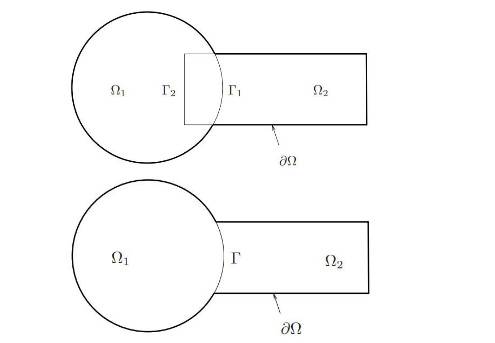
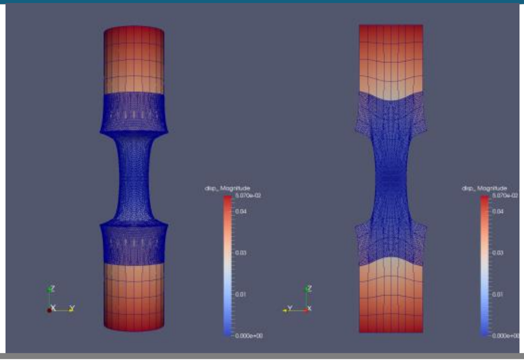
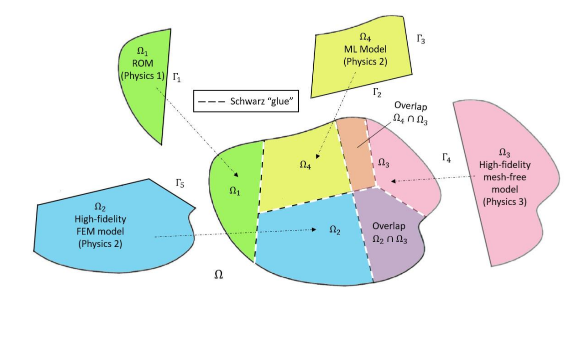
Domain decomposition-based coupling of intrusive and non-intrusive reduced order models via the Schwarz alternating method







Irina Tezaur[1], Chris Wentland[1], Francesco Rizzi[2], Joshua Barnett[3], Ian Moore[1], Eric Parish[1], Anthony Gruber[1], Alejandro Mota[1]

[1]Sandia National Laboratories, [2]NexGen Analytics, [3]Cadence Design Systems

Large-Scale Scientific Computations (LSSC) 2025
Sozopol, Bulgaria. June 16-20, 2025.

SAND2025-06760C

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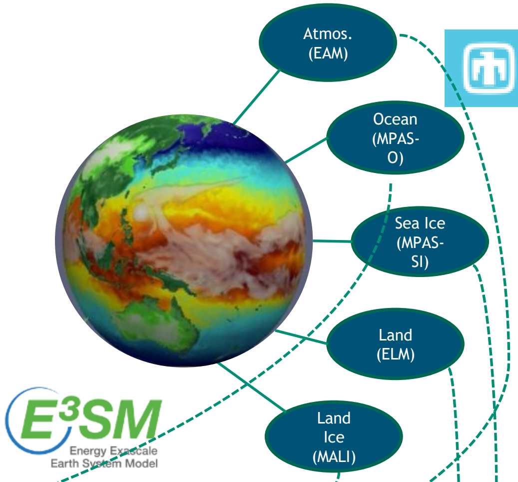
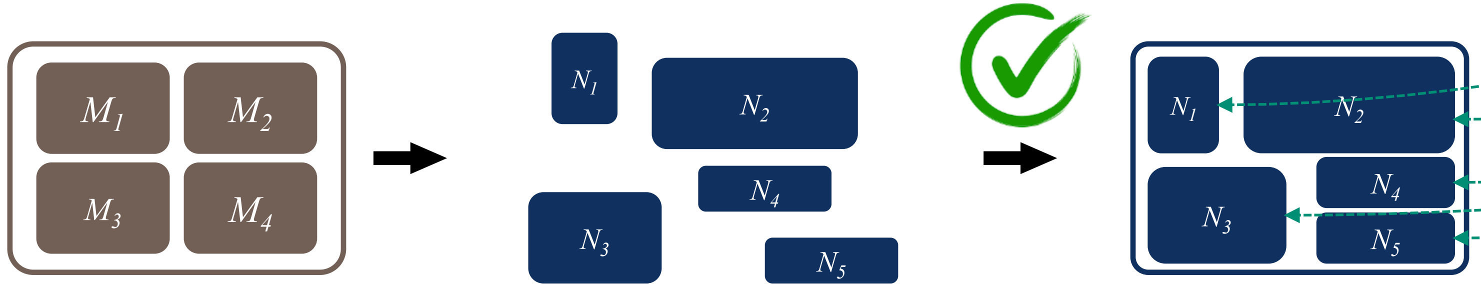
Motivation: Multi-scale & Multi-physics Coupling for Predictive Digital Twins



There exist established **rigorous mathematical theories** for **coupling** multi-scale and multi-physics components based on **traditional discretization methods** (“Full Order Models” or 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
- Iterative (Schwarz, optimization)

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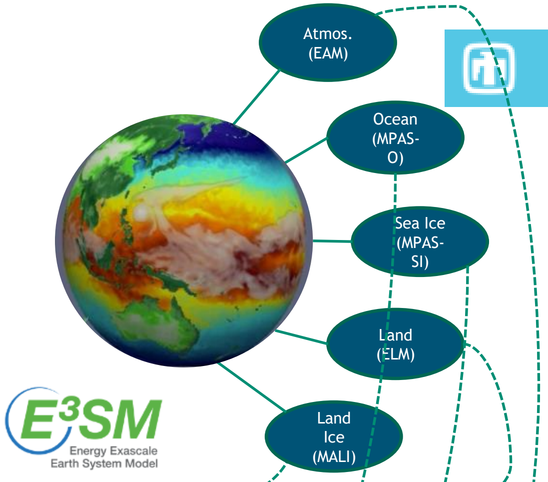

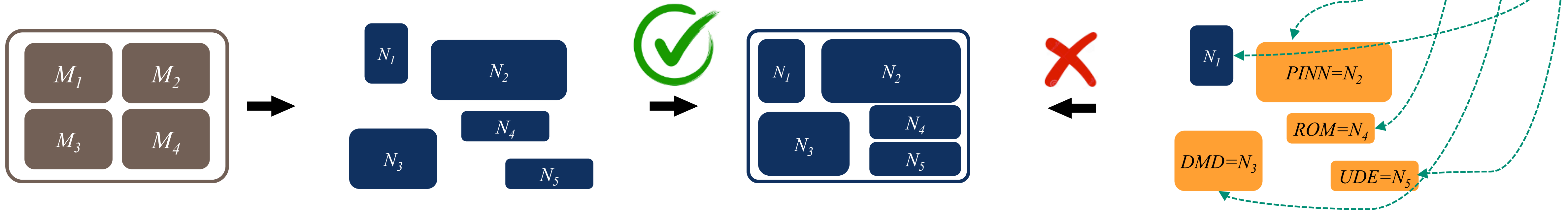

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Traditional + Data-Driven Methods

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

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

Projects on Coupling for Predictive Hybrid Models

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

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]

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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

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Three classes of coupling methods:

- Alternating **Schwarz**-based coupling [FHNM, M2dt, AHEAD]
- **Optimization**-based coupling [FHNM, M2dt]
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Three classes of coupling methods:

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- **Optimization**-based coupling → 2nd talk in MS (I. Prusak)
- Coupling via **generalized mortar methods** [FHNM, M2dt] → 3rd talk in MS (P. Kuberry)

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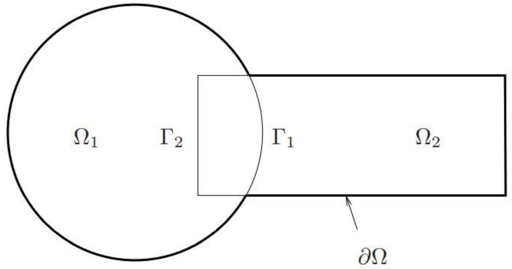

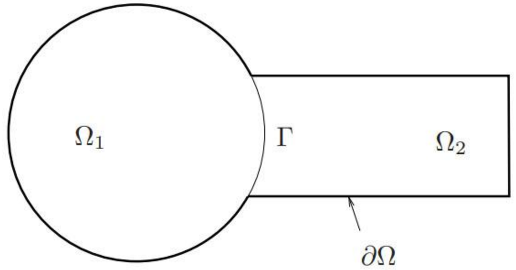

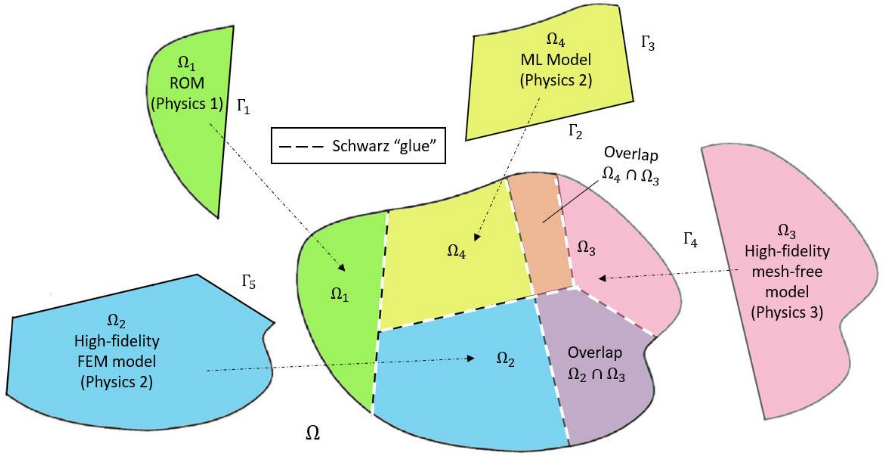

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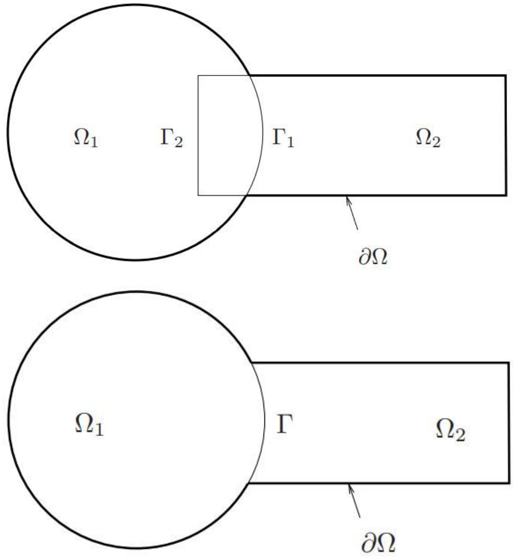
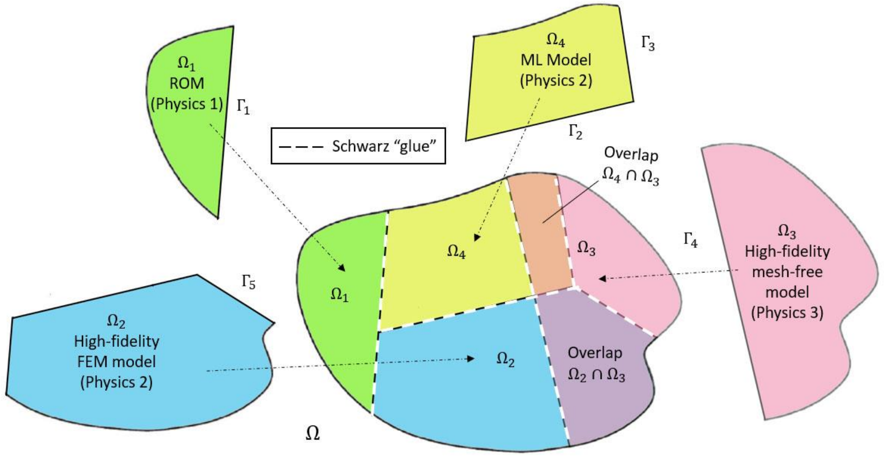
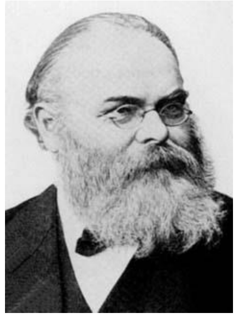




Schwarz Alternating Method for Domain Decomposition

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

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



H. Schwarz (1843–1921)

Basic Schwarz Algorithm

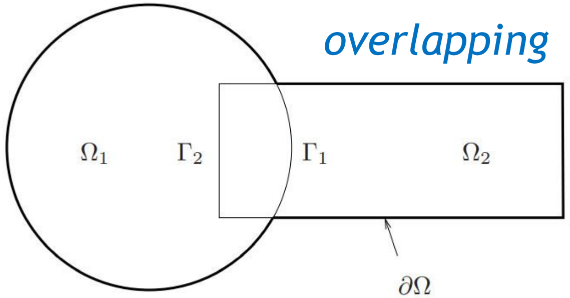
Initialize:

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

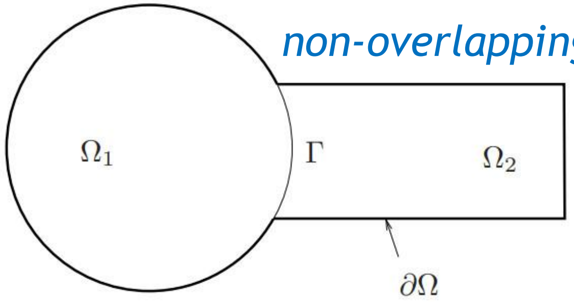
Iterate until convergence:

- 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



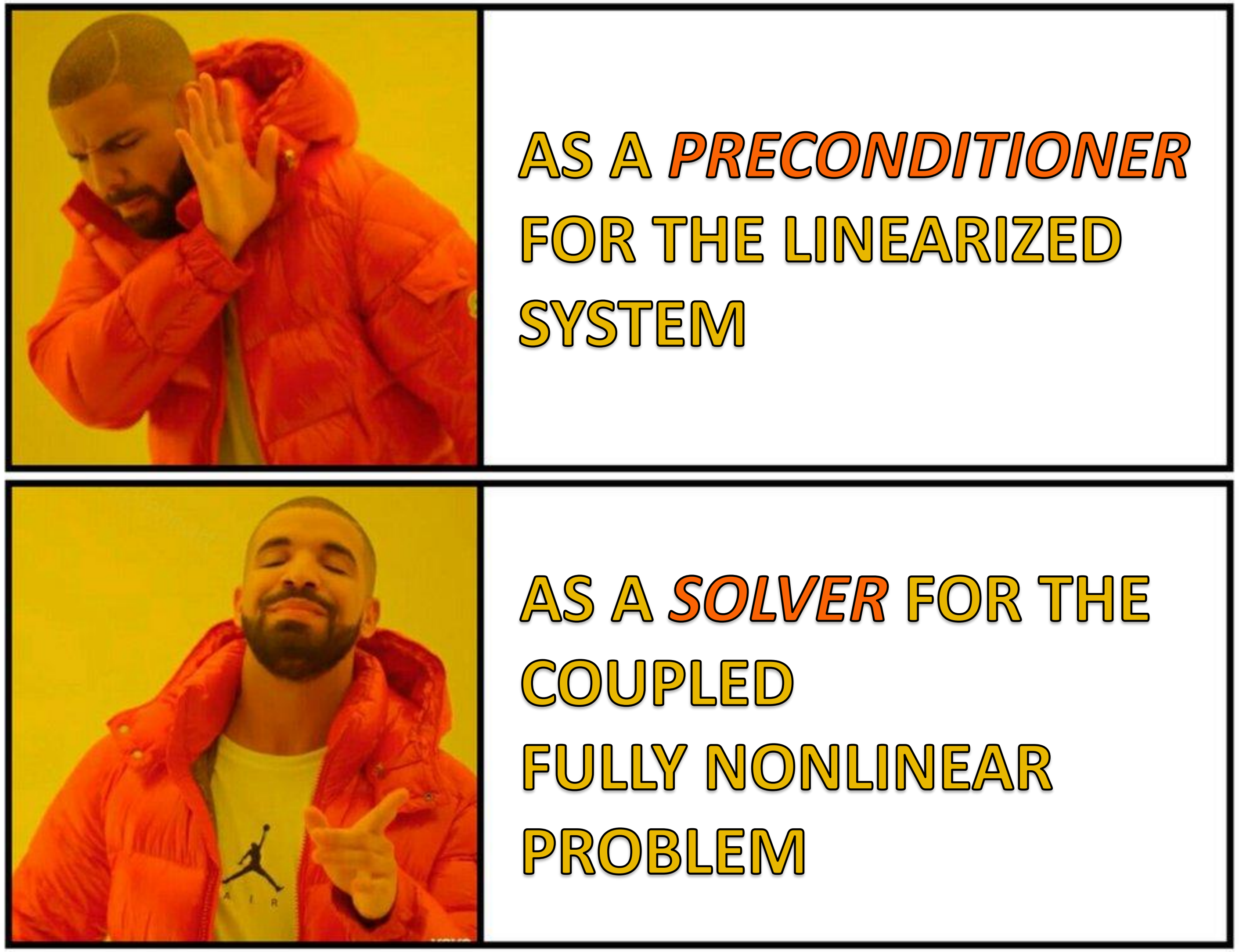
non-overlapping



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

Novelty: we are 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



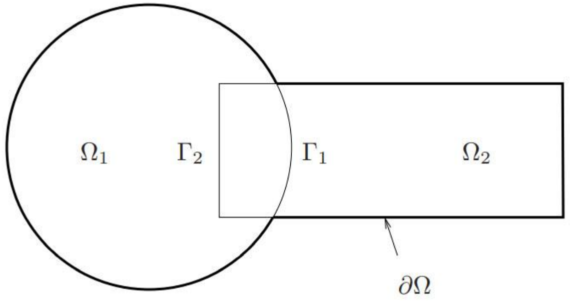
Transmission Boundary Conditions

Overlapping Domain Decomposition

$$\begin{cases} N\left(\boldsymbol{u}_1^{(n+1)}\right) = f \text{ , in } \Omega_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{g}, \text{ on } \partial\Omega_1 \backslash \Gamma_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{u}_2^{(n)} \quad \text{ on } \Gamma_1 \end{cases}$$

$$\begin{cases} N\left(\boldsymbol{u}_2^{(n+1)}\right) = f \text{ , in } \Omega_2 \\ \boldsymbol{u}_2^{(n+1)} = \boldsymbol{g}, \text{ on } \partial\Omega_2 \backslash \Gamma_2 \\ \boldsymbol{u}_2^{(n+1)} = \boldsymbol{u}_1^{(n+1)} \quad \text{ on } \Gamma_2 \end{cases}$$

Part 2 of Talk



Model PDE: $\begin{cases} N(\boldsymbol{u}) = \boldsymbol{f}, & \text{in } \Omega \\ \boldsymbol{u} = \boldsymbol{g}, & \text{on } \partial\Omega \end{cases}$

- Dirichlet-Dirichlet transmission BCs [Schwarz 1870; Lions 1988; Mota *et al.* 2017; Mota *et al.* 2022] guarantee convergence

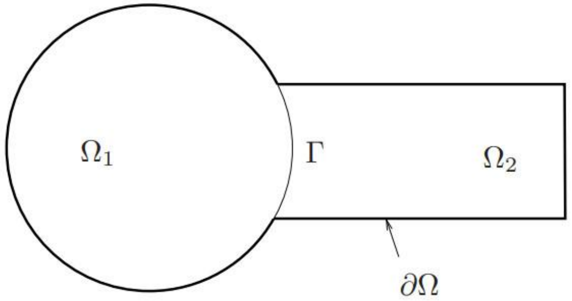
Non-overlapping Domain Decomposition

$$\begin{cases} N\left(\boldsymbol{u}_1^{(n+1)}\right) = f, & \text{in } \Omega_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{g}, & \text{on } \partial\Omega_1 \backslash \Gamma \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{\lambda}_{n+1}, & \text{on } \Gamma \end{cases}$$

$$\begin{cases} N\left(\boldsymbol{u}_2^{(n+1)}\right) = f \text{ ,} & \text{in } \Omega_2 \\ \boldsymbol{u}_2^{(n+1)} = \boldsymbol{g}, & \text{on } \partial\Omega_2 \backslash \Gamma \\ \nabla \boldsymbol{u}_2^{(n+1)} \cdot \boldsymbol{n} = \nabla \boldsymbol{u}_1^{(n+1)} \cdot \boldsymbol{n}, & \text{on } \Gamma \end{cases}$$

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

Part 1 of Talk



- Relevant for multi-material and multi-physics coupling*
- Usually requires alternating Dirichlet-Neumann [Zanolli *et al.* 1987] or Robin-Robin transmission BCs [Lions 1990] for convergence
- $\theta \in [0,1]$: relaxation parameter (can help convergence)

** For certain discretizations, **non-overlapping DD + Dirichlet-Dirichlet transmission BCs** is convergent [Wentland et al., 2025]!*

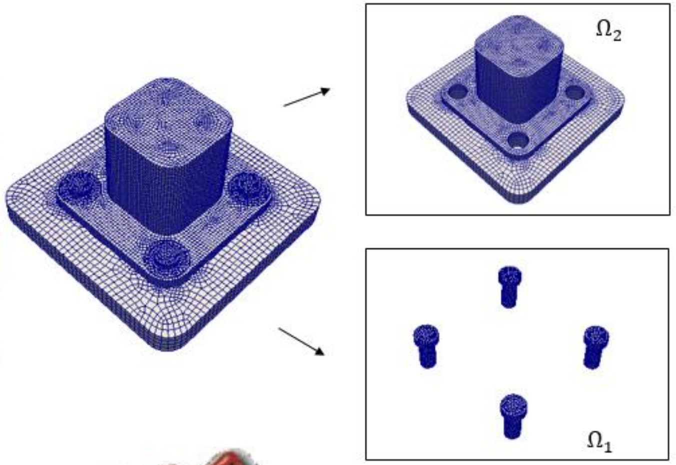
Schwarz for Multi-scale FOM-FOM Coupling in Solid Mechanics[1]

Model Solid Mechanics PDEs:

Quasistatic: $\mathrm{Div}\, \boldsymbol{P} + \rho_0 \boldsymbol{B} = \boldsymbol{0} \quad \text{in} \quad \Omega$

Dynamic: $\mathrm{Div}\, \boldsymbol{P} + \rho_0 \boldsymbol{B} = \rho_0 \ddot{\boldsymbol{\varphi}} \quad \text{in} \quad \Omega \times I$

- Coupling is ***concurrent*** (two-way).
- ***Ease of implementation*** into existing massively-parallel HPC codes.
- ***Scalable***, ***fast***, ***robust*** (we target ***real*** engineering problems, e.g., analyses involving failure of bolted components!).
- Coupling does not introduce ***nonphysical artifacts***.
- ***Theoretical*** convergence properties/guarantees[1].
- ***"Plug-and-play" framework***:
  - ➢ Ability to couple regions with ***different non-conformal meshes***, ***different element types*** and ***different levels of refinement*** to simplify task of ***meshing complex geometries***.
  - ➢ Ability to use ***different solvers/time-integrators*** in different regions.



Albany-LCM

SIERRA

[1] Mota *et al*. 2017; Mota *et al*. 2022. [2] https://github.com/sandialabs/LCM.

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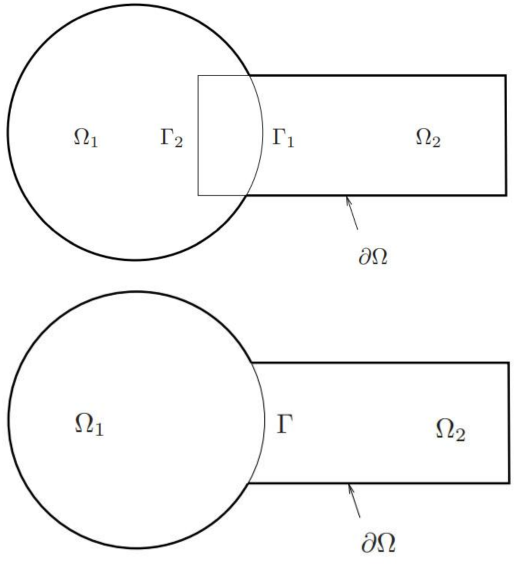
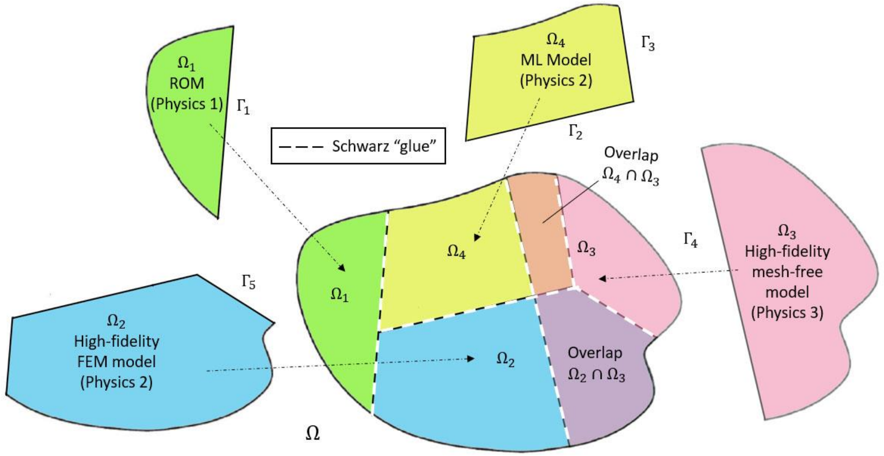


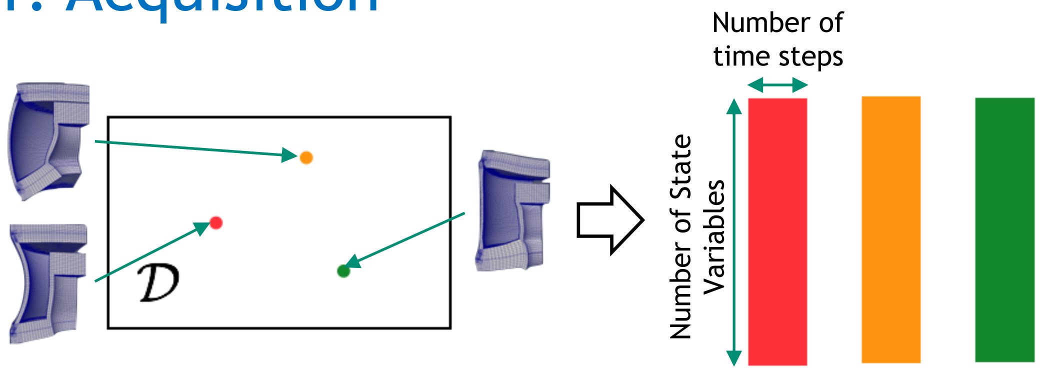


Intrusive Projection-Based Model Order Reduction via POD/LSPG*

Full Order Model (FOM): $\frac{d\boldsymbol{u}}{dt} = \boldsymbol{f}(\boldsymbol{u}; t, \boldsymbol{\mu})$

* Least-Squares Petrov-Galerkin

1. Acquisition

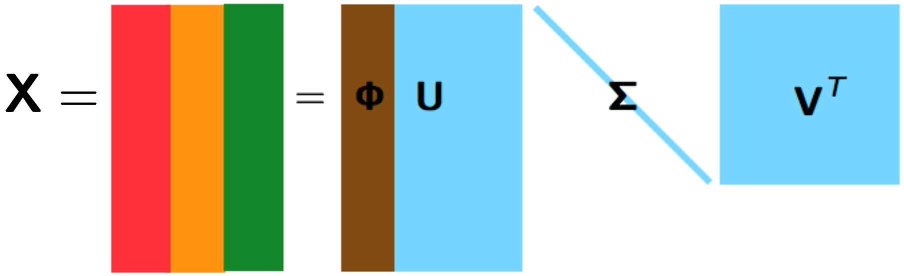


Solve ODE at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



ROM = projection-based Reduced Order Model

3. Projection-Based Reduction

Choose ODE temporal discretization

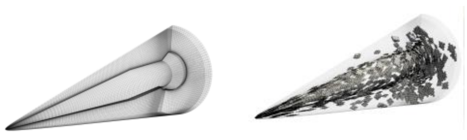
$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{f}(\boldsymbol{u}; t, \boldsymbol{\mu})$$
$$\Downarrow$$
$$\boldsymbol{r}^n(\boldsymbol{u}^n; \boldsymbol{\mu}) = \boldsymbol{0}, \qquad n = 1, \dots, T$$

Reduce the number of unknowns

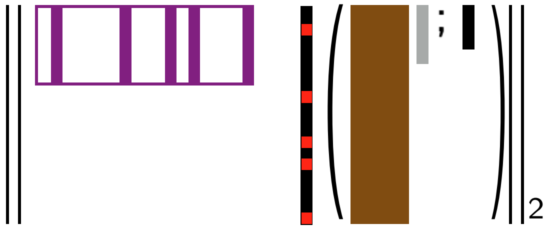
$$\boldsymbol{u}(t) \approx \tilde{\boldsymbol{u}}(t) = \boldsymbol{\Phi}\hat{\boldsymbol{u}}(t)$$

Minimize residual

$$\underset{\hat{v}}{\text{minimize}} \left\| \boldsymbol{S}\, \boldsymbol{r}^n(\boldsymbol{\Phi}\hat{\boldsymbol{v}}; \boldsymbol{\mu}) \right\|_2$$



Hyper-reduction/sample mesh

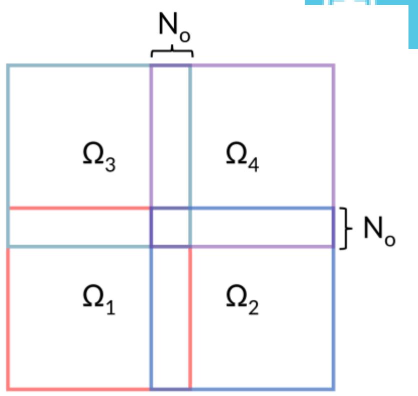


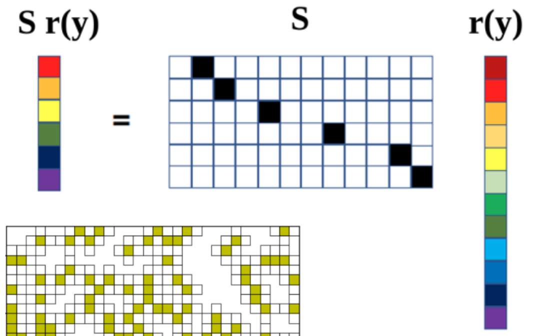
HROM = Hyper-reduced ROM

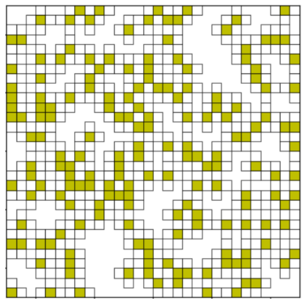
SAM-based Coupling for Intrusive Projection-based ROMs

Offline stage:

- Perform **FOM simulation** on a spatial domain Ω and **collect** s **snapshots**
- Create **domain decomposition** of Ω into d **overlapping** or **non-overlapping subdomains** Ω_i with N_o overlap cells (could be 0).
- Compute **POD basis** $\boldsymbol{\Phi}_i$ on each Ω_i by restricting the snapshots to Ω_i.
- For nonlinear problems, compute **sample mesh** S_i on each Ω_i.
  - ➢ **Collocation:** minimize the residual at a small subset of DOFs $N_s \ll N$.
  - ➢ ***Key question:*** *how to sample Schwarz boundaries given fixed budget of sample mesh points?*



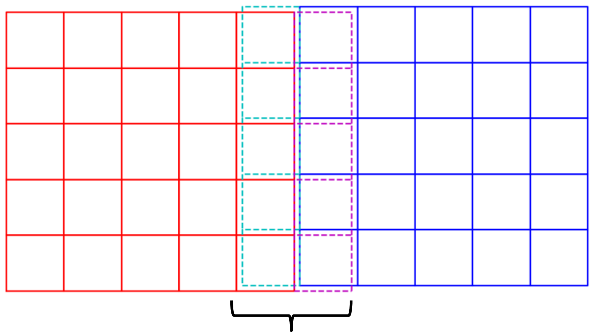




Yellow: residual cells, white: stencil cells

Online stage:

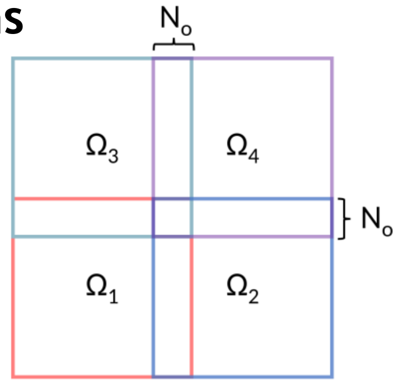
- **Construct POD/LSPG ROM** in each subdomain Ω_i, **transmit Schwarz BCs**, apply **Schwarz iteration procedure.**
  - ➢ ***Key question:*** *how to impose Schwarz BCs in ROMs?*
    - ❖ *Often* ***discretization specific***.
    - ❖ ***This talk:*** *cell-centered finite volume (CCFV) discretizations. BCs imposed* ***approximately*** *by* ***fictitious ghost cells***.

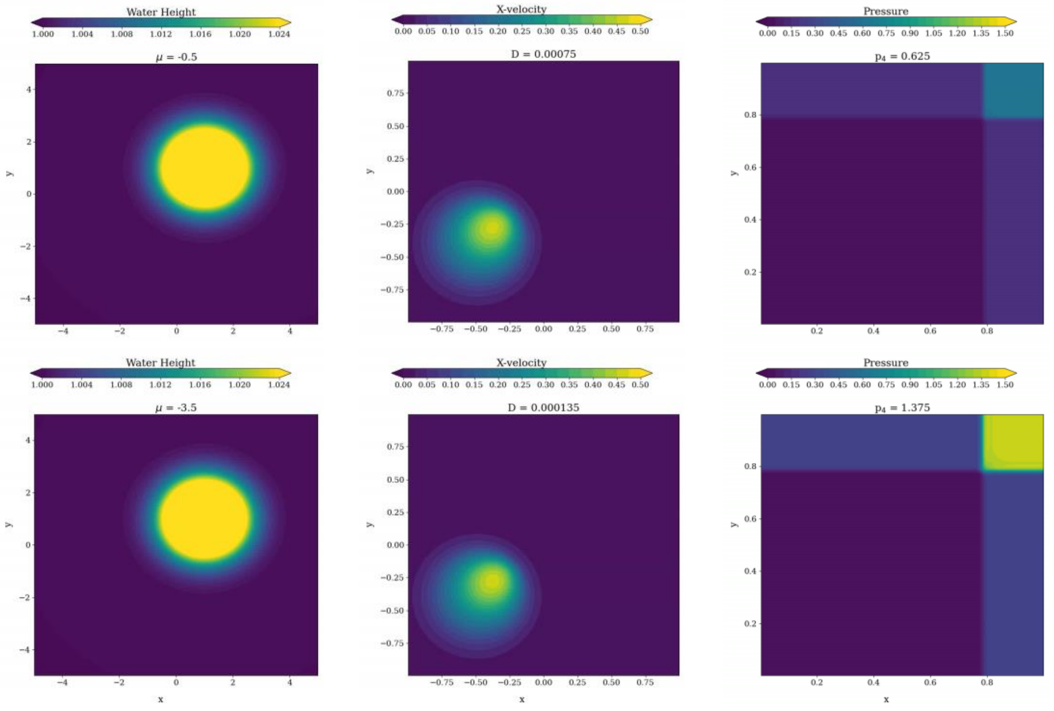


Ghost cells

Numerical Examples

- **Nonlinear hyperbolic fluid systems** in Pressio/Pressio demo-apps*
  - ➢ 2D **shallow water equations** (SWE), vary Coriolis parameter (μ)
  - ➢ 2D **viscous Burgers' equations**, vary diffusion parameter (D)
  - ➢ 2D **Euler equations**, vary upper right pressure (p_4) in IC
- **Wave/shock propagation** across interfaces ⇒ **high Kolmogorov n-width**
- **FOM discretization:** first-order **CCFV method,** 300x300 mesh, **BDF1**
- Consider **decompositions** of Ω into **four subdomains**





SWE | Burgers' | Euler

All results predictive: 5 training points, 4 (interpolative) testing points

SWE

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

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

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

Burgers'

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

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

Euler

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0$$

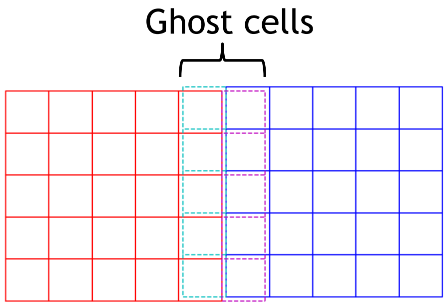
$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial}{\partial x}(\rho u^2 + p) + \frac{\partial (\rho u v)}{\partial y} = 0$$

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

$$\frac{\partial (\rho E)}{\partial t} + \frac{\partial}{\partial x}((E+p)u) + \frac{\partial}{\partial y}((E+p)v) = 0$$

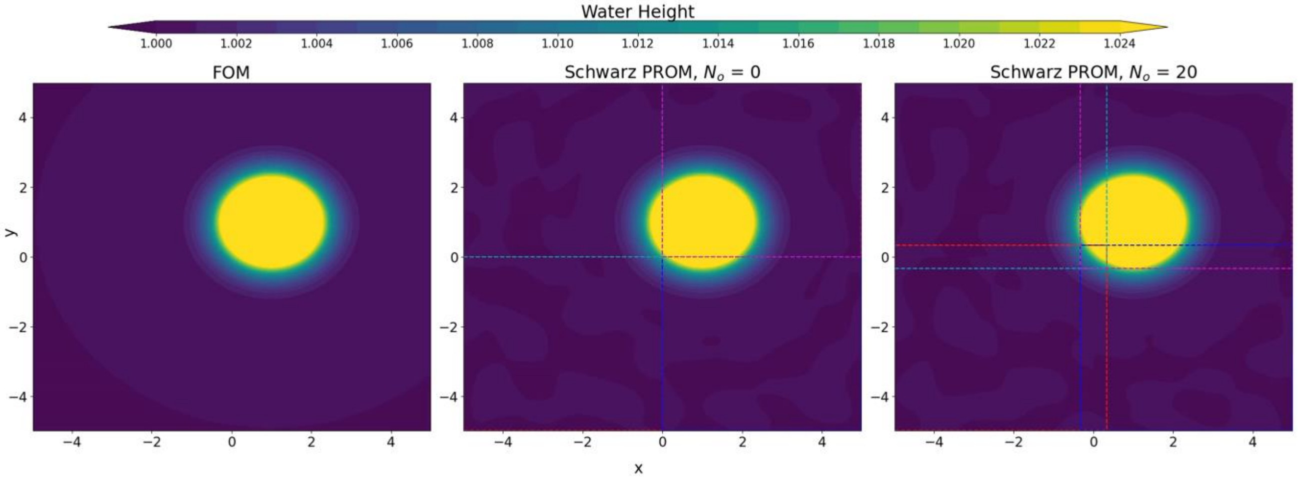
* https://pressio.github.io, https://github.com/Pressio/pressio-schwarz

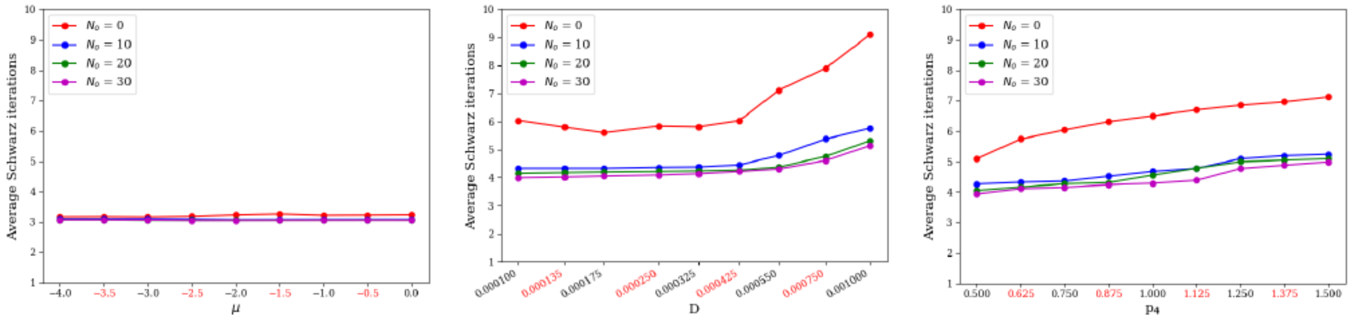
Impact of Subdomain Overlap*



Key result: **non-overlapping Schwarz** iteration converges without a degradation in accuracy when using **Dirichlet-Dirichlet Schwarz BCs!**

- This result is **not true** in general [Barnett et al., 2022; Mota et al., 2017; Mota et al. 2022]!
  - ➢ Generally need **alternating Dirichlet-Neumann** or **Robin-Robin BCs** for non-overlapping Schwarz convergence.
  - ➢ Dirichlet-Dirichlet works here due to **implied overlap** introduced into otherwise non-overlapping DD by ghost cells.
- **More Schwarz iterations** are required for convergence with no overlap (as expected)
- Non-overlapping incurs **negligible convergence penalty** for smooth problems (SWE)
- Non-overlapping Schwarz **avoids duplicate calculations** in overlap region
- It becomes **more difficult** to **transmit shock across non-overlapping interface** (Burgers, Euler)





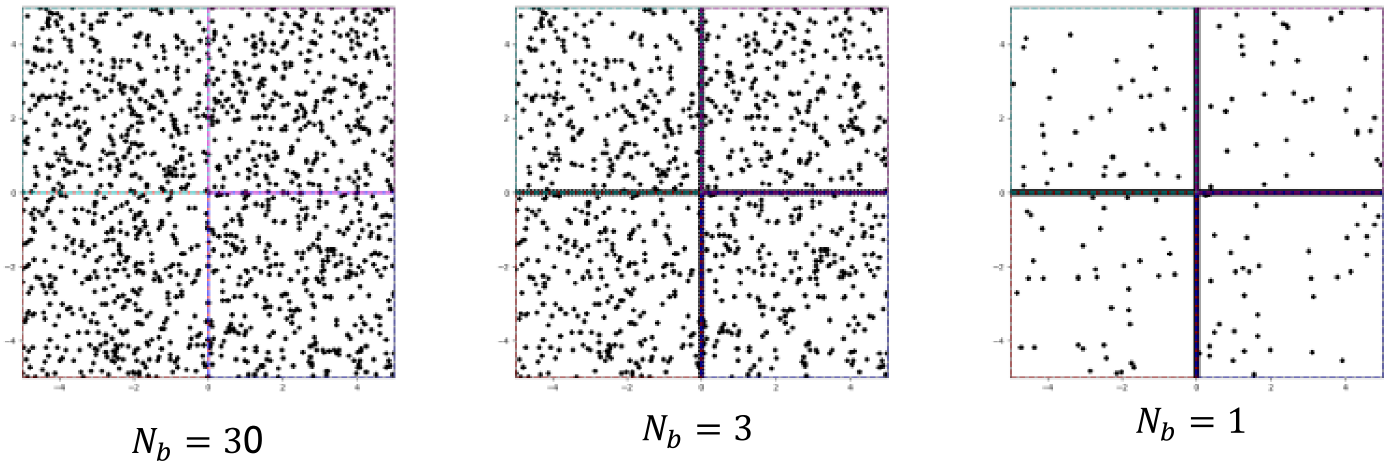
SWE, $K = 80$ Burgers', $K = 200$ Euler, $K = 200$

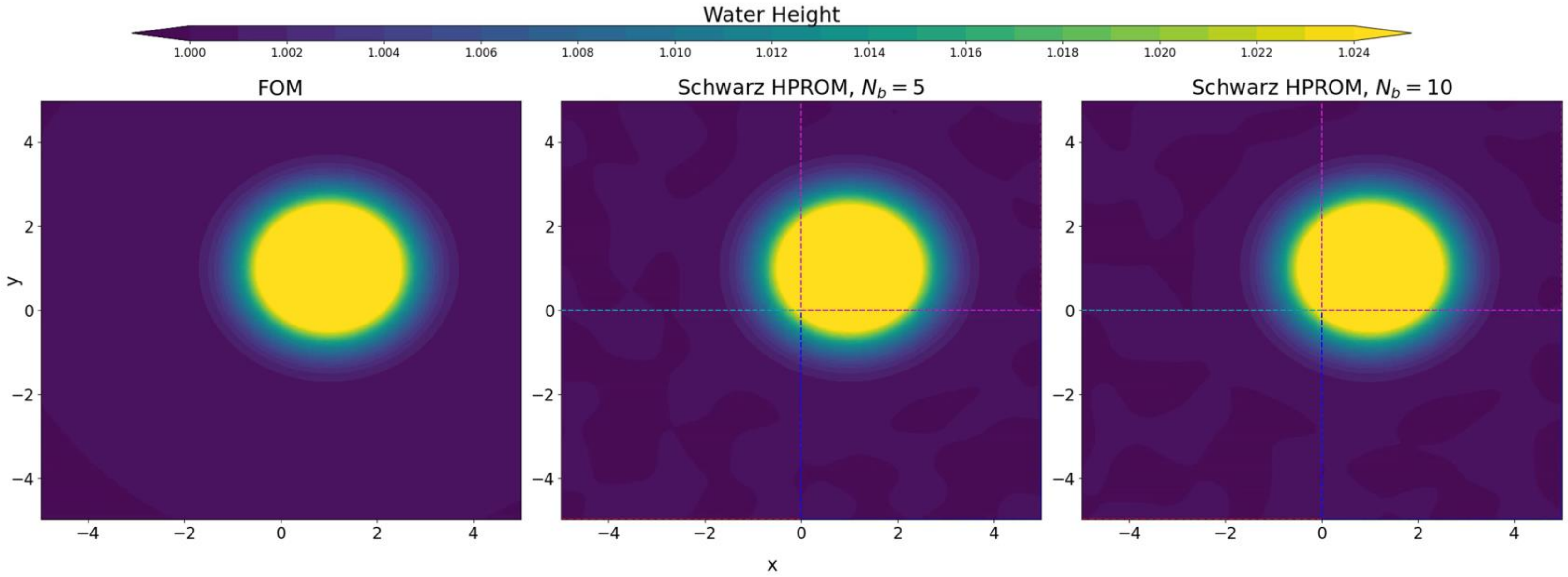
Red parameter values are predictive.

* See [Wentland et al., 2025] for more details.

Impact of Boundary Sampling for Hyper-Reduction*

Key result: given a **fixed "budget"** of **sample mesh points**, there is a (problem-dependent) **optimal number** of **sample mesh points** to allocate to the **Schwarz boundaries** vs. the **subdomain interiors**.

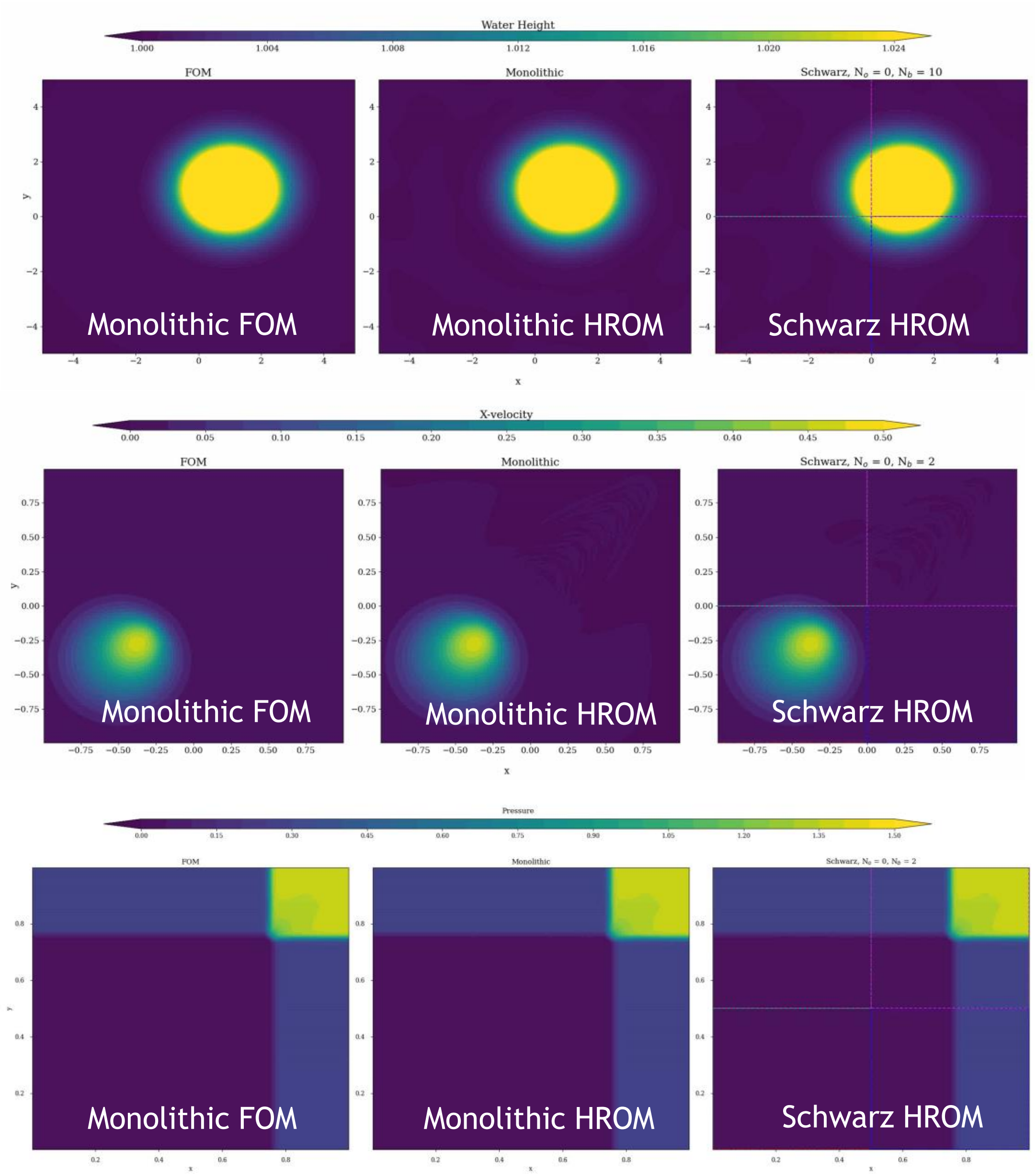




- N_b = **fixed interval** at which Schwarz boundaries are **sampled**
- For a **fixed budget** of sample mesh points N_s, boundary points draw points **away from interior** (figure left)
- Failure to **deliberately sample** the **Schwarz boundary** will also always lead to instabilities (movie left)

* See [Wentland et al., 2025] for more details.

Accuracy*



Top row: SWE
Middle row: Burgers'
Bottom row: Euler

***Key result:* predictive hyper-reduced ROMs (HROMs)** with **non-overlapping** Dirichlet-Dirichlet **Schwarz coupling** are indistinguishable from corresponding monolithic ROMs/FOMs.

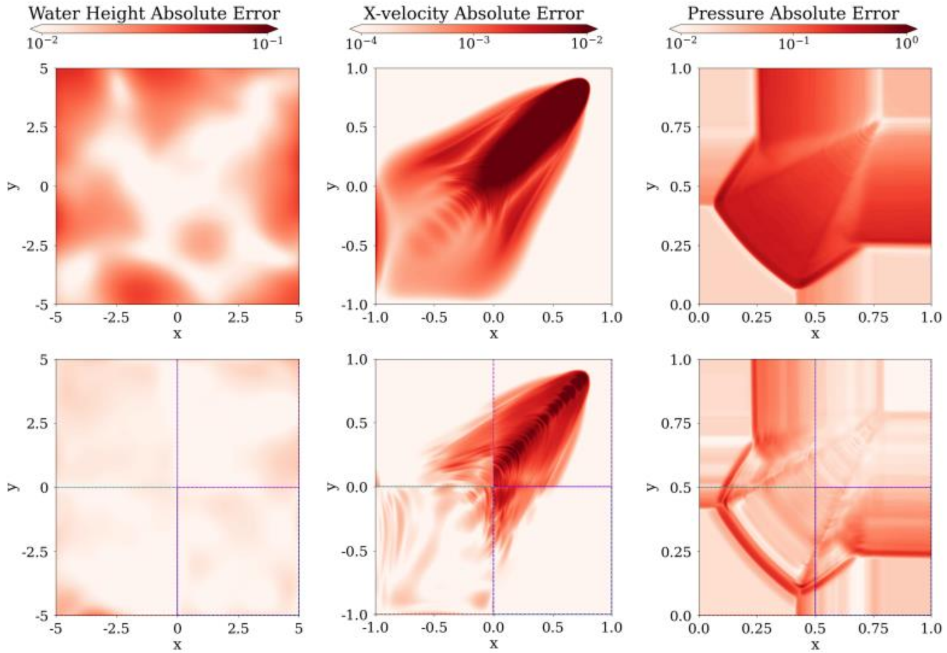


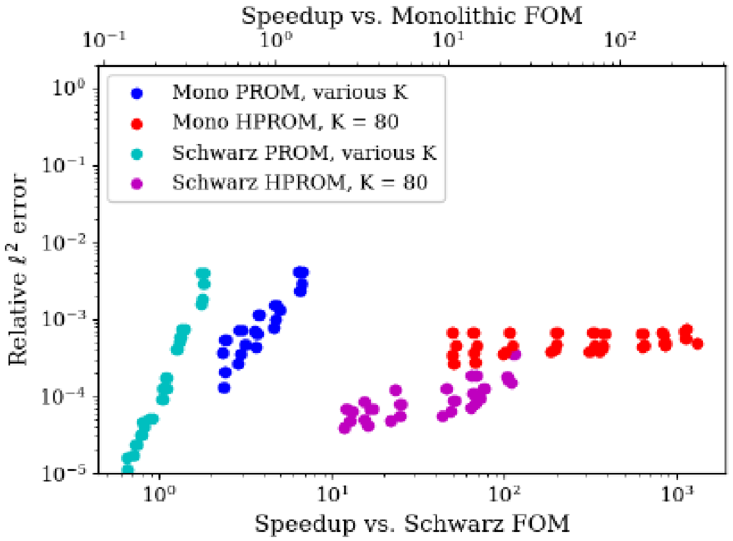
Figure above: **average absolute spatial error fields** for representative **monolithic** (top) and **decomposed** (bottom) hyper-reduced ROM with no overlap. Subdomain interfaces are marked with dashed lines.

* See [Wentland et al., 2025] for more details.

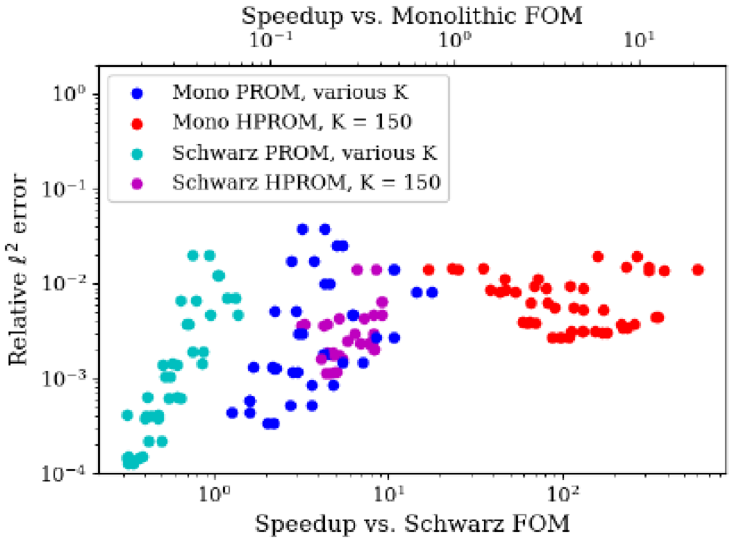
Computational Cost*

***Key result:* additive Schwarz** enables **speed-ups** over corresponding **coupled Schwarz FOM** and sometimes over **monolithic FOM**.

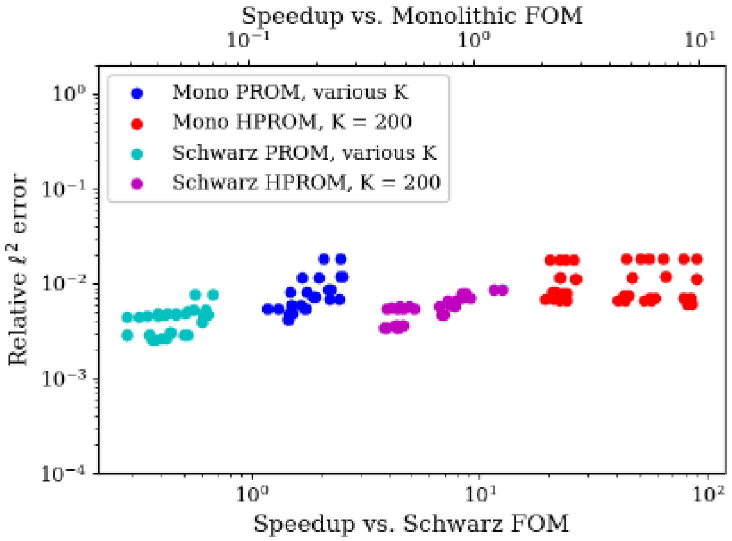
- Hyper-reduced ROMs generally achieve **cost savings** w.r.t. corresponding coupled Schwarz FOM
- **Cost savings** using Schwarz ROMs over corresponding **monolithic FOM** are possible for **SWE problem**
  - ➢ **Coupled Schwarz FOMs** are **often only viable options** for Sandia **analysts** due to **meshing challenges**
  - ➢ **Next step:** try to improve this via **adaptive Schwarz ROMs**



SWE



Burgers'



Euler

Red parameter values are predictive.

* See [Wentland et al., 2025] for more details.

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- Part 1: SAM-based Coupling of Intrusive Projection-based ROMs
  - Projection-based ROM Overview
  - SAM-based Coupling Workflow
  - Numerical Examples
- **Part 2: SAM-based Coupling of Non-Intrusive OpInf ROMs**
  - OpInf ROM Overview
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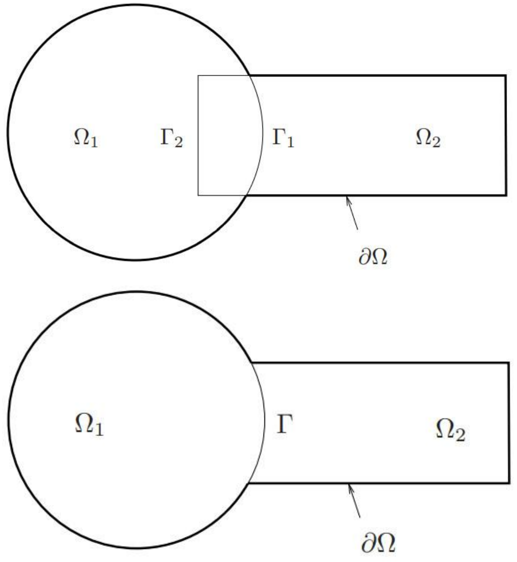
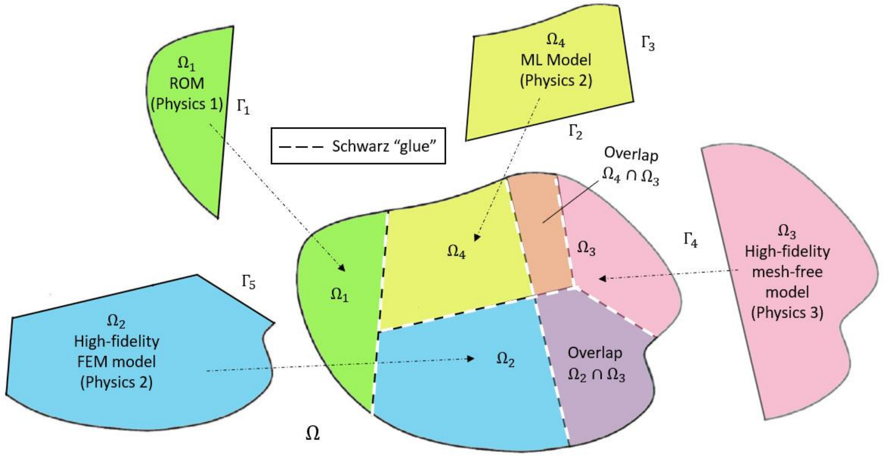
- Summary & Ongoing/Future Work





Non-Intrusive Model Order Reduction via OpInf*

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

Nuances:

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

FOM:

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

snapshots of $\boldsymbol{q}$

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

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

OpInf ROM:

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

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

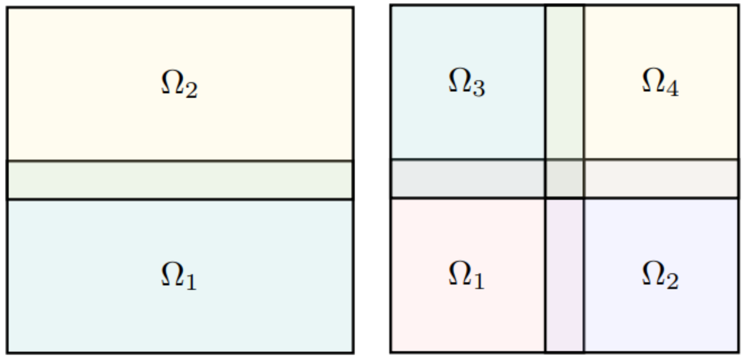
$\widehat{\boldsymbol{Q}}$: snapshots generated from projected simulation data $\boldsymbol{q}$

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

SAM-based Coupling for Non-Intrusive OpInf ROMs

Offline stage:

- Perform **FOM simulation** on a spatial domain Ω and **collect** s **snapshots**
- Create **DD** of Ω into d **overlapping subdomains** Ω_i.
- Compute **POD basis** $\boldsymbol{\Phi}_i$ on each Ω_i by restricting the snapshots to Ω_i.
- Assume a **functional form** for your ROM in Ω_i, informed by the functional form of the corresponding FOM
  - ➢ ***Key question****: how to impose Schwarz BCs in OpInf ROMs?*



OpInf ROM in Ω_i:

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

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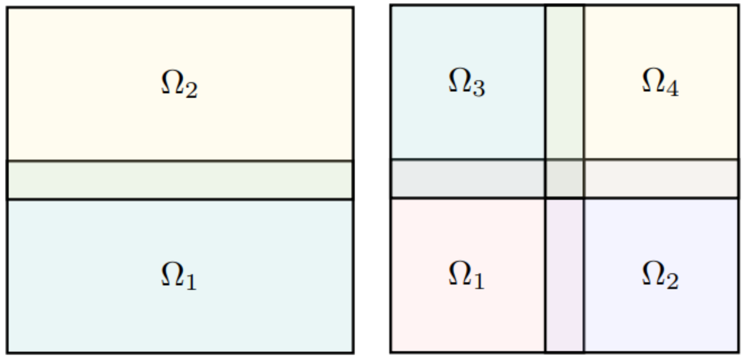
    - ❖ *Boundary transmission enters through* ***learned source term*** $\widehat{\boldsymbol{B}}_i\boldsymbol{g}_i$ *added to OpInf ROM dynamical system*



OpInf ROM + Schwarz BCs in Ω_i:

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

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

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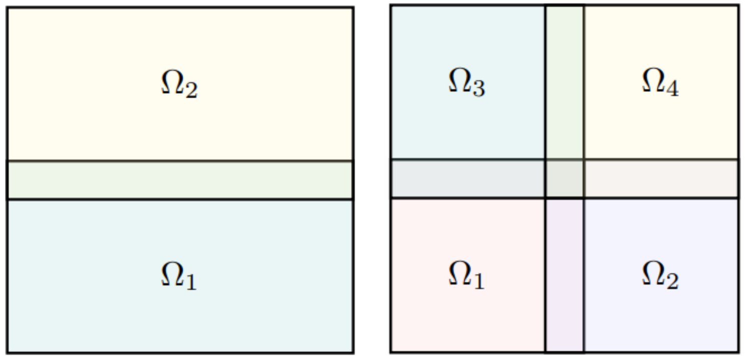
    - ❖ *Boundary transmission enters through **learned source term** $\widehat{\boldsymbol{B}}_i \boldsymbol{g}_i$ added to OpInf ROM dynamical system*
    - ❖ ***Further reduction** achieved by expanding $\boldsymbol{g}_i$* in its own POD basis $\boldsymbol{\Phi}_i^g$ and approximating $\widehat{\boldsymbol{B}}_i \boldsymbol{g}_i \approx \widehat{\boldsymbol{B}}_i \widehat{\boldsymbol{g}}_i = \widetilde{\boldsymbol{B}}_i \boldsymbol{g}_i$ where $\widehat{\boldsymbol{g}}_i = \boldsymbol{\Phi}_i^g \boldsymbol{g}_i$



OpInf ROM + Schwarz BCs in Ω_i:

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

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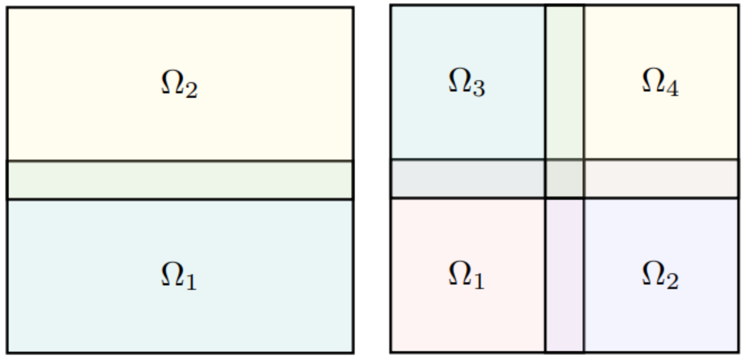
- Compute OpInf operators $\widehat{\boldsymbol{A}}_i, \widehat{\boldsymbol{H}}_i$ and $\widetilde{\boldsymbol{B}}_i$ in each subdomain Ω_i by solving regularized OpInf LS **minimization problem**

Online stage:

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



OpInf ROM + Schwarz BCs in Ω_i:

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

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

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

Numerical Examples

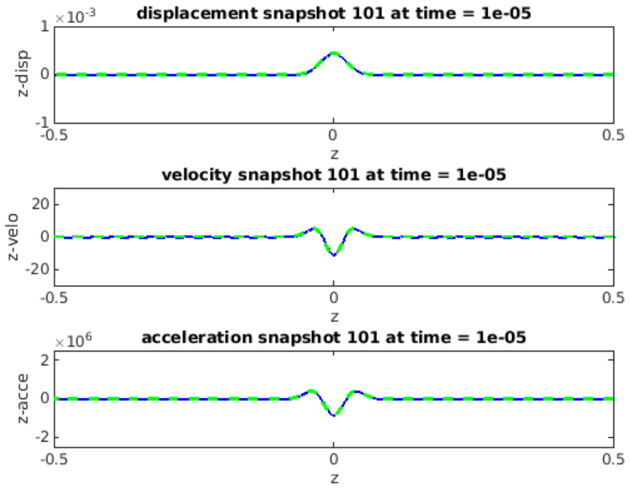
Solid dynamics weak variational form:

$$\int_I \left[\int_\Omega (\mathrm{Div}\, \boldsymbol{P} + \rho_0 \boldsymbol{B} - \rho_0 \ddot{\boldsymbol{\varphi}}) \cdot \boldsymbol{\xi} \; \mathrm{d}V + \int_{\partial_T \Omega} \boldsymbol{T} \cdot \boldsymbol{\xi} \; \mathrm{d}S \right] \mathrm{d}t = 0$$

- **Dynamic** finite deformation **solid mechanics** problem
  - 3D **linear elastic notched cylinder** problem
  - 3D **hyperelastic torsion** problem
- **Wave propagation** and **large deformation** ⇒ **difficult** for ROMs/coupling!
- **FOM discretization:** FEM in space, implicit Newmark in time
  - Implementation in ***Norma*** Julia code*, which relies on Python OpInf package**
- Consider **overlapping** DDs of Ω into **two** or **three subdomains**
- Evaluate **FOM-ROM** couplings only for now
- ROM = **linear**, **quadratic** or **cubic** OpInf model (OpInf, QOpInf, COpInf)

Semi-discrete form:

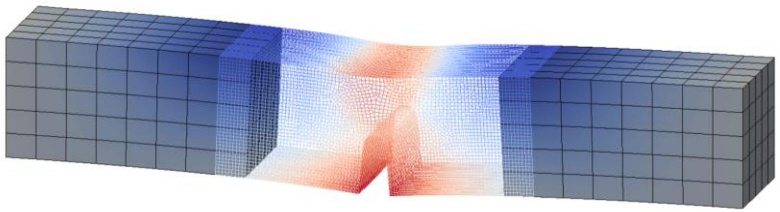
$$\boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{f}^{\mathrm{int}}(\boldsymbol{u}, \dot{\boldsymbol{u}}) = \boldsymbol{f}^{\mathrm{ext}}$$



1D linear elastic wave

3D notched cylinder

3D torsion



3D laser weld

Results are **preliminary** and focus on **verification/ initial prototyping** of OpInf ROMs and FOM-OpInf ROM coupling via **overlapping SAM** in *Norma*

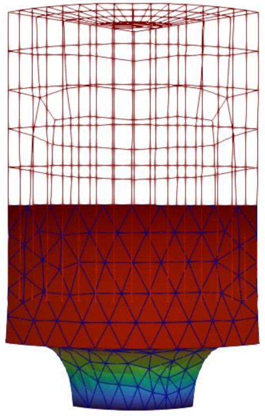
* https://github.com:sandialabs/Norma.jl
** https://pypi.org/project/opinf

3D Linear Elastic Notched Cylinder Problem

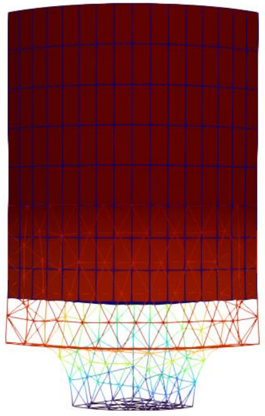
- Geometry is ***linear elastic notched cylinder*** pulled from top ***dynamically*** to time $T_{max} = 1.5$ at rate of $0.0064t$ with $\Delta t = 0.005$
- Demonstration of SAM's ability to ***couple disparate meshes***, ***element types*** and ***models***: TET10 + FOM (notched region) and HEX8 + Linear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

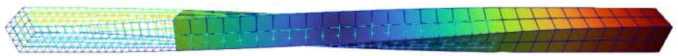
FOM-OpInf

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

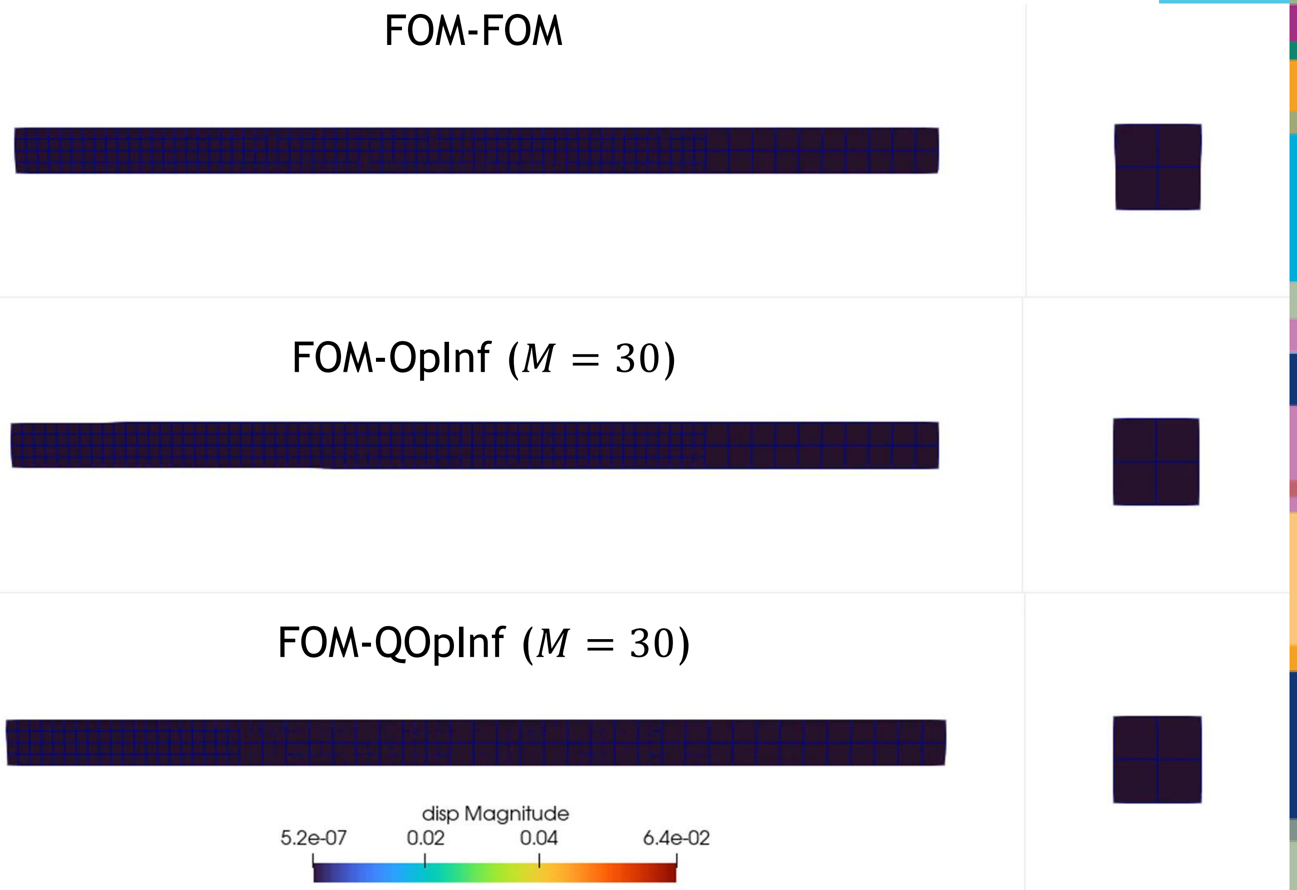
3D Hyperelastic Torsion Problem

- ***Dynamic nonlinear hyperelastic bar*** subjected to high degree of ***torsion*** (initial velocity = $(-ayz, axz, 0)$).
- ***Saint-Venant Kirchhoff*** material model, which gives rise to PDEs with ***cubic nonlinearities***.
- ***Overlapping*** DD of Ω into ***two subdomains***, discretized with ***nonconformal HEX8 meshes***
- Evaluated ***predictive FOM-OpInf*** couplings with ***linear***, ***quadratic*** and ***cubic OpInf ROMs*** built from 2K snapshots (train for $a = 5000,\ 6000,\ 7000,\ 8000$, predict for $a = 5500$)
- ***Displacement relative errors at final time*** ($M = 30$ QOpInf): 12.5% in Ω_1 and 9.38% in Ω_2

Ω_1 (HEX8 + FOM)



Ω_2 (HEX8 + OpInf)



Key result: **quadratic** and **cubic** OpInf models can produce **stable** and **accurate** solutions (whereas linear OpInf blows up) but are very **sensitive** to γ.

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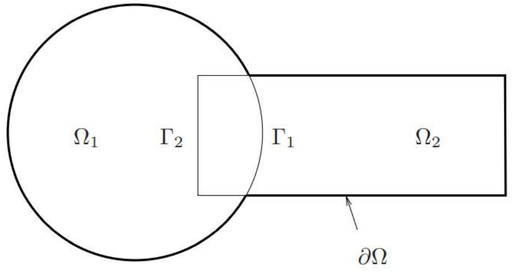
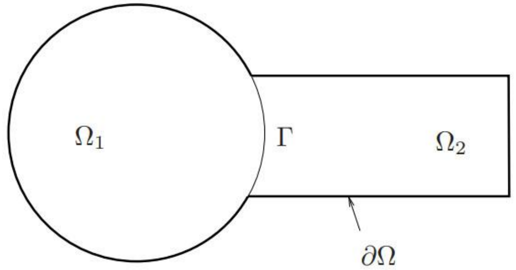
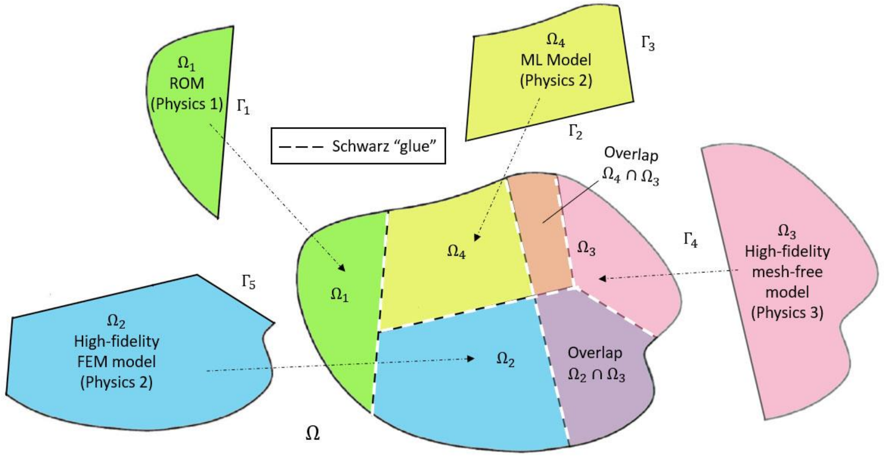




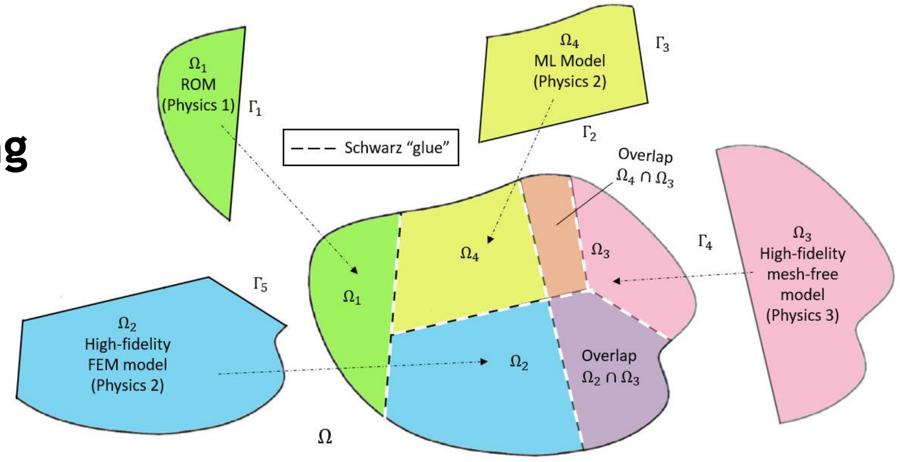


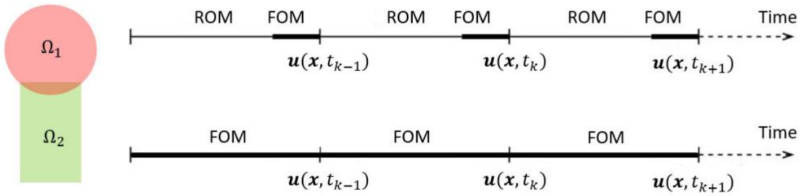
Summary & Ongoing/Future Work

Summary*:** the **Schwarz alternating method** is effective at coupling **subdomain-local FOMs** and (intrusive or nonintrusive) **ROMs** and does ***not introduce **artifacts** or **numerical instabilities** if applied correctly.

Ongoing & future work:

- Improve **robustness** and **stability** of OpInf ROMs + Schwarz via **filtering** and/or **stabilization** (with T. Iliescu, Virginia Tech)
- Develop **automated workflow** to **optimize** DD and SAM parameters
- Extend Schwarz + OpInf ROM to **parametric problems**
- Extend Schwarz + OpInf ROM to **non-intrusive kernel-based ROMs**
- Extend SAM to **fully nonlinear neural network-based ROMs**
- Develop **non-overlapping SAM** for non-intrusive ROMs
- Incorporate **structure preservation** into non-intrusive Schwarz ROMs
- **Implement** FOM-ROM coupling in **SIERRA/SM production code.**
- Development of **automated criteria** to determine appropriate use of less refined or reduced-order models without sacrificing accuracy, enabling **real-time transitions** between different model fidelities





→ ***Newest project*:** AHEAD LDRD

Team & Acknowledgments

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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[Schwarz + PINNs]

Ian Moore
Intern from Virginia Tech
[Schwarz + OpInf]

Eric Parish

Anthony Gruber

Cam Rodriguez
New Intern from Columbia U
[Schwarz + OpInf]

References & Codes

[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

[6] C. Wentland, F. Rizzi, J. Barnett, **I. Tezaur**. "The role of interface boundary conditions and sampling strategies for Schwarz-based coupling of projection-based reduced order models, *J. Comp. Appl. Math*, 2025 (in press). https://doi.org/10.1016/j.cam.2025.116584

[7] I. Moore, C. Wentland, A. Gruber, **I. Tezaur**. "Domain decomposition-based coupling of Operator Inference reduced order models via the Schwarz alternating method", ArXiv pre-print, 2024. https://arxiv.org/pdf/2409.01433

[8] Pressio: https://pressio.github.io

[9] Pressio demo-apps: https://github.com/Pressio/pressio-demoapps

[10] Pressio demo-apps + Schwarz: https://github.com/Pressio/pressio-schwarz

[11] Norma: https://sandialabs/Norma.jl

ikalash@sandia.gov
www.sandia.gov/~ikalash

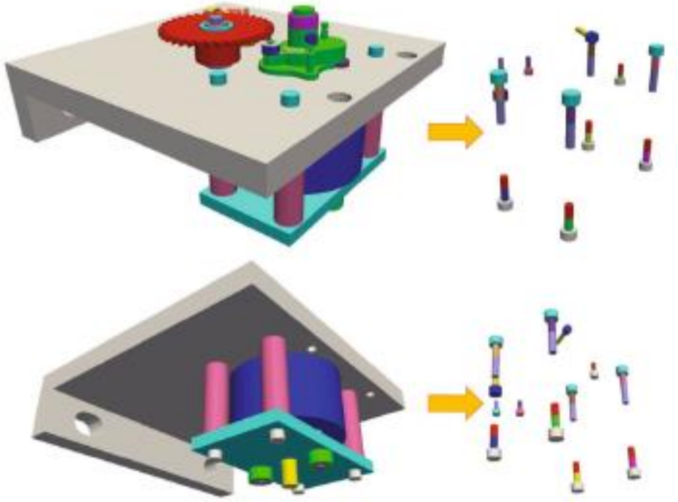
Start of Backup Slides

Motivation: Multi-scale & Multi-physics Modeling & Simulation

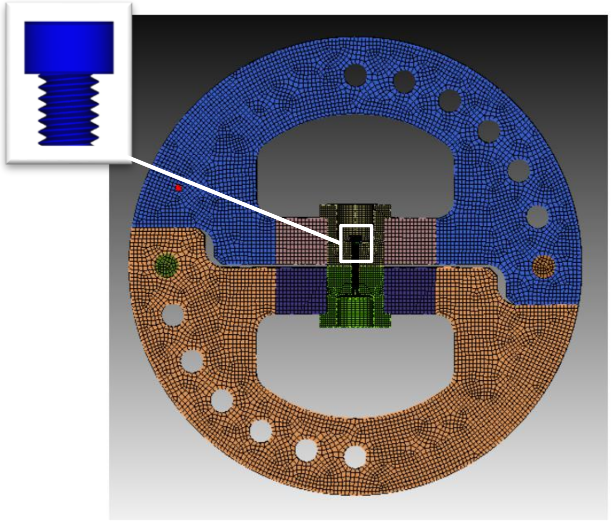
<u>**Key challenge**</u>: analysts using **high-fidelity models** to study multi-scale and/or multi-physics systems face **significant delays**.

Bottlenecks/Issues:

- **Mesh generation** is the "single biggest bottleneck in [mod/sim] analyses" [Sandia Lab News, 2020]
  - ➢ Generating a **single mesh** can take **weeks** → **months**
- High-fidelity full order model (FOM) simulations require **long runtimes**
  - ➢ Data-driven **reduced order models (ROMs)** can reduce runtime burdens, but:
    - ❖ Can suffer from **lack of robustness**, **stability** and **accuracy** in the predictive regime
    - ❖ **Cannot** be **easily refined** to achieve a specified level of accuracy like conventional discretizations
    - ❖ Can take **years** to **implement** in HPC codes



Ratcheting mechanism [Parish *et al.*, 2024]



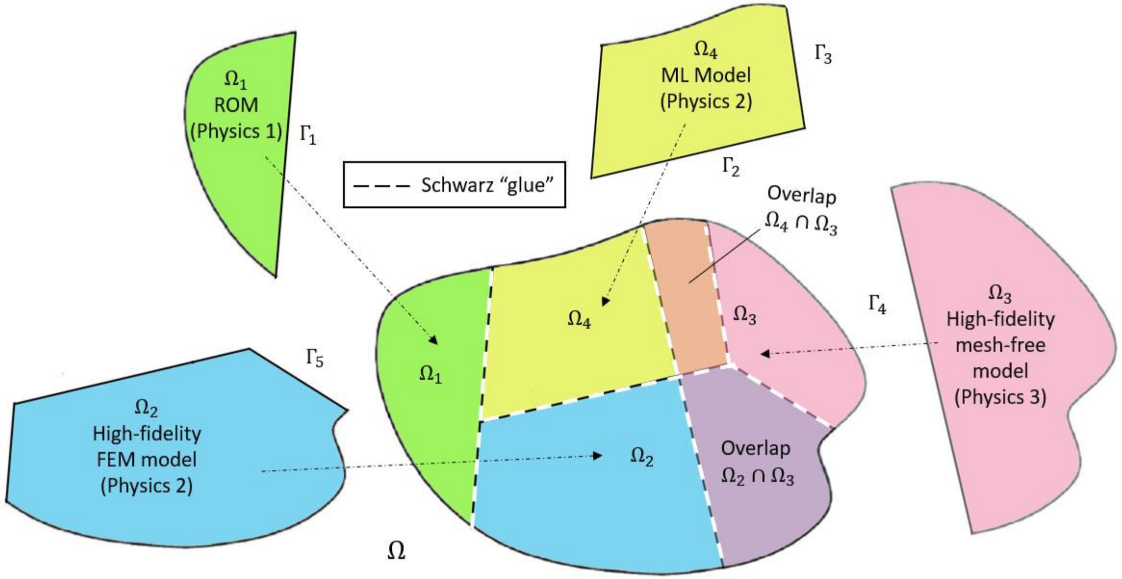
Fixture model with fastener held in by bushings [Murugesan *et al.*, 2020]

Solution: Hybrid Domain Decomposition-based Coupling

Hypothesis: the aforementioned hurdles can be **overcome** through the development of a **rigorous, minimally-intrusive coupling** method that creates **“hybrid” (ROM+FOM) models** based on an **optimal domain decomposition** (DD).

MESHING CHALLENGES *PRECLUDE* ANALYSES; DATA-DRIVEN ROMS *LACK STABILITY & ACCURACY* FOR PREDICTIONS

MITIGATE BOTH CHALLENGES WITH *OPTIMAL DOMAIN DECOMPOSITION-BASED HYBRID MODELS*



Example sample DD and ROM/FOM assignment.

Flexible Heterogeneous Numerical Methods (fHNM) and Multi-faceted Mathematics for Predictive Digital Twins (M2dt) Projects

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

Principal research objective:

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

U.S. DEPARTMENT OF ENERGY

Office of Science

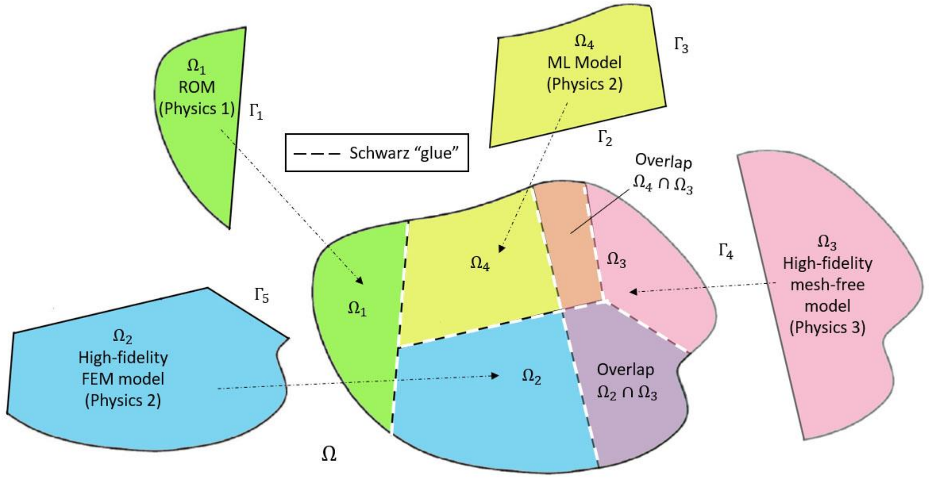
Principal research goals:

- **"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.

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Three coupling methods:

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



Additional Parallelism via Additive Schwarz

Multiplicative Overlapping Schwarz

$$\begin{cases} N\left(\boldsymbol{u}_1^{(n+1)}\right) = f \text{ , in } \Omega_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{g}, \text{ on } \partial\Omega_1 \backslash \Gamma_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{u}_2^{(n)} \quad \text{ on } \Gamma_1 \end{cases}$$

$$\begin{cases} N\left(\boldsymbol{u}_2^{(n+1)}\right) = f \text{ , in } \Omega_2 \\ \boldsymbol{u}_2^{(n+1)} = \boldsymbol{g}, \text{ on } \partial\Omega_2 \backslash \Gamma_2 \\ \boldsymbol{u}_2^{(n+1)} = \boldsymbol{u}_1^{(n+1)} \quad \text{ on } \Gamma_2 \end{cases}$$

Part 2 of Talk

Additive Overlapping Schwarz

$$\begin{cases} N\left(\boldsymbol{u}_1^{(n+1)}\right) = f \text{ , in } \Omega_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{g}, \text{ on } \partial\Omega_1 \backslash \Gamma_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{u}_2^{(n)} \quad \text{ on } \Gamma_1 \end{cases}$$

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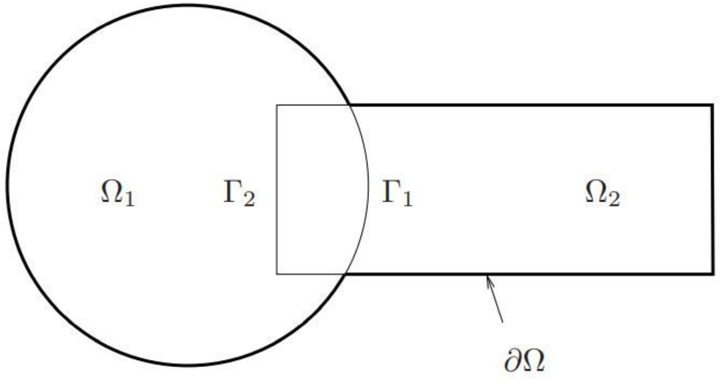
Part 1 of Talk

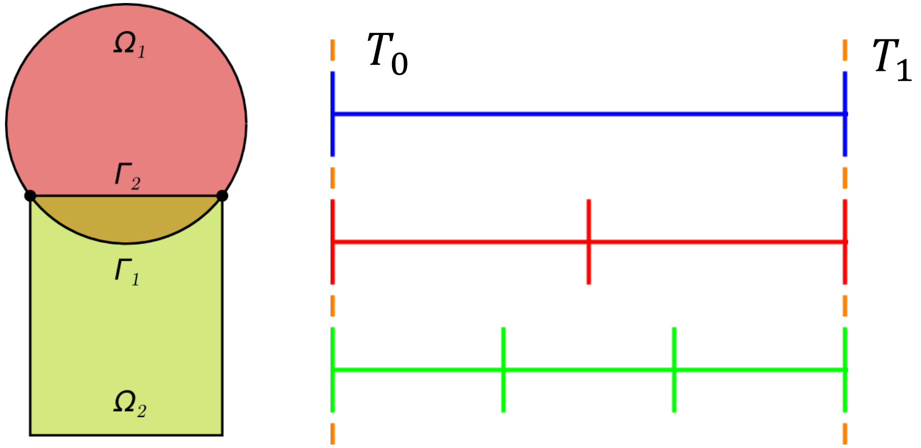
Model PDE:

$$\begin{cases} N(\boldsymbol{u}) = \boldsymbol{f}, \quad \text{in } \Omega \\ \boldsymbol{u} = \boldsymbol{g}, \quad \text{on } \partial\Omega \end{cases}$$



- **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

Time-Advancement Within the Schwarz Framework



Controller time stepper

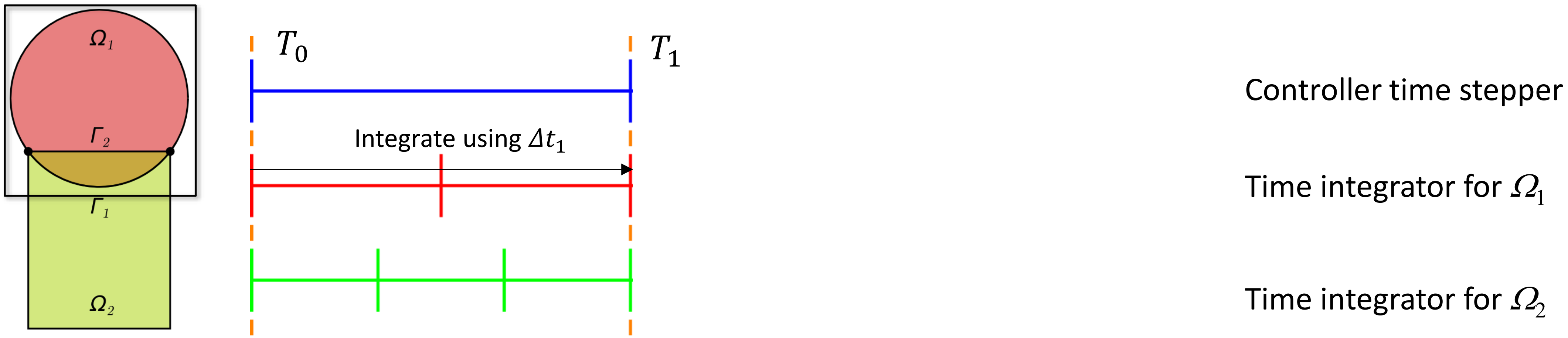
Time integrator for Ω_1

Time integrator for Ω_2

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

Model PDE:
$$\begin{cases} \dot{\boldsymbol{u}} + N(\boldsymbol{u}) = \boldsymbol{f}, & \text{in } \Omega \\ \boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{g}(t), & \text{on } \partial\Omega \\ \boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0, & \text{in } \Omega \end{cases}$$

Time-Advancement Within the Schwarz Framework



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

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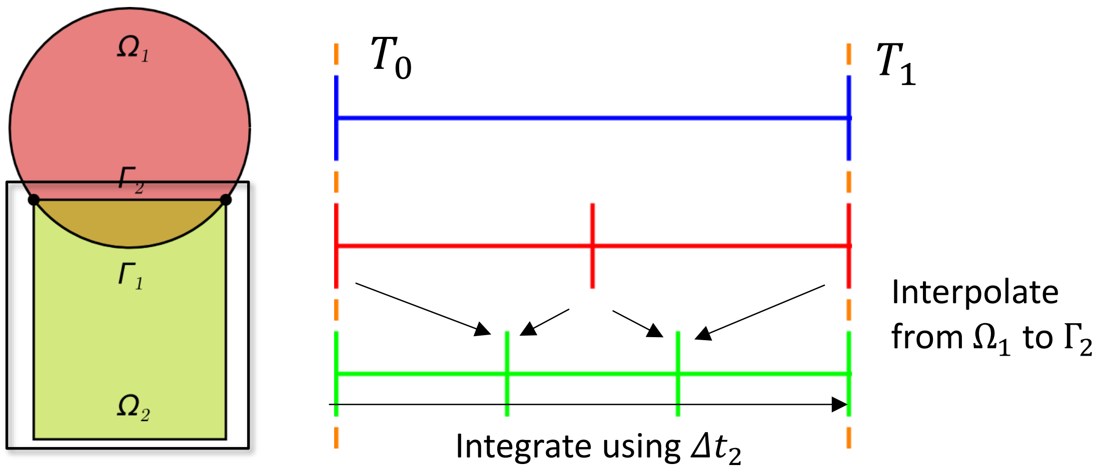

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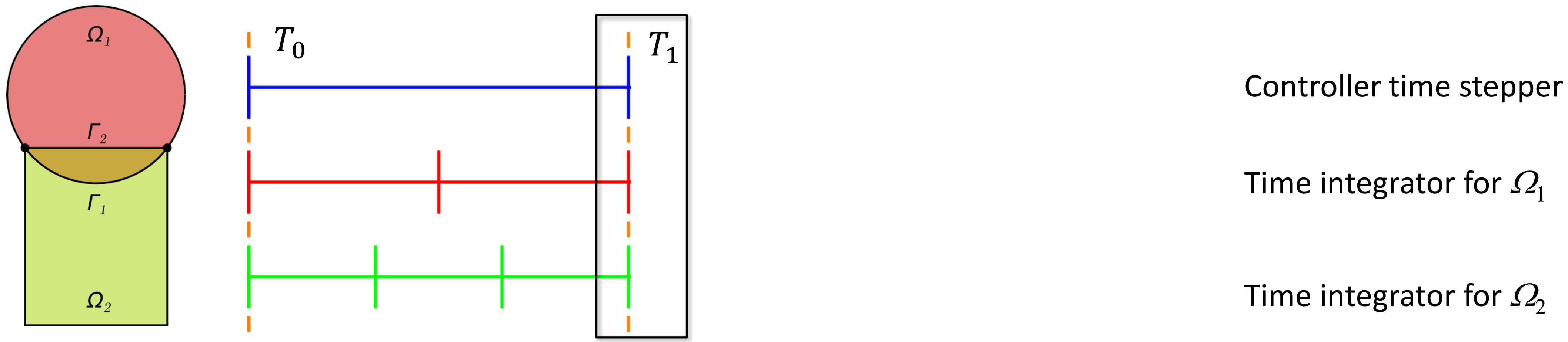
Time-Advancement Within the Schwarz Framework



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

Model PDE:
$$\begin{cases} \dot{\boldsymbol{u}} + N(\boldsymbol{u}) = \boldsymbol{f}, & \text{in } \Omega \\ \boldsymbol{u}(\boldsymbol{x},t) = \boldsymbol{g}(t), & \text{on } \partial\Omega \\ \boldsymbol{u}(\boldsymbol{x},0) = \boldsymbol{u}_0, & \text{in } \Omega \end{cases}$$

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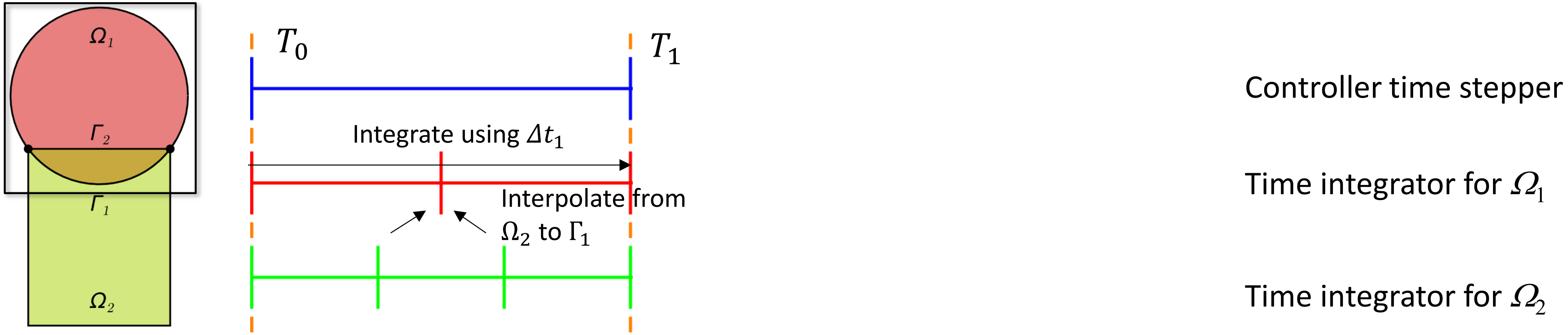

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- If unconverged, return to Step 1.

Model PDE:

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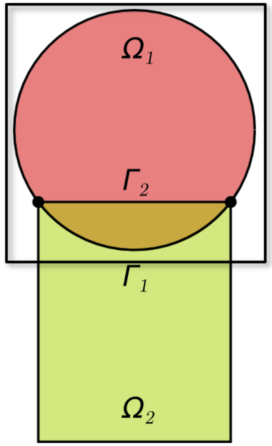
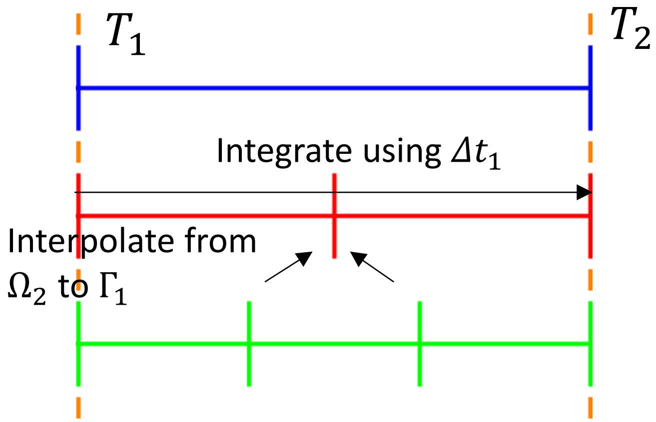
Time-Advancement Within the Schwarz Framework





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

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

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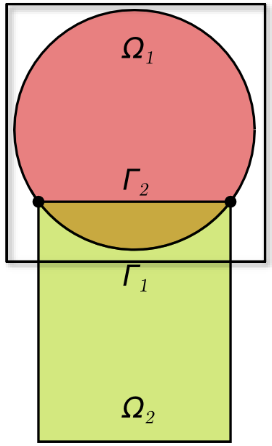
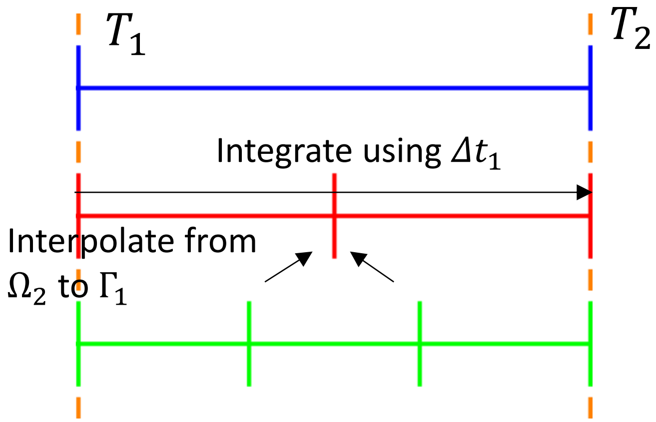
Time-Advancement Within the Schwarz Framework





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

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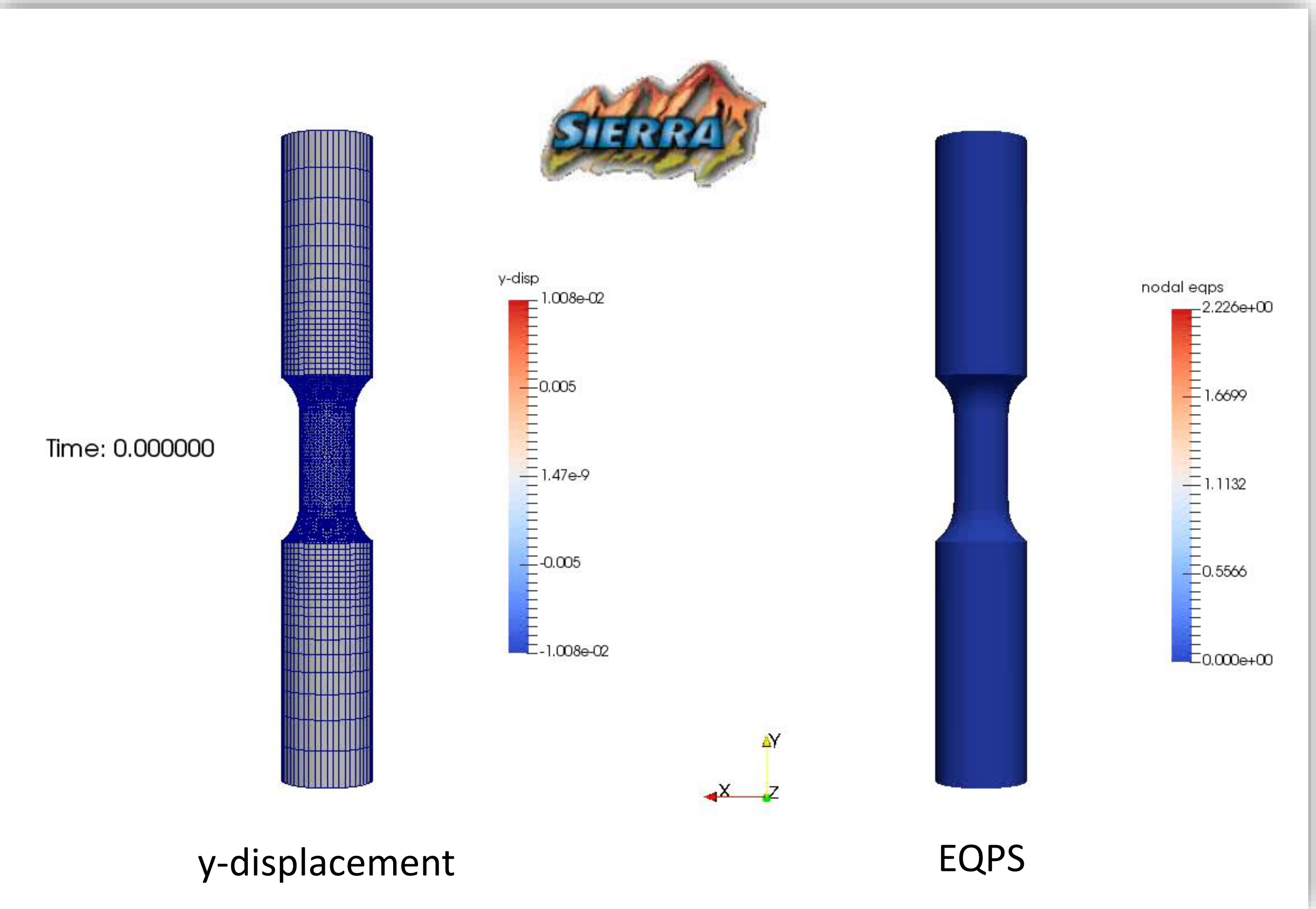
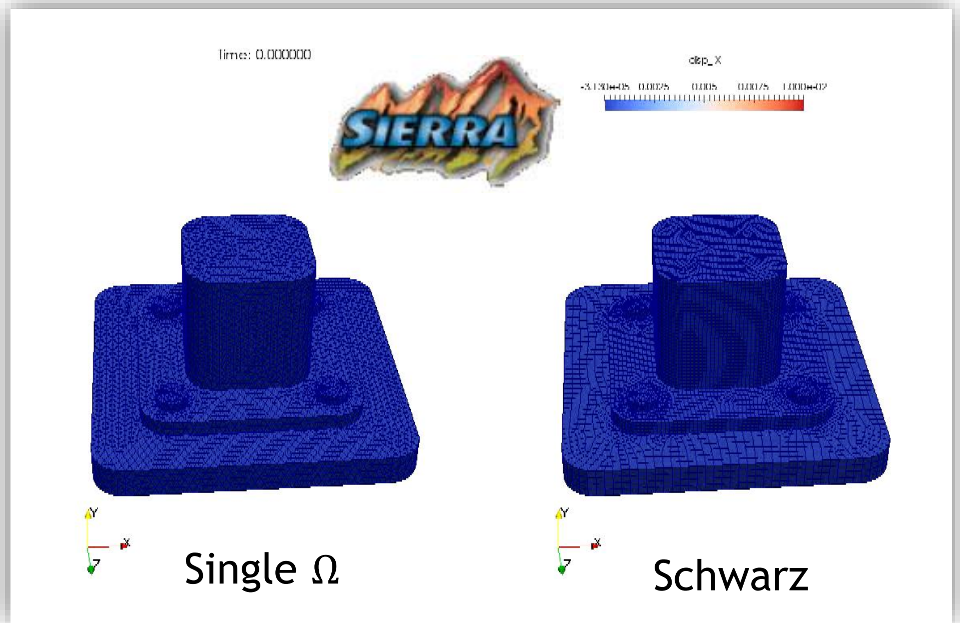
Schwarz for Multi-scale FOM-FOM Coupling in Solid Mechanics[1]





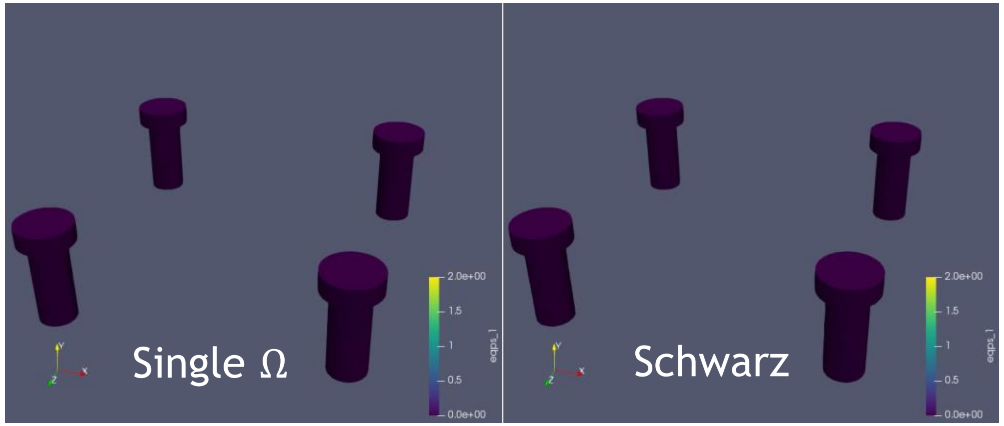


Figure above: tension specimen simulation coupling composite TET10 elements with HEX elements in Sierra/SM.

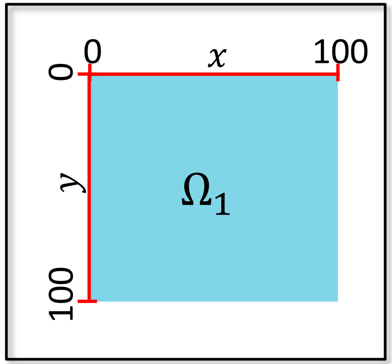
Figures right: bolted joint simulation coupling composite TET10 elements with HEX elements in Sierra/SM.

[1] Mota *et al*. 2017; Mota *et al*. 2022.

2D Inviscid Burgers Equation

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

$$\frac{\partial u}{\partial t} + \frac{1}{2}\left(\frac{\partial (u^2)}{\partial x} + \frac{\partial (uv)}{\partial y}\right) = 0.02\exp(\mu_2 x)$$
$$\frac{\partial v}{\partial t} + \frac{1}{2}\left(\frac{\partial (vu)}{\partial x} + \frac{\partial (v^2)}{\partial y}\right) = 0$$
$$u(0, y, t; \boldsymbol{\mu}) = \mu_1$$
$$u(x, y, 0) = v(x, y, 0) = 1$$



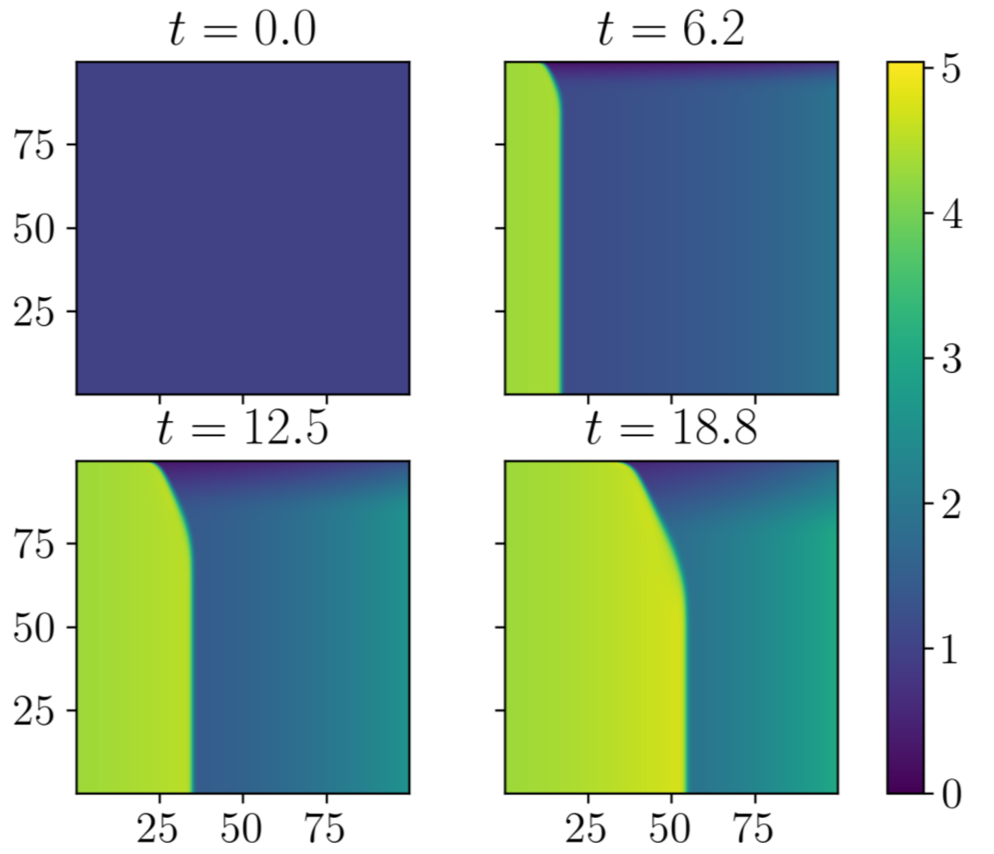


Figure above: solution of u component at various times

Problem setup:

- $\Omega = (0,100)^2$, $t \in [0, 25]$
- Two **parameters** $\boldsymbol{\mu} = (\mu_1, \mu_2)$. **Training:** uniform sampling of $\mu_1 \times \mu_2 = [4.25, 5.50] \times [0.015, 0.03]$ 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

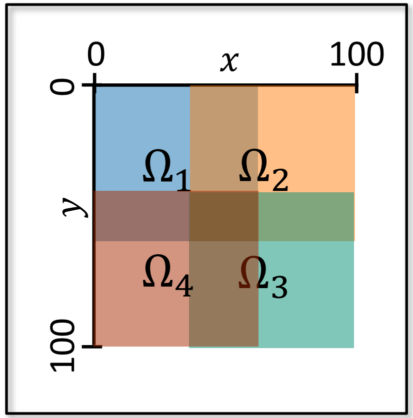


Figure above: 4 subdomain overlapping DD

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** via 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: $\boldsymbol{\Phi}(\boldsymbol{i}_{\text{Dir}}, :) = \mathbf{0}$
  - BCs imposed by modifying $\bar{\boldsymbol{q}}$: $\bar{\boldsymbol{q}}(\boldsymbol{i}_{\text{Dir}}) \leftarrow \boldsymbol{\chi}_{\boldsymbol{q}}$

Choice of hyper-reduction

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

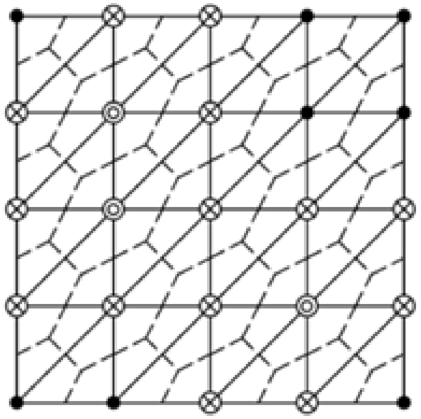
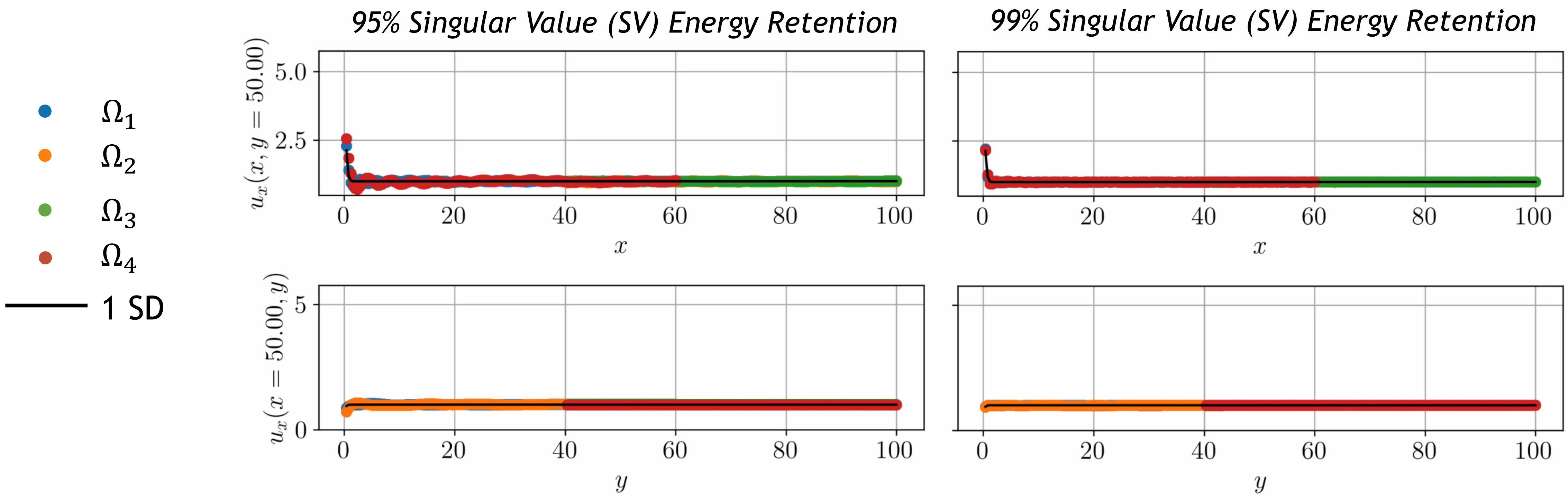


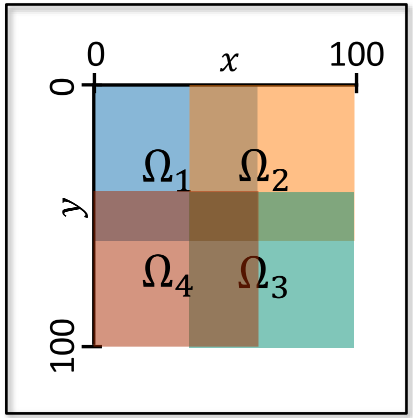
Figure above: ECSW augmented reduced mesh

All-ROM Coupling

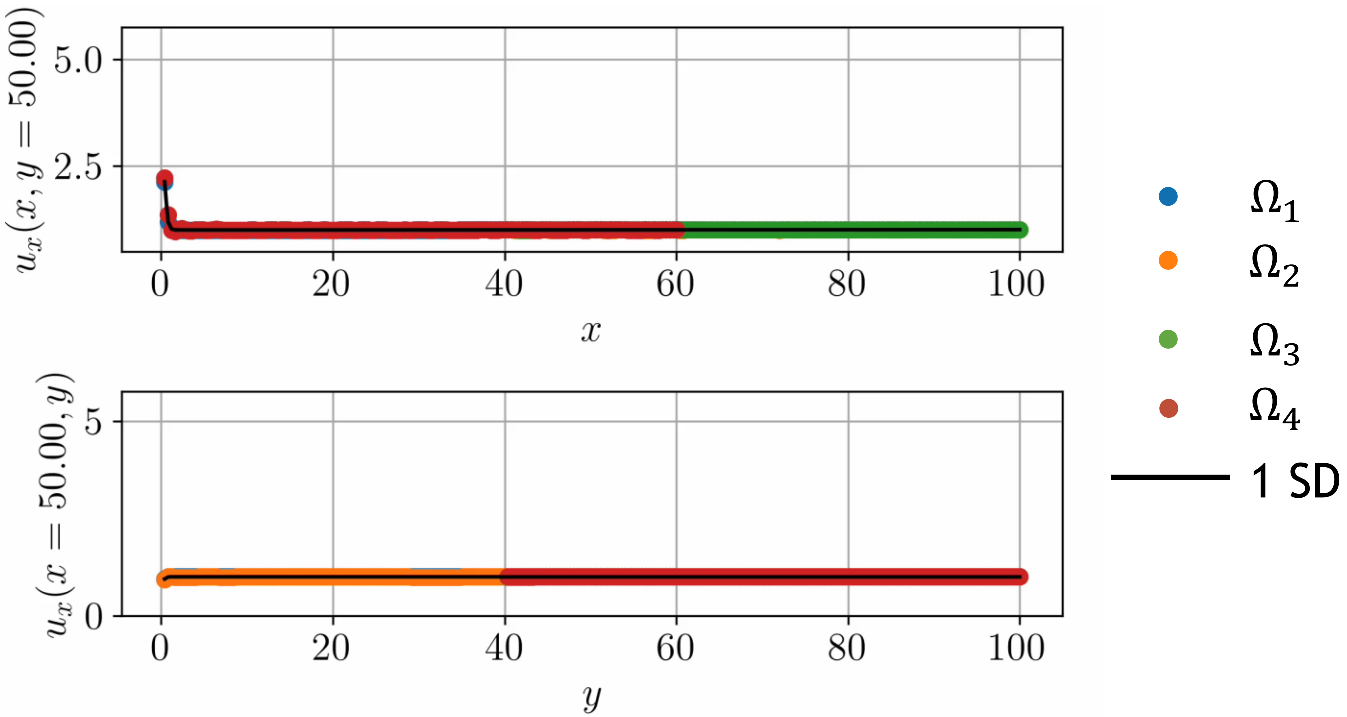


- Method converges in **only 3 Schwarz iterations** per controller time-step
- **Errors** $O(1\%)$ or less
- **1.47× speedup** over all-FOM coupling for 95% SV energy retention case

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**

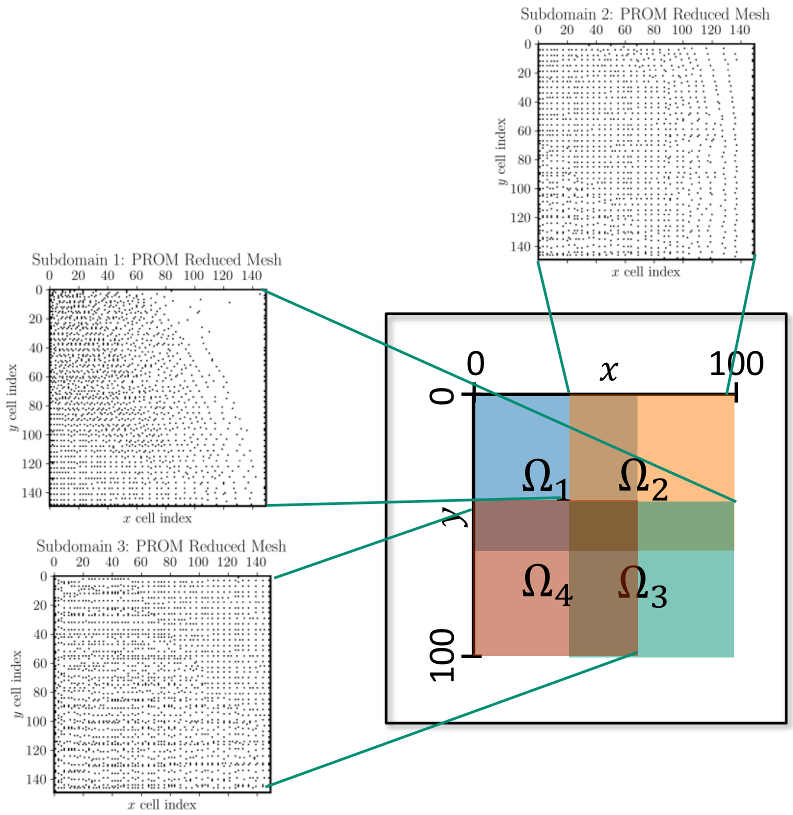


FOM-HROM-HROM-HROM Coupling



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.**

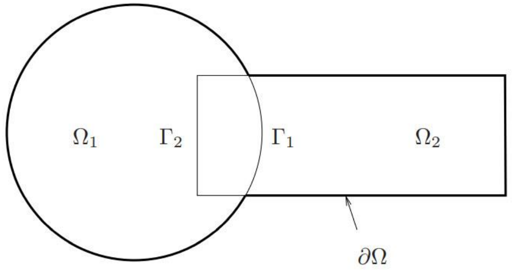
Outline

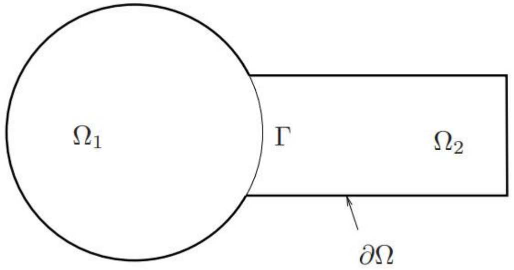
- The Schwarz Alternating Method for Domain Decomposition-Based Coupling

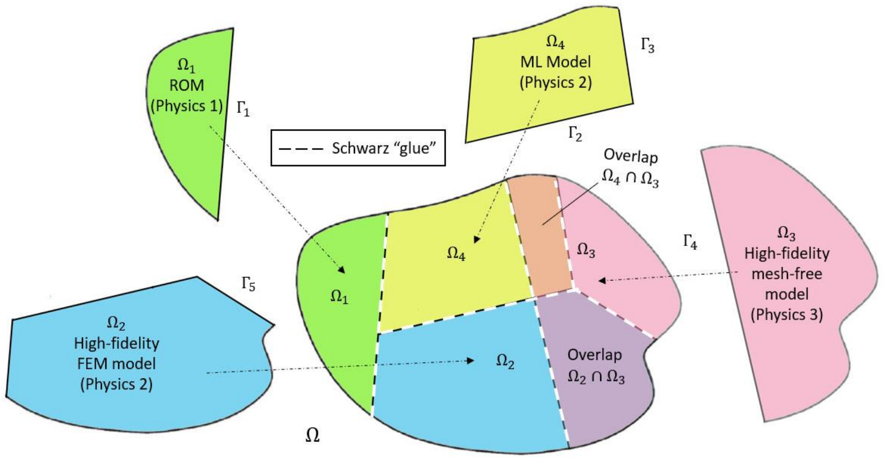
- Extension to FOM*-ROM# and ROM-ROM Coupling

- **Numerical Examples**
    - ➢ 2D Burgers Equation
    - ➢ **2D Shallow Water Equations**
    - ➢ Teaser: 2D Euler Equations Riemann Problem

- Summary & Future Work







*Full-Order Model. #Reduced Order Model.

2D Shallow Water Equations (SWE)

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

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

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

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

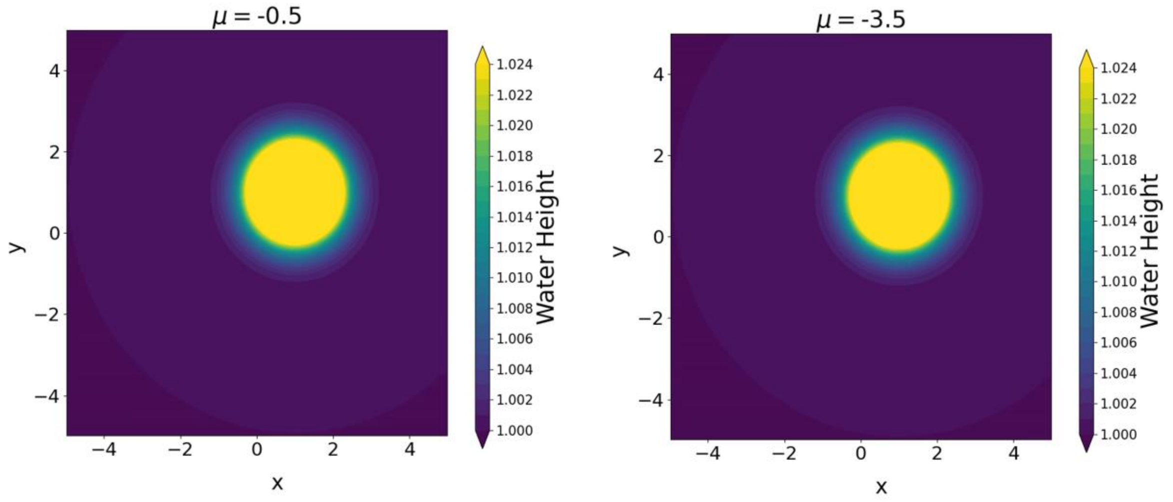


Figure above: FOM solutions to SWE for $\mu = -0.5$ (left) and $\mu = -3.5$ (right).

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)

Pressio

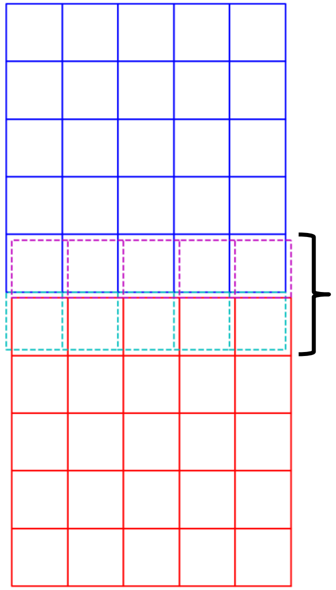
Schwarz Coupling Details

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!

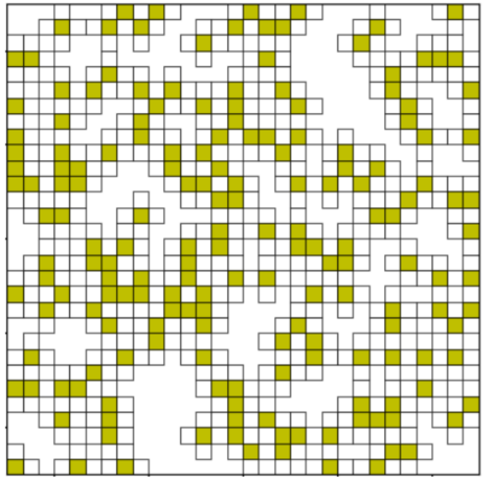


Figure above: sample mesh (yellow) and stencil (white) cells

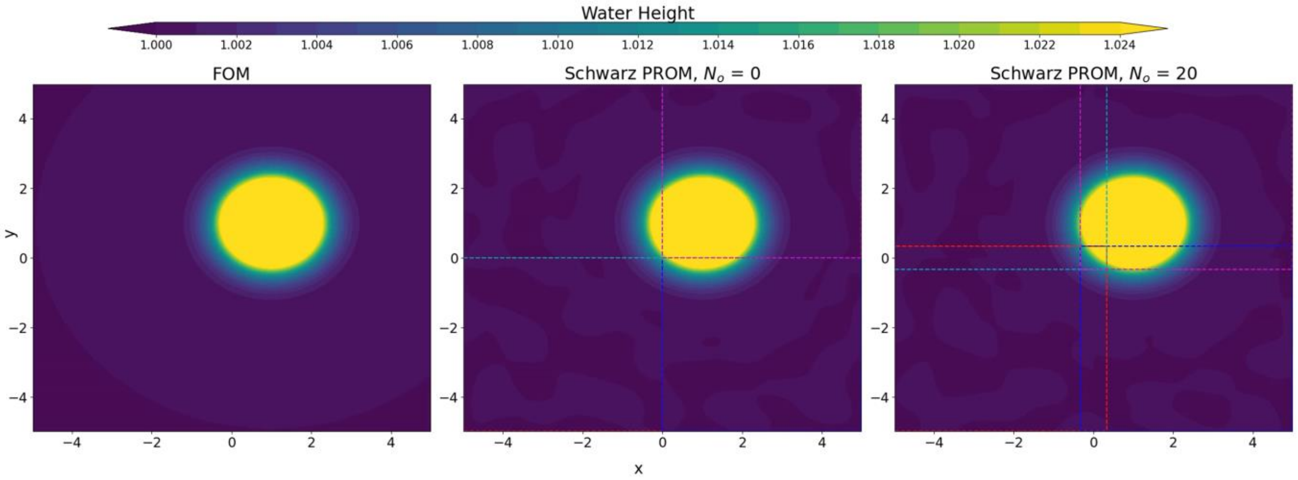
Choice of hyper-reduction

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

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

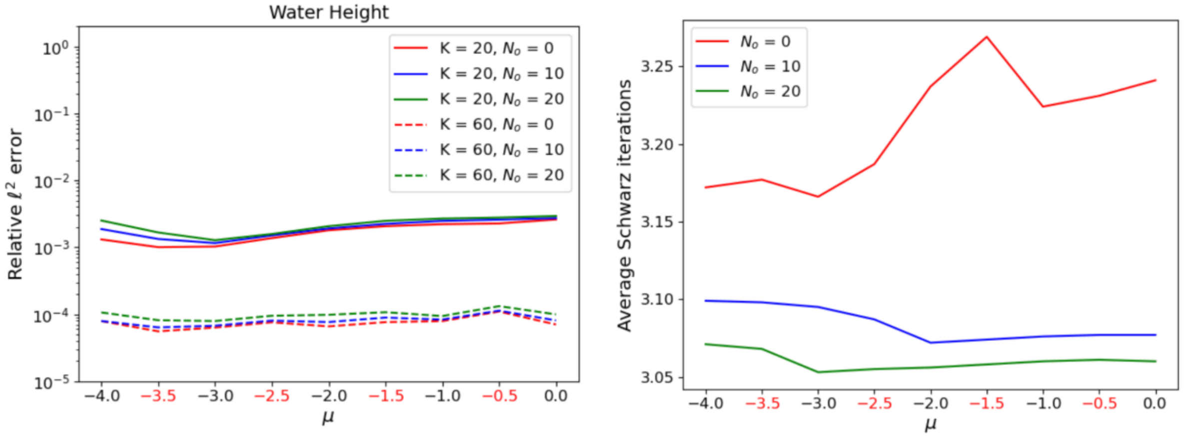
Schwarz All-ROM Domain Overlap Study

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)



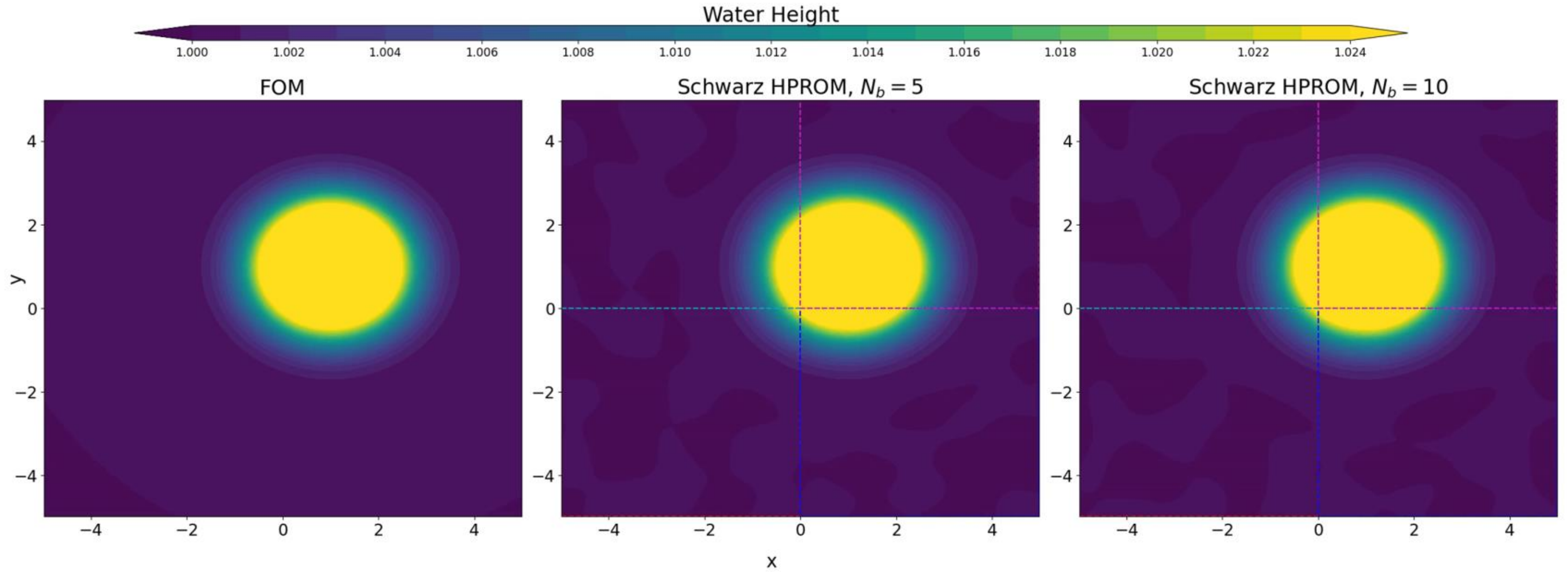
Figures above: relative error and average # Schwarz iterations as a function of μ and N_o. Black μ: training, red μ: testing.

- **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.

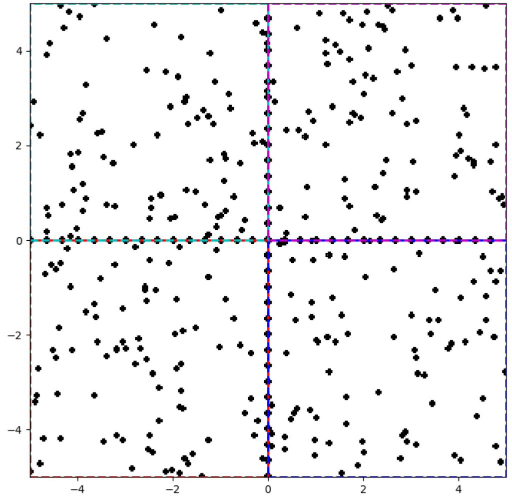
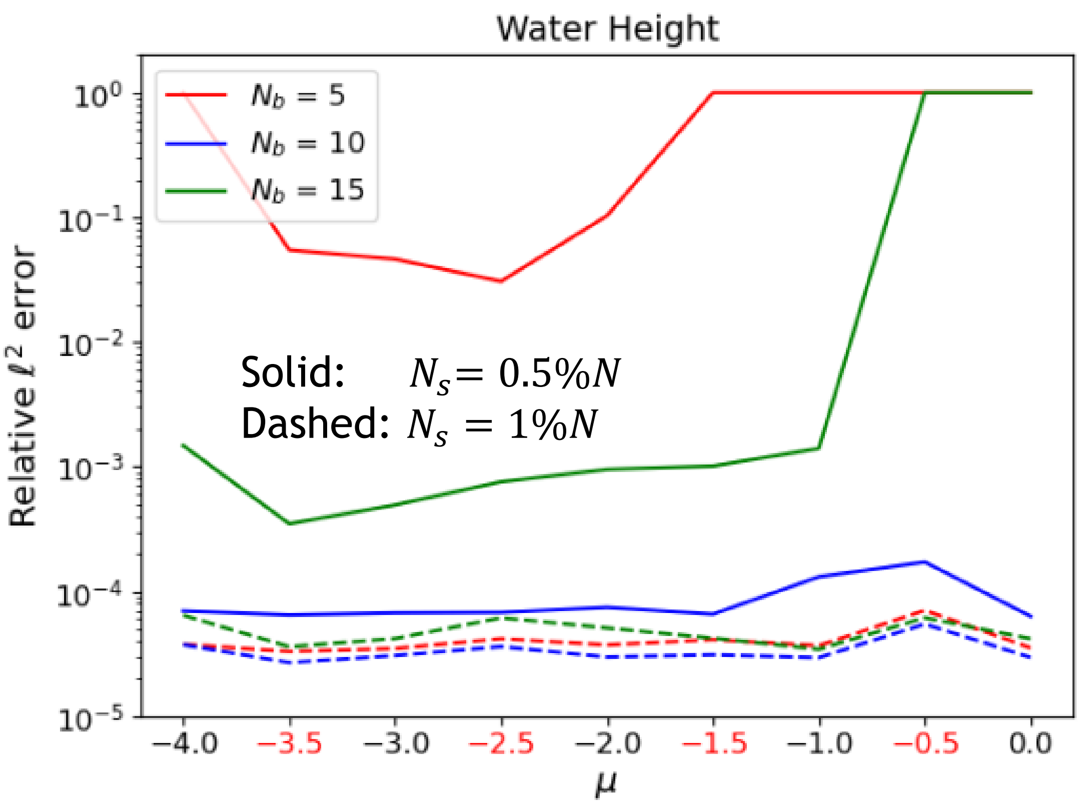
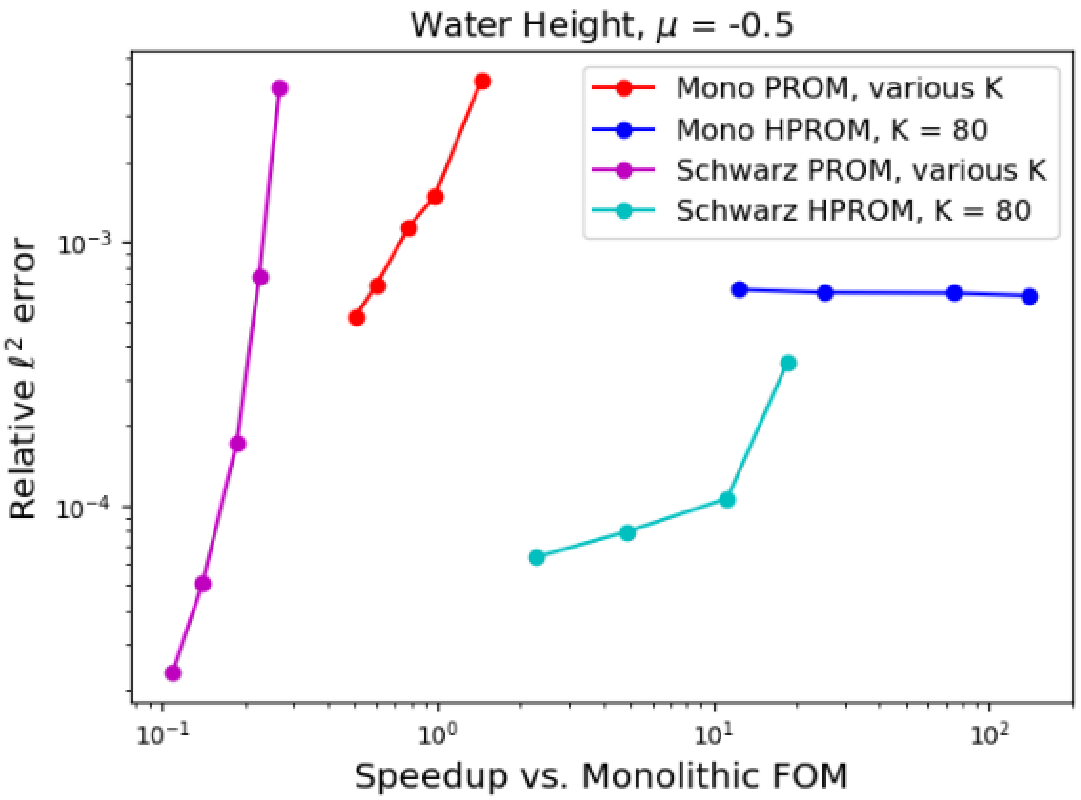


Figure above: example sample mesh with sampling rate $N_b = 10\%$

- 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 ~**10% boundary sampling** (movie above, right-most frame)

Coupled HROM Performance



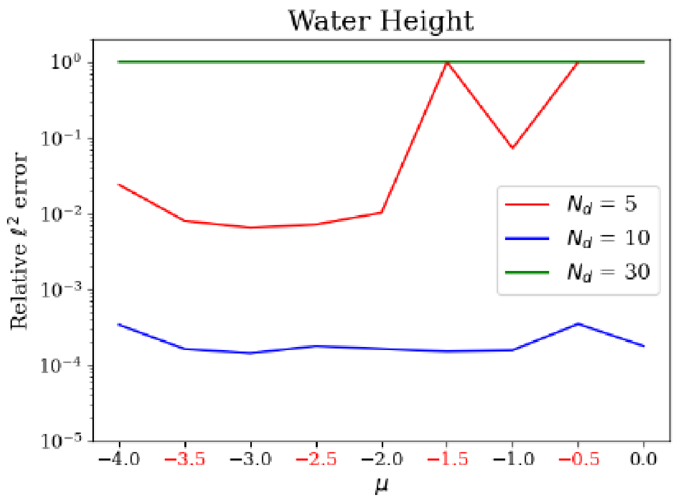


- For a fixed ROM dimension, Schwarz delivers **lower error** and **comparable cost!**
- There are noticeable **cost savings** relative to **monolithic FOM!**
- Accuracy similar for **predictive** μ (red) and **non-predictive** μ (black) cases.

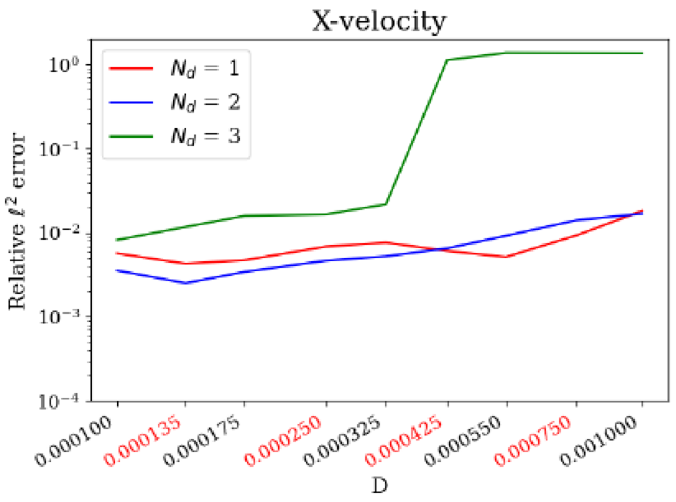
Hyper-reduced ROMs: Impact of Boundary Sampling

Key result: given a **fixed "budget"** of **sample mesh points**, there is a (problem-dependent) **optimal number** of **sample mesh points** to allocate to the **Schwarz boundaries** vs. the **subdomain interiors**.

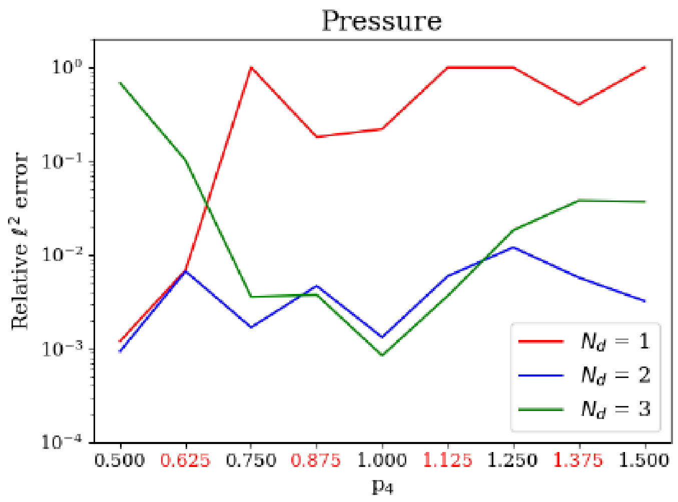
- There is a delicate balance of ensuring **BC transmission** together with an **accurate interior solutions**
- More **extensive boundary sampling** is required for problems with **shocks** (Burgers, Euler)



SWE, $N_s = 0.5\%N$



Burgers', $N_s = 3.75\%N$



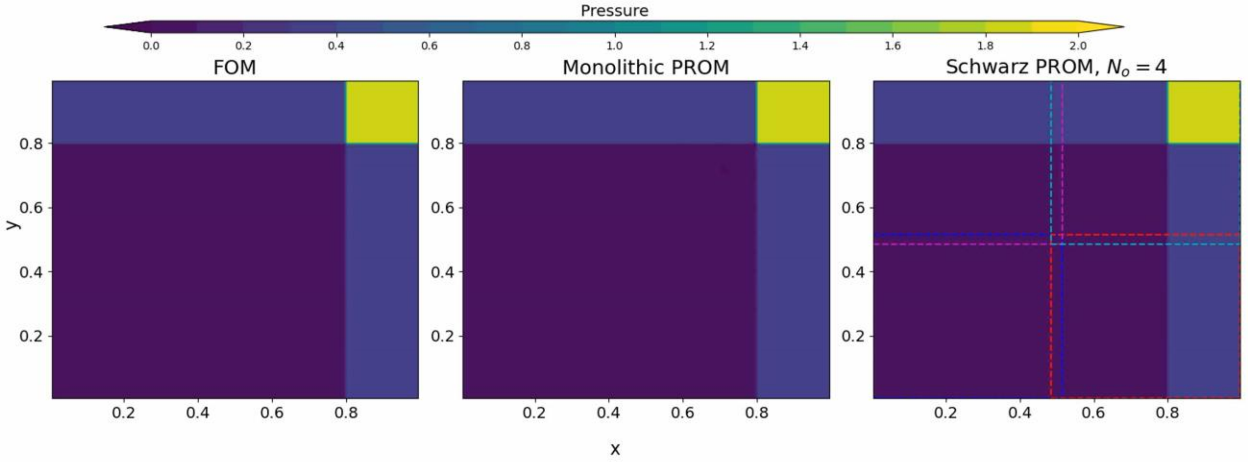
Euler, $N_s = 5\%N$

Red parameter values are predictive.

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**

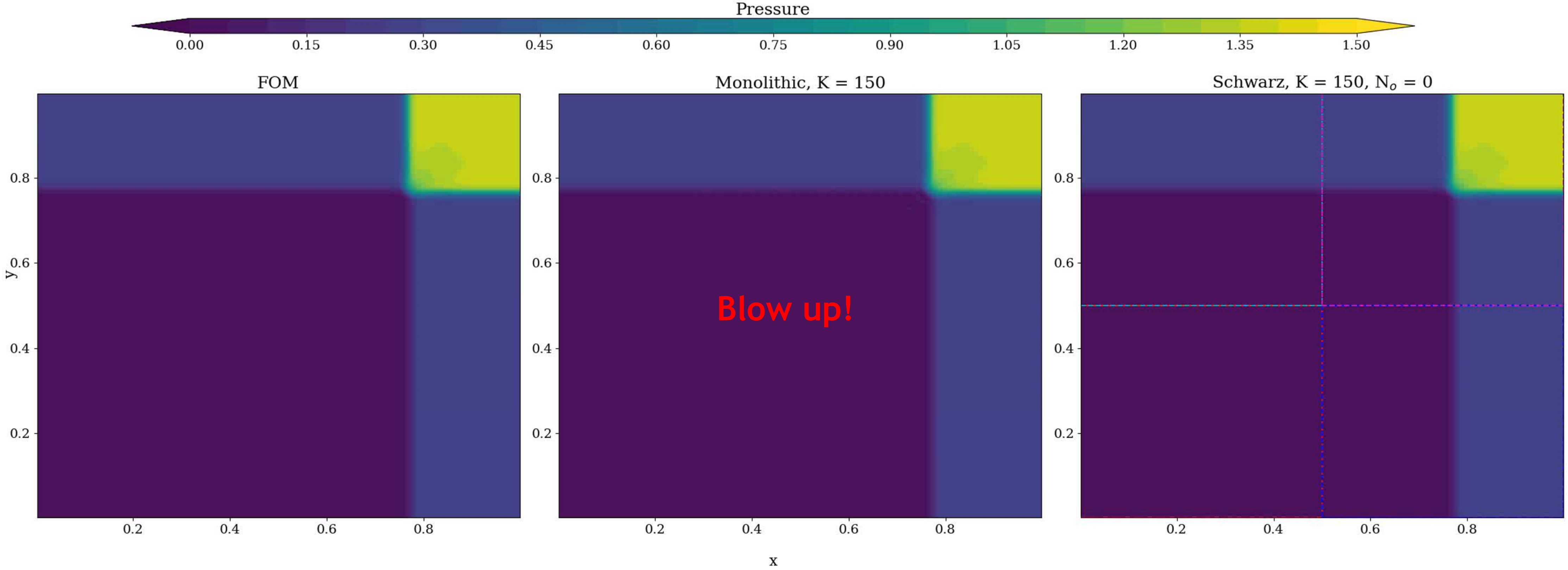
FOM discretization:

- 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.

Unsampled ROMs: Stabilization Effects

***Key result*: domain decomposition + Schwarz coupling** can **stabilize** an otherwise unstable monolithic solution



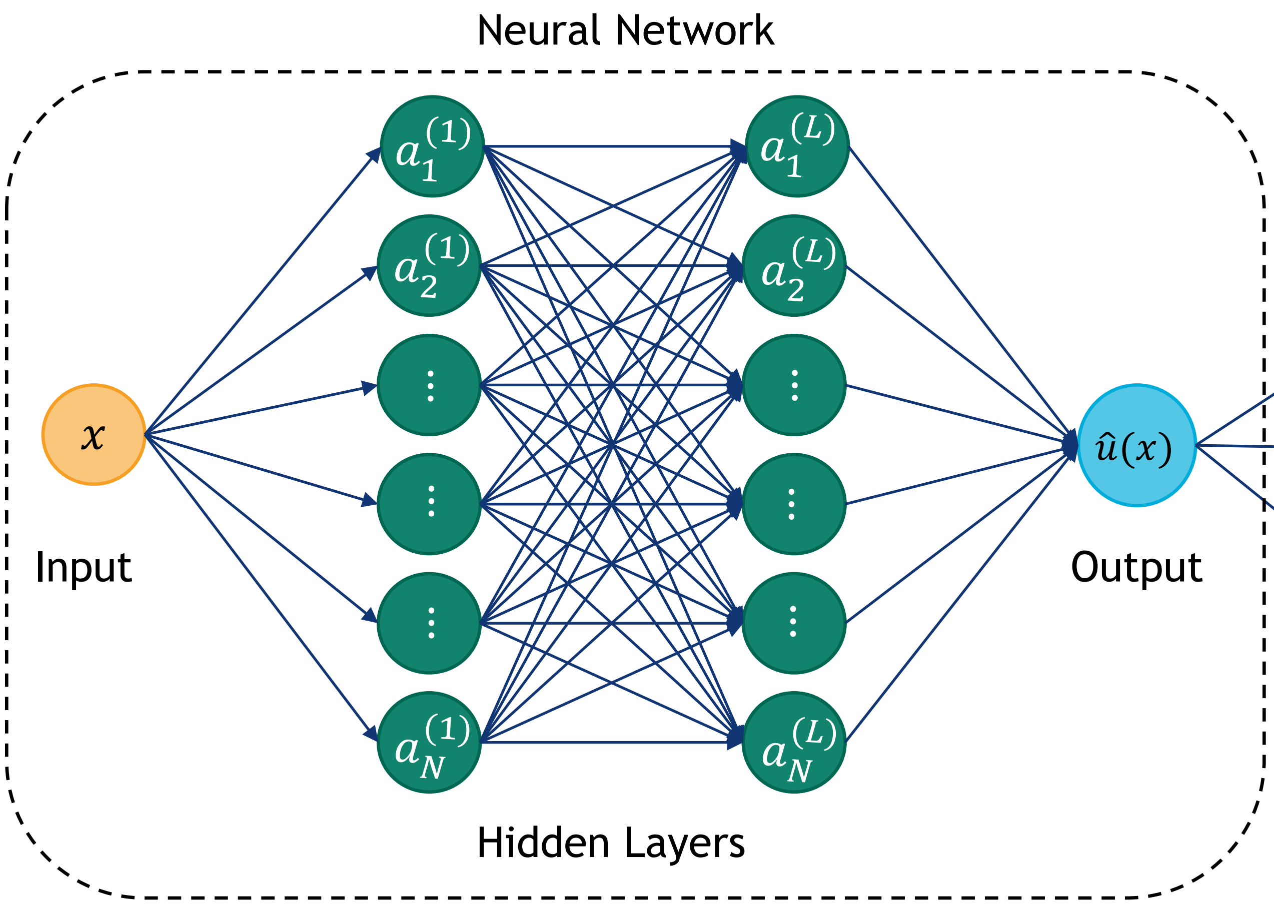
Movie above: monolithic vs. decomposed ROM for Euler problem with $p_4 = 1.375$ (predictive regime).

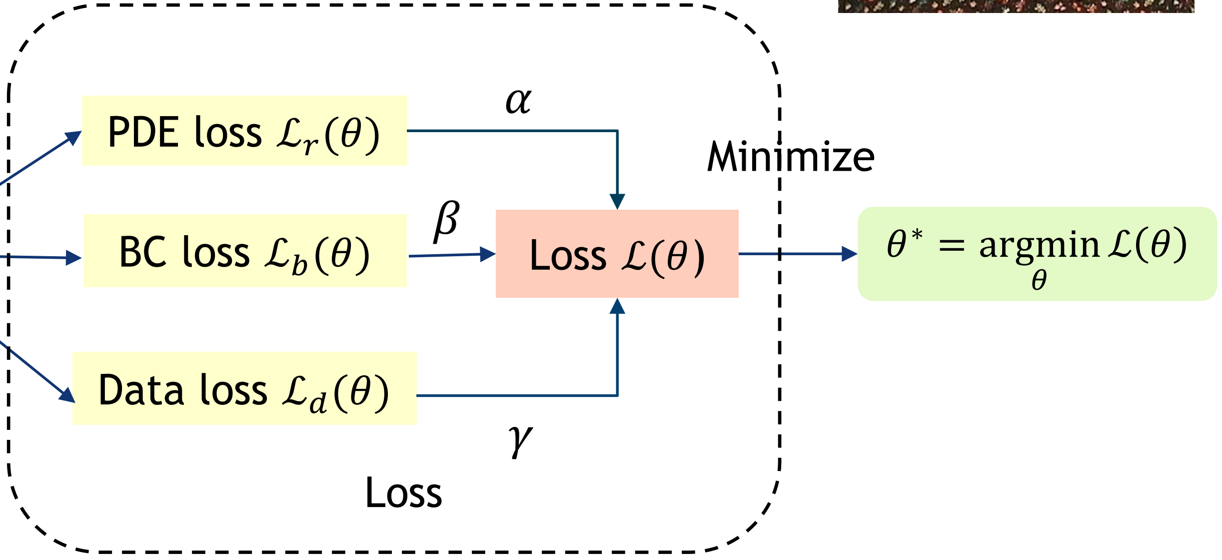
Summary

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.

Bonus: PINN-PINN and PINN-FOM coupling





$$\mathcal{L}(\theta) = \alpha_r \mathcal{L}_r(\theta) + \alpha_b \mathcal{L}_b(\theta) + \alpha_d \mathcal{L}_d(\theta)$$

Will Snyder
Summer Intern
Virginia Tech

Goal: investigate the use of the Schwarz alternating method as a means to couple **Physics-Informed Neural Networks (PINNs)**

Focus thus far

Scenario 1: use Schwarz to train subdomain PINNs (offline)

Scenario 2: use Schwarz to couple pre-trained subdomain PINNs/NNs (online)

Related work: Li et al., 2019, Li et al., 2020, Wang et al., 2022.

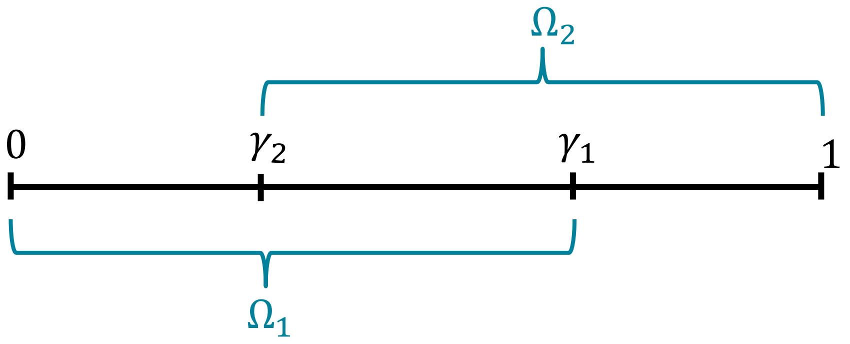
Bonus: PINN-PINN coupling

1D steady **advection-diffusion** equation on $\Omega = [0,1]$:

$$u_x - \nu u_{xx} = 1, \quad u(0) = u(1) = 0$$

PINNs are **notoriously difficult to train** for higher Peclet numbers!

Can Schwarz help?



Overlapping DD: $\Omega = \Omega_1 \cup \Omega_2$ with boundary $\partial\Omega = \{0,1\}$

$$\mathcal{L}_{r,i}(\theta) = MSE\left(-\nu\nabla_x^2 NN_{\Omega_i}(x,\theta) + \nabla_x NN_{\Omega_i}(x,\theta) - 1\right)$$

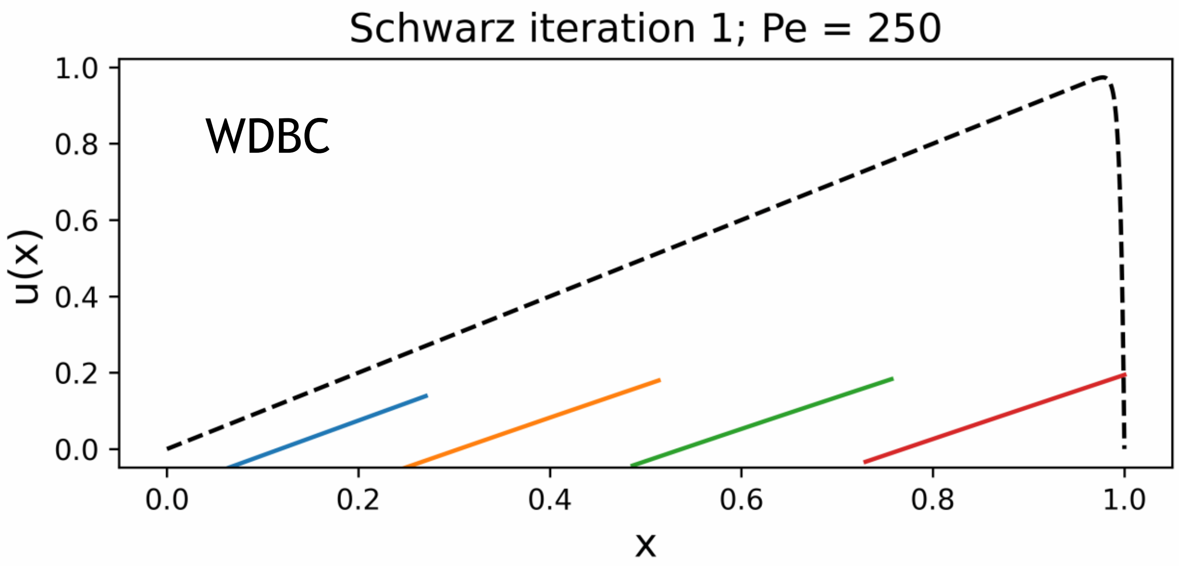
$$\mathcal{L}_{b,i}(\theta) = MSE\left(NN_{\Omega_i}(\partial\Omega,\theta)\right) + MSE\left(NN_{\Omega_i}(\gamma_i,\theta) - NN_{\Omega_j}(\gamma_i,\theta)\right)$$

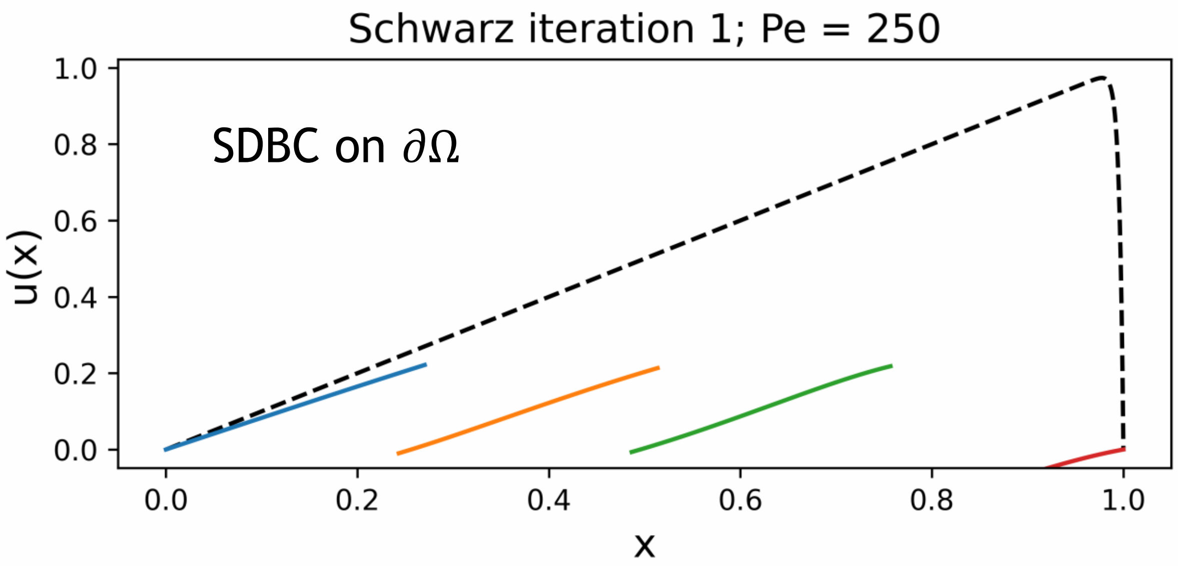
Schwarz PINN training algorithm:

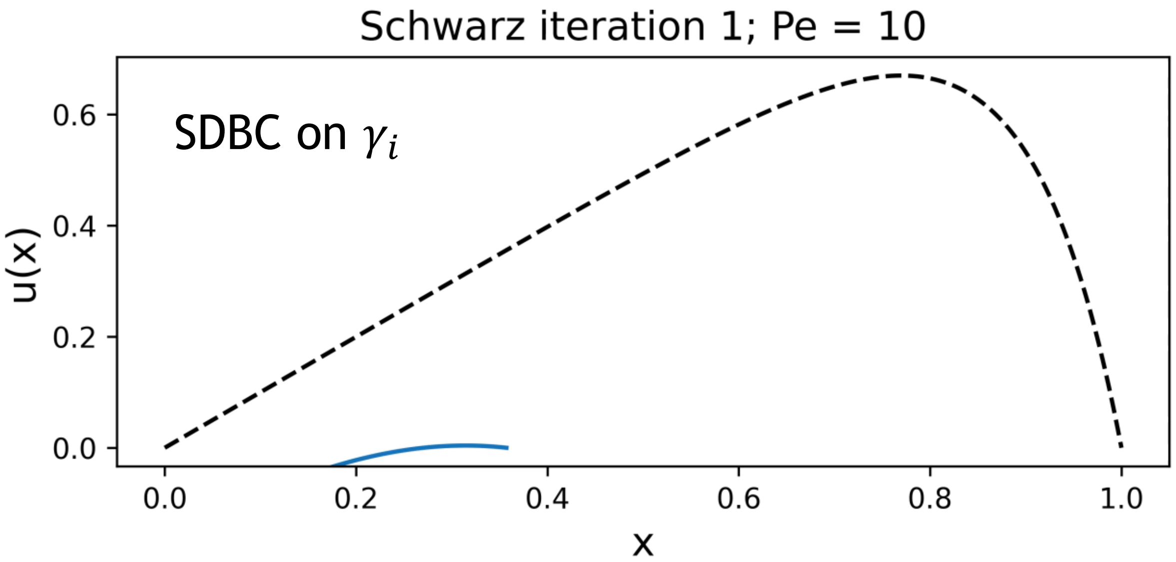
Loop over subdomains Ω_i until convergence of Schwarz method

- **Train** PINN in Ω_i with loss $\mathcal{L}_i(\theta) = \alpha\mathcal{L}_{r,i}(\theta) + \beta\mathcal{L}_{b,i}(\theta) + \gamma\mathcal{L}_{d,i}(\theta)$
- **Communicate** Dirichlet data between neighboring subdomains
- **Update** boundary data on γ_i from neighboring subdomains
- If **strong enforcement of Dirichlet BC (SDBC)**, set $\hat{u}_{\Omega_i}(x,\theta) = NN_{\Omega_i}(x,\theta)$
- If **weak enforcement of Dirichlet BC (WDBC)**, set $\beta = 0$ and $\hat{u}_{\Omega_i}(x,\theta) = v(x)NN_{\Omega_i}(x,\theta) + \psi(x)\hat{u}_{\Omega_j}(\gamma_j,\theta)$ where $v(x)$ is chosen s.t. $v(0) = v(\gamma_i) = v(1) = 0$ and $\psi(x)$ is chosen s.t. $v(\gamma_i) = 1$

Bonus: PINN-PINN coupling

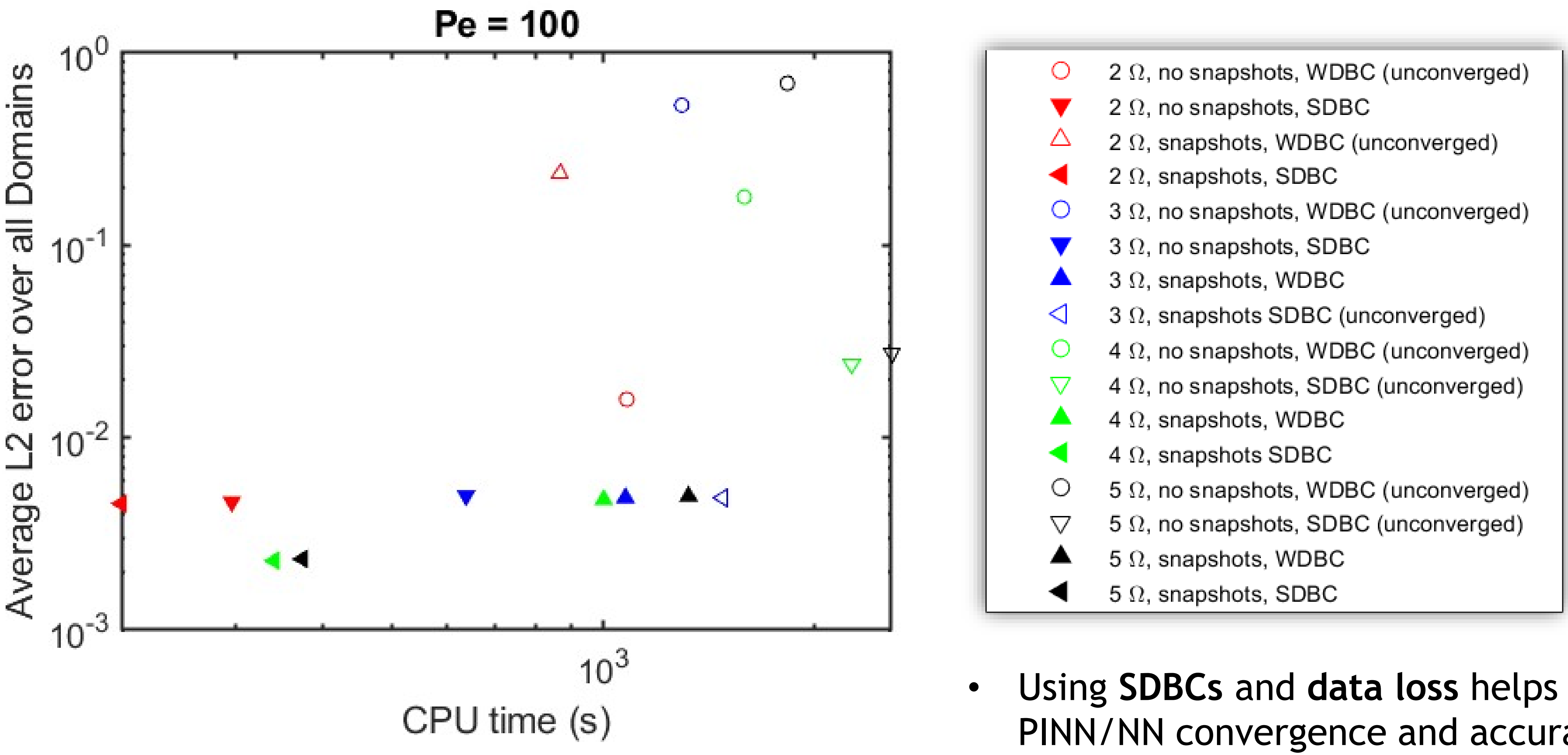






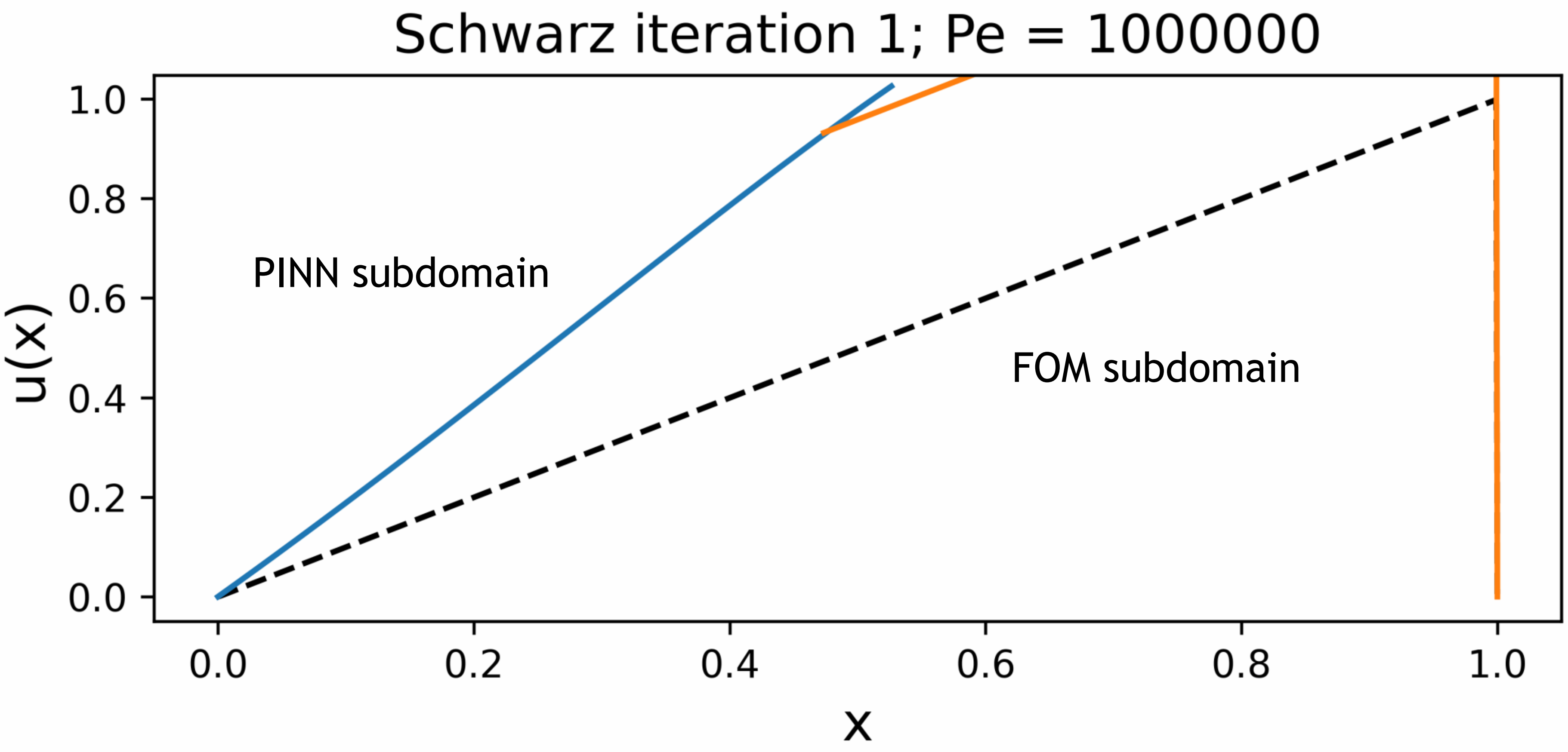
- How **Dirichlet boundary conditions** are handled has a large impact on PINN convergence
- Convergence not improved in general with **increasing overlap**
- Increasing **# subdomains** in general will increase CPU time

Bonus: PINN-PINN coupling



- Using **SDBCs** and **data loss** helps with PINN/NN convergence and accuracy

Bonus: PINN-FOM coupling



- PINN-FOM coupling gives **rapid PINN convergence** for **arbitrarily high Peclet numbers**
- PINN-FOM couplings works with **both WDBC and SDBC** configurations

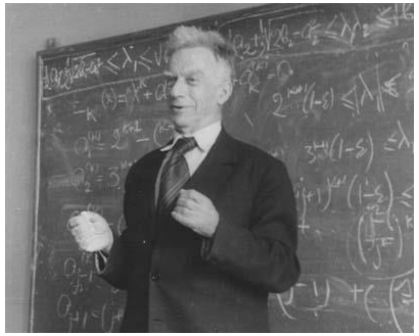
Theoretical Foundation

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

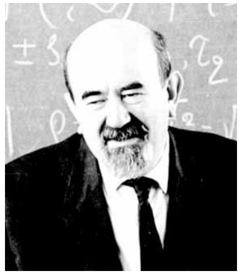
- **S.L. Sobolev (1936):** posed Schwarz method for ***linear elasticity*** in variational form and ***proved method's convergence*** by proposing a convergent sequence of energy functionals.
- **S.G. Mikhlin (1951):** ***proved convergence*** of Schwarz method for general linear elliptic PDEs.
- **P.-L. 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.***

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

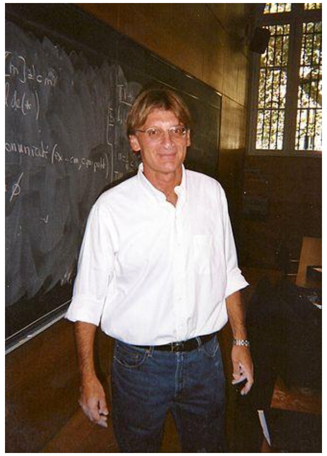
$$\nabla\cdot\boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



S.L. Sobolev (1908 – 1989)



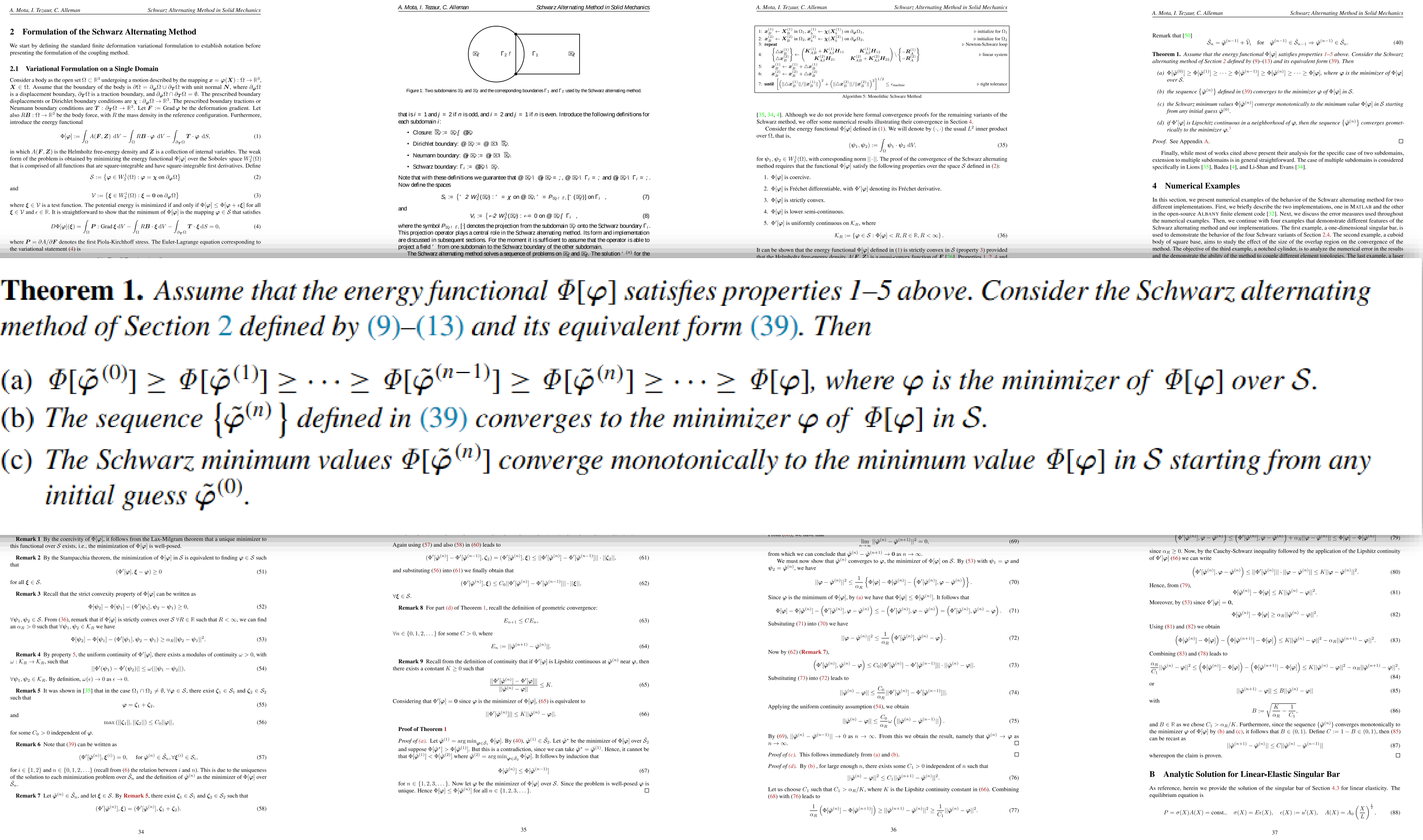
S.G. Mikhlin (1908 – 1990)



P.- L. Lions (1956-)

A. Mota, I. Tezaur, C. Alleman

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

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

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:

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

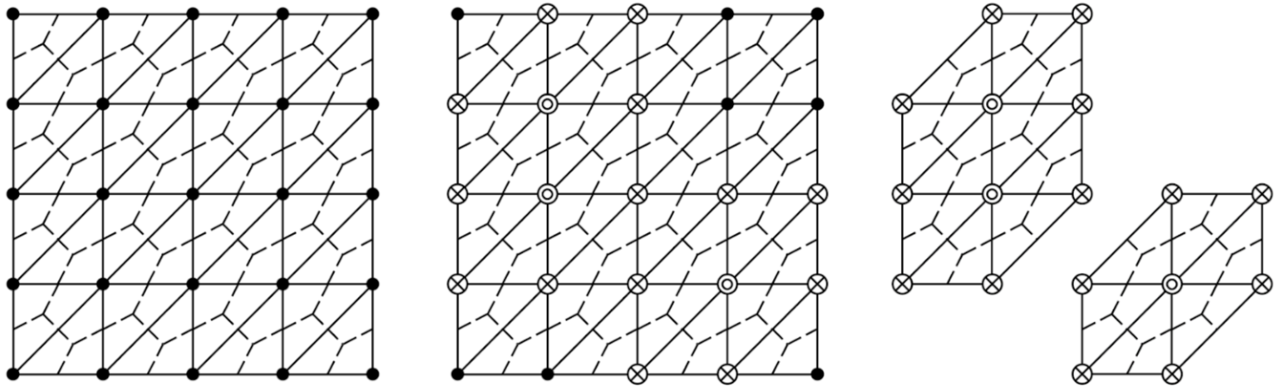
  - $\delta^2 S[\boldsymbol{\varphi}_h]$ can always be made positive by choosing a ***sufficiently small*** Δt
  - Numerical experiments reveal that Δt requirements for ***stability/accuracy*** typically lead to automatic satisfaction of this bound.

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

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

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

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

- Solve the above optimization problem using a **non-negative least squares solver** with an **early termination condition** to **promote sparsity** of the vector $\boldsymbol{\xi}$

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).

- Start with a physics-based FOM that can be written to have a specific structure, e.g., quadratic structure:

$$\dot{\boldsymbol{q}} + \boldsymbol{A}\boldsymbol{q} + \boldsymbol{H}(\boldsymbol{q} \times \boldsymbol{q}) = \boldsymbol{0}$$

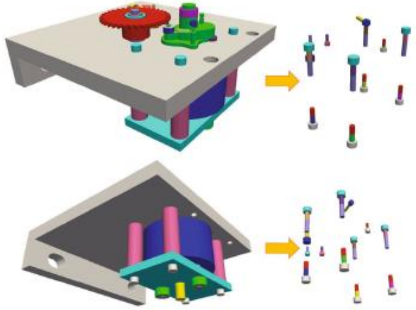
- Use lens of projection to define the functional form of a ROM for (1):

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

- Learn ROM operators in (2) from FOM data by solving the following least-squares minimization problem:

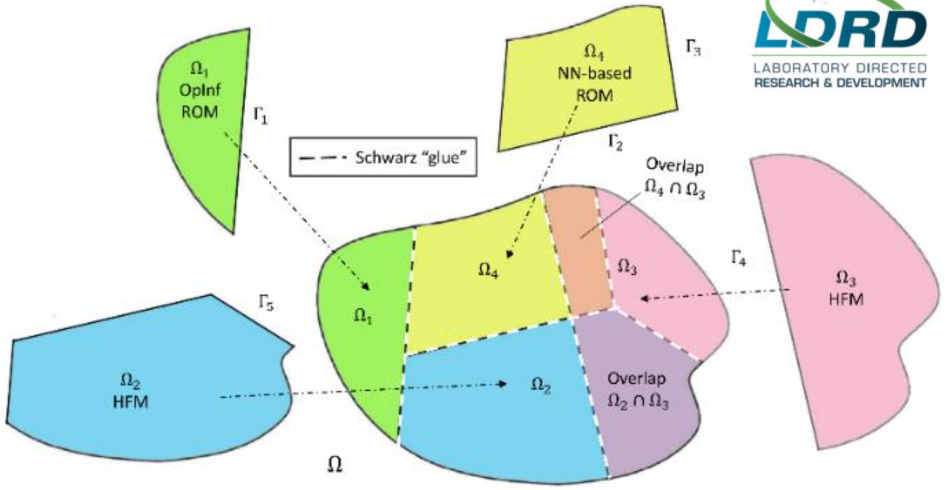
$$\min_{\widehat{\boldsymbol{A}},\widehat{\boldsymbol{H}}} \left\| \dot{\widehat{\boldsymbol{Q}}}^T + \widehat{\boldsymbol{Q}}^T \widehat{\boldsymbol{A}}^T + (\widehat{\boldsymbol{Q}} \otimes \widehat{\boldsymbol{Q}})^T \widehat{\boldsymbol{H}}^T \right\|_F^2$$

New Project: Adaptive Hybrid modEls via domAin Decomposition (AHEAD)

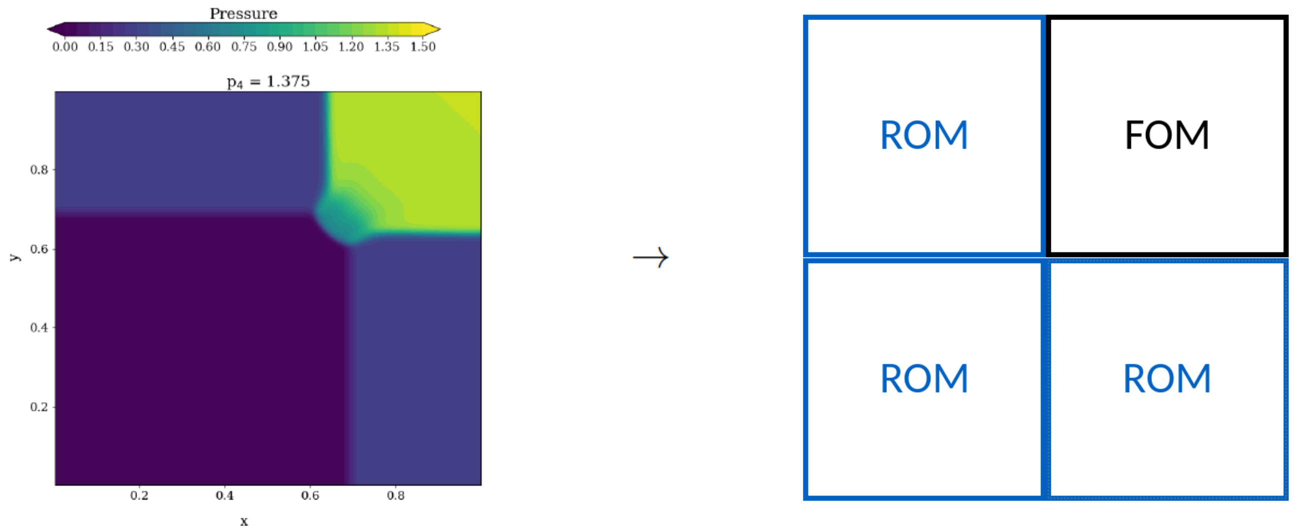


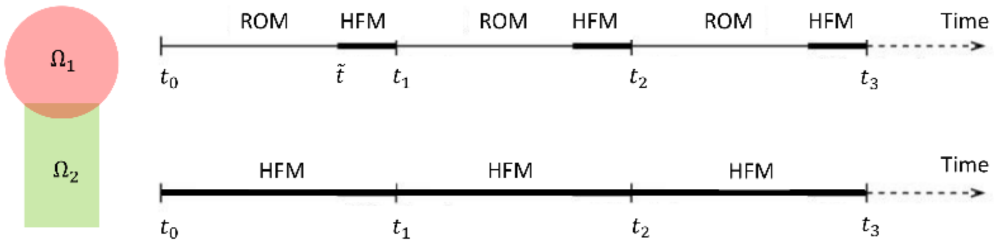
Goals (for solid mechanics exemplars):

- **Simplify meshing** via Schwarz + DD
- Extend Schwarz to **non-intrusive ROMs** (Operator Inference, NN)
- Development of **automated criteria** to determine appropriate use of less refined or reduced-order models without sacrificing accuracy, enabling **real-time transitions** between different model fidelities



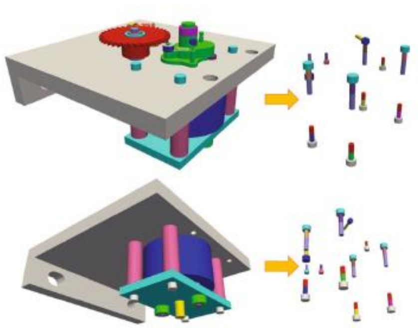
Example sample DD and ROM/FOM assignment.





On-the-fly model switching in our DD workflow.

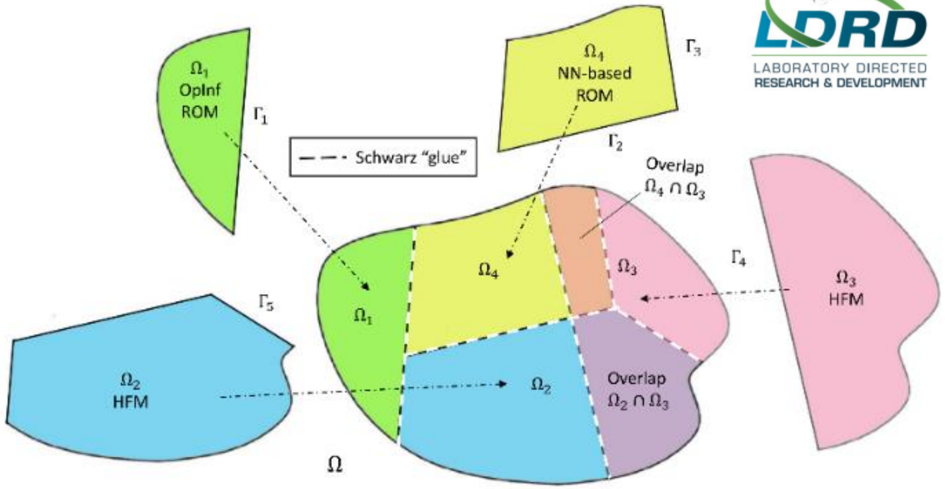
New Project: Adaptive Hybrid modEls via domAin Decomposition (AHEAD)



LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Goals (for solid mechanics exemplars):

- **Simplify meshing** via Schwarz + DD
- Extend Schwarz to **non-intrusive ROMs** (Operator Inference, NN)
- Development of **automated criteria** to determine appropriate use of less refined or reduced-order models without sacrificing accuracy, enabling **real-time transitions** between different model fidelities



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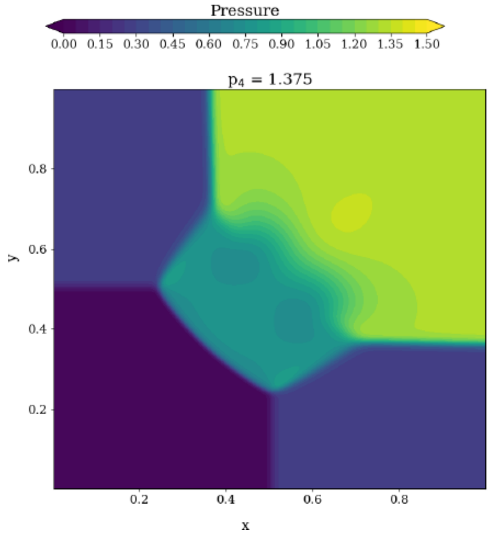

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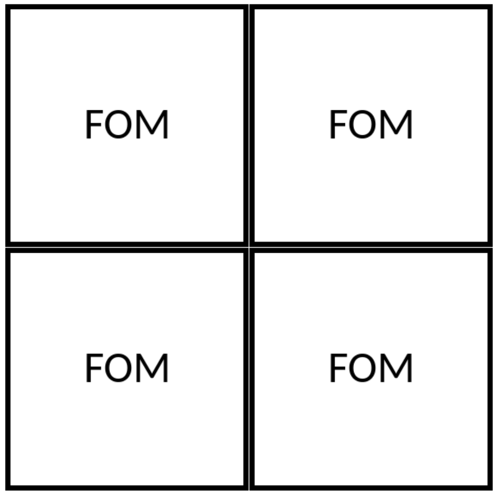

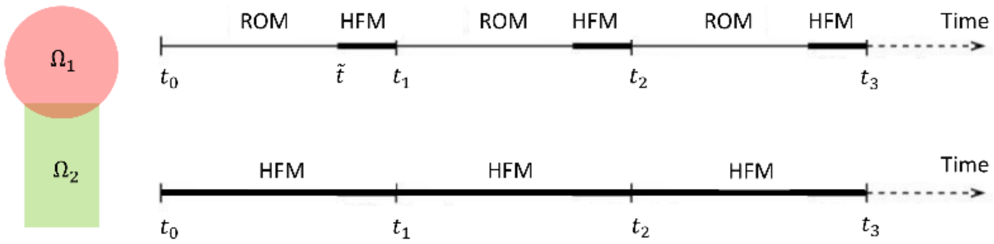

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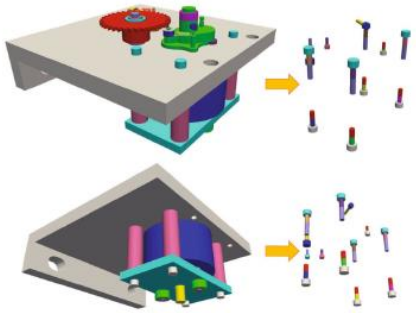

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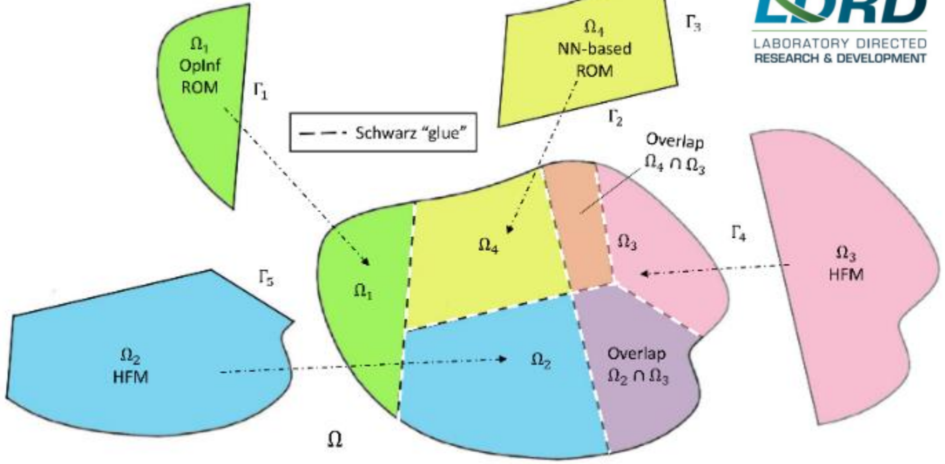

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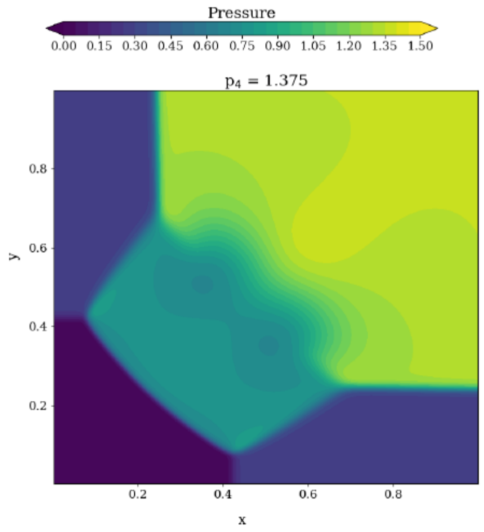
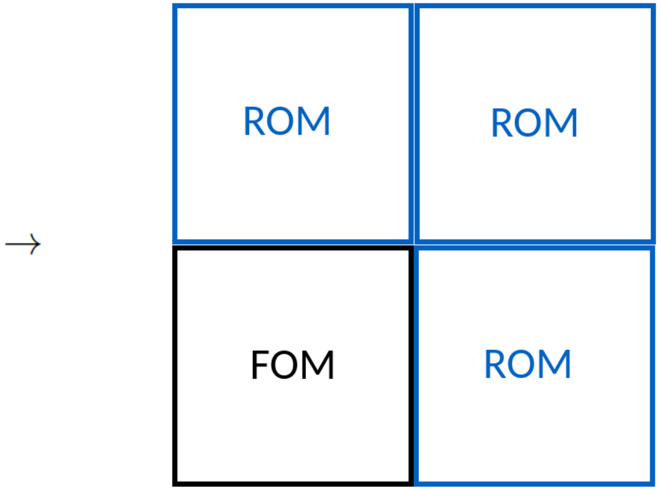
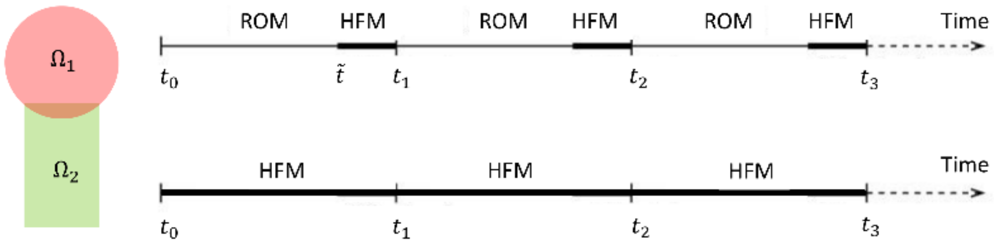






On-the-fly model switching in our DD workflow.

1D Linear Elastic Wave Propagation in a Clamped Beam

- ***1D linear elastic beam*** geometry $\Omega = (-0.5, 0.5)$, clamped at both ends, with prescribed initial condition, $\Delta x = 1 \times 10^{-3}$, $\Delta t = 1 \times 10^{-7}$, $T_{max} = 1 \times 10^{-3}$ and $\nu = 0$.
- Very ***stringent test*** for discretization/coupling methods and ROMs.
- ***Overlapping DD***: $\Omega_1 = (-0.5, 0.25)$ and $\Omega_2 = (-0.25, 0.5)$
- ***Prediction*** across ***different initial conditions (ICs)***:
  - ➢ Train with data from symmetric Gaussian IC (10K snapshots)
  - ➢ Predict with rounded square initial condition
- ***Linear OpInf***, with ***regularization*** $\gamma = 1 \times 10^{-11}$

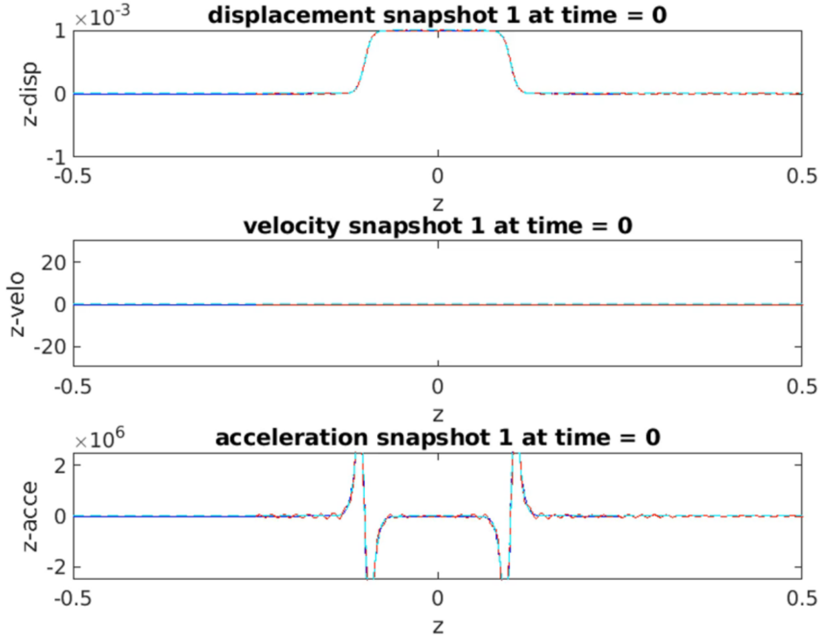


Figure above: cyan = exact analytical, blue/red = FOM/OpInf computed.

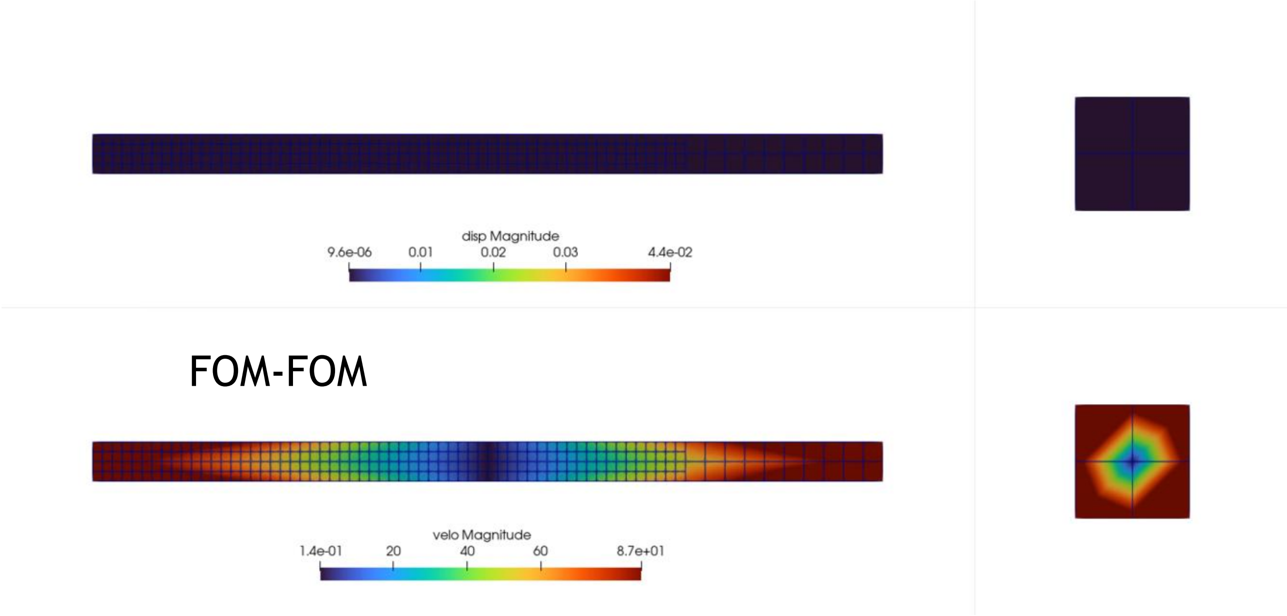
Key result: similar **accuracy** for predictive and reproductive cases. **Convergence** with basis size M is observed

	Reproductive			**Predictive**		
	Displacement	**Velocity**	**Acceleration**	**Displacement**	**Velocity**	**Acceleration**
FOM-FOM	6.50e-3	8.02e-2	2.5e-1	6.5e-3	8.02e-2	2.52e-1
FOM-OpInf ($M = 15$)	6.30e-2	4.50e-1	8.18e-1	7.48e-2	5.21e-1	8.82e-1
FOM-OpInf ($M = 30$)	1.44e-2	1.66e-1	4.46e-1	1.70e-2	2.01e-1	5.25e-1
FOM-OpInf ($M = 60$)	6.11e-3	7.67e-2	2.38e-1	6.53e-3	8.02e-2	2.60e-1

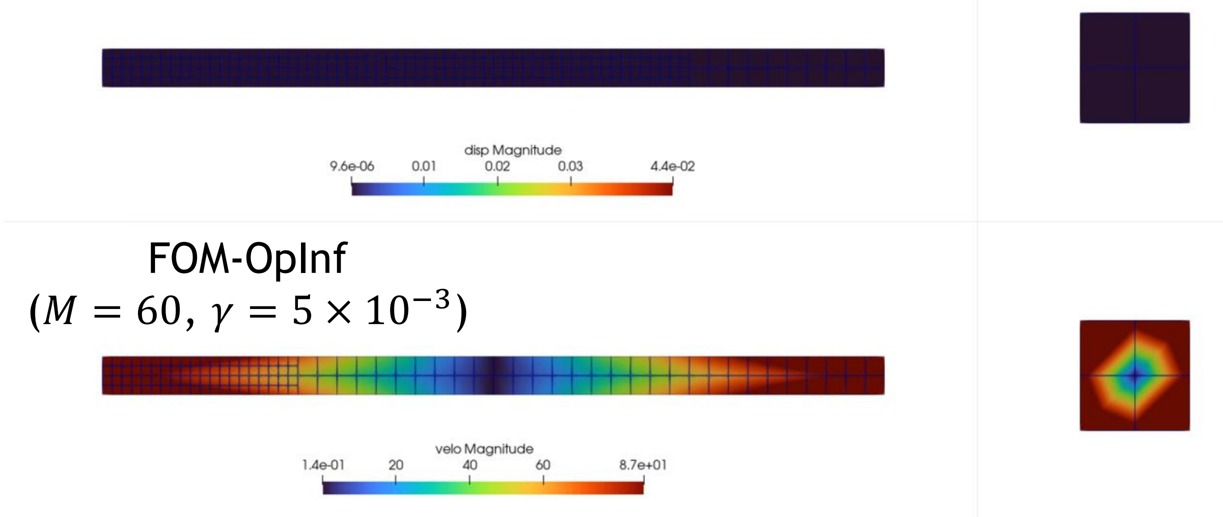
Table left: relative errors w.r.t. exact analytical solution

3D Hyperelastic Torsion Problem

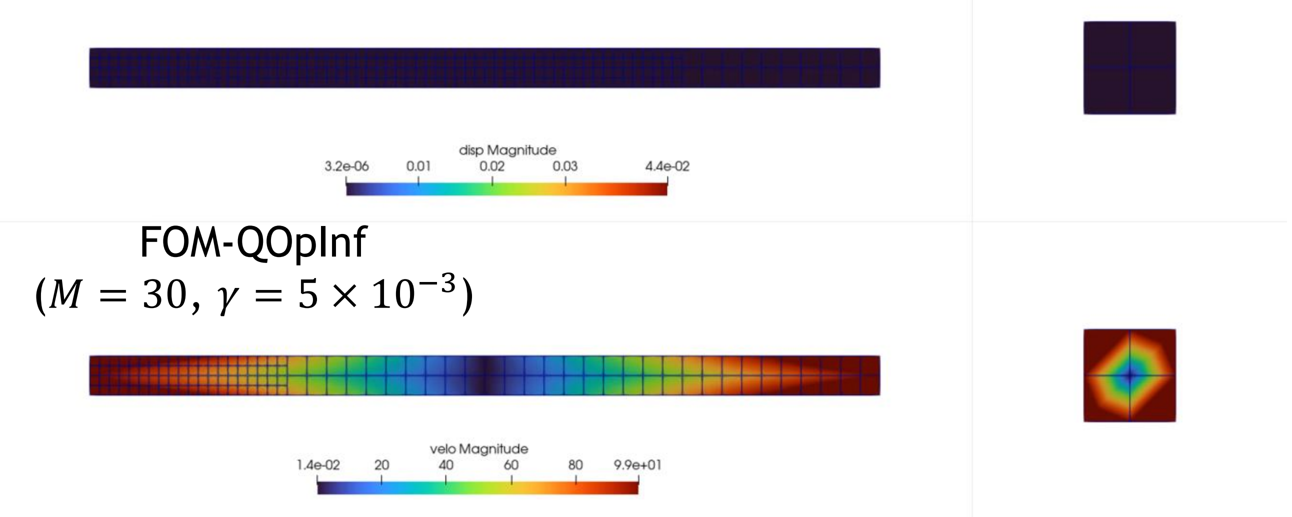
- ***Dynamic nonlinear hyperelastic bar*** subjected to high degree of ***torsion***
- ***Saint-Venant Kirchhoff*** material model, which gives rise to PDEs with ***cubic nonlinearities***.
- ***Overlapping*** DD of Ω into ***two subdomains***, discretized with ***nonconformal HEX8 meshes***
- Evaluated ***reproductive FOM-OpInf*** couplings with ***linear***, ***quadratic*** and ***cubic OpInf ROMs*** built from 2K snapshots.
- ***Best displacement relative errors*** (quadratic OpInf): 1.94% in Ω_1 and 3.78% in Ω_2



Key result: **quadratic** and **cubic** OpInf models can produce **stable** and **accurate** solutions (whereas linear OpInf blows up) but are extremely **sensitive** to γ.



FOM-OpInf ($M = 60$, $\gamma = 5 \times 10^{-3}$)

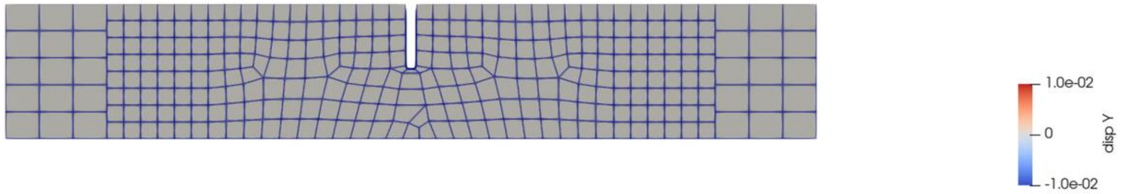


FOM-QOpInf ($M = 30$, $\gamma = 5 \times 10^{-3}$)

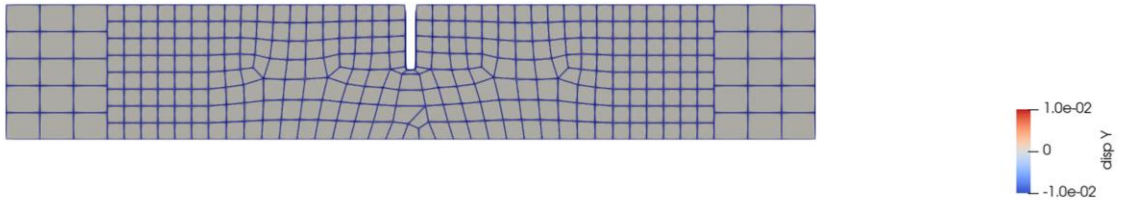
3D Hyperelastic Laser Weld Problem

- ***Nonlinear hyperelastic laser weld*** geometry pulled dynamically from both ends at rate of $0.1t$ and run to $T_{max} = 0.1$ with $\Delta t = 0.001$.
- ***Neohookean material model***, which gives rise to PDE with ***non-polynomial nonlinearities***
- ***Overlapping*** DD of Ω into ***three subdomains***, discretized with ***nonconformal HEX8 meshes***
- FOM in Ω_1 and Ω_2, ***linear OpInf*** ROM with $M = 20$ in Ω_3
  - ➢ Problem is ***nonlinear*** but dynamics away from laser weld are ***linear***.
- ***Reproductive*** problem, ***regularization*** $\gamma = 1 \times 10^{-4}$
- ***Relative errors in y-displacement***: 0.61% in Ω_1, 4.4% in Ω_2 and 14% in Ω_3

FOM-FOM-FOM



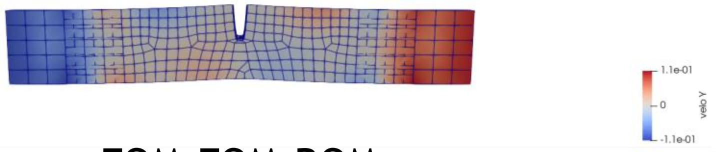
FOM-FOM-ROM



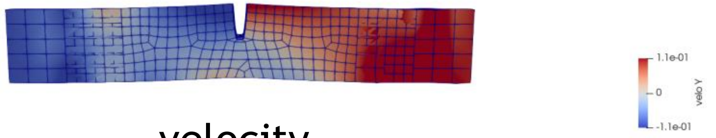
Movies above: y-displacement for coupled models.

***Key result:* linear OpInf ROMs** within coupled FOM-ROM models can give **reasonably accurate results** for nonlinear problems if used in appropriate (linear dynamics) regions.

FOM-FOM-FOM

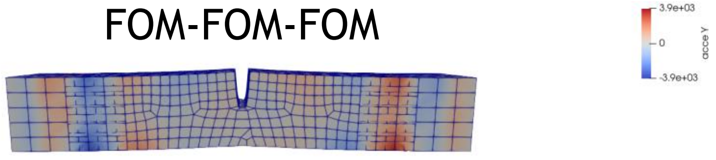


FOM-FOM-ROM

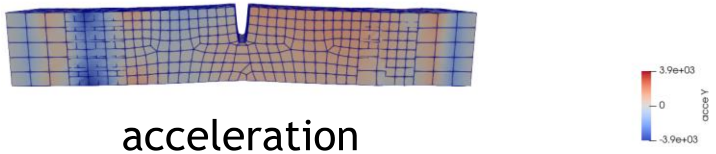


velocity

FOM-FOM-FOM



FOM-FOM-ROM



acceleration

Figures left: y-velocity and y-acceleration solutions at final time.

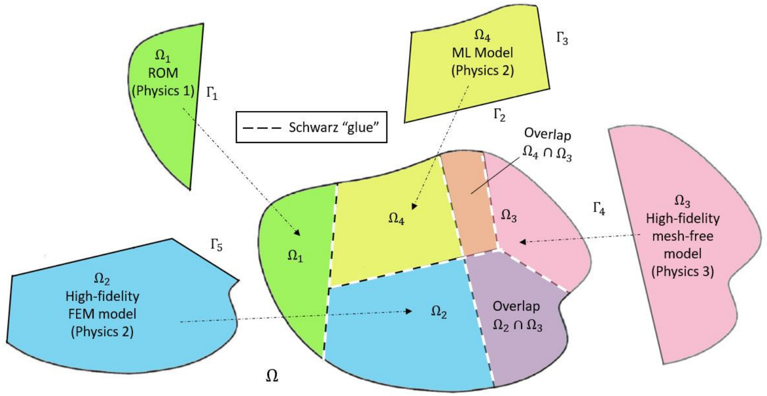
Summary and Ongoing/Future Work

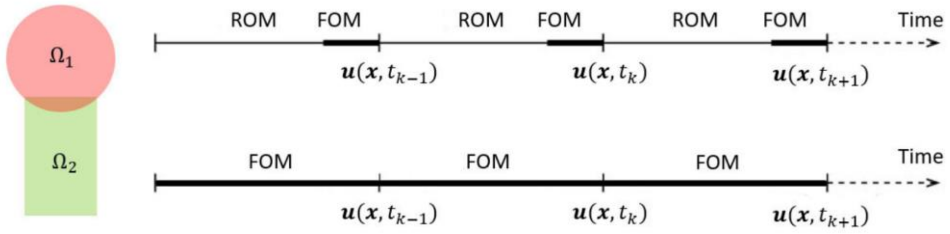
Summary:

- Schwarz has been **demonstrated** for **coupling** of FOMs and (H)ROMs
- **Computational gains** can be achieved by coupling **HROMs** and using the **additive Schwarz** variant
- Interesting **new results** regarding **interface sampling** & **non-overlapping transmission BCs** for CCFV

Ongoing & future work:

- Extension to **other applications** (fasteners, laser welds)
- **Rigorous analysis** of why Dirichlet-Dirichlet BC "work" when employing non-overlapping Schwarz with discretizations that employ ghost cells
- **Learning** of **"optimal" transmission conditions** to ensure **structure preservation**
- Extension of Schwarz to enabling coupling of **non-intrusive ROMs** (e.g., OpInf, Neural Networks)
- Development of **automated criteria** to determine appropriate use of less refined or reduced-order models without sacrificing accuracy, enabling **real-time transitions** between different model fidelities → ***New project***: AHEAD LDRD





* https://pressio.github.io