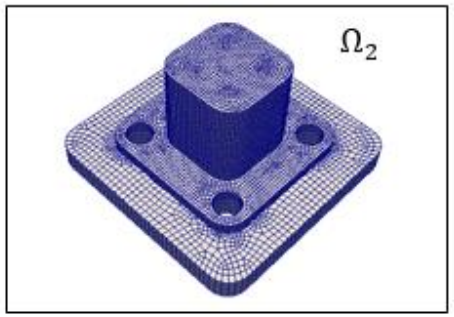
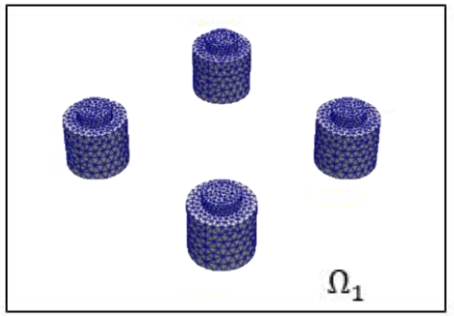
Bolted Joint (Overlapping SAM, Reproductive)

- **Hyper-elastic** (Saint-Venant Kirchhoff) problem with **TET10 - HEX8 meshes**
- **Loading** is applied to top part of bolted join
- **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 (right)







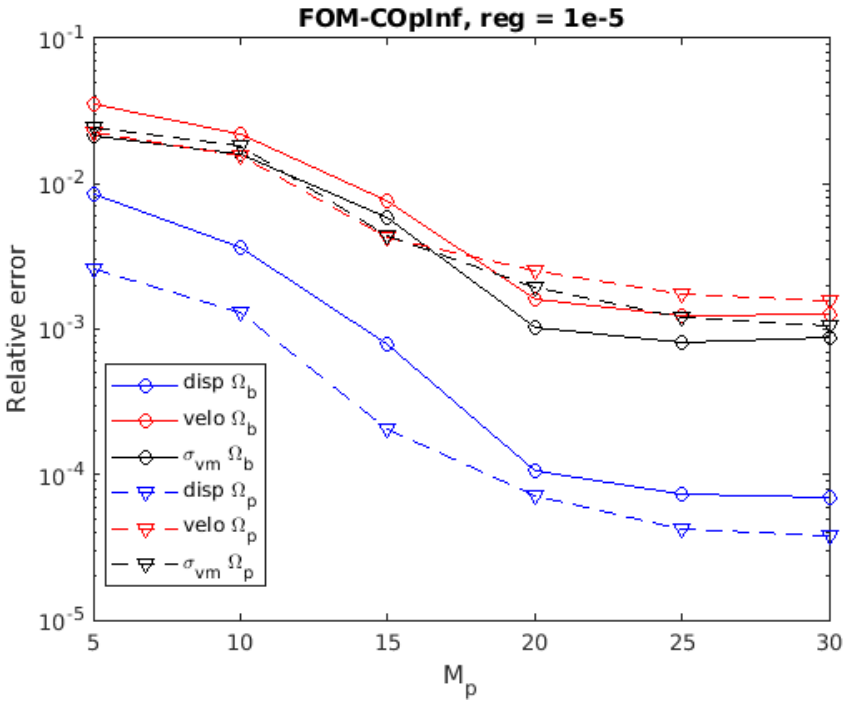


Figure above: convergence w.r.t. basis size for reproductive FOM-COpInf coupling

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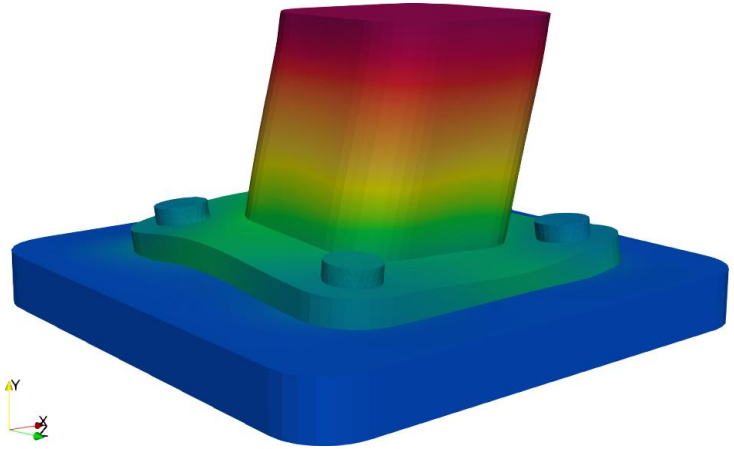
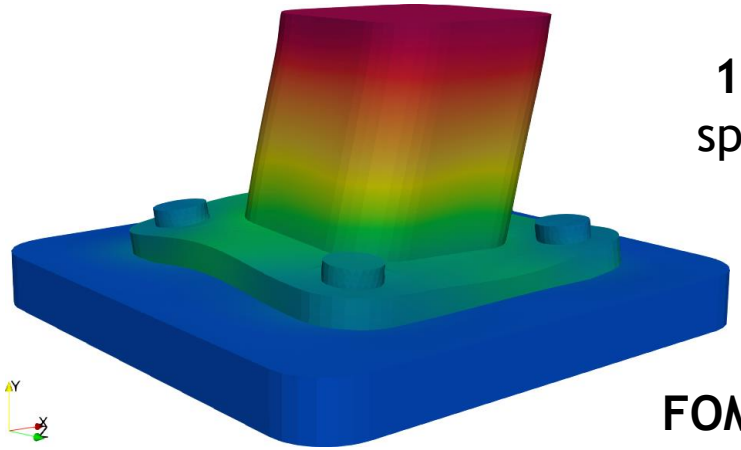
Bolted Joint (Overlapping SAM, Predictive): Displacements

COpInf = Cubic OpInf



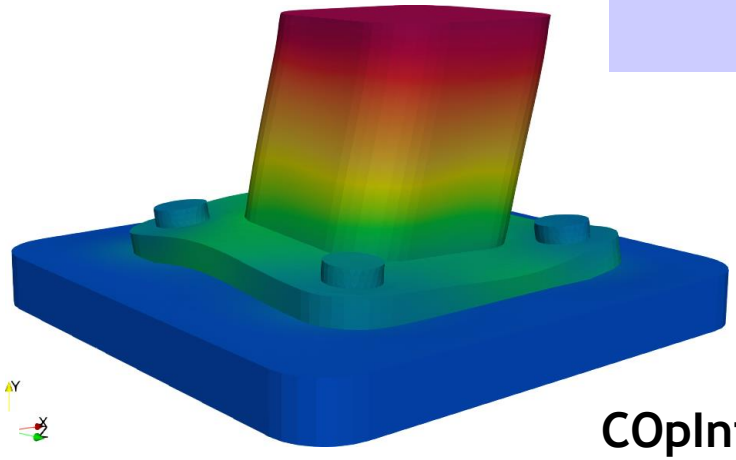
FOM-FOM



1.65×
speedup

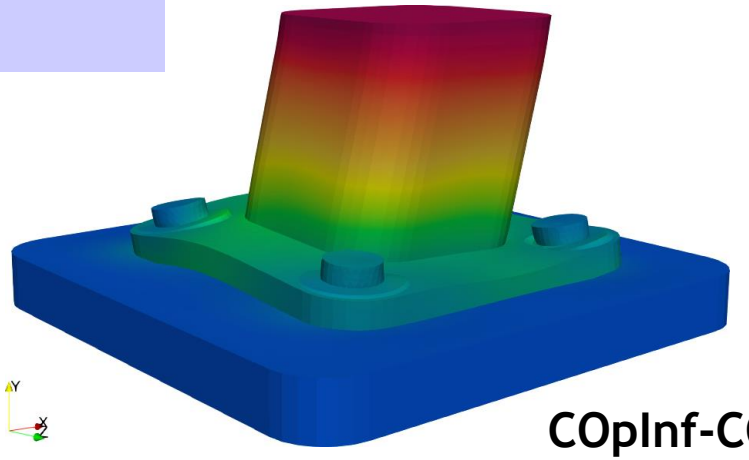
FOM-COpInf
0.69% rel err (parts)
3.51% rel err (bolts)

Models generally 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)

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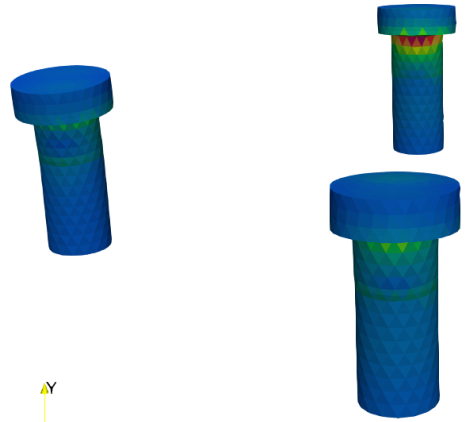
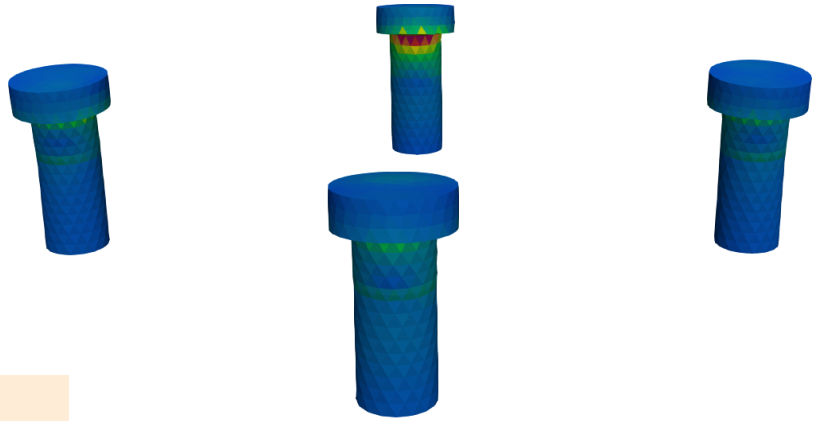
Bolted Joint (Overlapping SAM, Predictive): von Mises Stresses

COpInf = Cubic OpInf



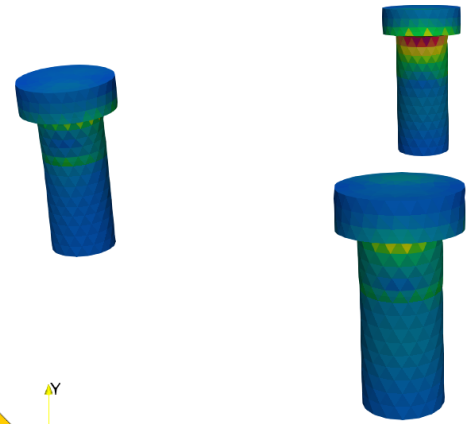
FOM-FOM

1.65×
speedup



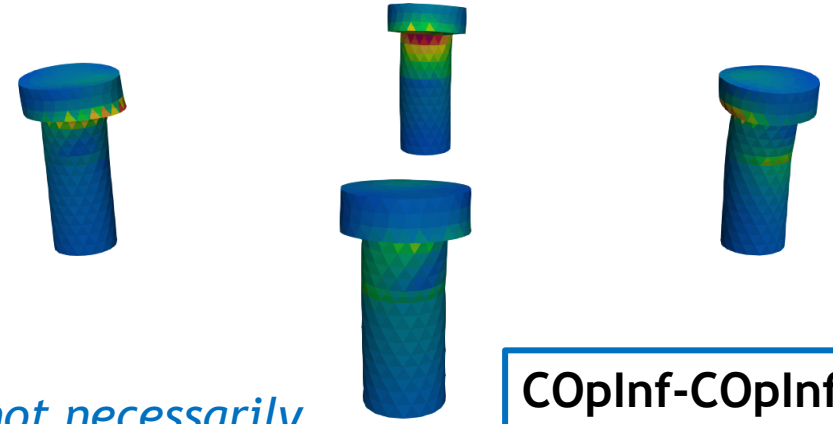
FOM-COpInf
7.74% rel err

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



COpInf-COpInf (best)
12.4% rel error

6.12×
speedup



COpInf-COpInf (worst)
30.9% rel error

High errors do not necessarily mean result cannot be informative.

NORMA.JL

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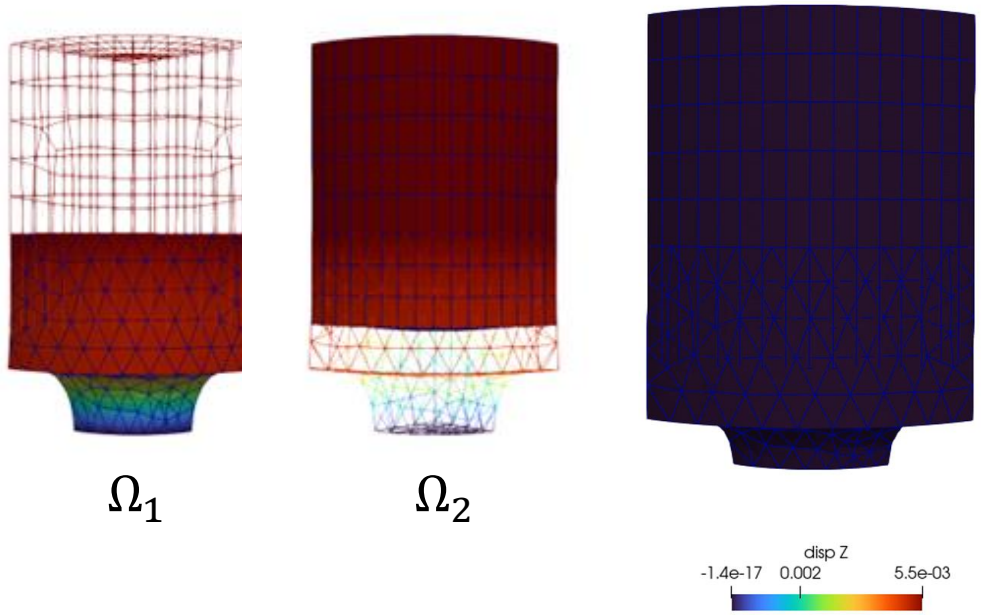
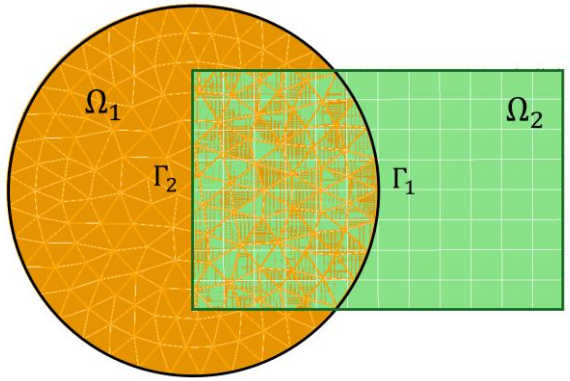


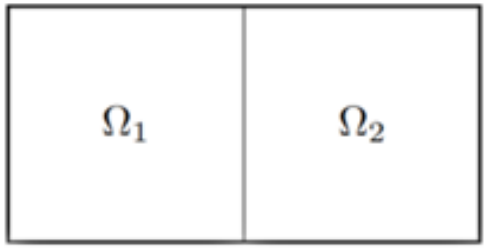


Non-overlapping SAM-based Coupling for Non-Intrusive OpInf ROMs

Alternating Dirichlet-Neumann non-overlapping SAM (dynamic linear elastic problem)

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

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



Non-overlapping SAM-based Coupling for Non-Intrusive OpInf ROMs

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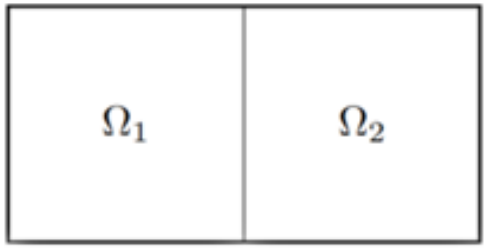
$$\begin{cases} \text{Div}\, \boldsymbol{P}_1^{(n+1)} = \rho \ddot{\boldsymbol{\varphi}}_1^{(n+1)}, & \text{in } \Omega_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\chi}, & \text{on } \partial\Omega_1 \backslash \Gamma \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\varphi}_2^{(n)}, & \text{on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

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



$$\int_I \left[\int_{\Omega_1} \left(\rho \ddot{\boldsymbol{\varphi}}_1^{(n+1)} \cdot \boldsymbol{\xi} + \boldsymbol{P}_1^{(n+1)} : \nabla \boldsymbol{\xi} \right) d\Omega \right] dt = 0$$

$$\int_I \left[\int_{\Omega_2} \left(\rho \ddot{\boldsymbol{\varphi}}_2^{(n+1)} \cdot \boldsymbol{\xi} + \boldsymbol{P}_2^{(n+1)} : \nabla \boldsymbol{\xi} \right) d\Omega - \int_\Gamma \left(\boldsymbol{P}_1^{(n+1)} \boldsymbol{n} \right) \cdot \boldsymbol{\xi} dS \right] dt = 0$$

Non-overlapping SAM-based Coupling for Non-Intrusive OpInf ROMs

Alternating Dirichlet-Neumann non-overlapping SAM (dynamic linear elastic problem)

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

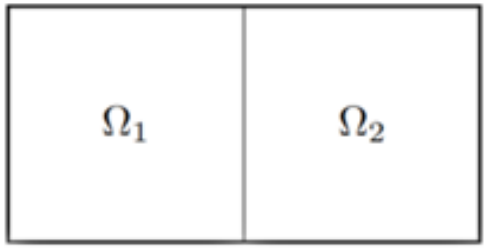
$$\int_I \left[\int_{\Omega_1} \left(\rho \ddot{\boldsymbol{\varphi}}_1^{(n+1)} \cdot \boldsymbol{\xi} + \boldsymbol{P}_1^{(n+1)} : \nabla \boldsymbol{\xi} \right) d\Omega \right] dt = 0$$

$$\widehat{\boldsymbol{M}}_1 \ddot{\widehat{\boldsymbol{q}}}_1 + \widehat{\boldsymbol{K}}_1 \widehat{\boldsymbol{q}}_1 + \widehat{\boldsymbol{B}}_1 \boldsymbol{g}_1 = \boldsymbol{0}$$

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

$$\int_I \left[\int_{\Omega_2} \left(\rho \ddot{\boldsymbol{\varphi}}_2^{(n+1)} \cdot \boldsymbol{\xi} + \boldsymbol{P}_2^{(n+1)} : \nabla \boldsymbol{\xi} \right) d\Omega - \int_\Gamma \left(\boldsymbol{P}_1^{(n+1)} \boldsymbol{n} \right) \cdot \boldsymbol{\xi} dS \right] dt = 0$$

$$\widehat{\boldsymbol{M}}_2 \ddot{\widehat{\boldsymbol{q}}}_2 + \widehat{\boldsymbol{K}}_2 \widehat{\boldsymbol{q}}_2 + \widehat{\boldsymbol{B}}_2 \boldsymbol{g}_2 + \widehat{\boldsymbol{H}}_2 \boldsymbol{t}_2 = \boldsymbol{0}$$



OpInf ROMs

Dirichlet problem: learn $\widehat{\boldsymbol{M}}_1$, $\widehat{\boldsymbol{K}}_1$, $\widehat{\boldsymbol{B}}_1$

- Use snapshots of displacement, acceleration and Dirichlet data to train ROM

Neumann problem: learn $\widehat{\boldsymbol{M}}_2$, $\widehat{\boldsymbol{K}}_2$, $\widehat{\boldsymbol{B}}_2$, $\widehat{\boldsymbol{H}}_2$

- Use snapshots of displacement, acceleration, Dirichlet data and tractions to train ROM

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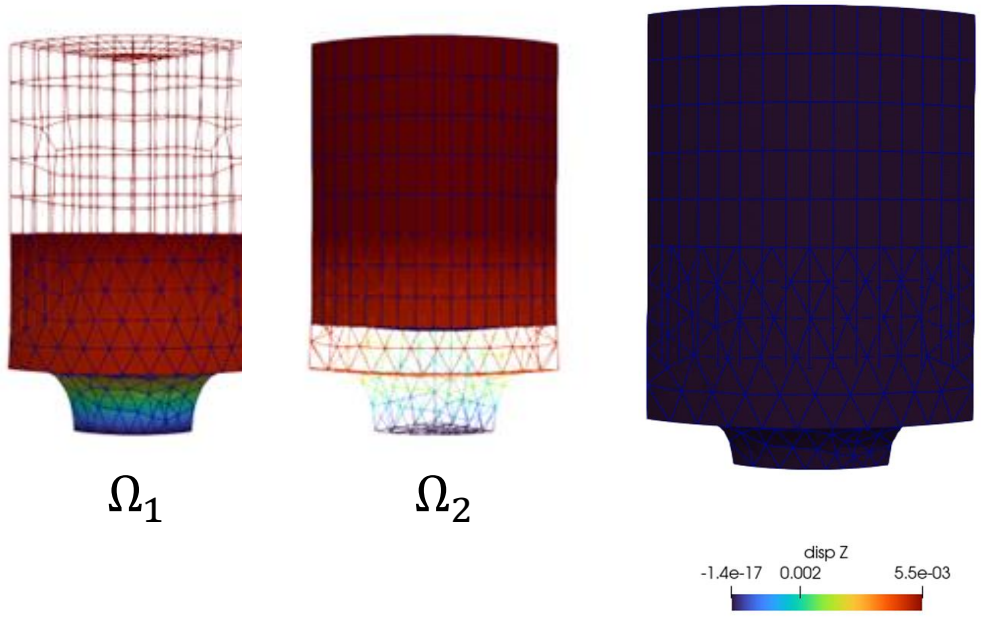
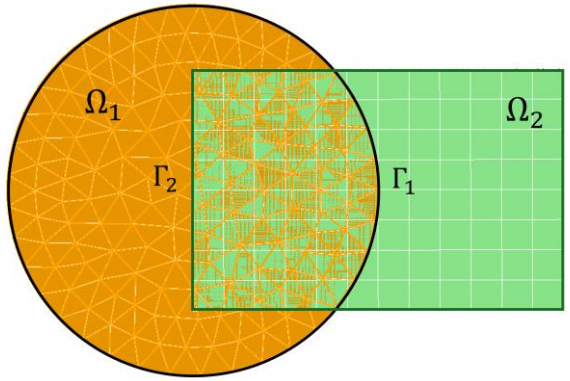
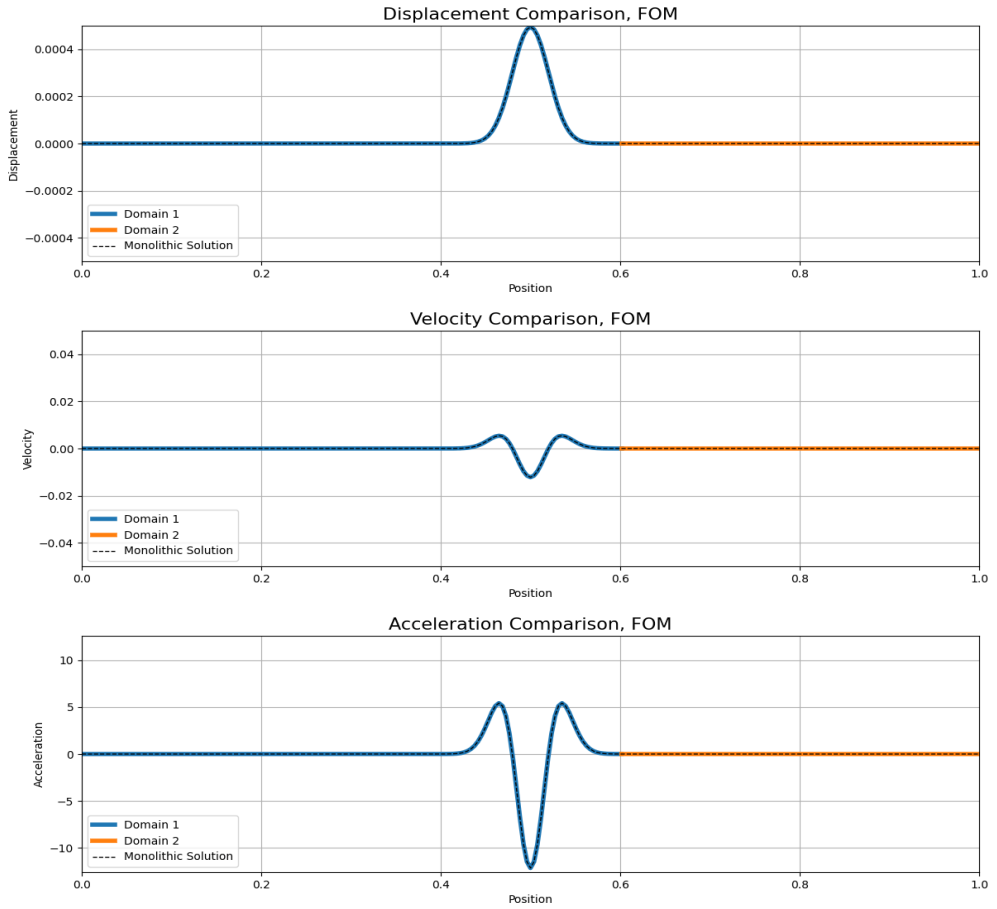




Linear Elastic Wave Propagation (Non-Overlapping SAM, Reproductive)

- 1D linear elastic ***clamped beam*** with Gaussian initial condition for the displacement.
- Simple problem with analytical exact solution but very ***stringent test*** for discretization methods.
- Test non-overlapping SAM w/ ***2 subdomains***: $\Omega_1 = (0,0.6), \Omega_2 = (0.6,1)$.

Transmission Type	Model	M_1 / M_2	Error	Iterations	CPU time (s)
Dirichlet-Neumann	FOM-FOM	– / –	3.43×10^{-4}	3.73	52
Dirichlet-Neumann	OpInf-FOM	20 / –	7.37×10^{-4}	6.08	64
Dirichlet-Neumann	FOM-OpInf	– / 17	7.31×10^{-4}	4.10	47
Dirichlet-Neumann	OpInf-OpInf	20 / 17	9.63×10^{-4}	4.12	37
Dirichlet-Neumann	OpInf-FOM	34 / –	1.29×10^{-4}	5.45	60
Dirichlet-Neumann	FOM-OpInf	– / 29	1.53×10^{-4}	4.19	51
Dirichlet-Neumann	OpInf-OpInf	34 / 29	2.03×10^{-4}	4.10	39



Above: representative OpInf-FOM coupling result

Good accuracy and ***moderate speedups*** over FOM-FOM coupling are possible. Larger speedups expected in ***multi-D***.

Work in Progress: Accelerating Non-Overlapping SAM via Transmission Condition Design

C. Rodriguez
(Columbia U)

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

$$
\begin{cases}
M_1\ddot{\boldsymbol{u}}_1^{(s+1)} + \boldsymbol{K}_1\boldsymbol{u}_1^{(s+1)} = \boldsymbol{F}_1^{(s+1)} & \text{in } \Omega_1 \\
\boldsymbol{u}_1^{(s+1)} = \boldsymbol{u}_D & \text{on } \partial_\Psi\Omega_1\backslash\Gamma \\
\alpha_{12}\boldsymbol{T}_1^{(s+1)} + \beta_{12}\boldsymbol{u}_1^{(s+1)} = \boldsymbol{\lambda}_1^{(s+1)} & \text{on } \Gamma
\end{cases}
$$

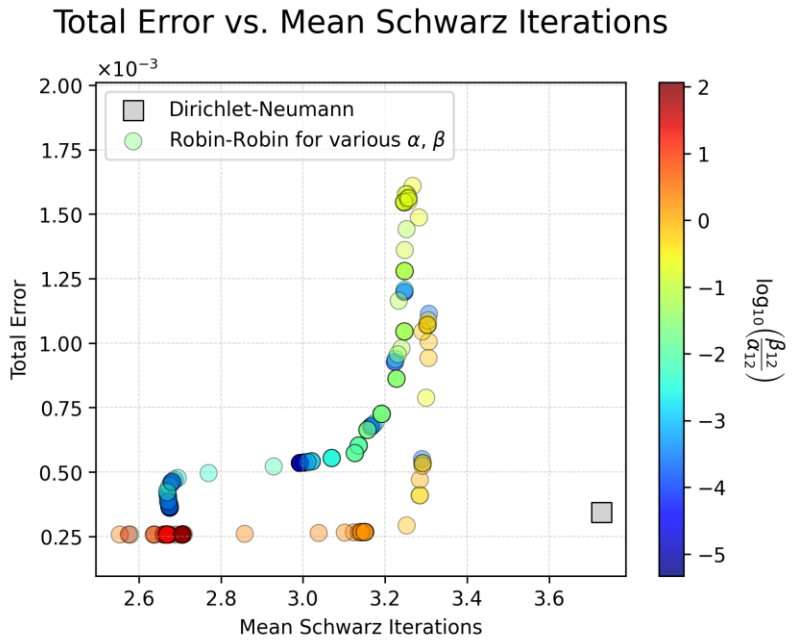
$$
\begin{cases}
M_2\ddot{\boldsymbol{u}}_2^{(s+1)} + \boldsymbol{K}_2\boldsymbol{u}_2^{(s+1)} = \boldsymbol{F}_2^{(s+1)} & \text{in } \Omega_2 \\
\boldsymbol{u}_2^{(s+1)} = \boldsymbol{u}_D & \text{on } \partial_\Psi\Omega_2\backslash\Gamma \\
\alpha_{21}\boldsymbol{T}_2^{(s+1)} + \beta_{21}\boldsymbol{u}_2^{(s+1)} = \boldsymbol{\lambda}_2^{(s+1)} & \text{on } \Gamma
\end{cases}
$$

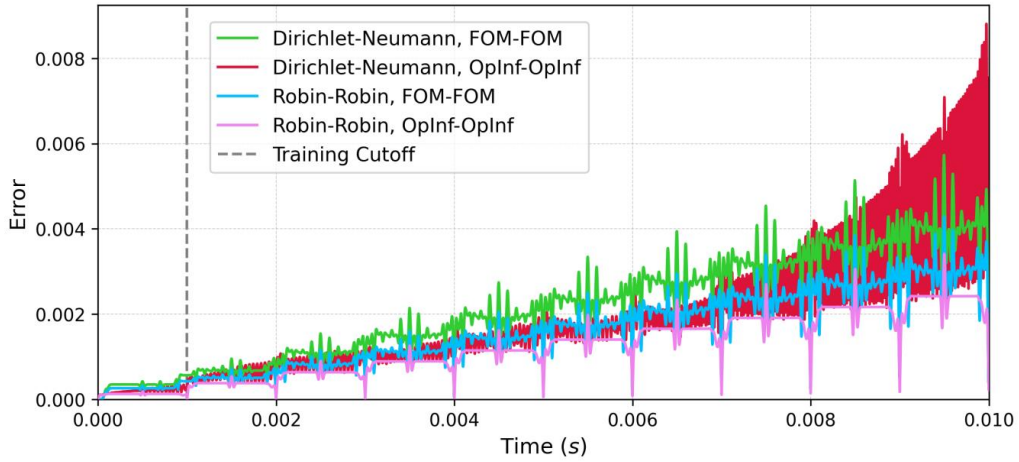
$$\boldsymbol{\lambda}_1^{(s+1)} = \alpha_{12}\boldsymbol{T}_2^{(s)} + \beta_{12}\boldsymbol{u}_2^{(s)}$$

$$\boldsymbol{\lambda}_2^{(s+1)} = \alpha_{21}\boldsymbol{T}_1^{(s+1)} + \beta_{21}\boldsymbol{u}_1^{(s+1)}$$

α_{ij}, β_{ij}: tuning parameters

Automatic tuning of α_{ij}, β_{ij} possible using ***Bayesian optimization*** via ***GPTune***.





Non-overlapping SAM with **optimized Robin-Robin TCs** can give to **faster convergence (29% less Schwarz iterations), lower errors (by up to 25%),** and **more stable/accurate time-predictive ROMs** than non-overlapping SAM with Dirichlet-Neumann TCs.

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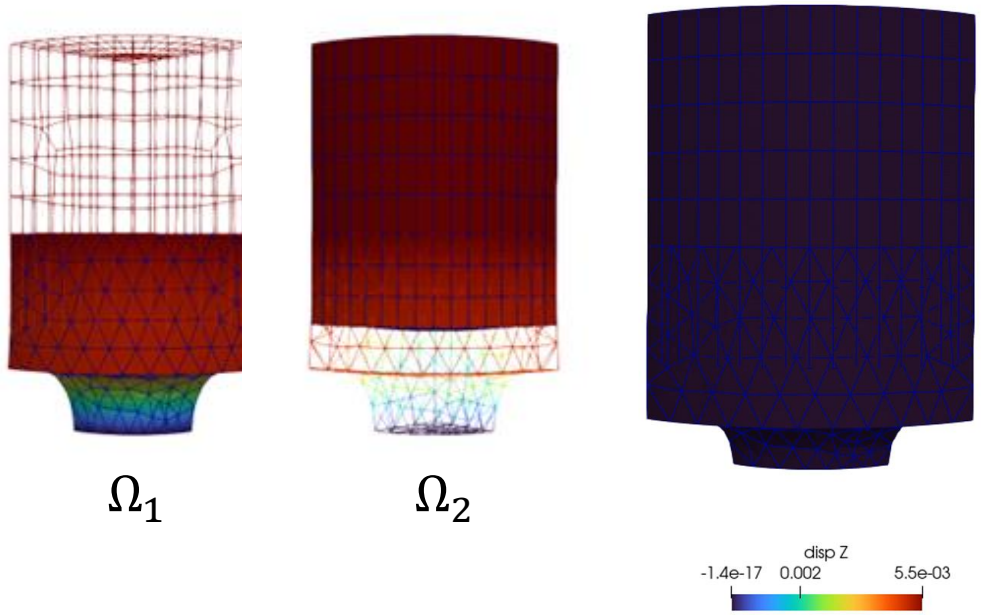

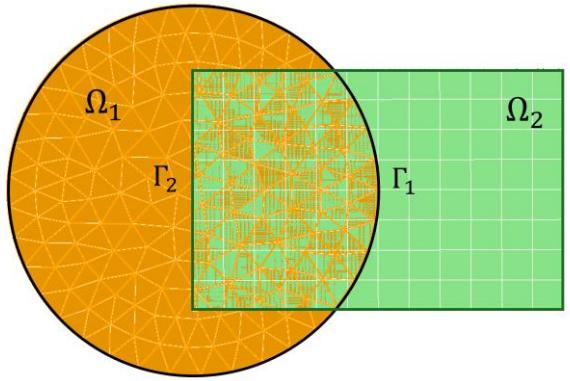

Summary

The **Schwarz alternating method** has been developed for concurrent multiscale 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.

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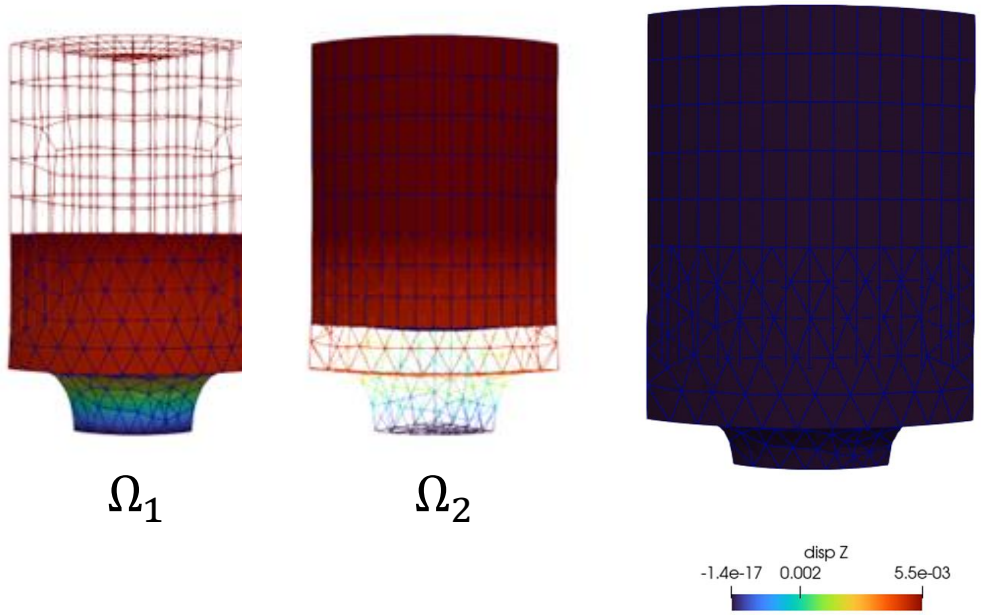
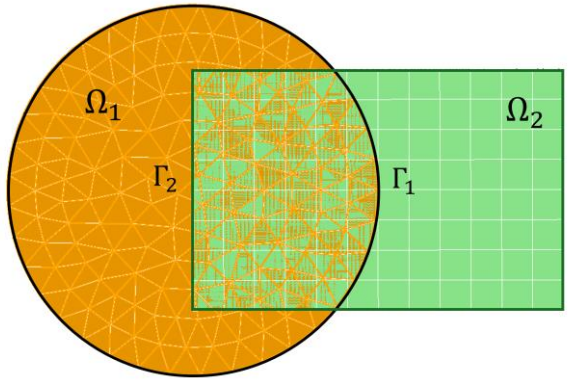




Ongoing & Future Work

Performance Improvements

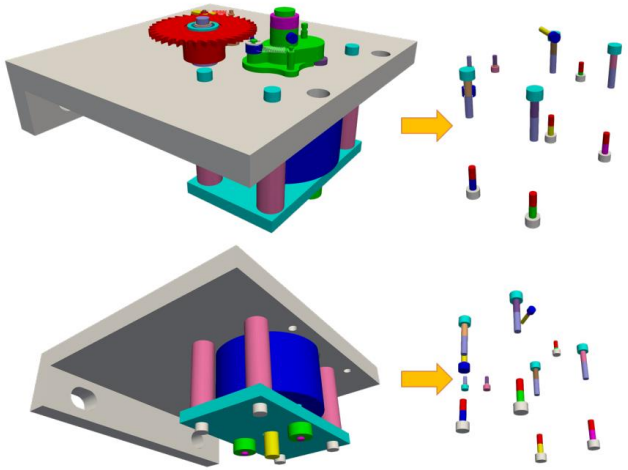
- Acceleration of Schwarz via optimized Robin-Robin TCs
- Acceleration of Schwarz via Aitken and Anderson Acceleration
- Asynchronous additive Schwarz on GPUs

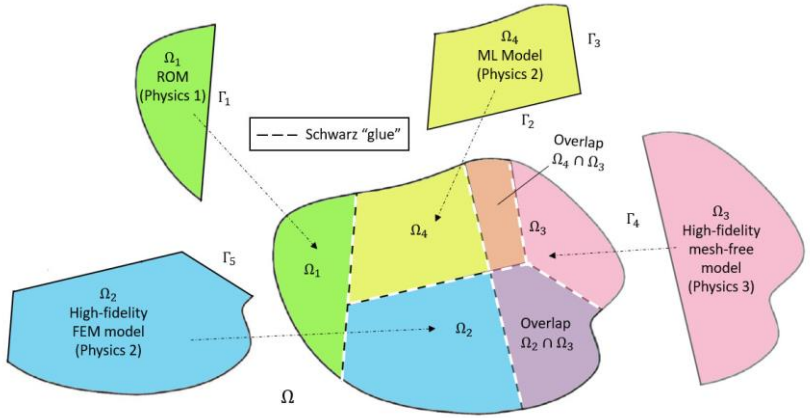
Automated & Adaptive Schwarz

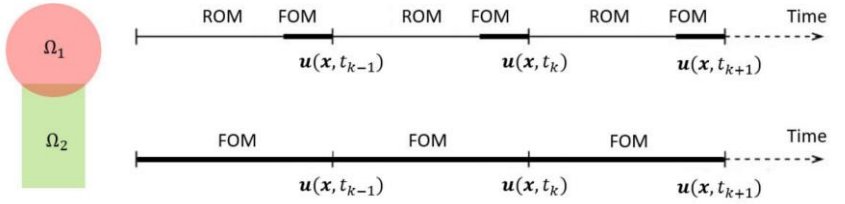
- Automated optimization of meshes/DD with multiple constraints
- Automated criteria to determine appropriate use of less refined or reduced-order models w/o sacrificing accuracy

Schwarz for ROM/Data-Driven Model Coupling

- Non-overlapping Schwarz + OpInf
- Schwarz + Deep NN-OpInf ROMs
- Schwarz + kernel-based ROMs (w/ Ionut Farcas, Virginia Tech)
- Fully non-intrusive adaptive ROM-FOM coupling (w/ K. Willcox & N. Aretz, UT Austin)
- On-the-fly switching between ROMs and FOMs
- Implementation in Sandia's production code, SIERRA/SM
- Schwarz + multiphysics coupling







Thank you! Questions?

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Schwarz Couplings Involving Non-Intrusive OpInf ROMs:

- **I. Tezaur,** E. Parish, A. Gruber, I. Moore, C. Wentland, A. Mota. "Hybrid coupling with operator inference and the overlapping Schwarz alternating method". ArXiv pre-print, 2025. https://arxiv.org/abs/2511.20687
  - **Implementation:** Norma.jl Julia code (https://github.com/sandialabs/Norma.jl)
- 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 that we are aware of

NORMA.JL

Contact: Irina Tezaur (ikalash@sandia.gov)


I. Tezaur


J. Barnett


I. Moore


E. Parish


C. Wentland

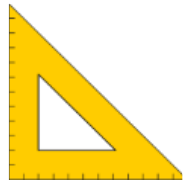

A. Gruber


C. Rodriguez


W. Snyder


G. Sambataro

Contact



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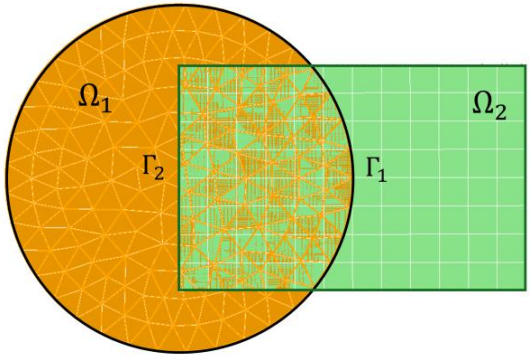

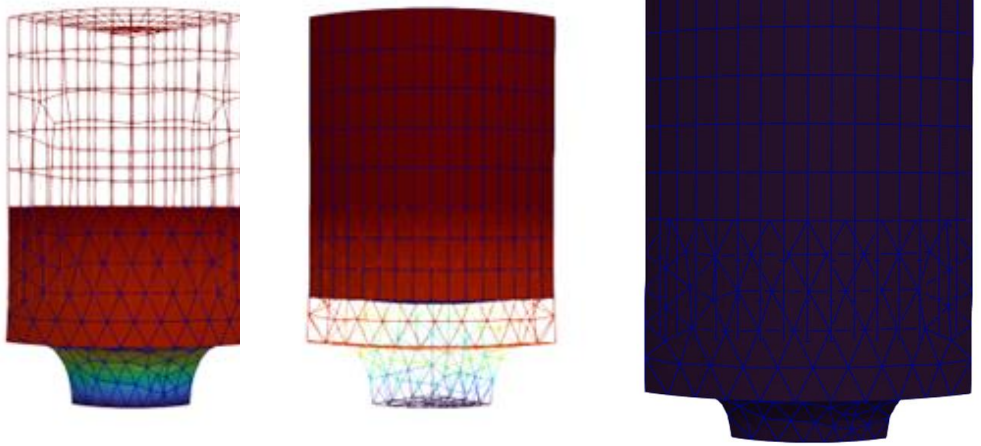

Ω_1 Ω_2

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LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT
ASC
U.S. DEPARTMENT OF ENERGY
Office of Science

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Start of Backup Slides

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
  - Ability to mix-and-match ***conventional*** and ***data-driven models*** 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

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

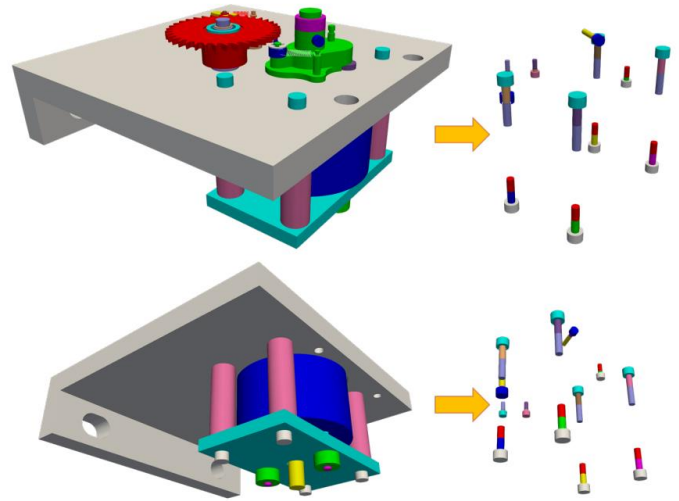

Figure above: schematic of difficult-to-mesh ratcheting mechanism with multiple threaded fasteners. From Parish *et al.*, 2024.

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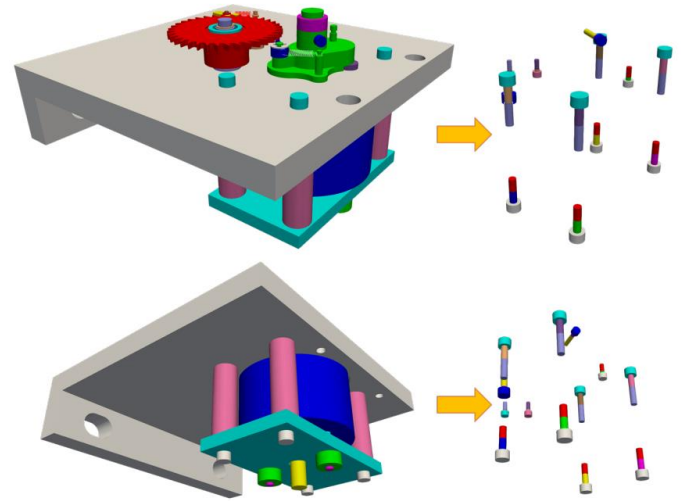
*Creating a **high-quality mesh** can take **weeks** or longer, making it "the **single biggest bottleneck** in [mod/sim] analyses" [Sandia Lab News, 2020]*



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

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]

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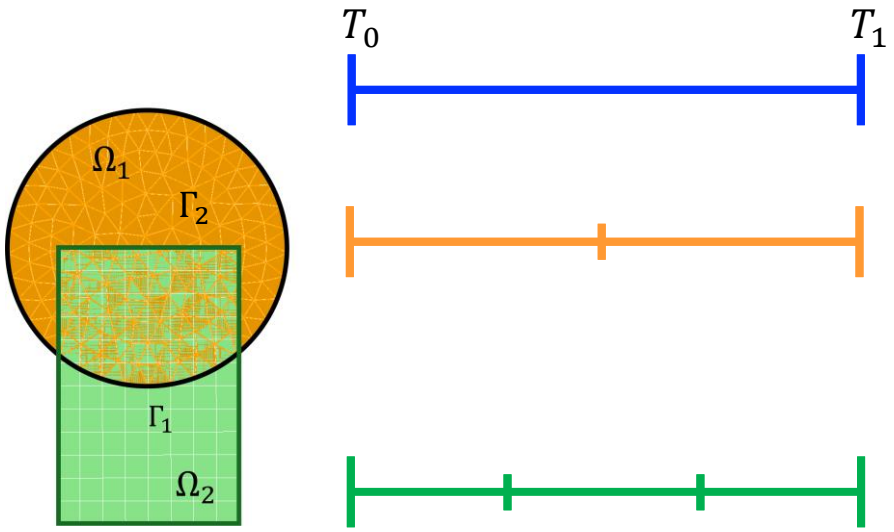
Why? **Less intrusive** to integrate into **production codes.**

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

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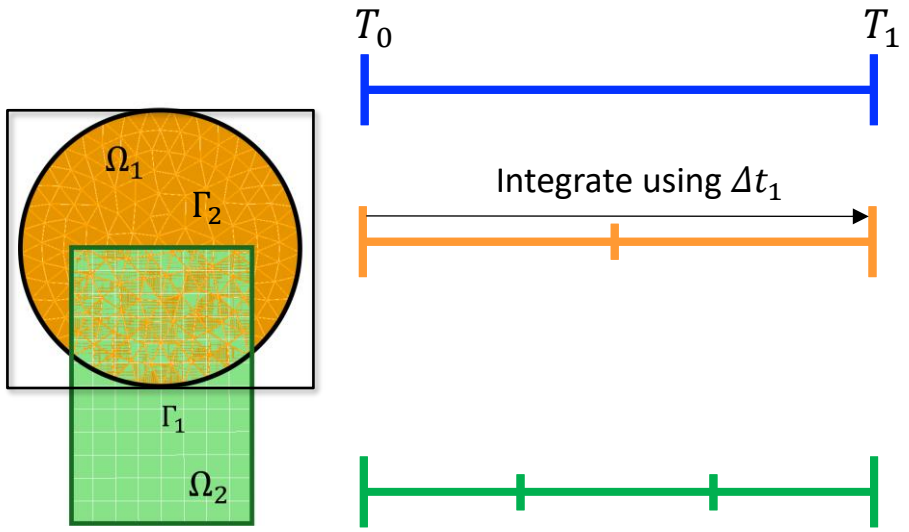

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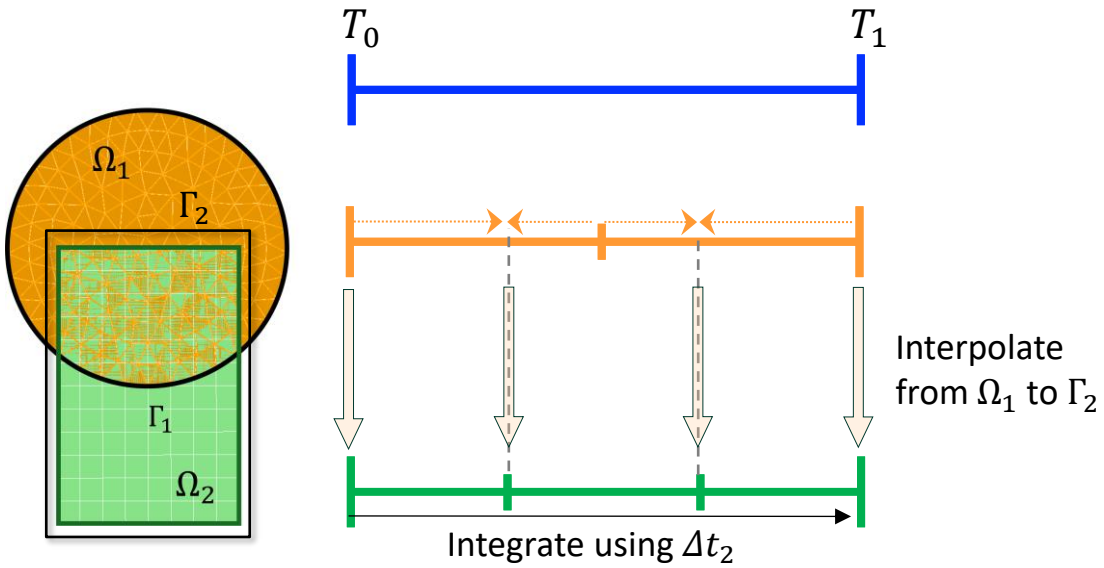

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.

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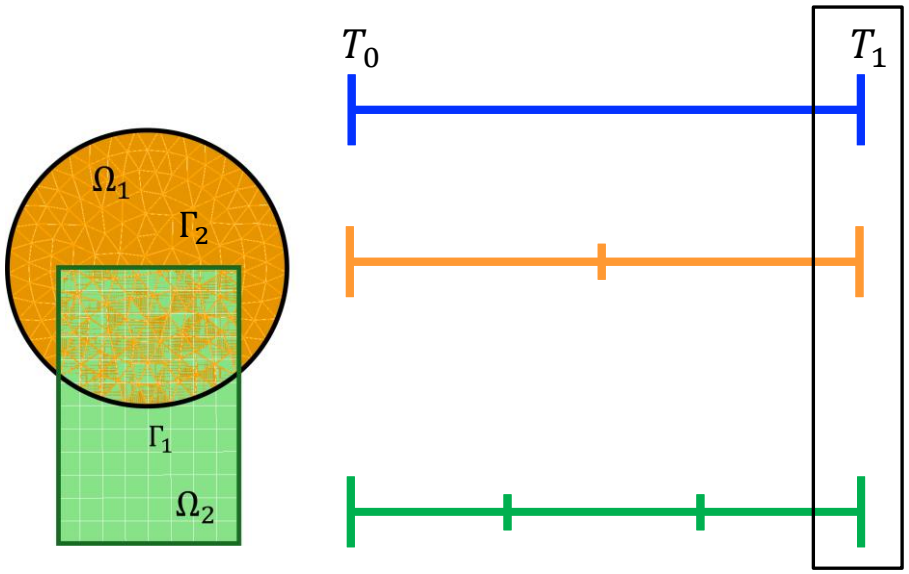

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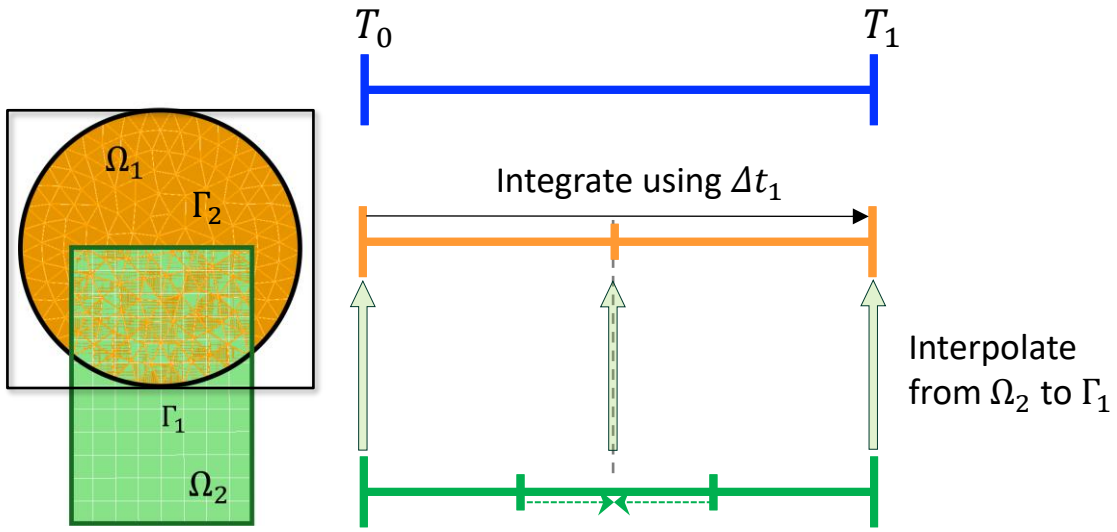

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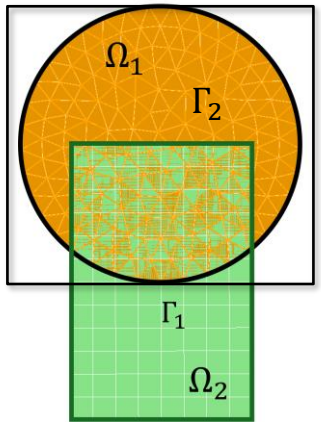

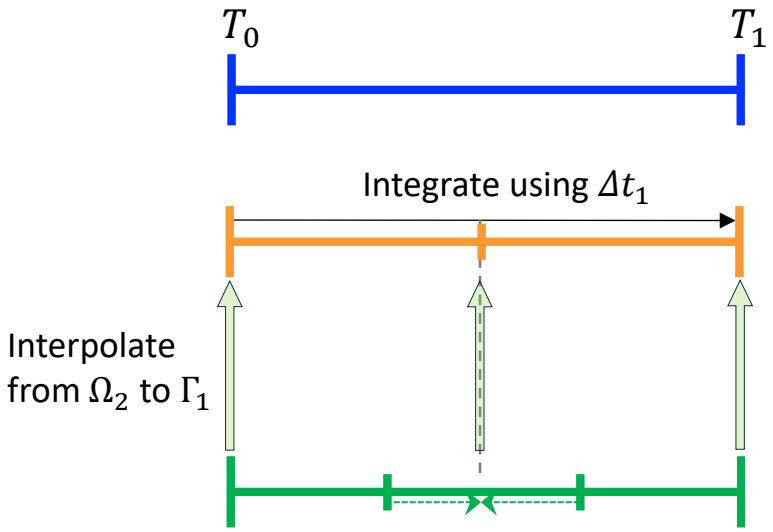

Controller time stepper

Time integrator in Ω_1

Time integrator in Ω_2

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].

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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.

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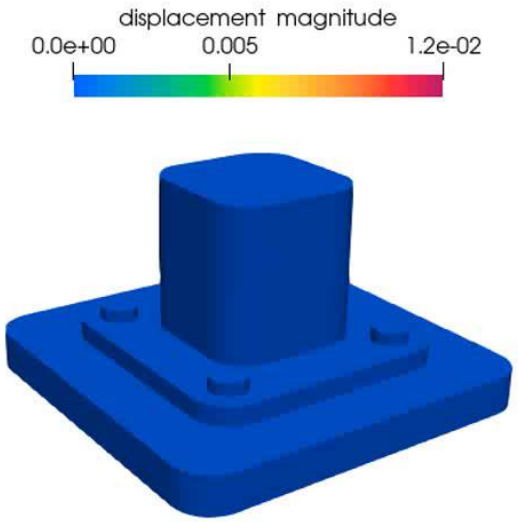
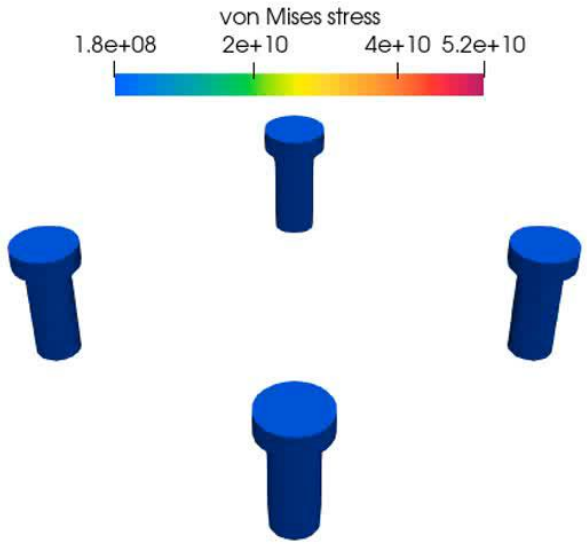
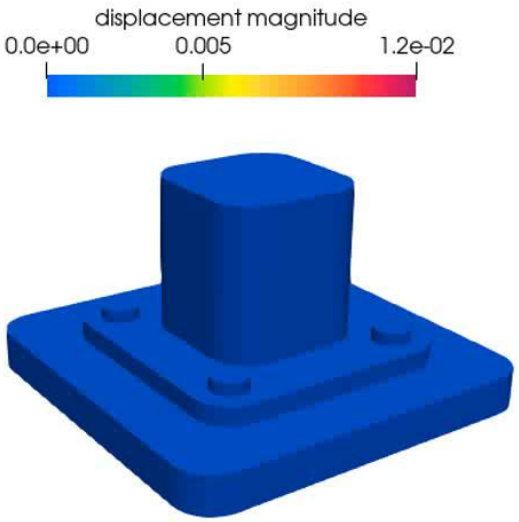
Bolted Joint (Overlapping SAM, Predictive): Animations

COpInf = Cubic OpInf

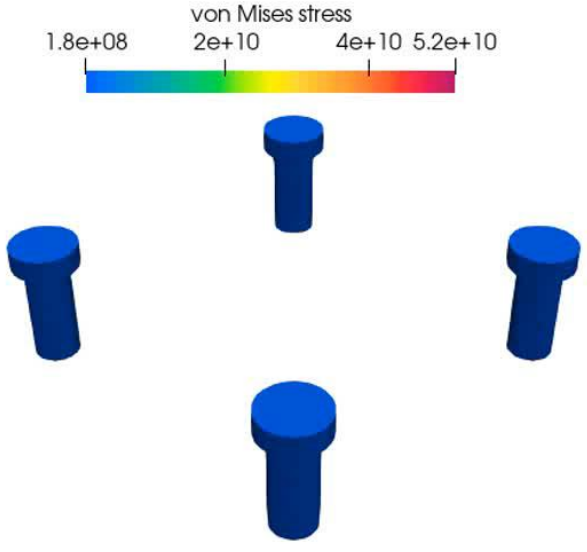


FOM-FOM
~53m





COpInf-COpInf
~8.5m



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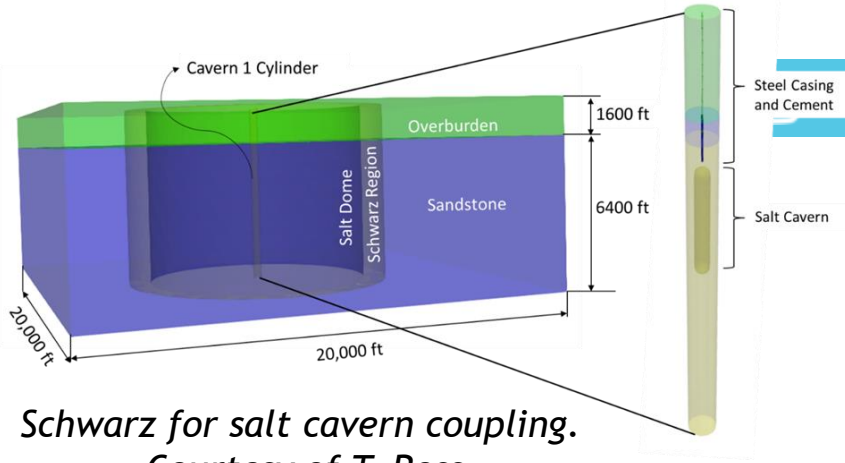
Current Research Directions

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
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- Automated optimization of meshes/DD with multiple constraints
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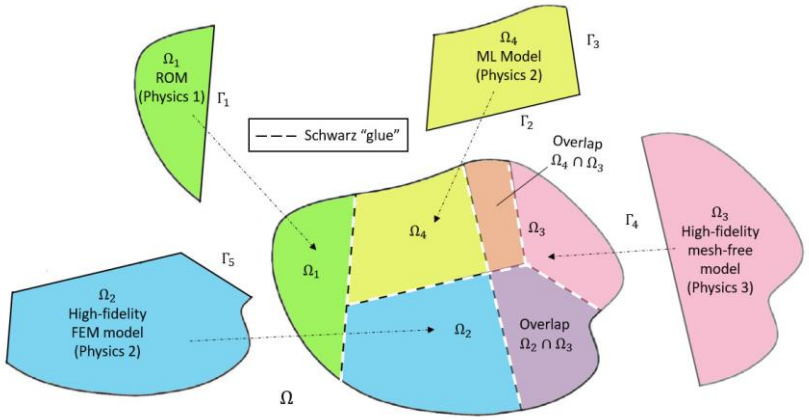

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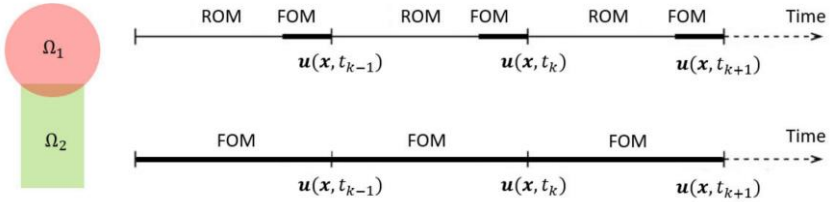
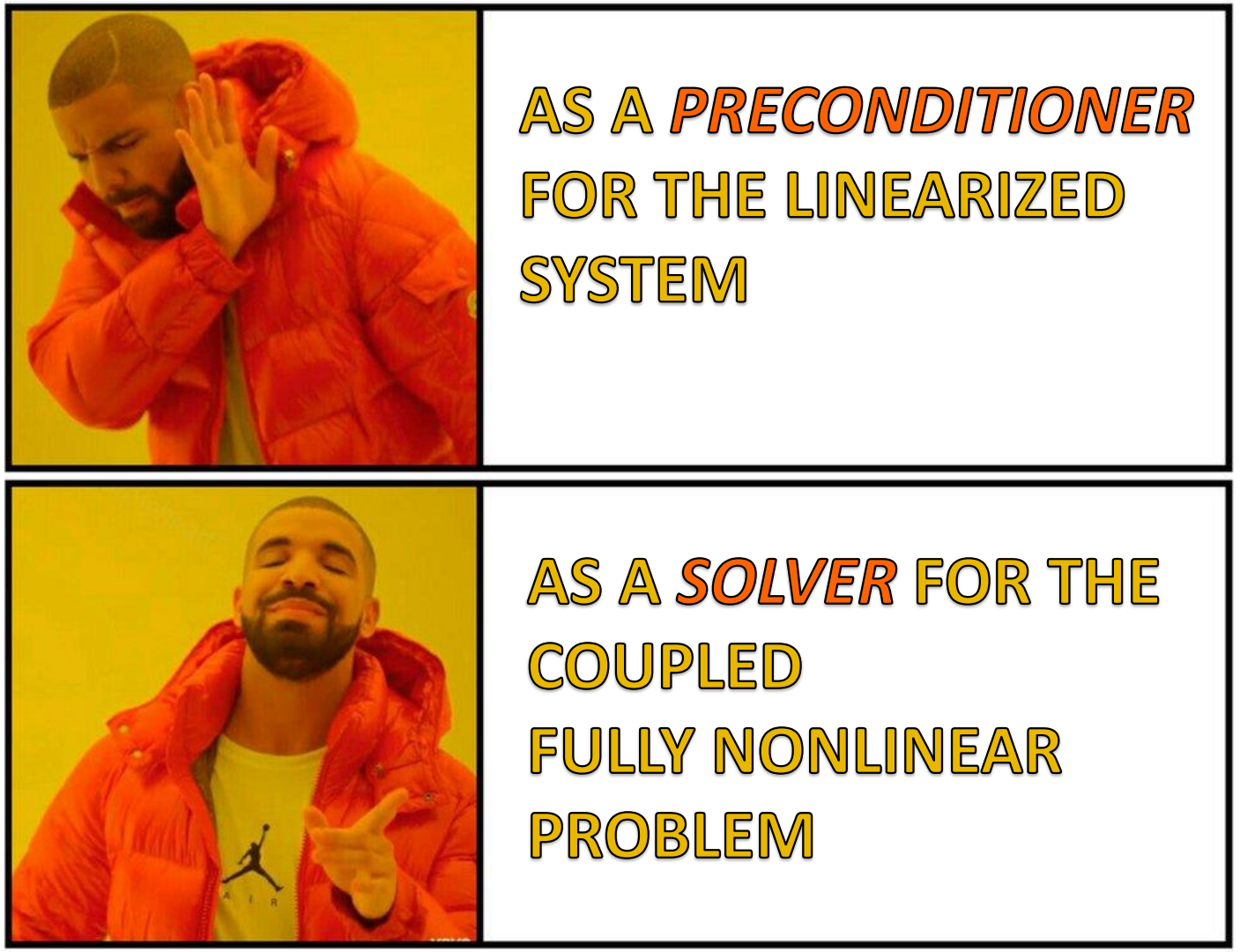
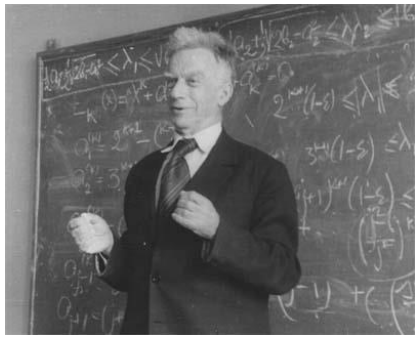


How We Use the Schwarz Alternating Method



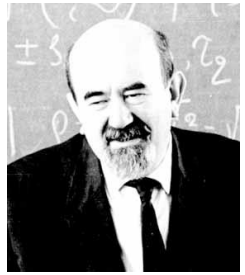
Theoretical Foundation

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

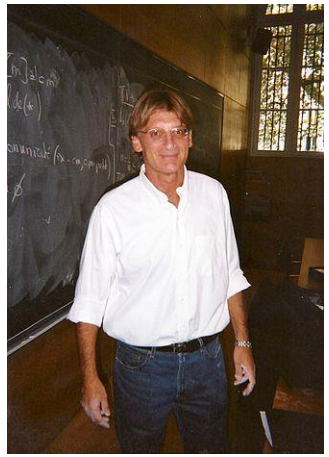


S.L. Sobolev (1908 – 1989)

- 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***.



S.G. Mikhlin
(1908 – 1990)

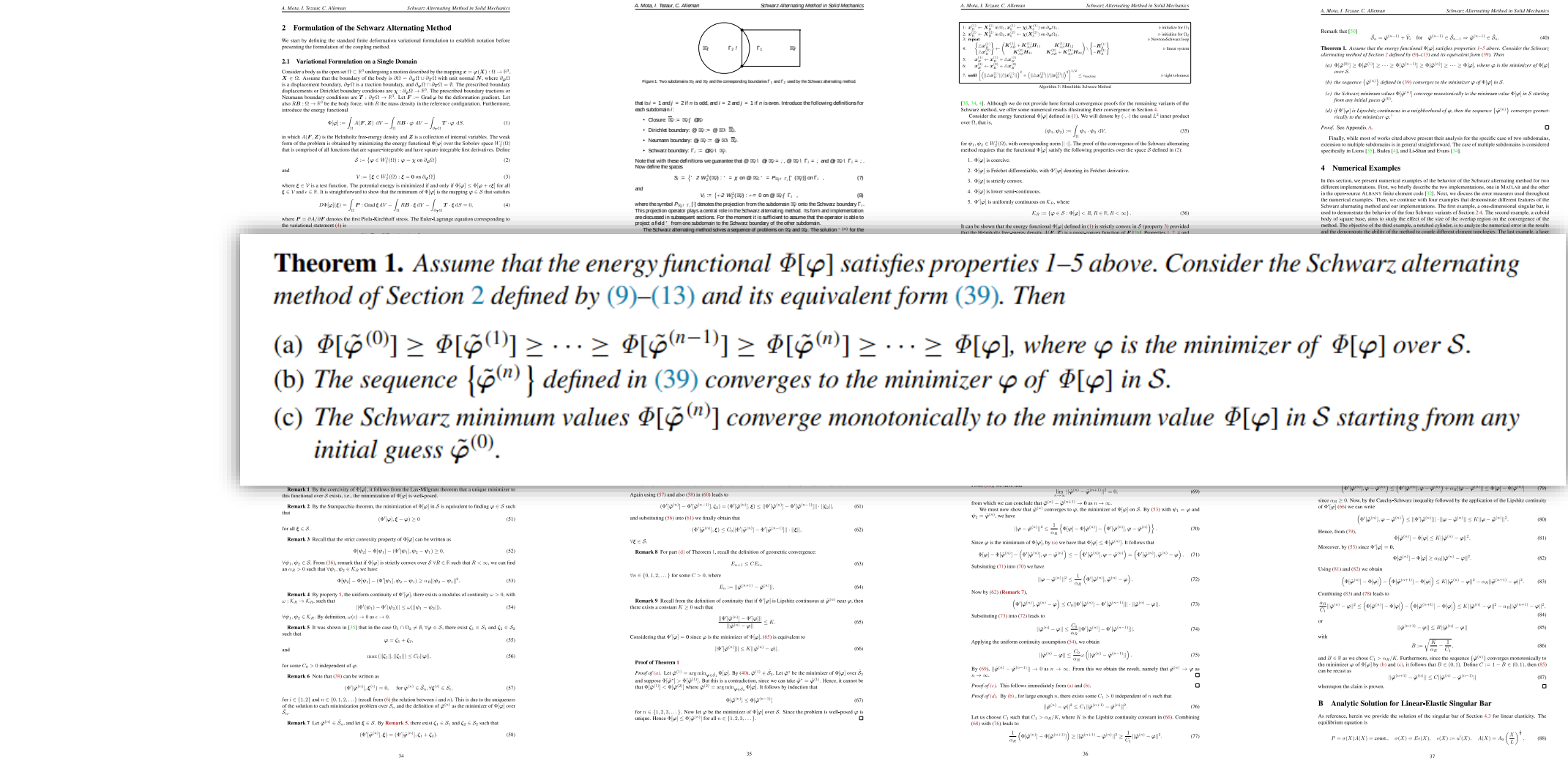


P.- L. Lions (1956-)

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

A. Mota, I. Tezaur, C. Alleman

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

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

* 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 $S[\boldsymbol{\varphi}] \coloneqq \int_I \int_\Omega L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) dV dt$ be ***strictly convex*** or ***strictly concave***, where $L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) \coloneqq T(\dot{\boldsymbol{\varphi}}) + V(\boldsymbol{\varphi})$ 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.

Additional Parallelism via Additive Schwarz

This talk

Multiplicative Overlapping Schwarz

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

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

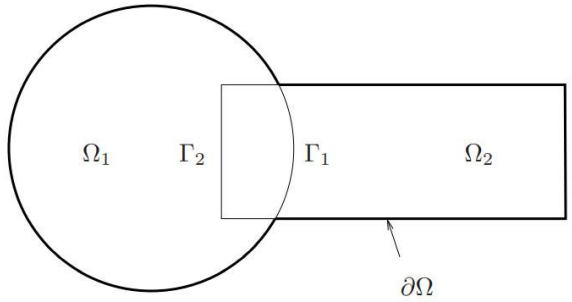
Additive Overlapping Schwarz

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

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

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

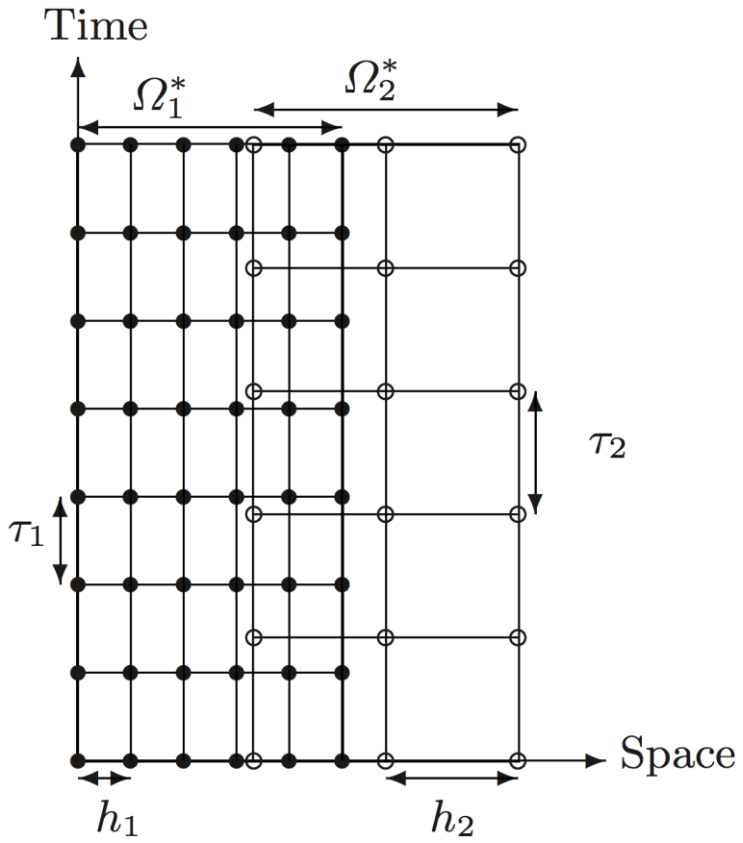
How to Apply Schwarz to Dynamics?

- 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).

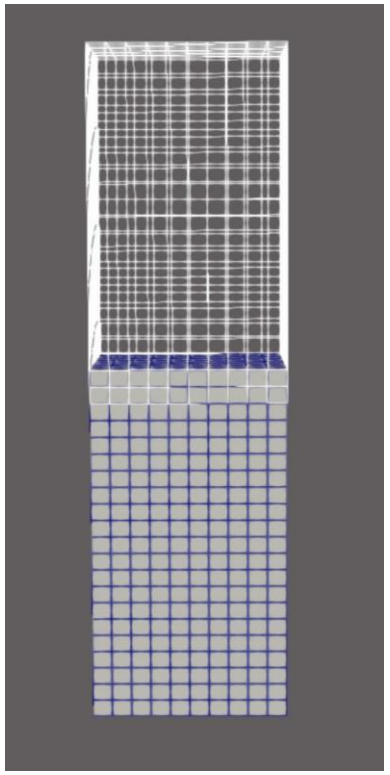
Con ☹: ***Unfeasible*** given the design of our current codes and size of simulations.

Ease of implementation is a very important requirement!

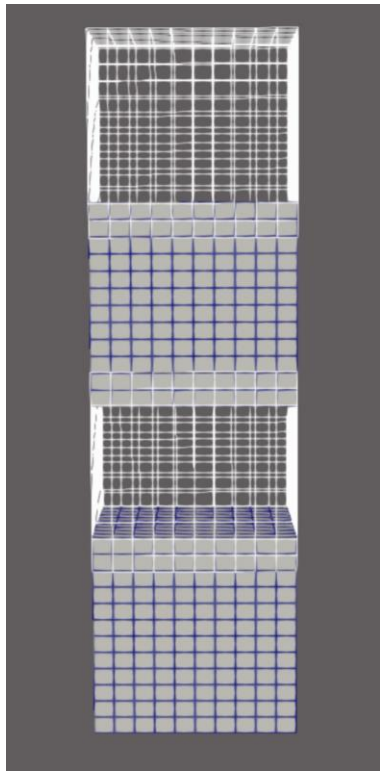


Overlapping non-matching meshes and time steps in dynamics.

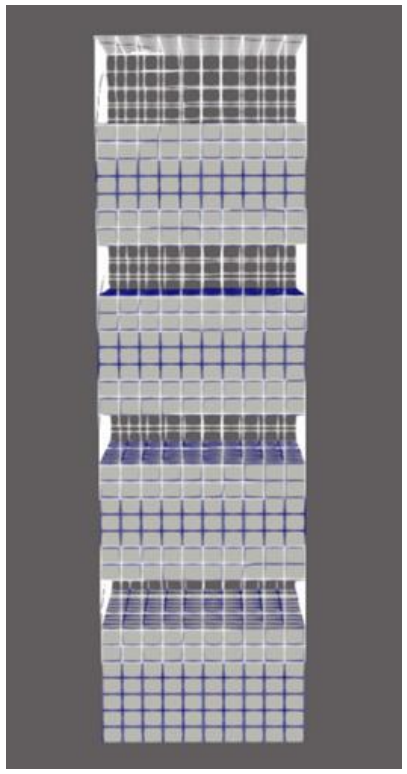
Scaling with Respect to the Number of Subdomains



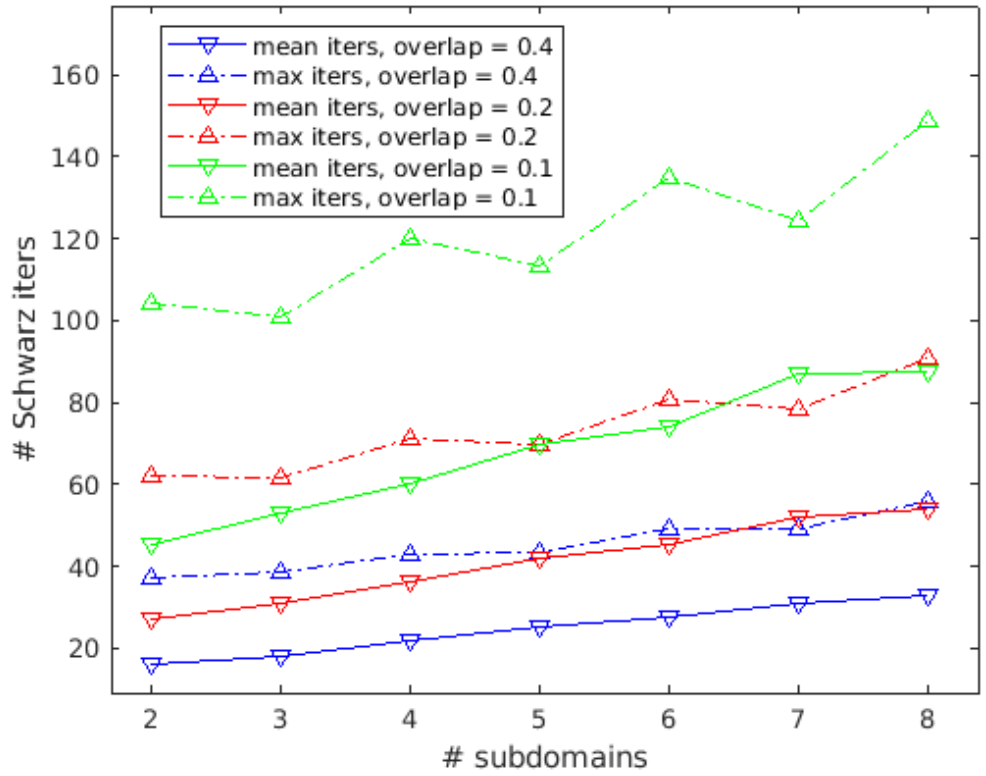
2 subdomains



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

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

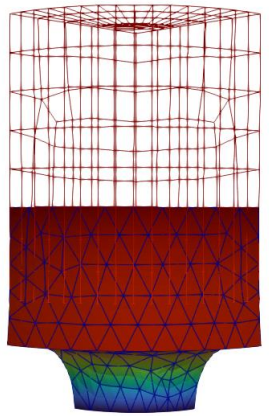
- What **hyper-reduction** method to use?
  - Application may require particular method (e.g., ECSW for solid mechanics problems)
- How to **sample Schwarz boundaries** in applying hyper-reduction?
  - Need to have enough sample mesh points at Schwarz boundaries to apply Schwarz

3D Linear Elastic Notched Cylinder Problem

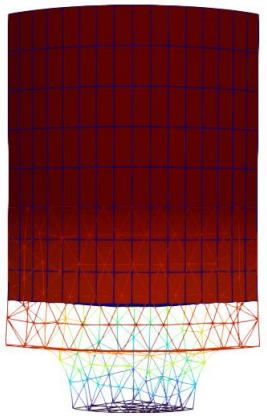
- Geometry is ***linear elastic notched cylinder*** pulled from top ***dynamically*** to time $T_{max} = 1.5$ at rate of $0.0064t$ with $\Delta t = 0.005$
- Demonstration of SAM's ability to ***couple disparate meshes***, ***element types*** and ***models***: TET10 + FOM (notched region) and HEX8 + Linear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



Ω_1 (TET10 + FOM)



Ω_2 (HEX8 + OpInf)

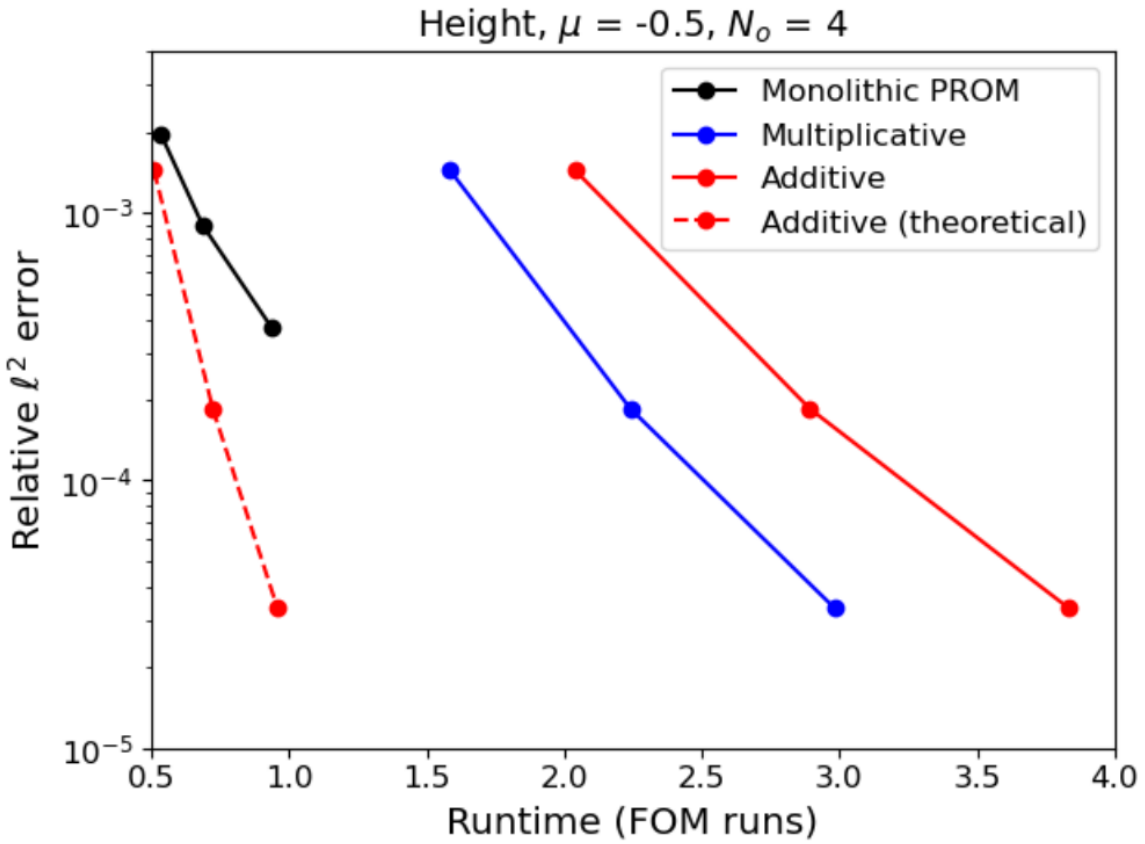
FOM-FOM

FOM-OpInf

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

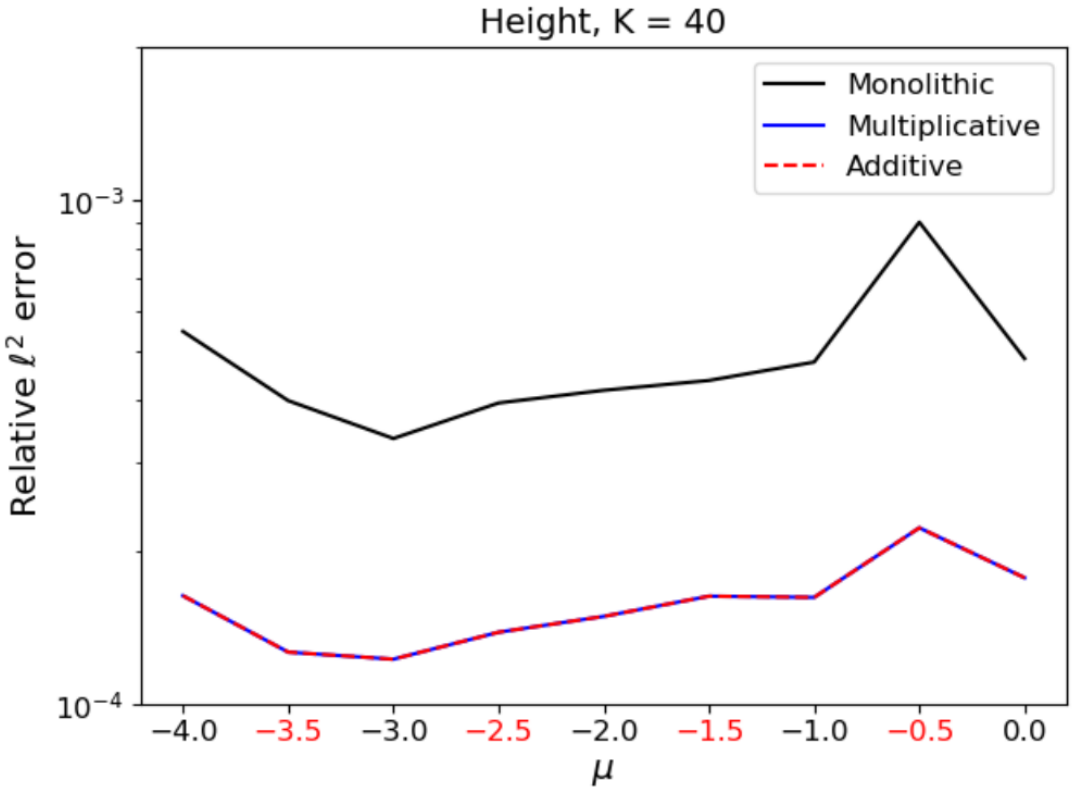
2D SWE: Takeaways

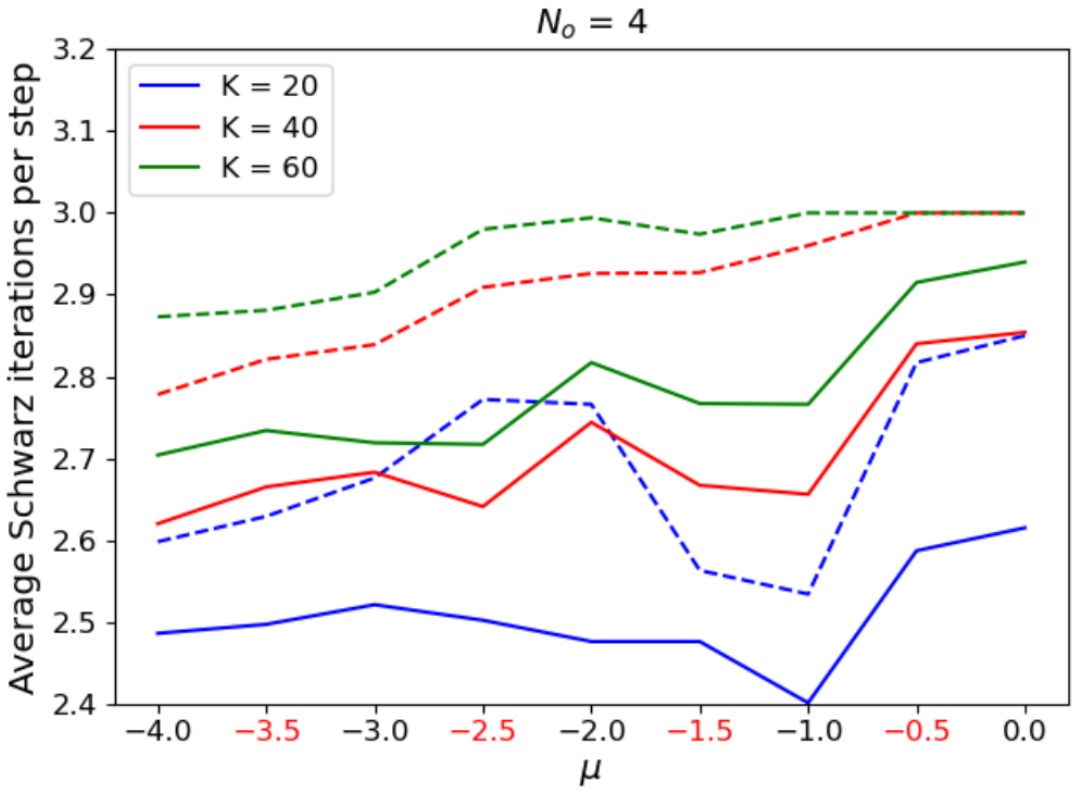
- Resolving overlap region discrepancy is critical
- Additive Schwarz exacerbates PROM dimension costs
- Available parallel cost savings
- Unexpected overlap error requires further investigation



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

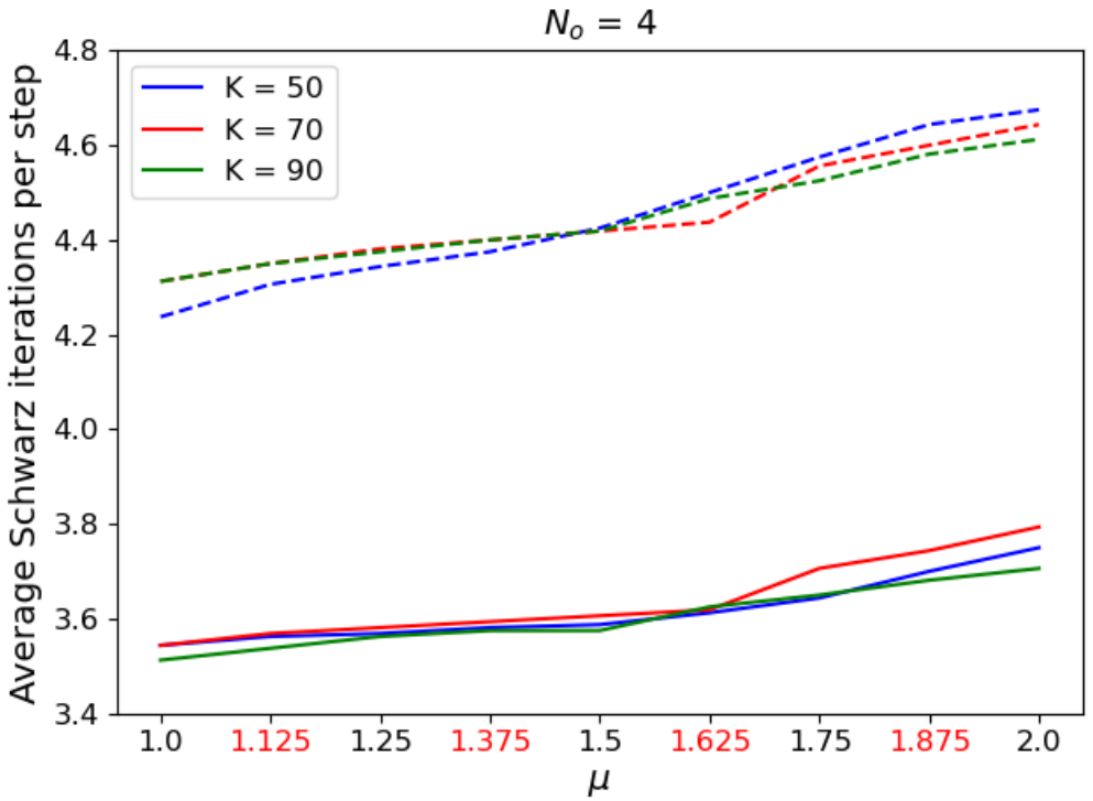


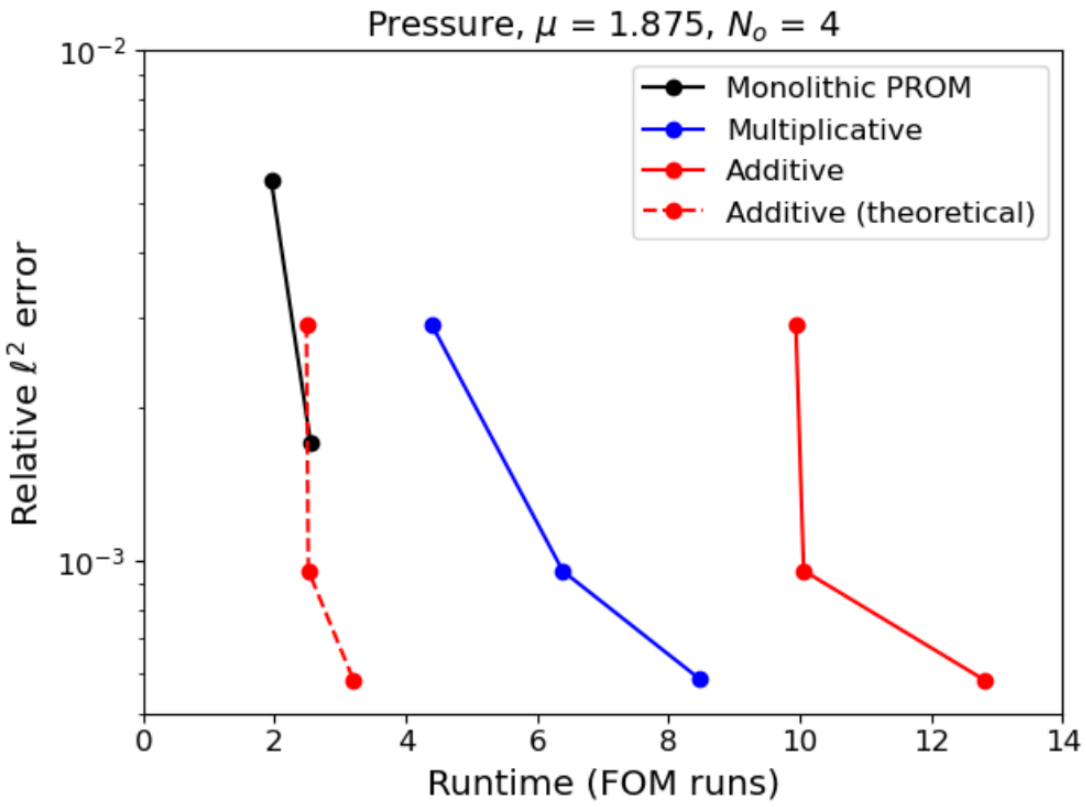


Solid: multiplicative, Dashed: additive

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

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.**

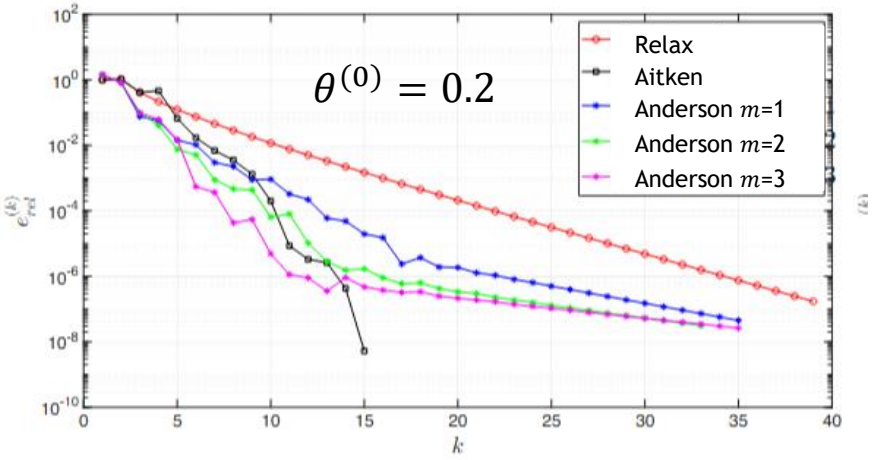
Non-overlapping Dirichlet-Neumann Schwarz

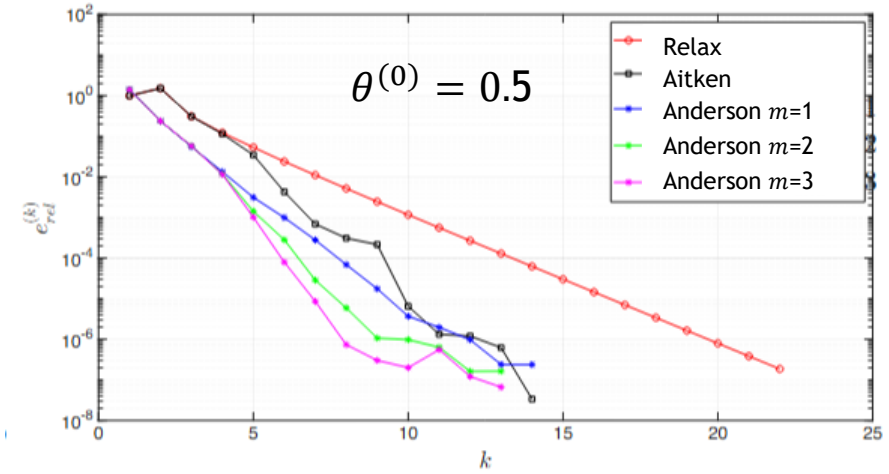
$$\begin{cases} \text{Div}\, \boldsymbol{P}_1^{(n+1)} + \rho \boldsymbol{B}(t_i) = \boldsymbol{0}\,, \text{ in } \Omega_1 \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\chi}, \qquad \text{on } \partial\Omega_1 \backslash \Gamma \\ \boldsymbol{\varphi}_1^{(n+1)} = \boldsymbol{\lambda}_{n+1} \qquad \text{on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

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

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

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

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***

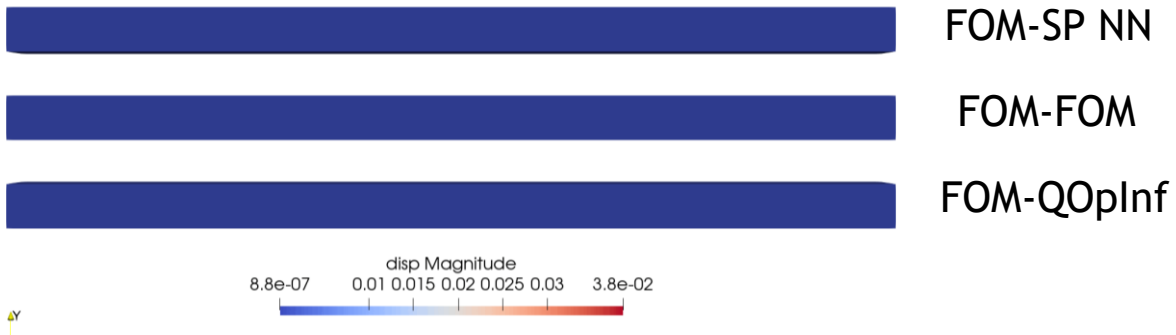
- Limits capacity of polynomial-based OpInf models

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

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

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

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

Structure is enforced via SPD parameterization of stiffness:

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

Enforced structure significantly improves performance

Future work: Hamiltonian parameterizations

Training paradigms

Offline (traditional) training

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

Dynamics-constrained training (rollout)

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

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