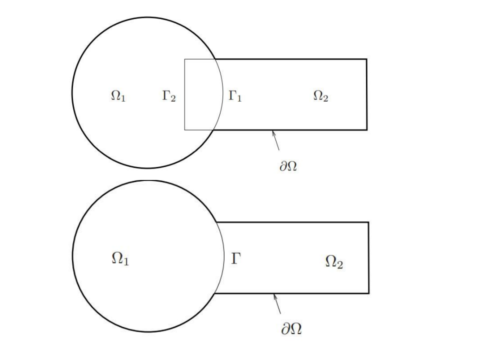
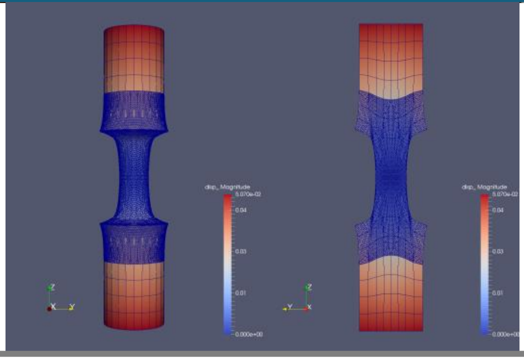
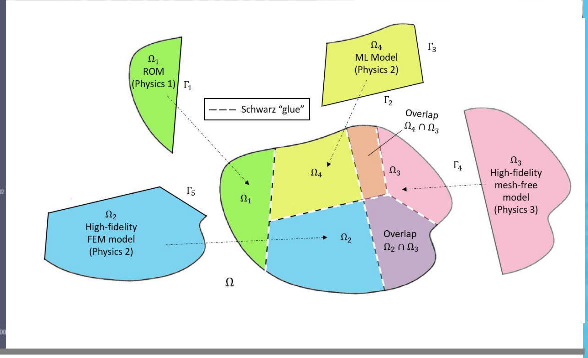
Rigorous component-based coupling of first-principles and data-driven models







Irina Tezaur[1], Chris Wentland[1], Francesco Rizzi[2], Joshua Barnett[3], Alejandro Mota[1], Amy de Castro[1,4], Paul Kuberry[1], Pavel Bochev[1]

[1]Sandia National Laboratories, [2]NexGen Analytics, [3]Cadence Design Systems, [4]Clemson University

NA-GROM Webinar

April 30, 2024

Sandia National Laboratories

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U.S. Department of Energy ENERGY NNSA

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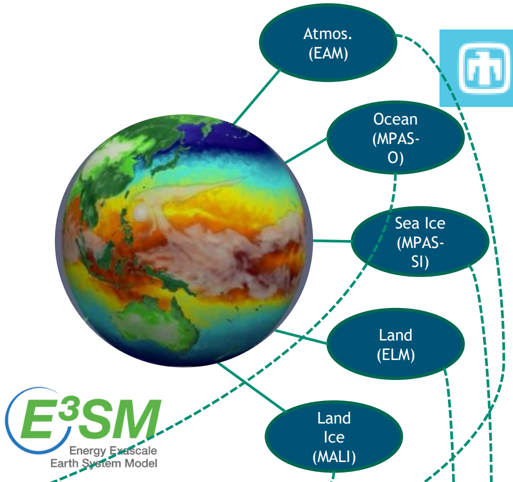
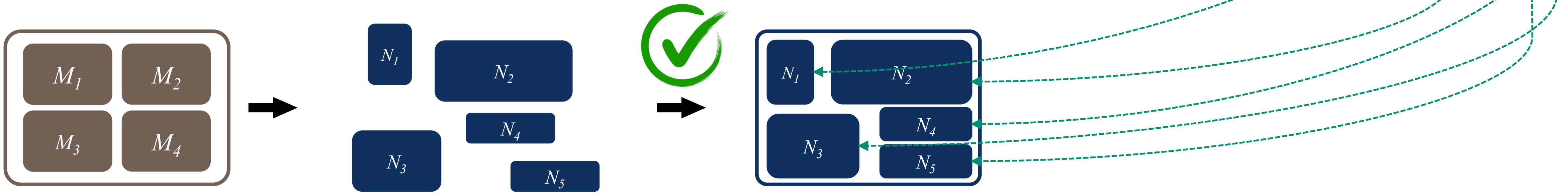
Motivation

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



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



Complex System Model

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

Traditional Methods

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

Coupled Numerical Model

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

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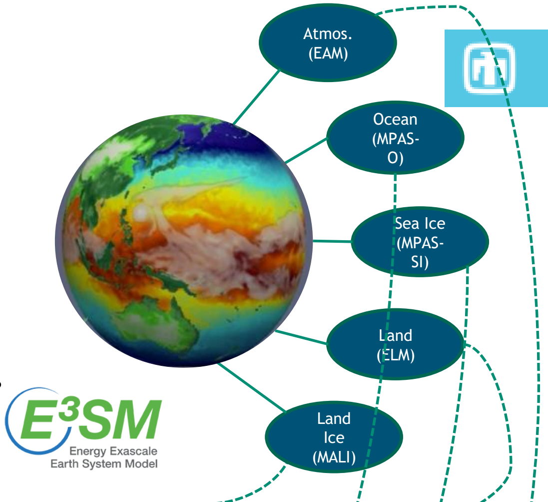

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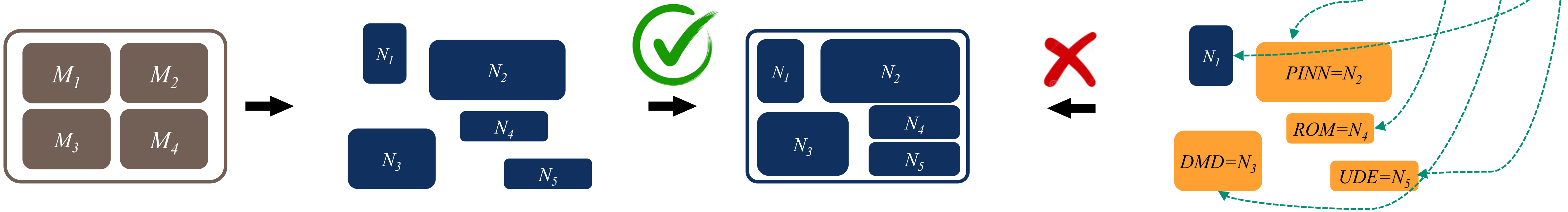

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Traditional + Data-Driven Methods
- PINNs
- Neural ODEs
- Projection-based ROMs, …

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

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

Current Projects on Coupling for Predictive Heterogeneous Models

fHNM: flexible Heterogeneous Numerical Methods

- **Sandia Laboratory Directed Research & Development (LDRD)** project (FY22-FY24)
  - Co-PIs: Pavel Bochev & Irina Tezaur; Team: 5 staff, 2 post docs, 3 students, 2 consultants
  - Academic Alliance: Prof. Arif Masud (UIUC)
- ***Primary research objective:*** discover the **mathematical principles** guiding the **assembly** of **standard** and **data-driven numerical models** in stable, accurate and physically consistent ways

M2dt: Multi-faceted Mathematics for Predictive Digital Twins

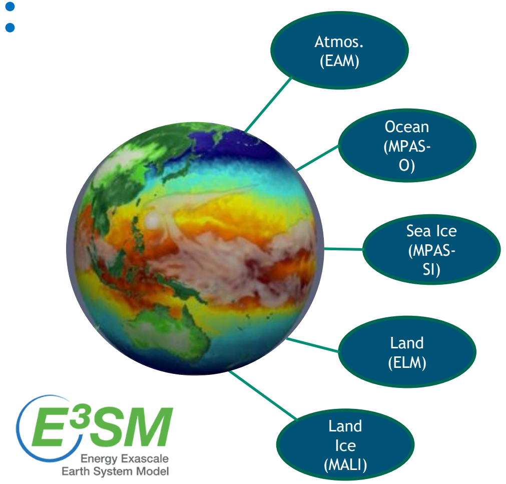
$\int \mathcal{M}^2 dt$

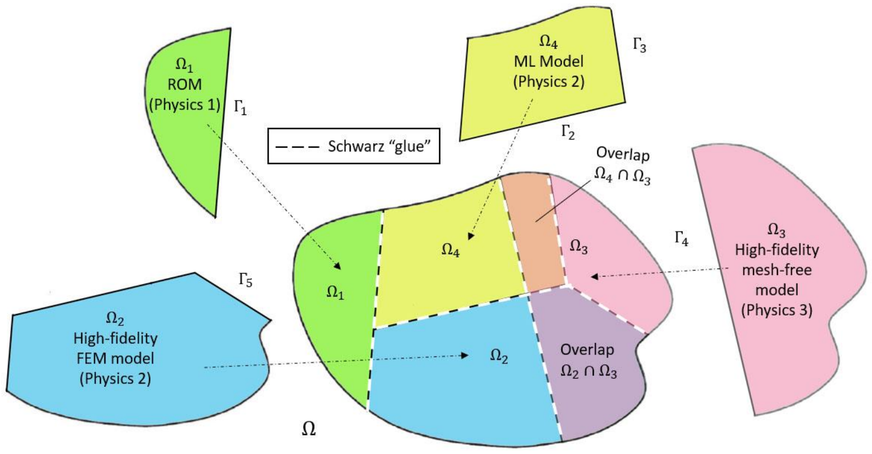
- Funded by DOE's **Advanced Scientific Computing Research (ASCR) Mathematical Multifaceted Integrated Capability Centers (MMICC)** Program (FY23-FY27)
- **Partnership** between UT Austin (Lead Institution), Sandia National Labs (SNL), Argonne National Lab (ANL), Brookhaven National Lab (BNL) and MIT
  - Directors: Karen Willcox & Omar Ghattas (UT Austin)
  - Sandia co-PIs: Irina Tezaur & Pavel Bochev; Sandia team: 6 staff, 1 post doc
- ***Primary research objective:*** establish a center for research and education on multifaceted **mathematical foundations** for **predictive digital twins (DTs)** for complex energy systems
  - Central to DTs is: (1) tight **two-way coupling** of data and models, (2) **structure preservation** and (3) **dynamic data assimilation**

Coupling Scenarios, Models and Methods

Coupling scenarios:

Scenario I: multi-component coupling with a given domain/component decomposition (for reuse of single-component codes)





Scenario II: multi-scale coupling where decomposition can be chosen to maximize accuracy, robustness & efficiency of coupled model

Data-driven models: to be "mixed-and-matched" with each other and first-principles models

- *Class A*: projection-based reduced order models (ROMs)
- *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

Coupling methods:

- *Method 1*: Alternating Schwarz-based coupling
- *Method 2*: Optimization-based coupling
- *Method 3*: Coupling via generalized mortar methods (GMMs)

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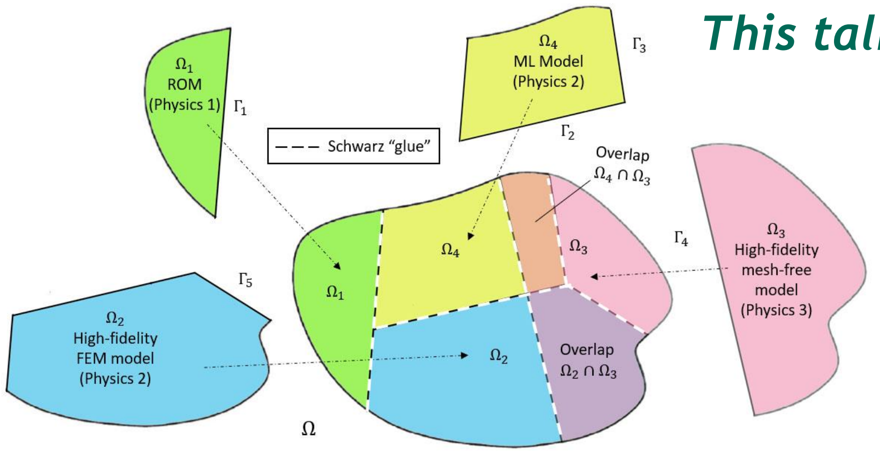

This talk

Scenario II: multi-scale coupling where decomposition can be chosen to maximize accuracy, robustness & efficiency of coupled model

Data-driven models: to be "mixed-and-matched" with each other and first-principles models

- *Class A:* projection-based reduced order models (ROMs) — ***This talk***
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Coupling methods:

- *Method 1:* Alternating Schwarz-based coupling — ***This talk***
- *Method 2:* Optimization-based coupling
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Outline

1. The Alternating Schwarz Method for FOM*-ROM# and ROM-ROM Coupling
   - Method Formulation
   - ROM Construction and Implementation
   - Numerical Examples

2. A Lagrange Multiplier-based Partitioned Scheme for FOM-ROM and ROM-ROM Coupling
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   - ROM Construction and Implementation
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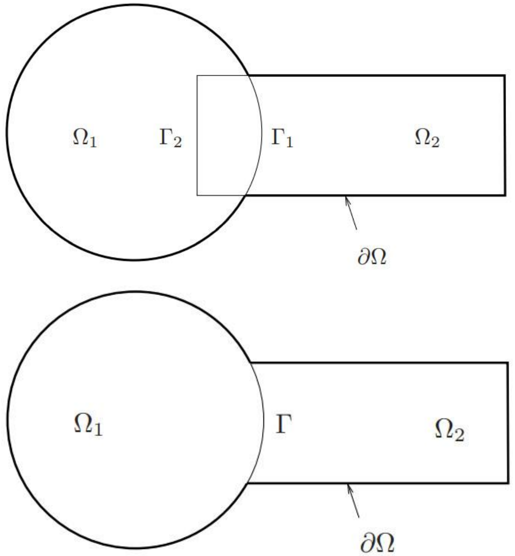
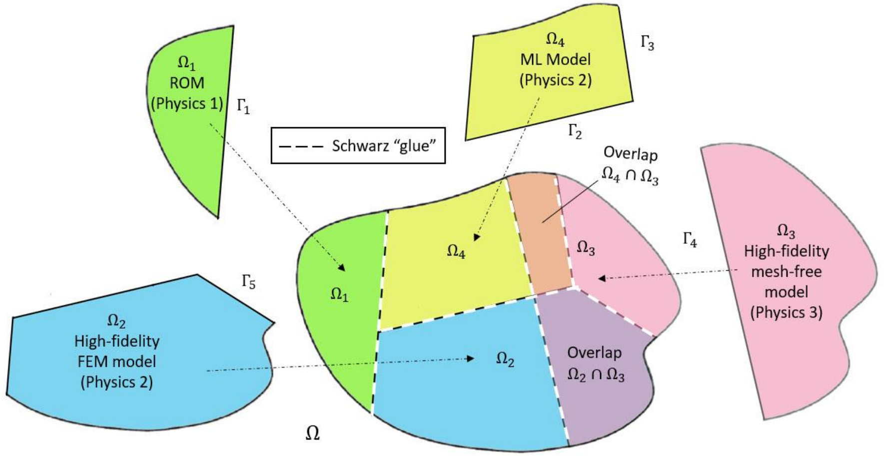
3. Summary and Future Work





*Full-Order Model. #Reduced Order Model.

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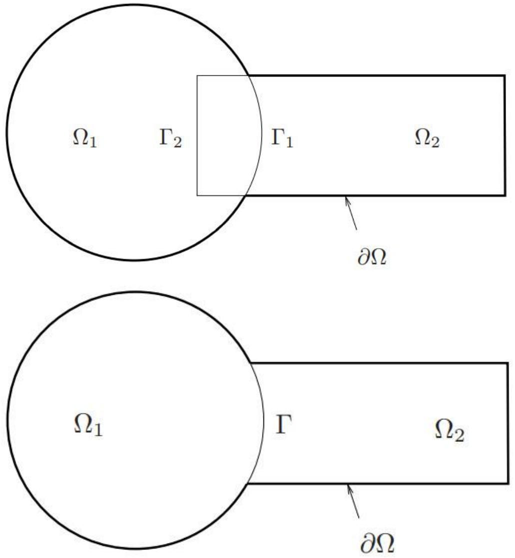

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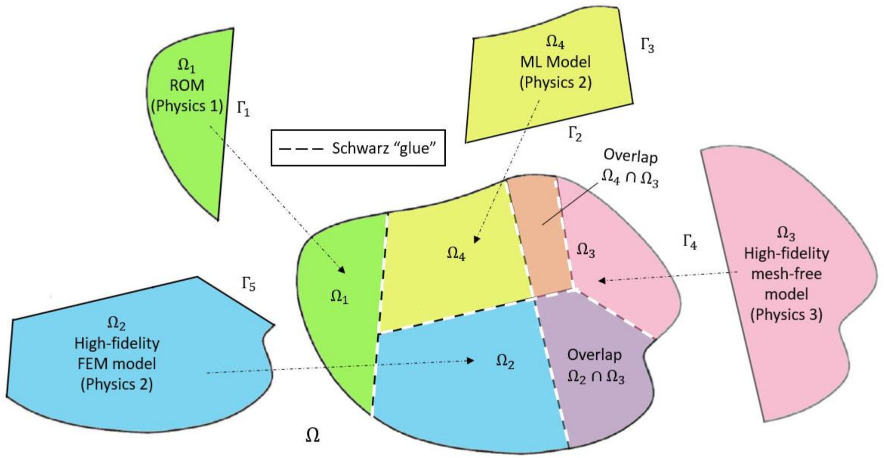
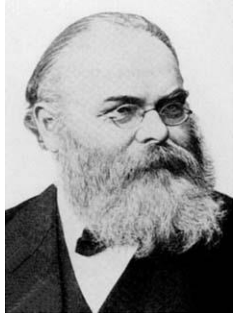


*Full-Order Model. #Reduced Order Model.

Schwarz Alternating Method for Domain Decomposition



H. Schwarz (1843–1921)

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

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

Basic Schwarz Algorithm

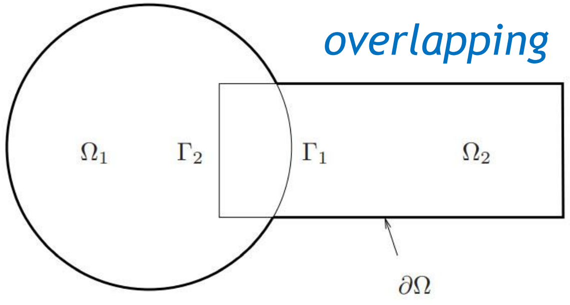
Initialize:

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

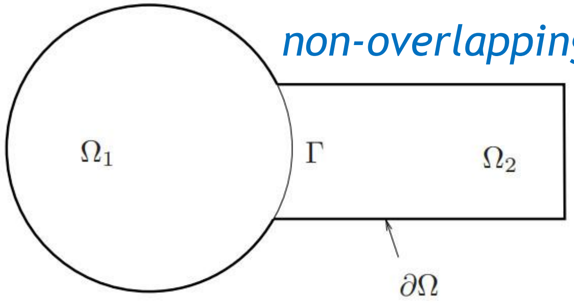
Iterate until convergence:

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

overlapping



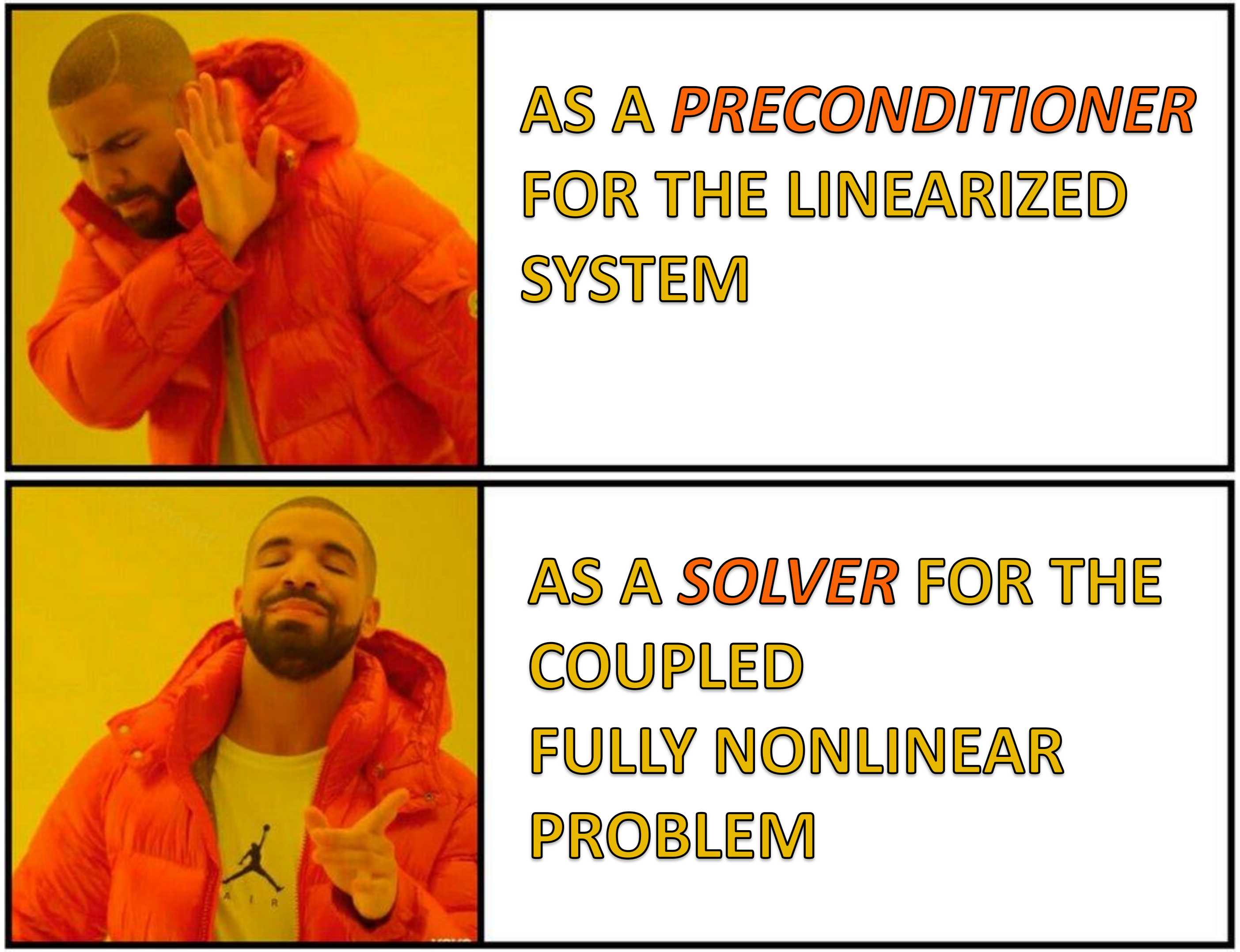
non-overlapping



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

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

How We Use the Schwarz Alternating Method

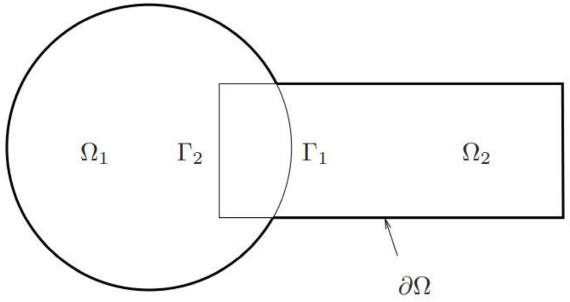


Spatial Coupling via (Multiplicative) Alternating Schwarz

Overlapping Domain Decomposition

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

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



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

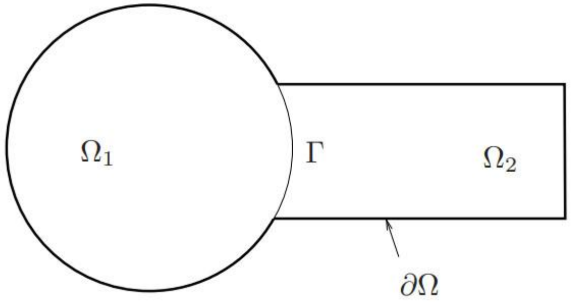
- Dirichlet-Dirichlet transmission BCs [Schwarz 1870; Lions 1988; Mota *et al*. 2017; Mota *et al*. 2022]

Non-overlapping Domain Decomposition

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

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

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



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

Additional Parallelism via Additive Schwarz

Multiplicative Overlapping Schwarz

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

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Additive Overlapping Schwarz

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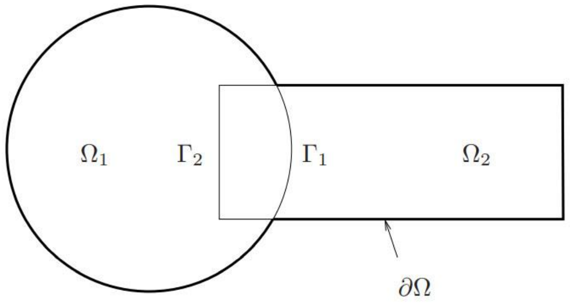
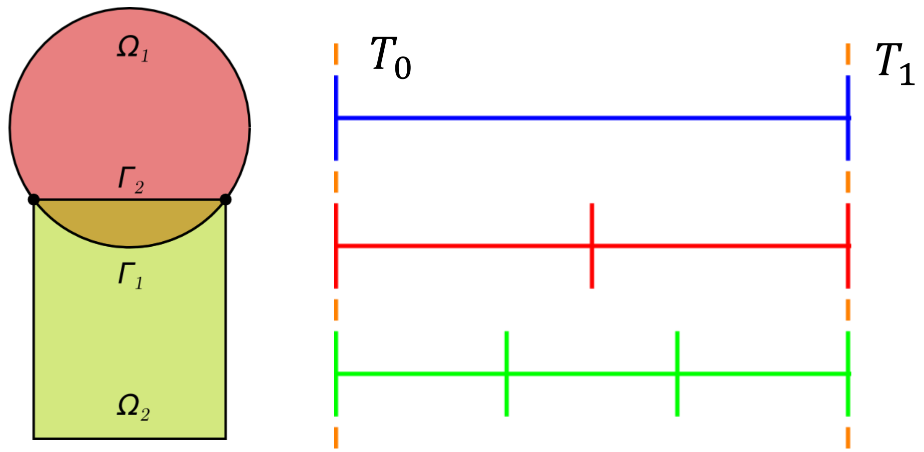


- **Multiplicative Schwarz:** solves subdomain problems **sequentially** (in serial)
- **Additive Schwarz:** advance subdomains in **parallel**, communicate boundary condition data later
  - ➢ Typically requires a few more **Schwarz iterations**, but does not degrade **accuracy**
  - ➢ **Parallelism**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

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

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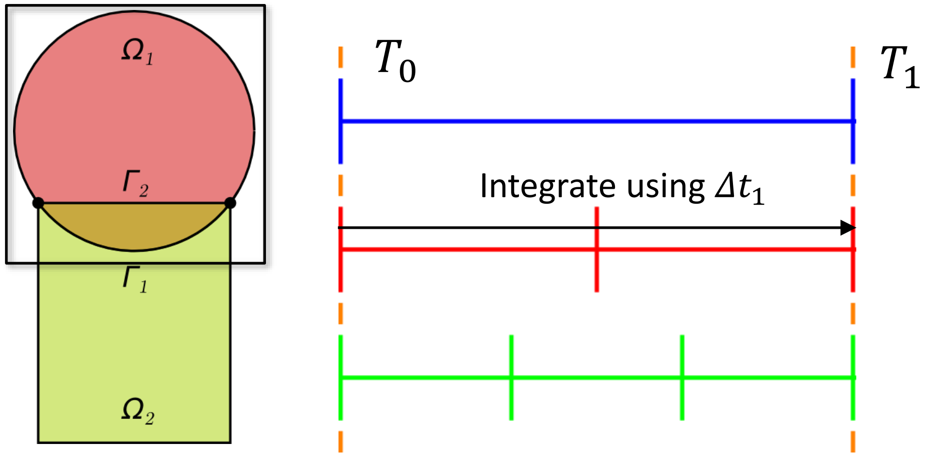

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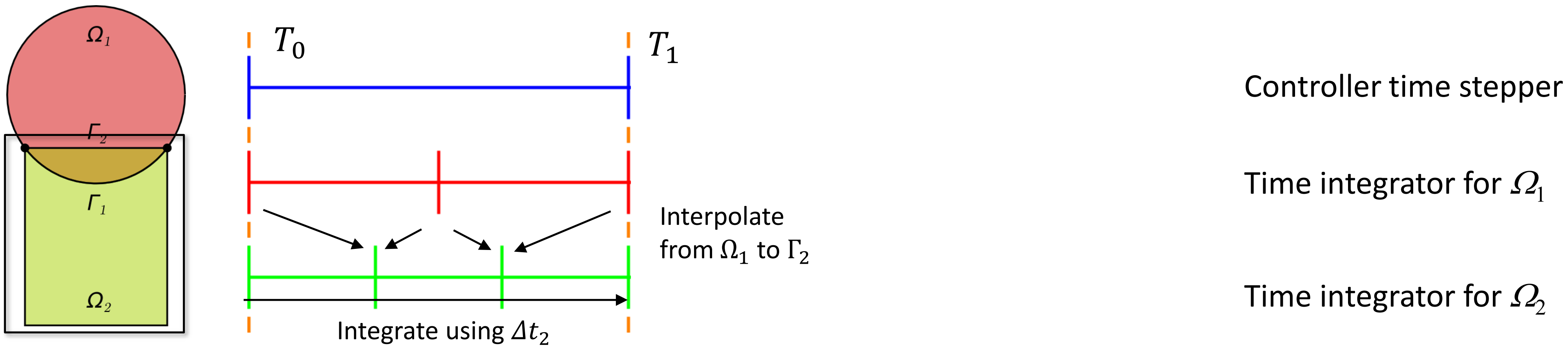

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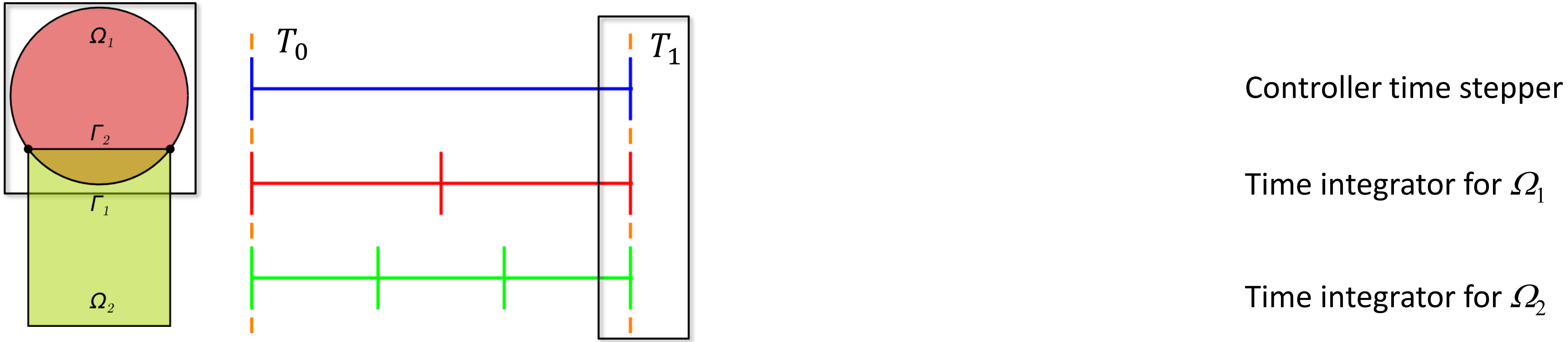

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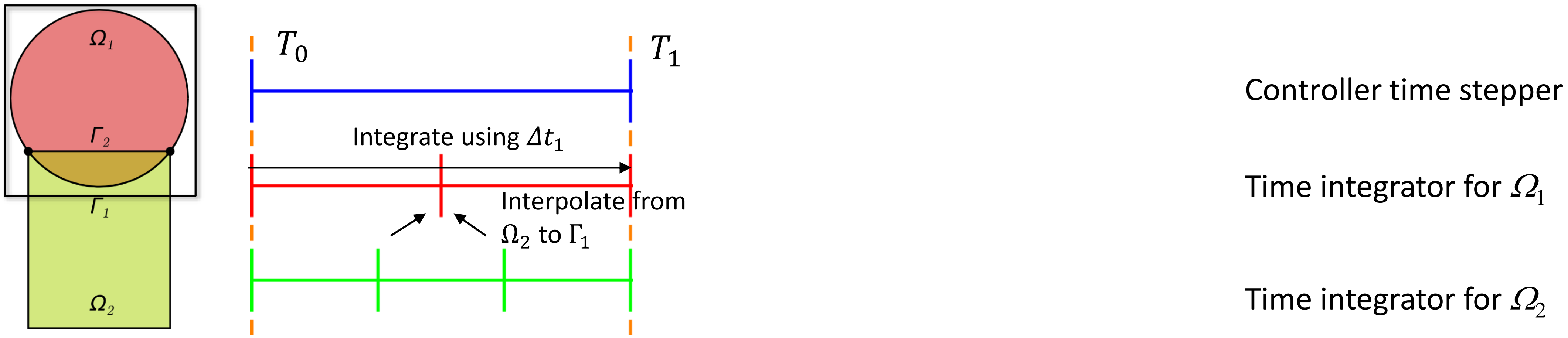

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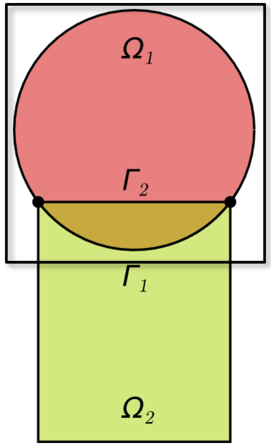

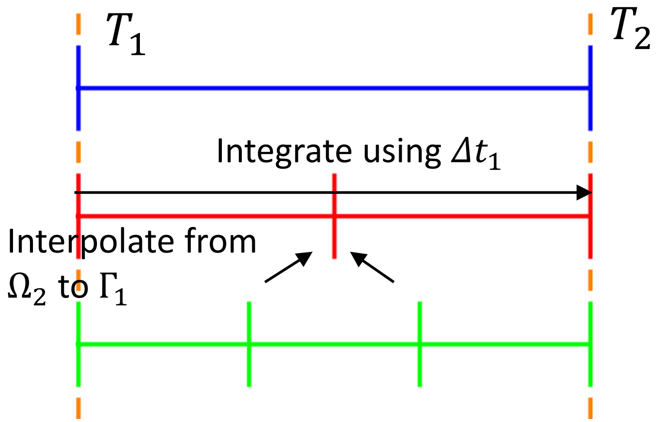

Can use ***different integrators*** with ***different time steps*** within each domain!

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- If unconverged, return to Step 1.
- If converged, set $i = i + 1$ and return to Step 1.

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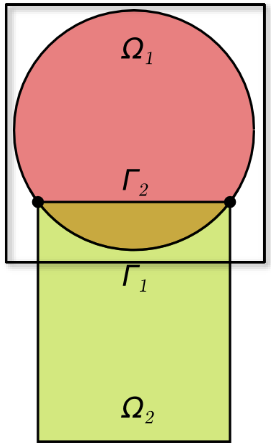
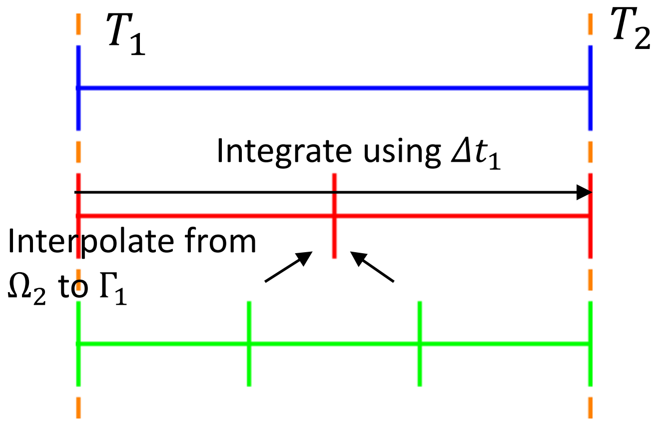




Controller time stepper

Time integrator for Ω_1

Time integrator for Ω_2

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

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

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

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

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

- If unconverged, return to Step 1.
- If converged, set $i = i + 1$ and return to Step 1.

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

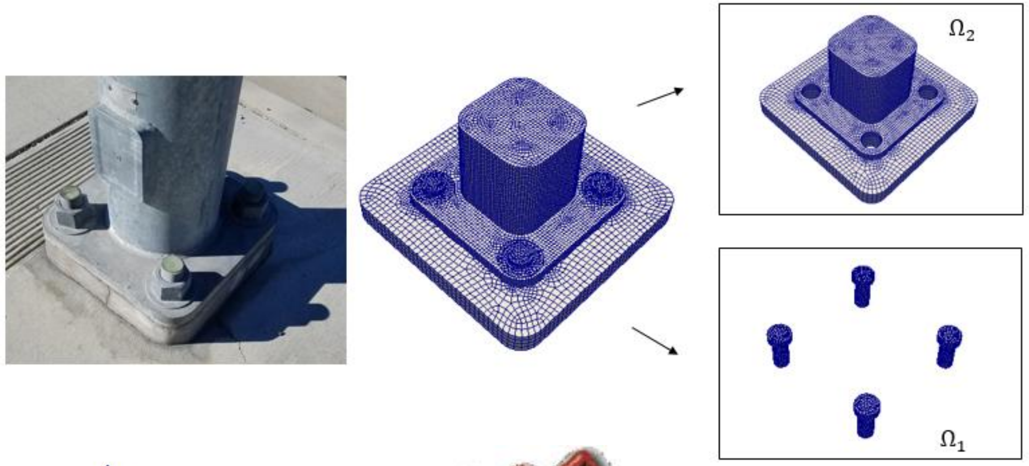
Schwarz for Multiscale FOM-FOM Coupling in Solid Mechanics[1]

- 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.

Model Solid Mechanics PDEs:

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

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



Albany-LCM[2]

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

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*

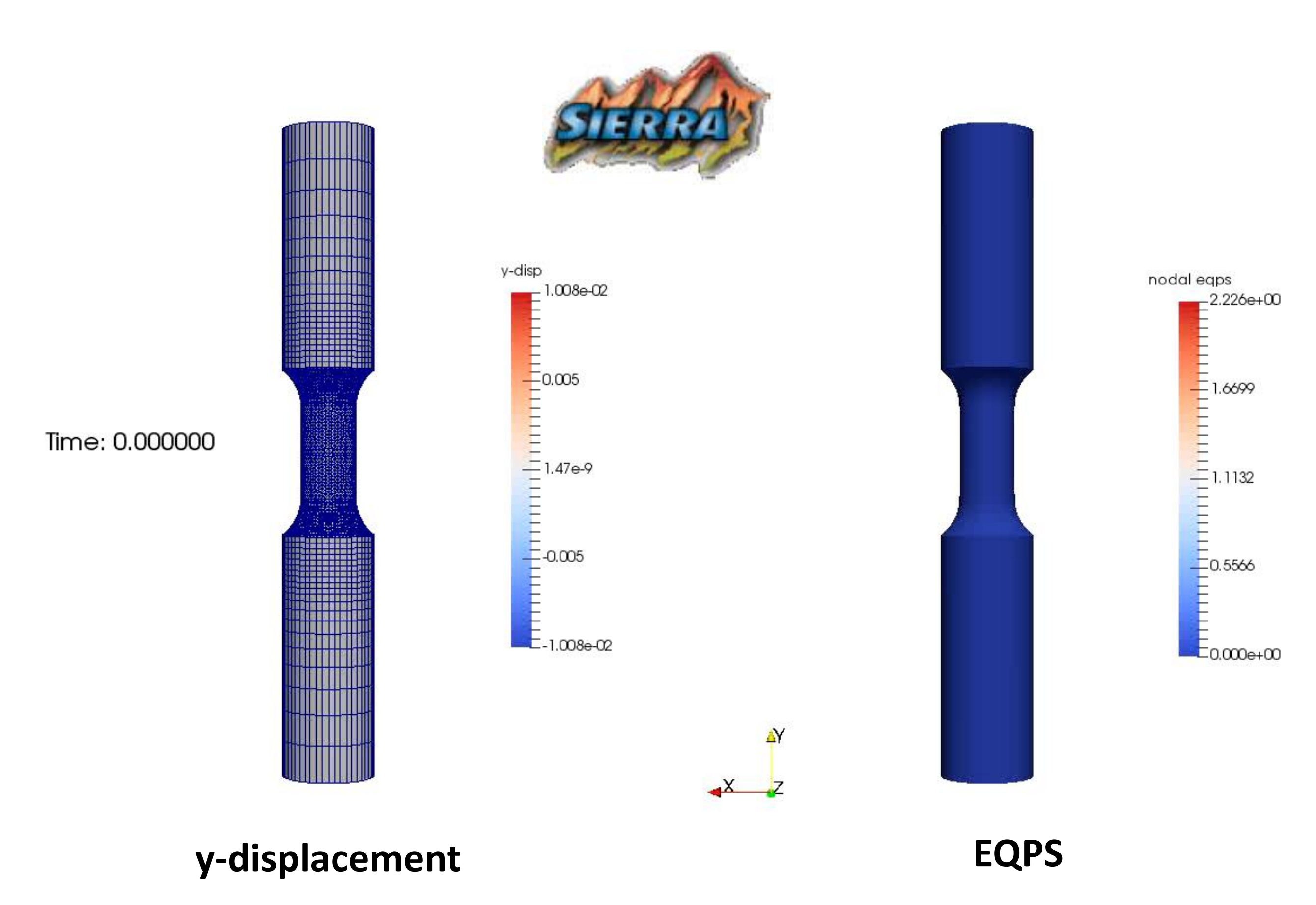
(a) $\Phi[\tilde{\varphi}^{(0)}] \geq \Phi[\tilde{\varphi}^{(1)}] \geq \cdots \geq \Phi[\tilde{\varphi}^{(n-1)}] \geq \Phi[\tilde{\varphi}^{(n)}] \geq \cdots \geq \Phi[\varphi]$, *where φ is the minimizer of $\Phi[\varphi]$ over $\mathcal{S}$.*

(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 for Multiscale FOM-FOM Coupling in Solid Mechanics*



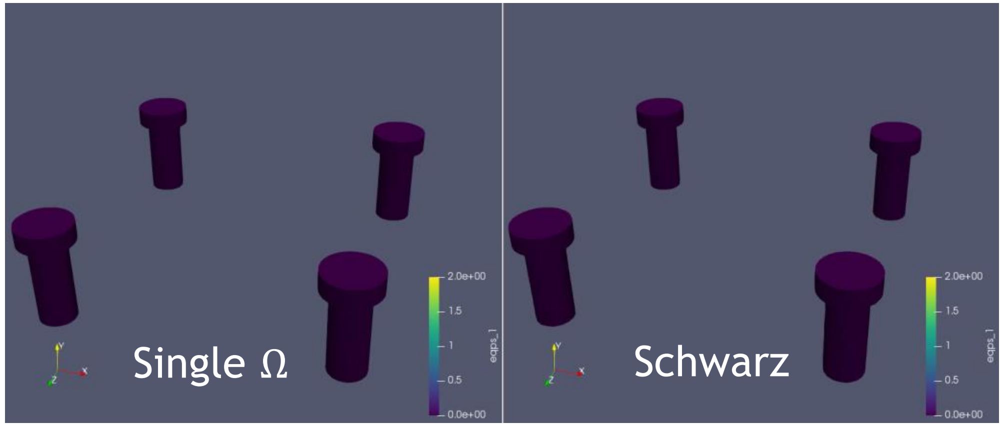


Figure above: tension specimen simulation coupling composite TET10 elements with HEX elements in Sierra/SM.

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

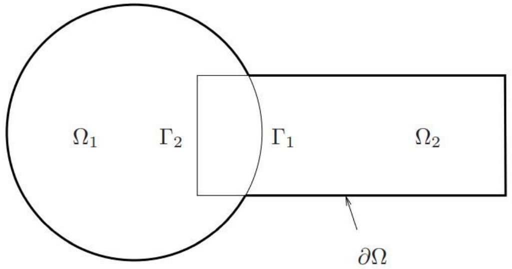
*Mota *et al*. 2017; Mota *et al*. 2022.

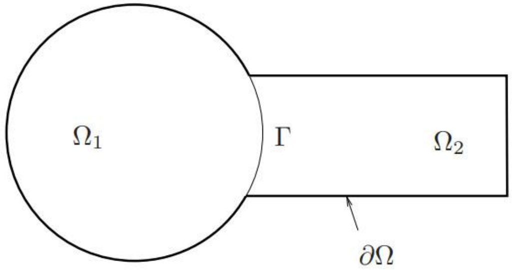
Outline

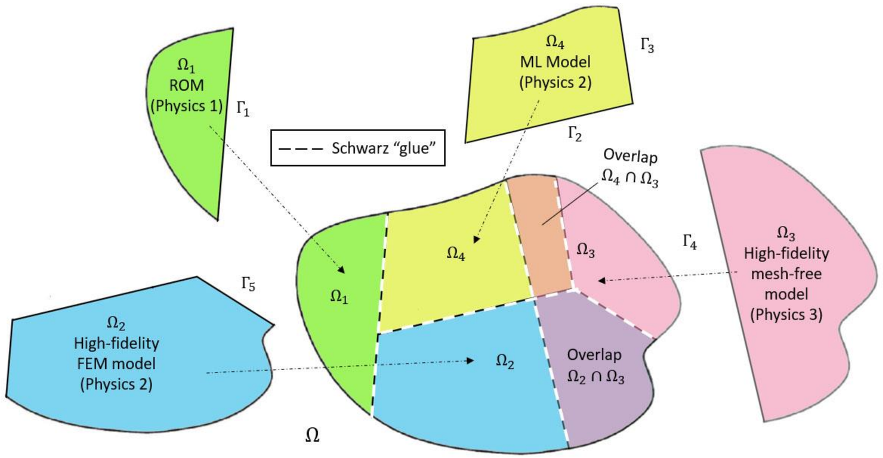
1. **The Alternating Schwarz Method for FOM*-ROM# and ROM-ROM Coupling**
   - Method Formulation
   - **ROM Construction and Implementation**
   - Numerical Examples

2. A Lagrange Multiplier-based Partitioned Scheme for FOM-ROM and ROM-ROM Coupling
   - Method Formulation
   - ROM Construction and Implementation
   - Numerical Examples

3. Summary and Future Work







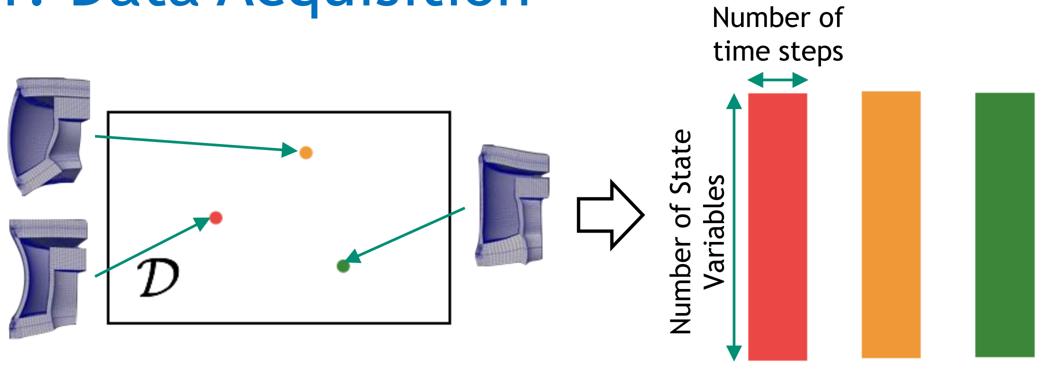
*Full-Order Model. #Reduced Order Model.

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

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

*Least-Squares Petrov-Galerkin

1. Data Acquisition

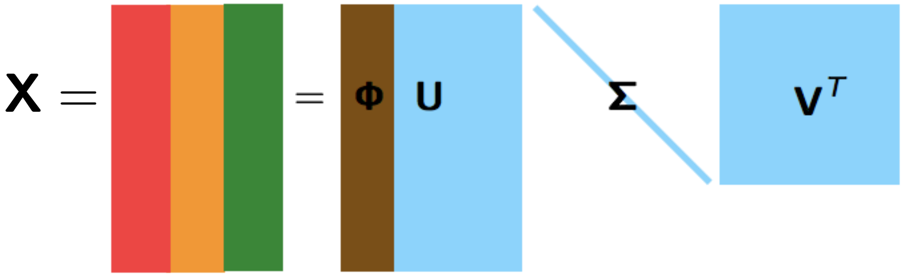


Solve ODE at different design points

Save solution data

2. Learning of Reduced Basis

Proper Orthogonal Decomposition (POD):



ROM = projection-based Reduced Order Model

3. Projection-Based Reduction

Discretize FOM in time

$$\dot{\boldsymbol{q}} = \boldsymbol{f}(\boldsymbol{q}, t; \boldsymbol{\mu})$$

$$\Downarrow$$

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

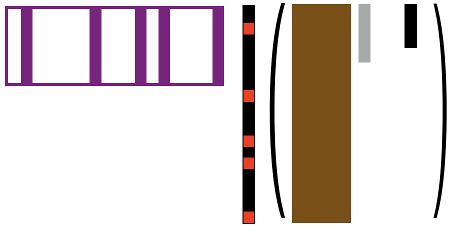
Reduce the number of unknowns

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

Apply hyper-reduction and minimize residual

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

Hyper-reduction/sample mesh



HROM = Hyper-reduced ROM

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 (Scenario I) or together?

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

- **Strong** vs. **weak** BC enforcement?
  - ➢ Strong BC enforcement difficult for some models (e.g., cell-centered finite volume, PINNs)
- **Optimizing parameters** in Schwarz BCs for non-overlapping Schwarz?

Choice of hyper-reduction

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

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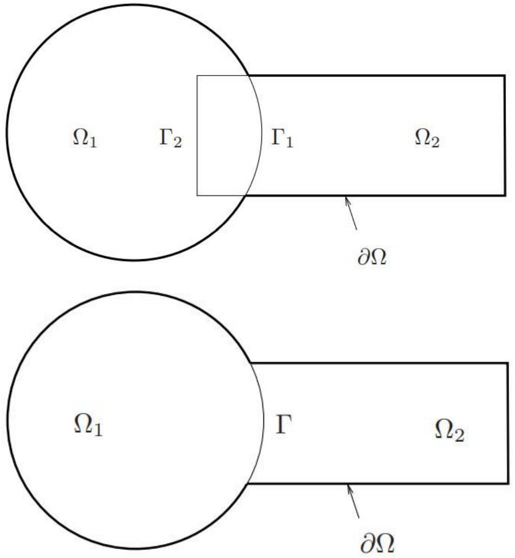
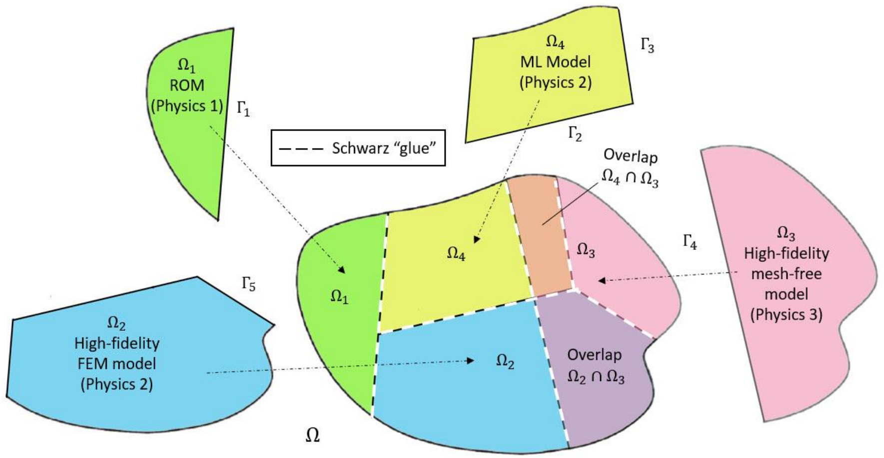


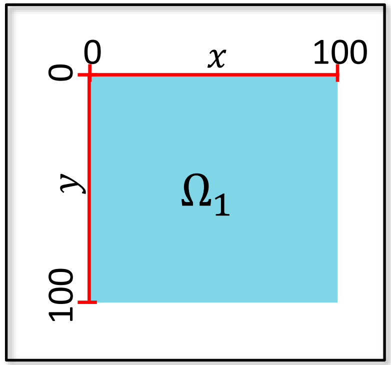


*Full-Order Model. #Reduced Order Model.

Model Problem 1: 2D Inviscid Burgers Equation

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

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



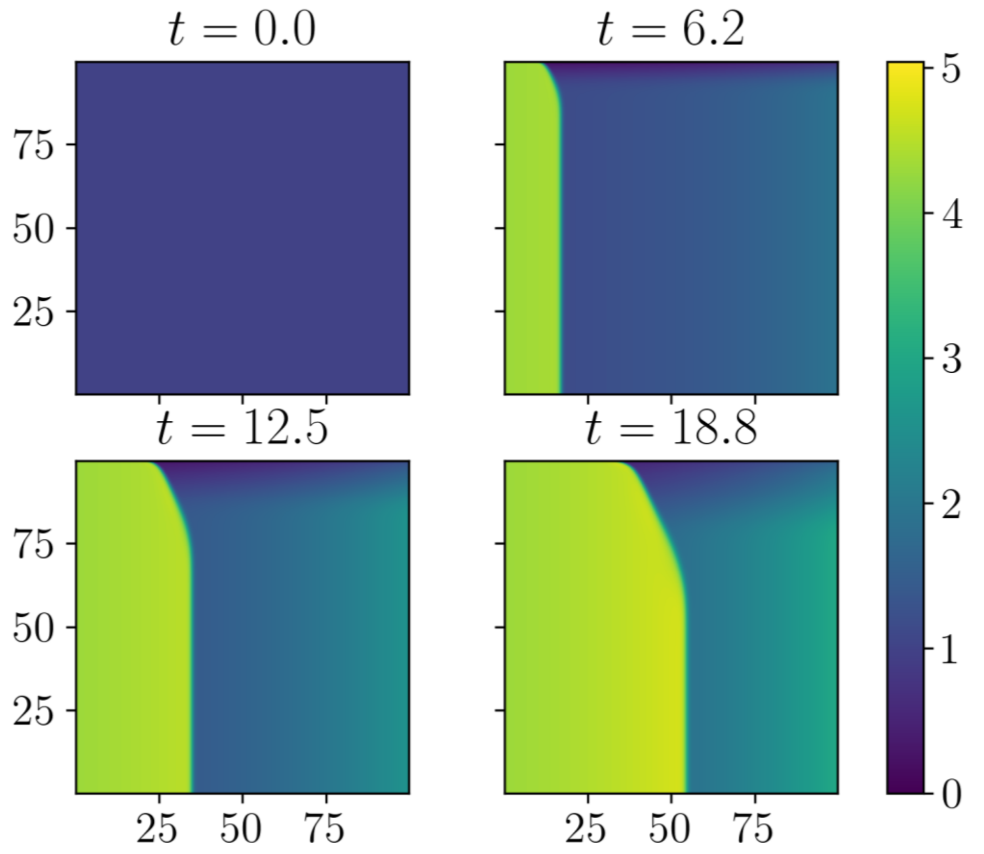


Figure above: solution of u component at various times

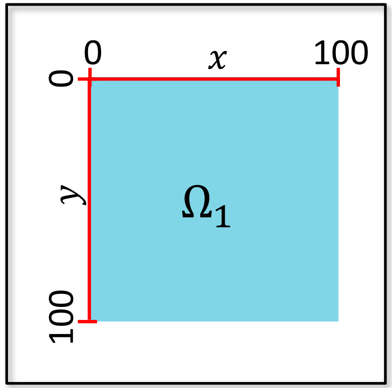
Problem setup:

- $\Omega = (0{,}100)^2$, $t \in [0, 25]$
- Two **parameters** $\boldsymbol{\mu} = (\mu_1, \mu_2)$ defining source and BC terms, respectively

FOM discretization:

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

Single Domain Predictive ROM



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

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

* Numbers in table are w/o hyper-reduction

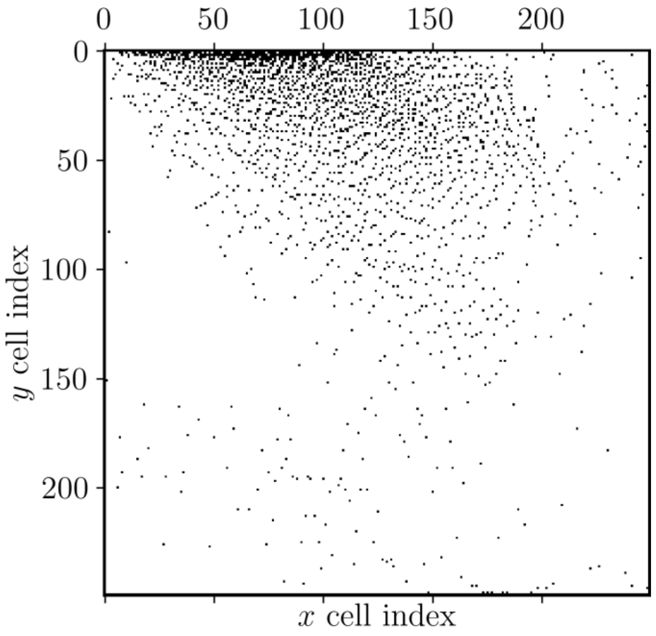


Figure above: Reduced mesh of single domain HROM

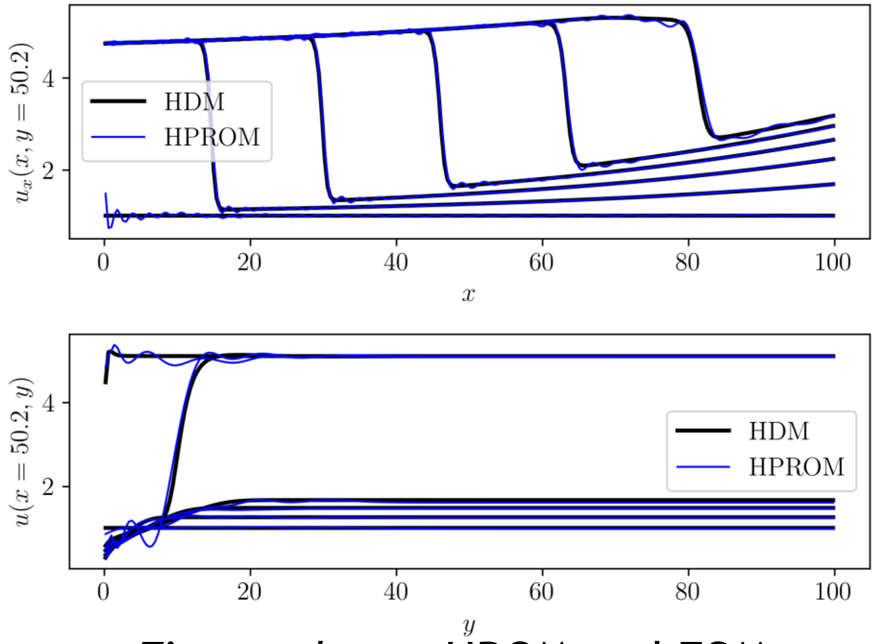
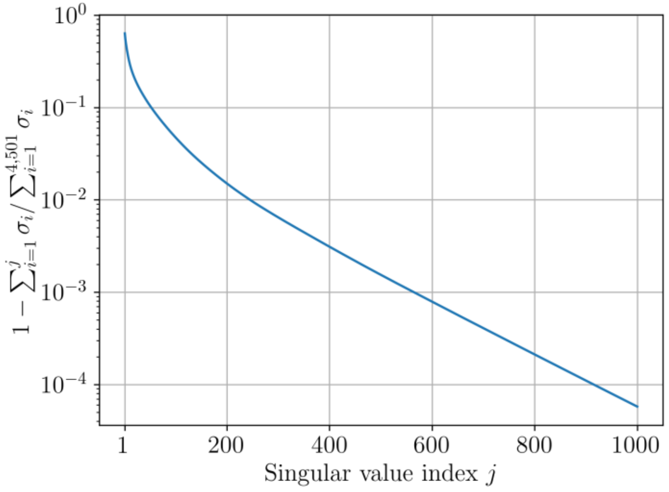
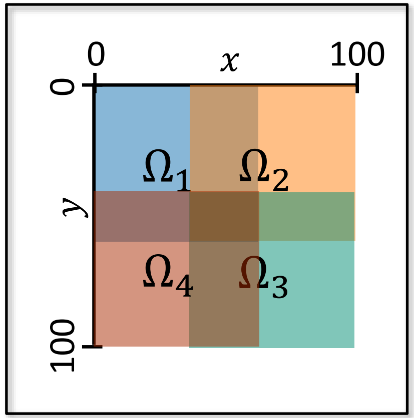


Figure above: HROM and FOM results at various time steps



Schwarz Coupling Details



Choice of domain decomposition

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

Snapshot collection and reduced basis construction

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

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

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

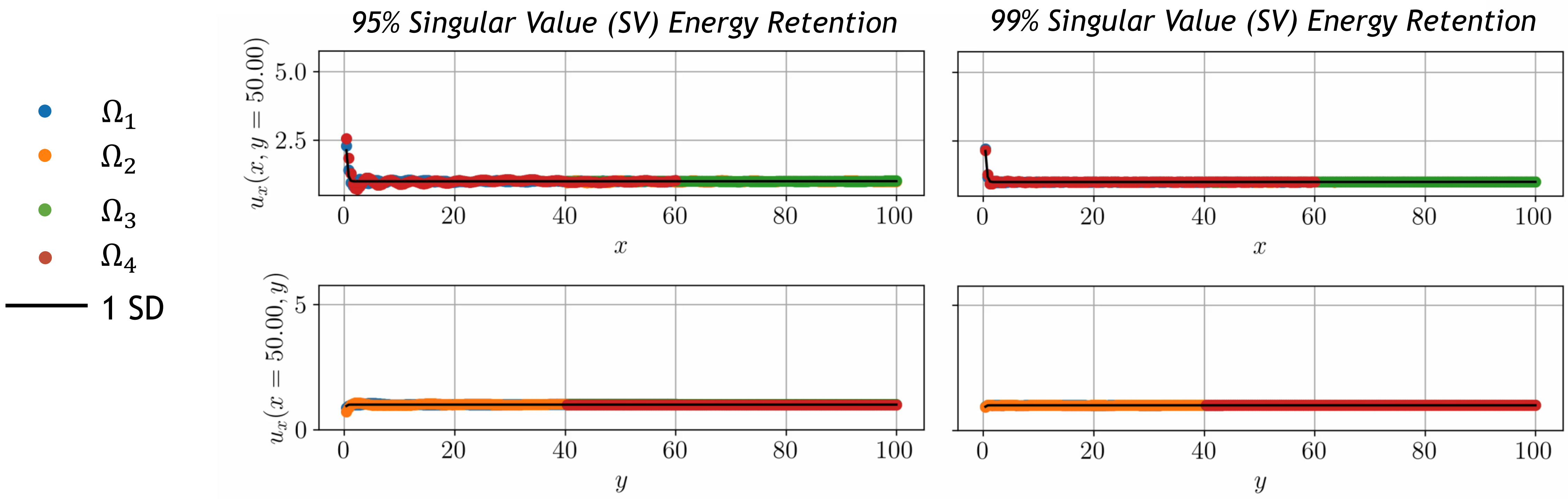
$$\boldsymbol{q}(t) \approx \overline{\boldsymbol{q}} + \boldsymbol{\Phi}\hat{\boldsymbol{q}}(t)$$

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

Choice of hyper-reduction

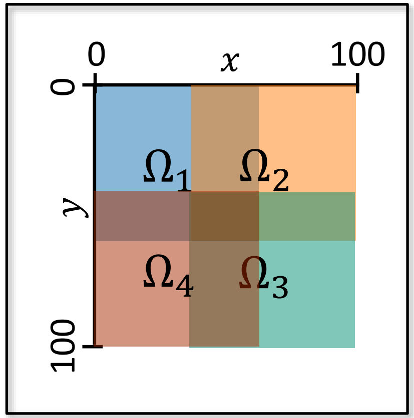
- **Energy Conserving Sampling & Weighting** (ECSW) method for hyper-reduction
- **All points** on Schwarz boundaries are included in the sample mesh

All-ROM Coupling

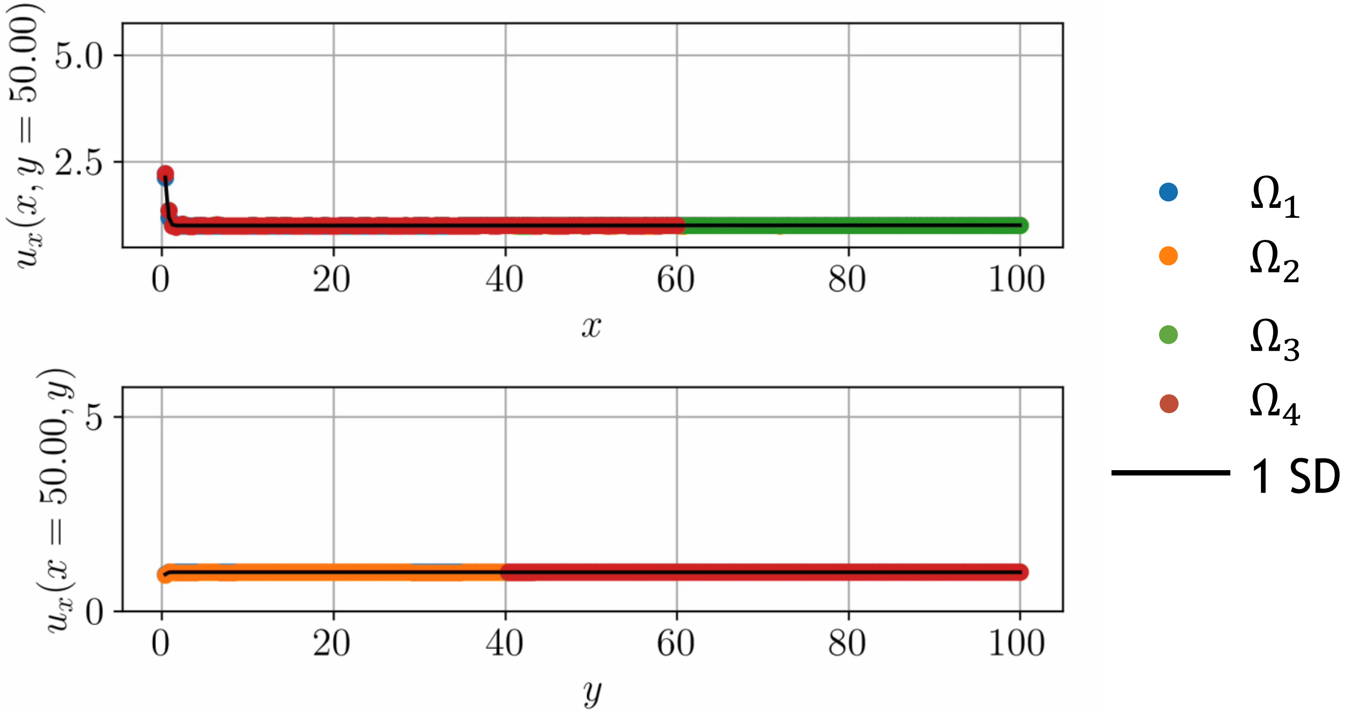


- Method converges in **only 3 Schwarz iterations** per controller time-step
- **Errors** $O(1\%)$ or less
- **1.47× speedup** over all-FOM coupling for 95% SV energy retention case

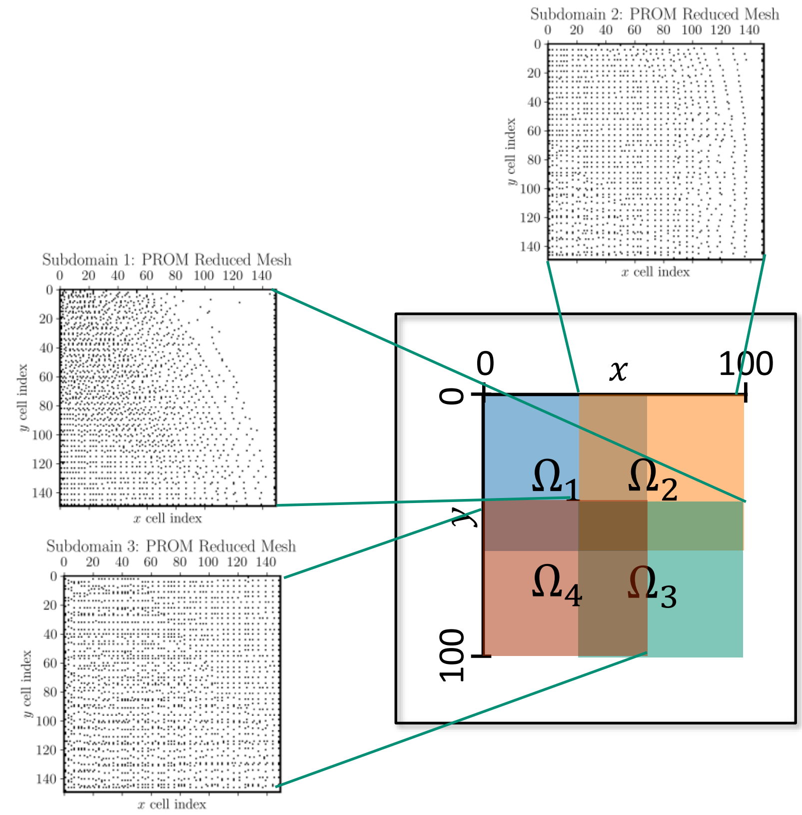
Subdomains	95% SV Energy			99% SV Energy		
	M	MSE (%)	CPU time (s)	M	MSE (%)	CPU time (s)
Ω_1	57	1.1	85	146	0.18	295
Ω_2	44	1.2	56	120	0.18	216
Ω_3	24	1.4	43	60	0.16	89
Ω_4	32	1.9	61	66	0.25	100
Total			245			**700**



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.**

Model Problem 2: 2D Shallow Water Equations (SWE)

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

$$\frac{\partial h}{\partial t} + \frac{\partial (hu)}{\partial x} + \frac{\partial (hv)}{\partial y} = 0$$
$$\frac{\partial (hu)}{\partial t} + \frac{\partial}{\partial x}\left(hu^2 + \frac{1}{2}gh^2\right) + \frac{\partial}{\partial y}(huv) = -\mu v$$
$$\frac{\partial (hv)}{\partial t} + \frac{\partial}{\partial x}(huv) + \frac{\partial}{\partial y}\left(hv^2 + \frac{1}{2}gh^2\right) = \mu u$$

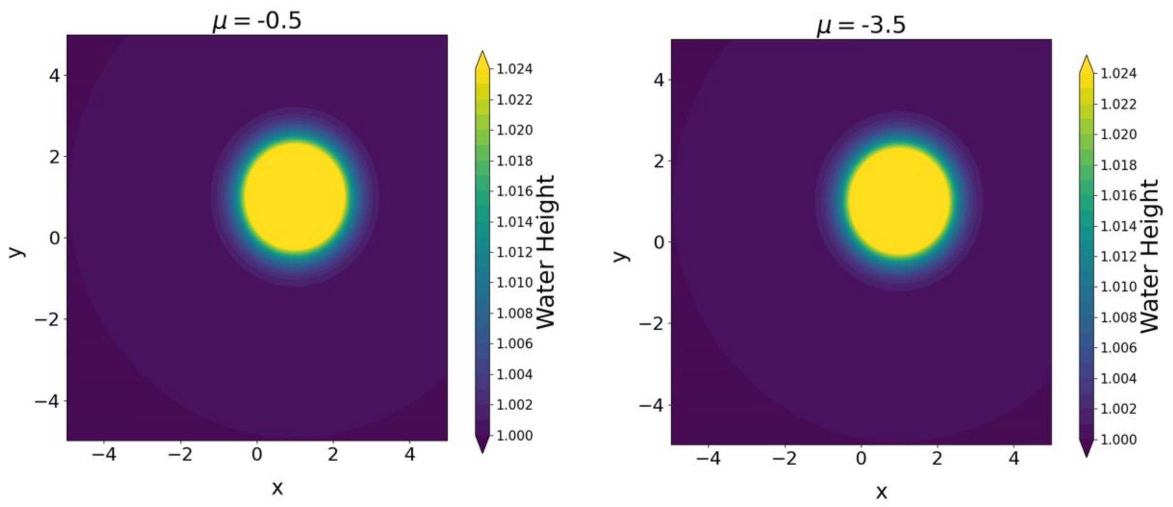


Figure above: FOM solutions to SWE for $\mu = -0.5$ (left) and $\mu = -3.5$ (right).

Problem setup:

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

FOM discretization:

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

Schwarz Coupling Details

Green: different from Model Problem 1

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*

Snapshot collection and reduced basis construction

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

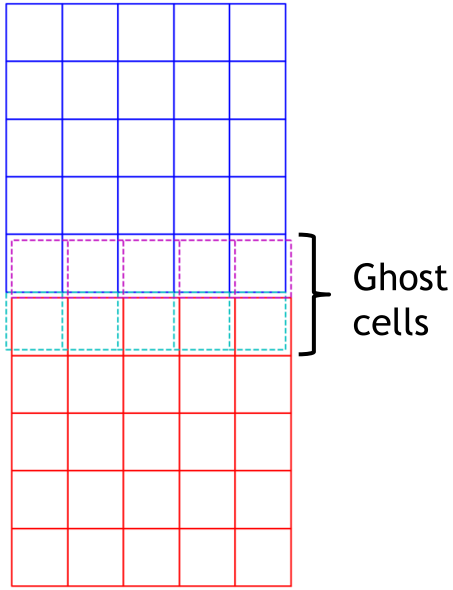
Enforcement of boundary conditions (BCs) in ROM at Schwarz boundaries

- 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
  - ➢ ⇒ **Dirichlet-Dirichlet non-overlapping Schwarz** is stable/convergent!

Choice of hyper-reduction

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

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



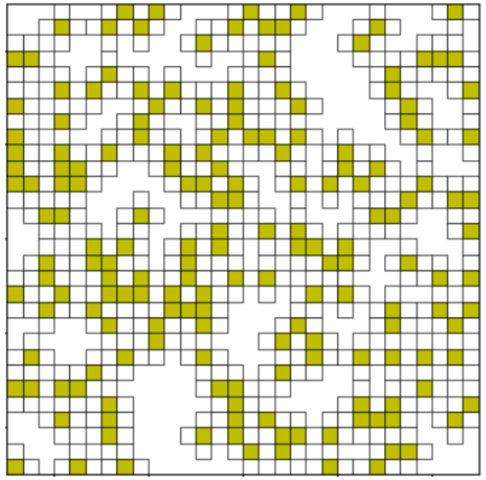
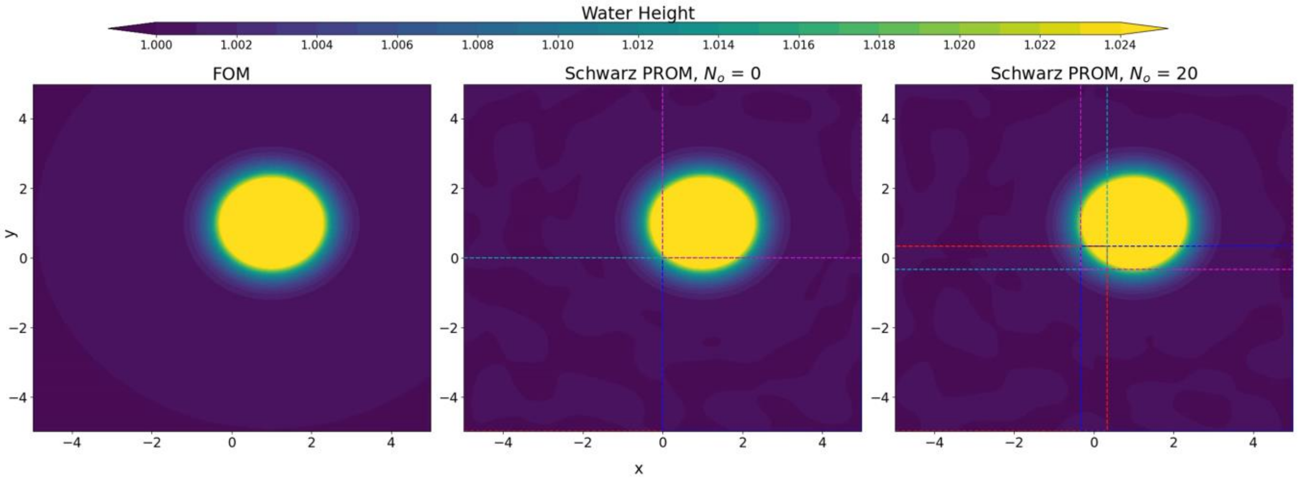


Figure above: sample mesh (yellow) and stencil (white) cells

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

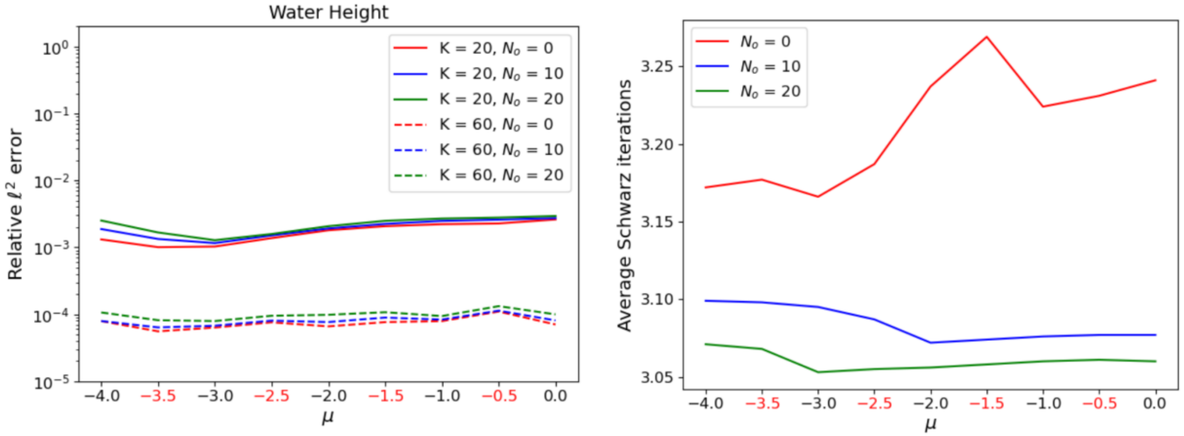
Schwarz All-ROM Domain Overlap Study

Study of **Schwarz convergence** for **all-ROM coupling** as a function of 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

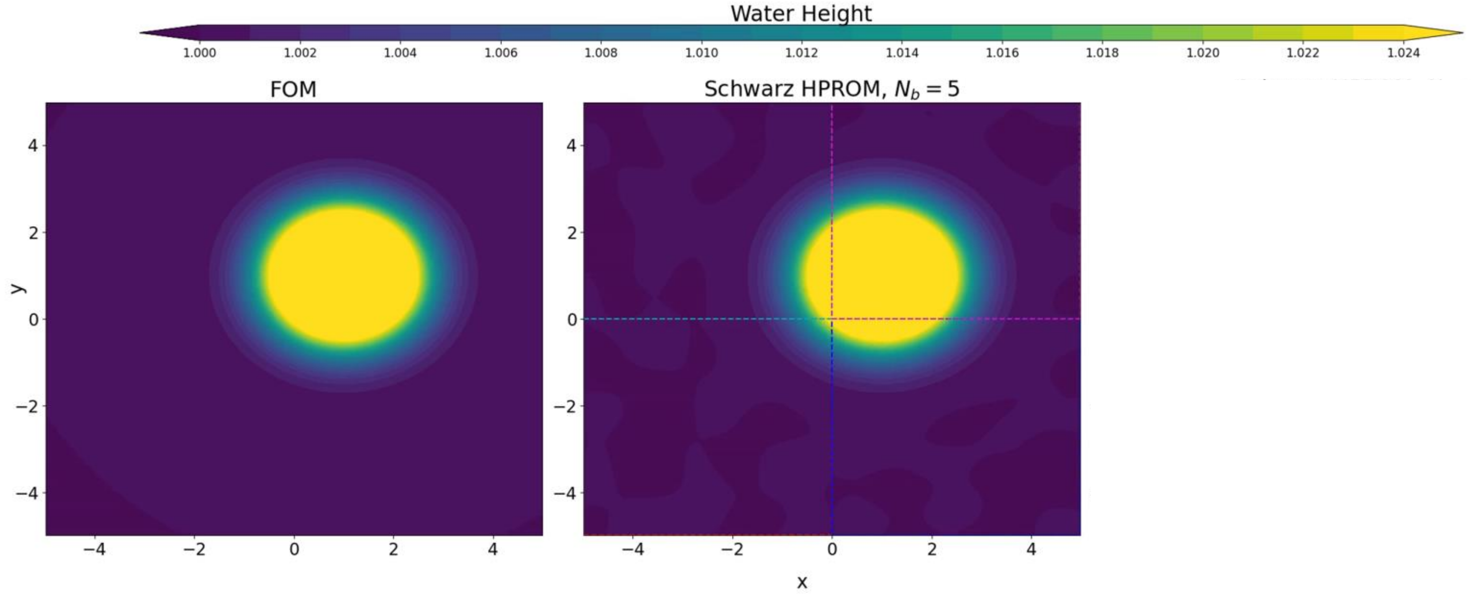
Schwarz Boundary Sampling for All-HROM Coupling

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

Schwarz Boundary Sampling for All-HROM Coupling

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

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



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

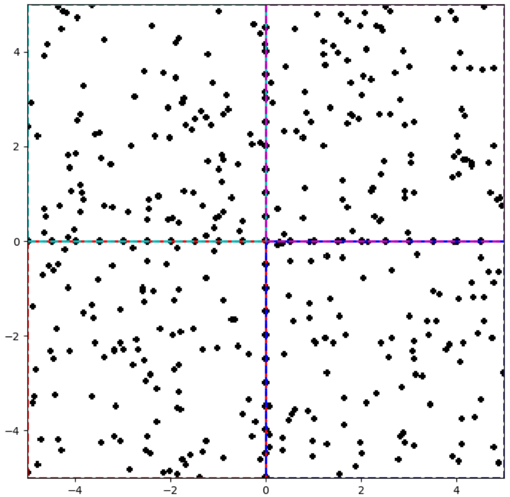
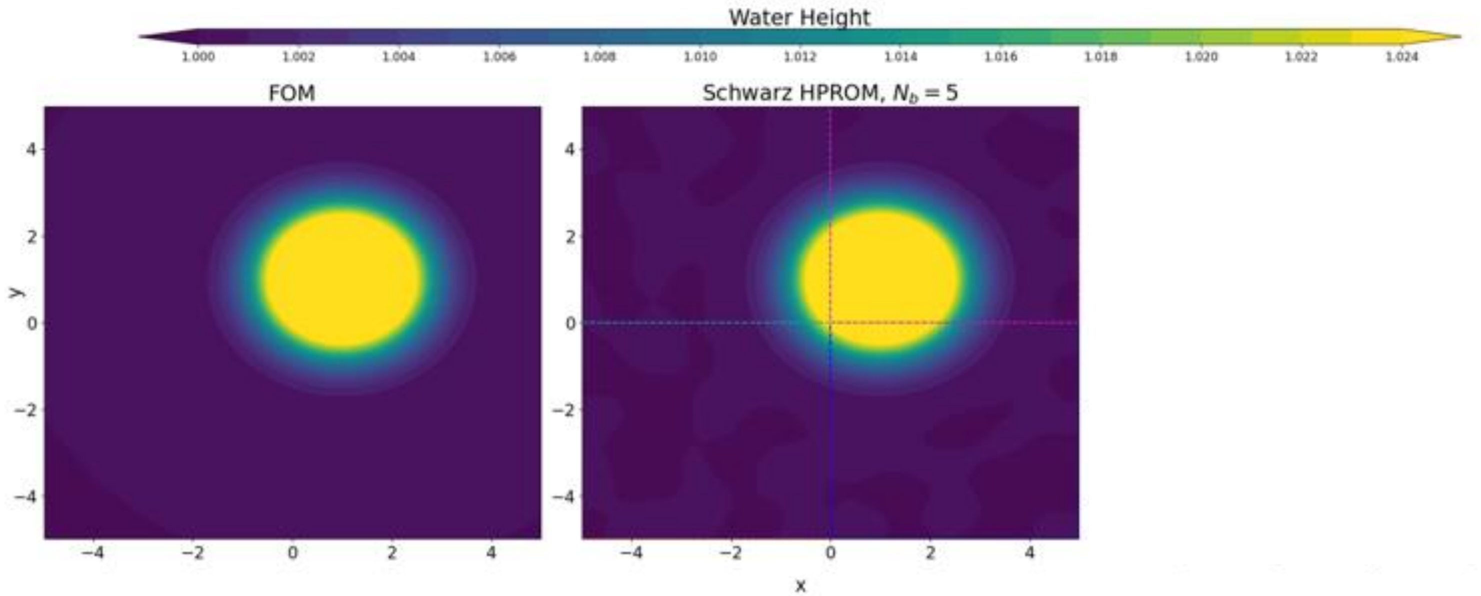


Figure above: example sample mesh with sampling rate $N_b = 5\%$.

Schwarz Boundary Sampling for All-HROM Coupling

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

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



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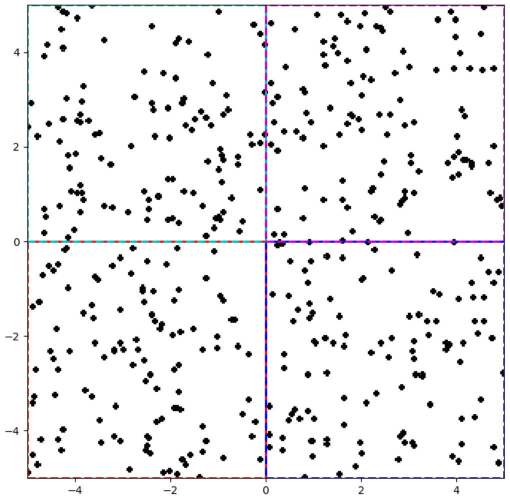


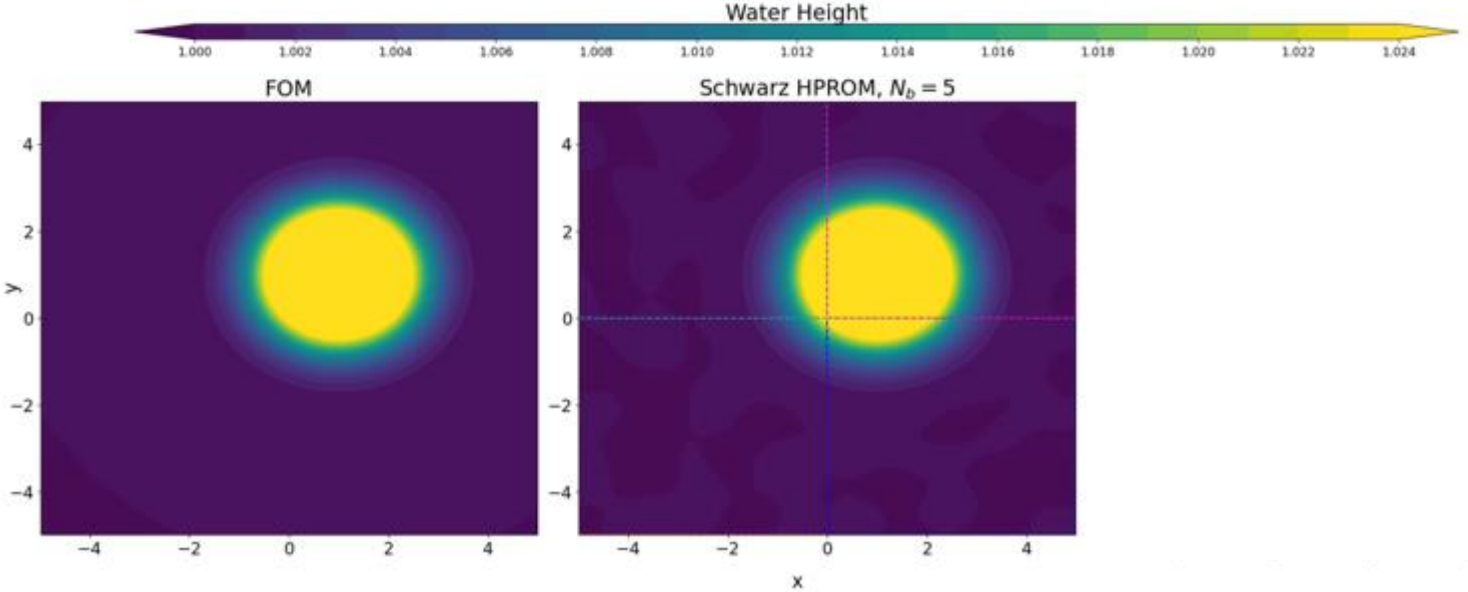
Figure above: example sample mesh with sampling rate $N_b = 0$.

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

Schwarz Boundary Sampling for All-HROM Coupling

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

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



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

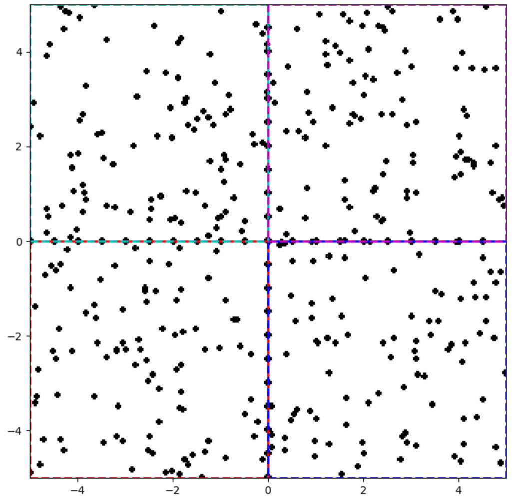


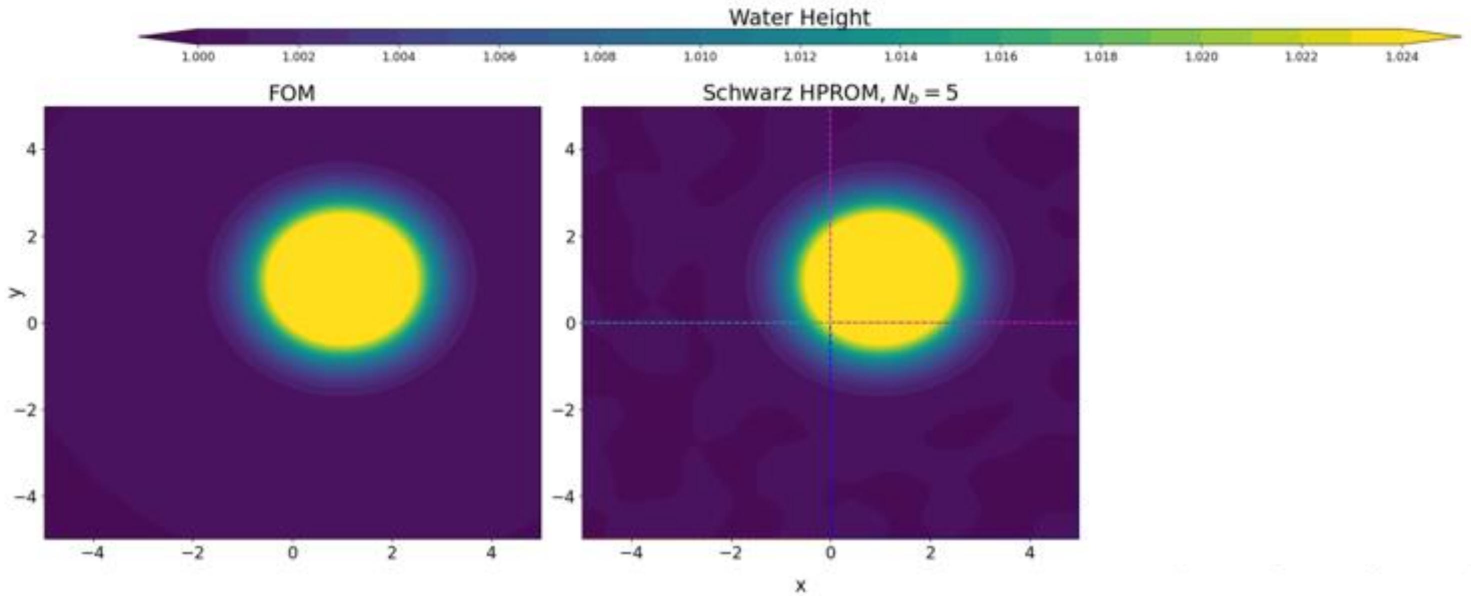
Figure above: example sample mesh with sampling rate $N_b = 5\%$.

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

Schwarz Boundary Sampling for All-HROM Coupling

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

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



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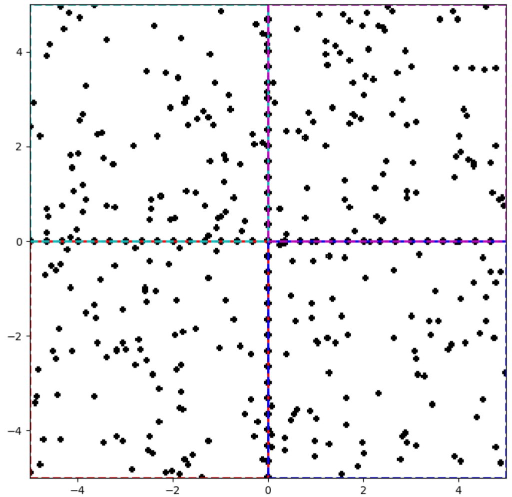

Figure above: example sample mesh with sampling rate $N_b = 10\%$.

- 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**

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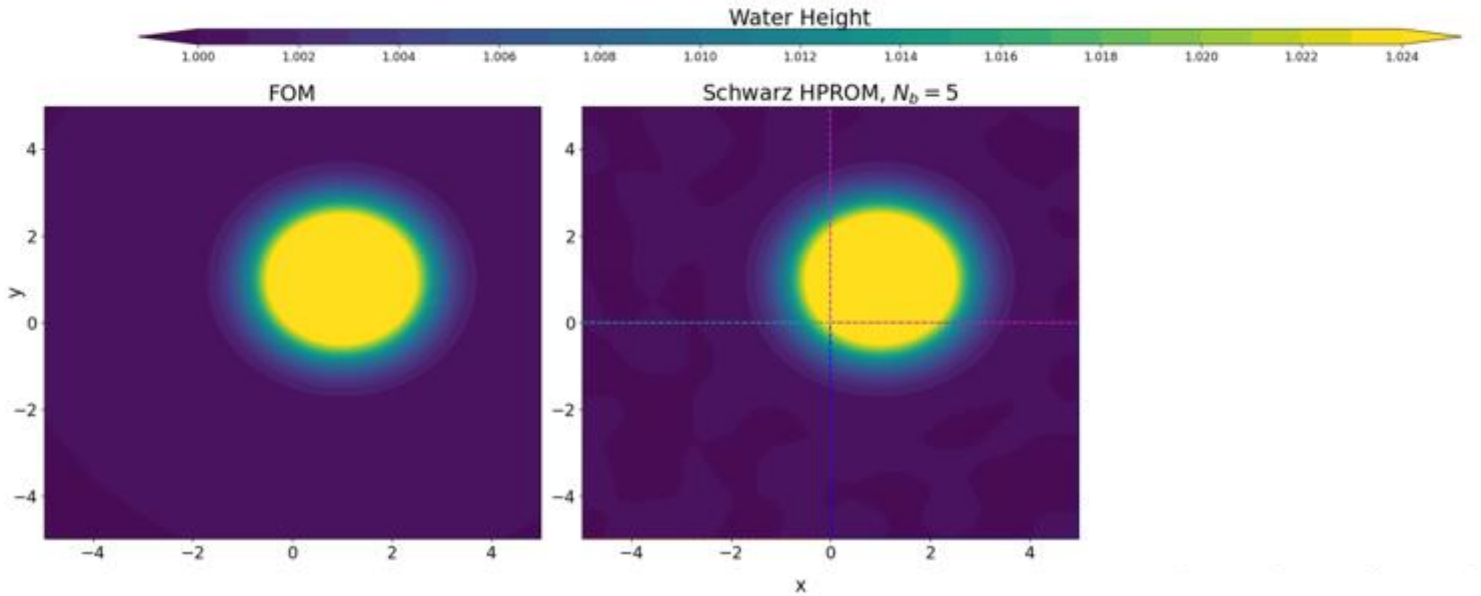

Movie above: FOM (left) and all HROM with $N_b = 5\%$ (right). ROMs have $K = 100$ modes and $N_s = 0.5\% N$ sample mesh points.

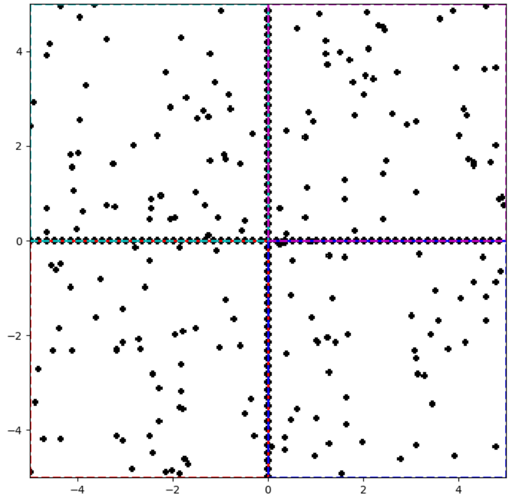

Figure above: example sample mesh with sampling rate $N_b = 15\%$.

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

Schwarz Boundary Sampling for All-HROM Coupling

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

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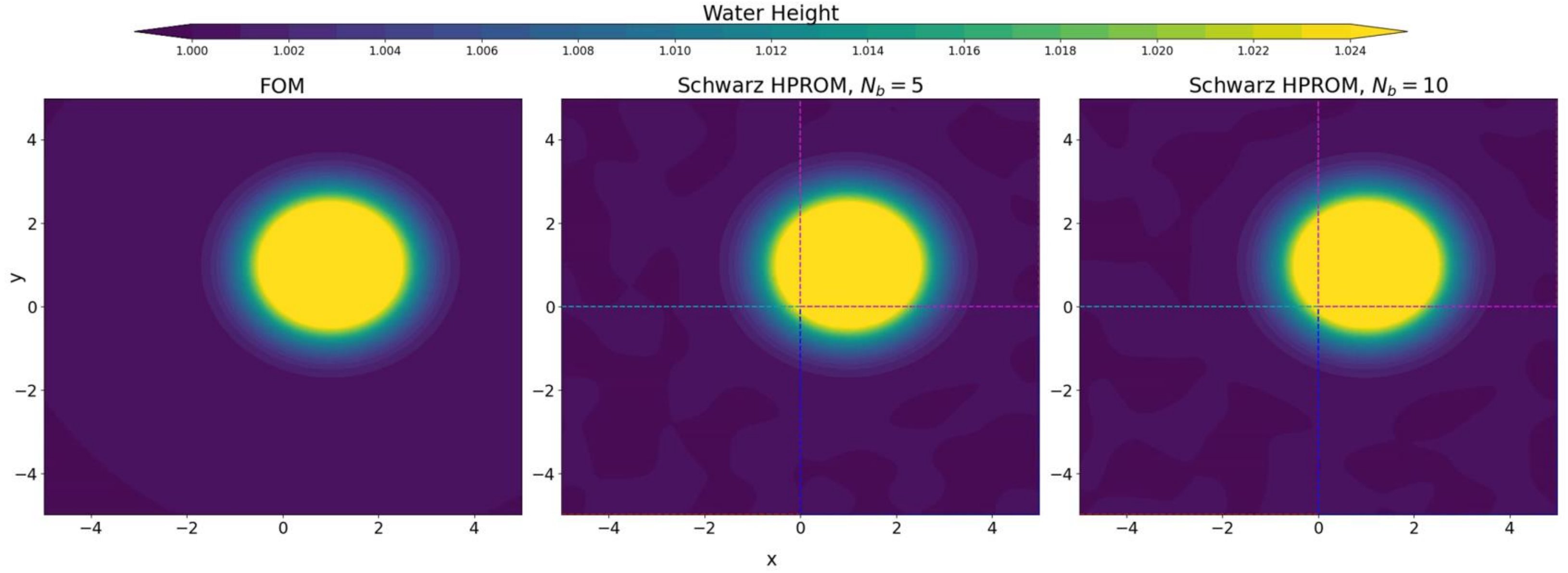


Movie above: FOM (left), all HROM with $N_b = 5\%$ (middle) and all HROM with $N_b = 10\%$ (left). ROMs have $K = 100$ modes and $N_s = 0.5\% N$ sample mesh points.

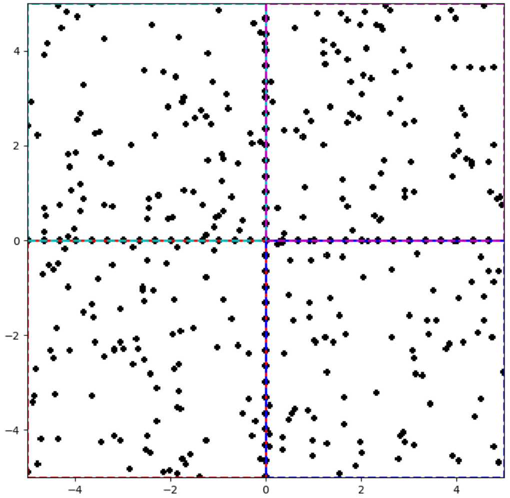
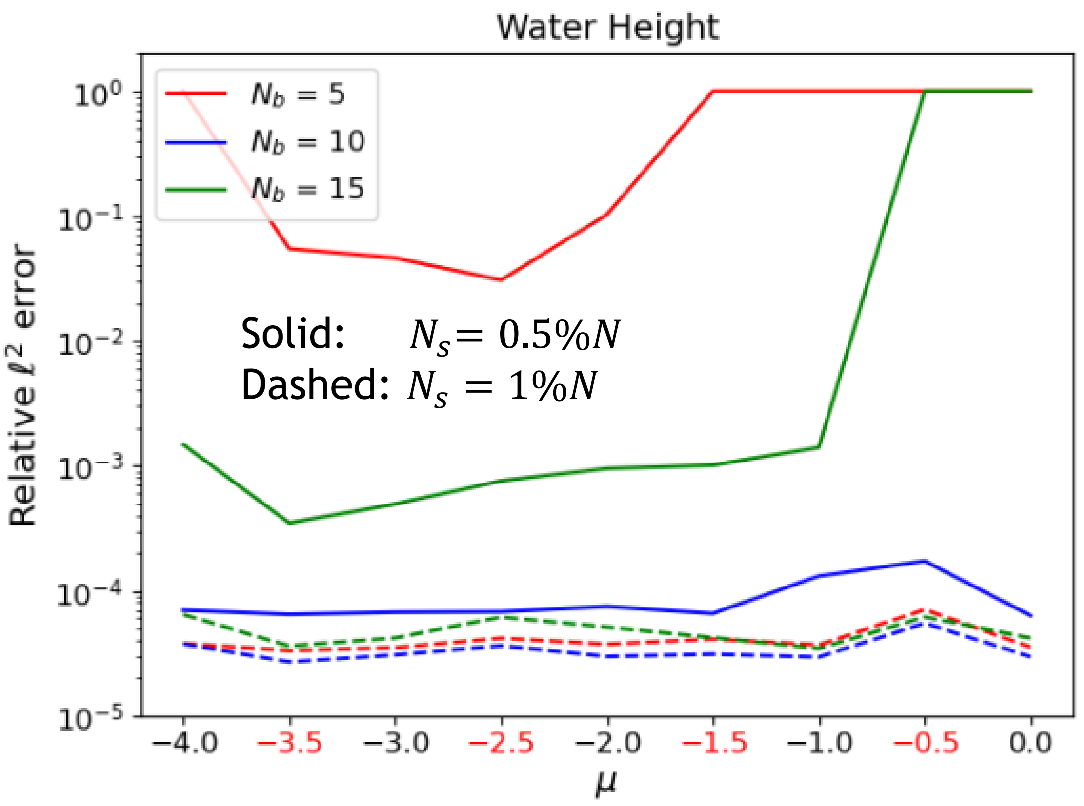
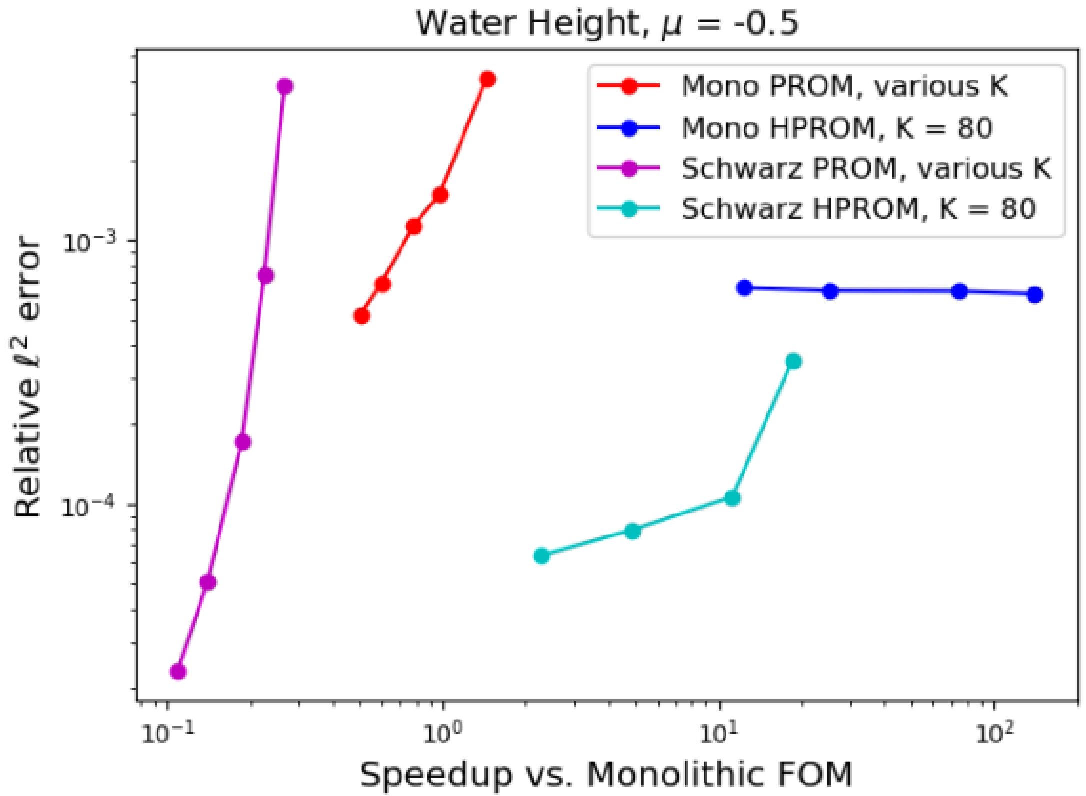


Figure above: example sample mesh with sampling rate $N_b = 10\%$

- 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

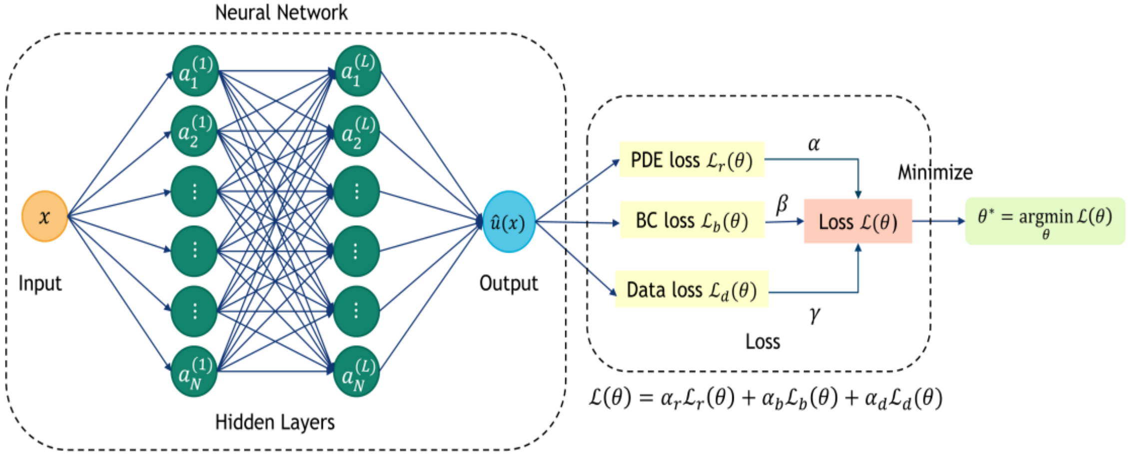




- For a fixed ROM dimension, Schwarz delivers **lower error** and **comparable cost!**
- There are noticeable **cost savings** relative to **monolithic FOM**!
- Accuracy similar for **predictive** μ (red) and **non-predictive** μ (black) cases.

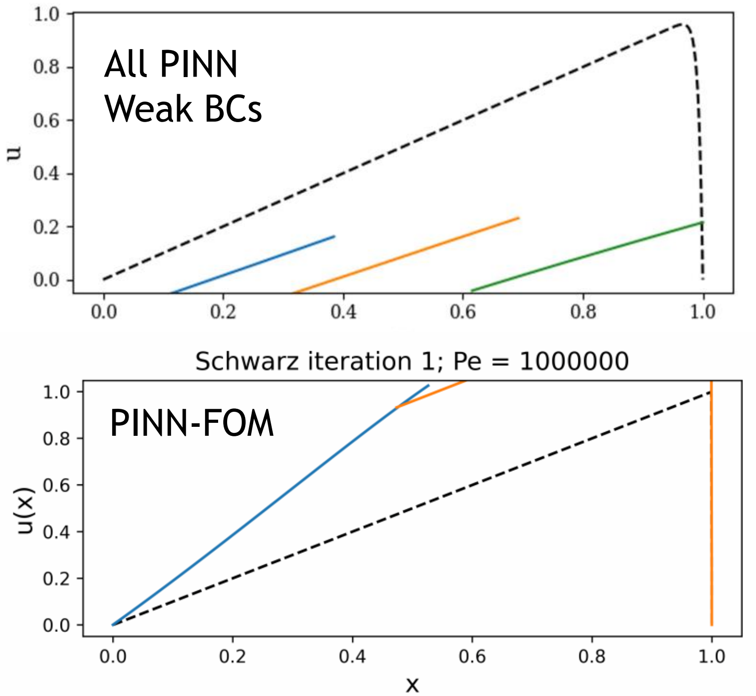
Extension to PINN-PINN Coupling

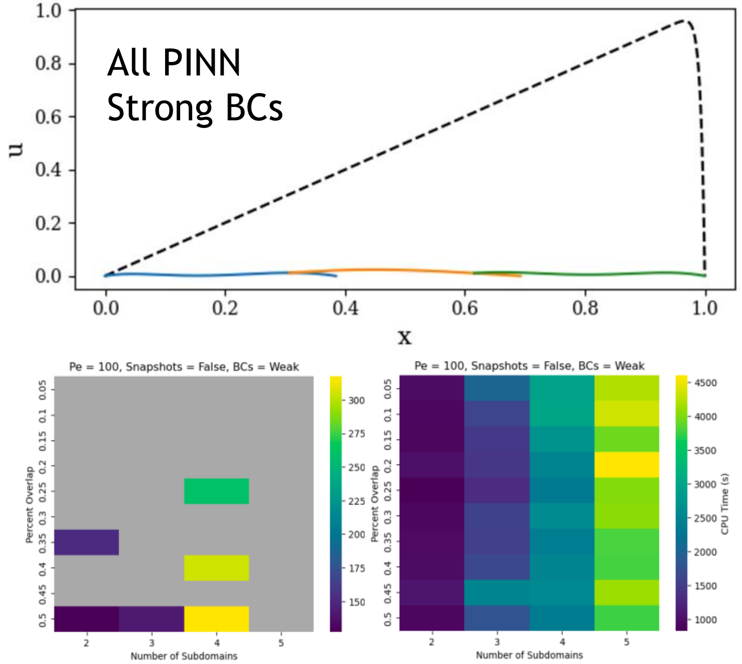
Goal: investigate the use of the Schwarz alternating method as a means to couple **Physics-Informed Neural Networks (PINNs)**



Learnings (using Schwarz to facilitate PINN training for 1D advection-diffusion PDE):

- PINNs are **very difficult to train** even for 1D linear advection-diffusion PDE, if Pe > 100!
- Schwarz convergence is **sensitive** to how **BCs** are enforced in the PINN.
- Training can be facilitated greatly through **PINN-FOM coupling.**
- **Tuning libraries** like RayTune and HyperOpt can autotune PINN/Schwarz parameters to **improve performance.**
- Could not get **non-overlapping Schwarz** to work.





Figures above: untuned (left) & tuned (right) results. Gray = no convergence.

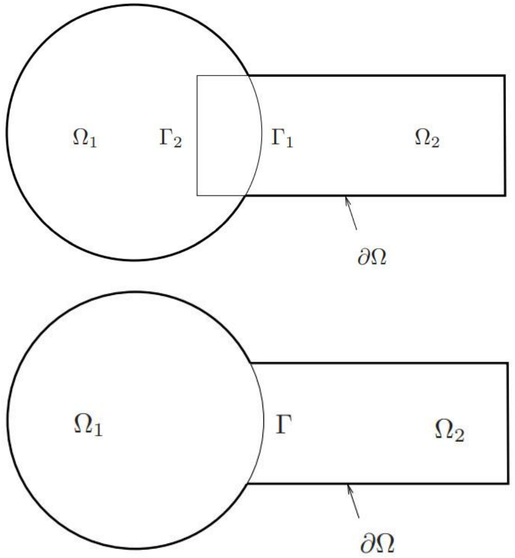
with Will Snyder (Virginia Tech), and Siqi Ma, Jinny Chung, Peter Krenek (Stanford U)

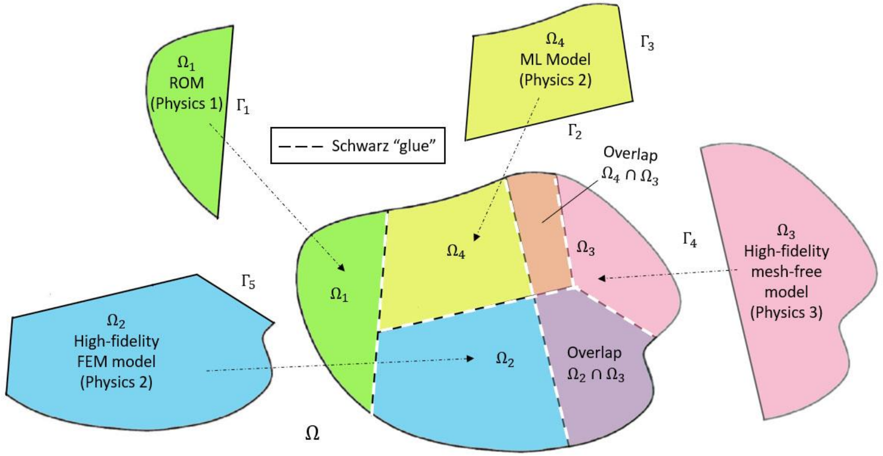
Outline

1. The Alternating Schwarz Method for FOM*-ROM# and ROM-ROM Coupling
   - Method Formulation
   - ROM Construction and Implementation
   - Numerical Examples

2. **A Lagrange Multiplier-based Partitioned Scheme for FOM-ROM and ROM-ROM Coupling**
   - **Method Formulation**
   - ROM Construction and Implementation
   - Numerical Examples

3. Summary and Future Work





*Full-Order Model. #Reduced Order Model.

Lagrange Multiplier-Based Partitioned Coupling Formulation

Model problem: time-dependent **advection-diffusion** problem on $\Omega = \Omega_1 \cup \Omega_2$ with $\Omega_1 \cap \Omega_2 = \emptyset$

$$\begin{aligned} &\dot{c}_i - \nabla \cdot F_i(c_i) = f_i, && \text{in} \quad \Omega_i \times [0,T] \\ &c_i = g_i, && \text{on} \quad \Gamma_i \times [0,T] \\ &c_i(\boldsymbol{x}, 0) = c_{i,0}(x), && \text{in} \quad \Omega_i \end{aligned} \qquad (1)$$

- $i \in \{1,2\}$
- c_i: unknown scalar solution field
- f_i: body force, g_i: boundary data on Γ_i
- $F_i(c_i) \coloneqq \kappa_i \nabla c_i - \boldsymbol{u} c_i$: total flux function
- κ_i: non-negative diffusion coefficient
- $\boldsymbol{u}$: given advection velocity field

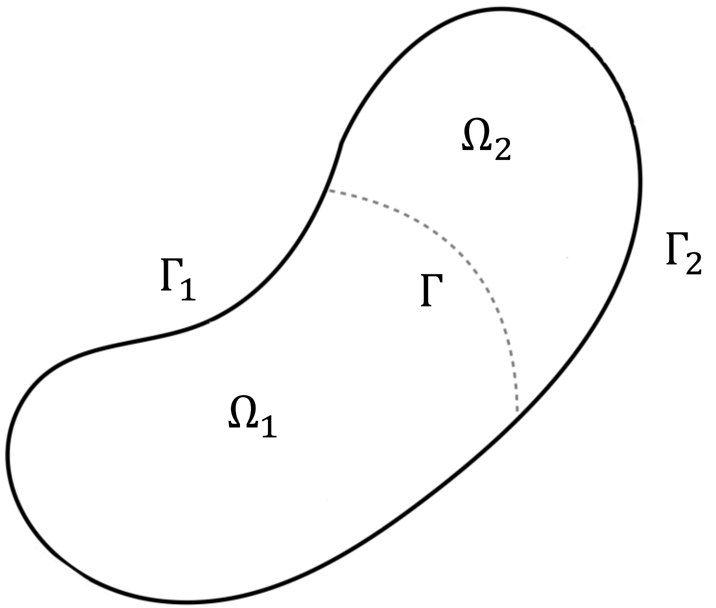


Figure above: example non-overlapping domain decomposition (DD) of $\Omega = \Omega_1 \cup \Omega_2$

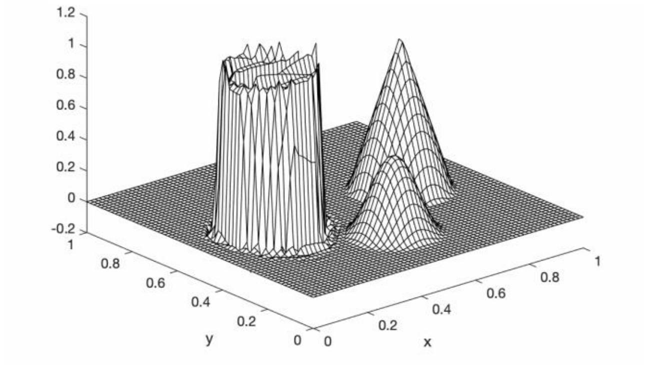
Compatibility conditions: on interface $\Gamma \times [0,T]$

- ***Continuity of states***: $c_1(\boldsymbol{x},t) - c_2(\boldsymbol{x},t) = 0$
- ***Continuity of total flux***: $F_1(\boldsymbol{x},t) \cdot \boldsymbol{n}_\Gamma = F_1(\boldsymbol{x},t) \cdot \boldsymbol{n}_\Gamma$

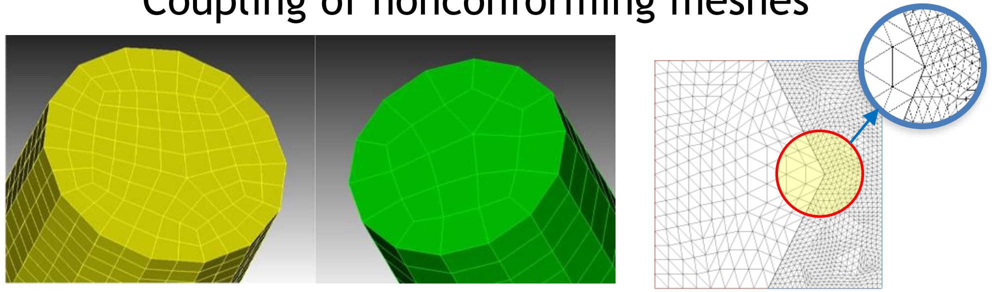
$\Rightarrow$ *Imposed weakly using Lagrange multiplier (LM)* λ

Lagrange Multiplier-Based Partitioned FOM-FOM Coupling

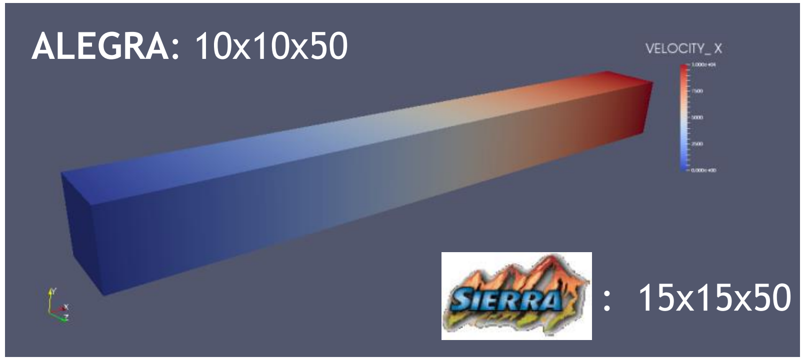
FEM-FEM coupling for high Peclet transport problem



Coupling of nonconforming meshes



Patch test (ALEGRA-Sierra/SM coupling)



"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[1,2]
- Coupling is ***non-iterative*** (single pass)

Method is theoretically rigorous[3]:

- Coupling does not introduce ***nonphysical artifacts***
- ***Theoretical convergence*** properties/guarantees including well-posedness of coupling force system
- ***Preserves*** the ***exact solution*** for conformal meshes

Method has been applied to several application spaces:

- ***Transport*** (unsteady advection-diffusion)
- ***Ocean-atmosphere coupling***
- ***Elasticity*** (e.g., ALEGRA-Sierra/SM coupling)

[1]Connors *et al*. 2022. [2]Sockwell *et al*. 2023. [3]Peterson *et al*. 2019.

A Lagrange Multiplier-Based Partitioned Scheme

Hybrid semi-discrete coupled formulation: obtained by differentiating interface conditions in time and discretizing hybrid problem using FEM in space

$$\begin{pmatrix} \boldsymbol{M}_1 & \boldsymbol{0} & \boldsymbol{G}_1^T \\ \boldsymbol{0} & \boldsymbol{M}_2 & -\boldsymbol{G}_2^T \\ \boldsymbol{G}_1 & -\boldsymbol{G}_2 & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \dot{\boldsymbol{c}}_1 \\ \dot{\boldsymbol{c}}_2 \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_1 - \boldsymbol{K}_1 \boldsymbol{c}_1 \\ \boldsymbol{f}_2 - \boldsymbol{K}_2 \boldsymbol{c}_2 \\ \boldsymbol{0} \end{pmatrix} \qquad (2)$$

- $\boldsymbol{M}_i$: mass matrices
- $\boldsymbol{K}_i := \boldsymbol{D}_i + \boldsymbol{A}_i$: stiffness matrices, where $\boldsymbol{D}_i$ and $\boldsymbol{A}_i$ are matrices for diffusive and advective terms, respectively
- $\boldsymbol{G}_i$: constraints matrices enforcing constraints in weak sense

Decoupling via Schur complement: equation (2) is equivalent to

*Equations **decouple** if using **explicit** or **IMEX** time-integration!*

$$\begin{pmatrix} \boldsymbol{M}_1 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{M}_2 \end{pmatrix} \begin{pmatrix} \dot{\boldsymbol{c}}_1 \\ \dot{\boldsymbol{c}}_2 \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_1 - \boldsymbol{K}_1 \boldsymbol{c}_1 - \boldsymbol{G}_1^T \boldsymbol{\lambda} \\ \boldsymbol{f}_2 - \boldsymbol{K}_2 \boldsymbol{c}_2 + \boldsymbol{G}_2^T \boldsymbol{\lambda} \end{pmatrix} \qquad (3)$$

where $(\boldsymbol{G}_1 \boldsymbol{M}_1^{-1} \boldsymbol{G}_1^T + \boldsymbol{G}_2 \boldsymbol{M}_2^{-1} \boldsymbol{G}_2^T)\boldsymbol{\lambda} = \boldsymbol{G}_1 \boldsymbol{M}_1^{-1}(\boldsymbol{f}_1 - \boldsymbol{K}_1 \boldsymbol{c}_1) - \boldsymbol{G}_2 \boldsymbol{M}_2^{-1}(\boldsymbol{f}_2 - \boldsymbol{K}_2 \boldsymbol{c}_2)$ (4)

Time integration schemes** and **time-steps** in Ω_1 and Ω_2 can be **different!

Implicit Value Recovery (IVR) Algorithm [Peterson *et al*. 2019]

- Pick explicit or IMEX time-integration scheme for Ω_1 and Ω_2
- Approximate LM space as trace of FE space on Ω_1 or Ω_2*
- Compute matrices $\boldsymbol{M}_i, \boldsymbol{K}_i$, $\boldsymbol{G}_i$ and vectors $\boldsymbol{f}_i$
- For each timestep t^n:
  - ➢ Solve Schur complement system (4) for the LM $\boldsymbol{\lambda}^n$
  - ➢ Update the state variables $\boldsymbol{c}_i^n$ by advancing (3) in time

* Ensures that dual Schur complement of (2) is s.p.d.

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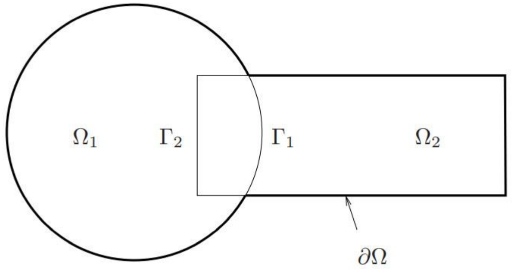
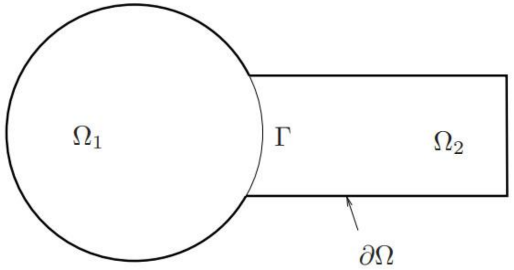
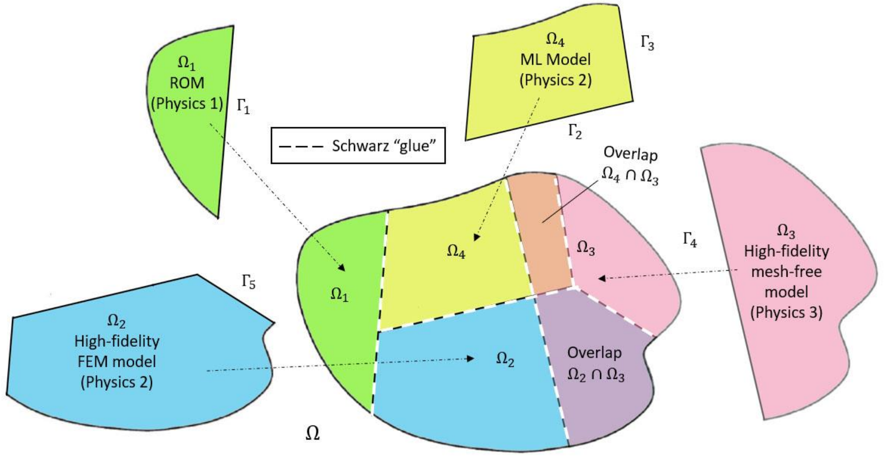




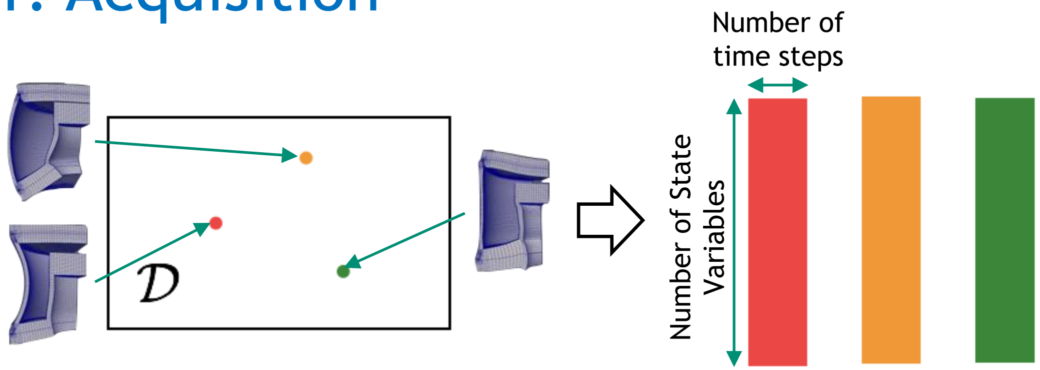


*Full-Order Model. #Reduced Order Model.

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

Full Order Model (FOM): $\boldsymbol{M}\frac{d\boldsymbol{u}}{dt} + \boldsymbol{K}\boldsymbol{u} = \boldsymbol{f}$

1. Acquisition

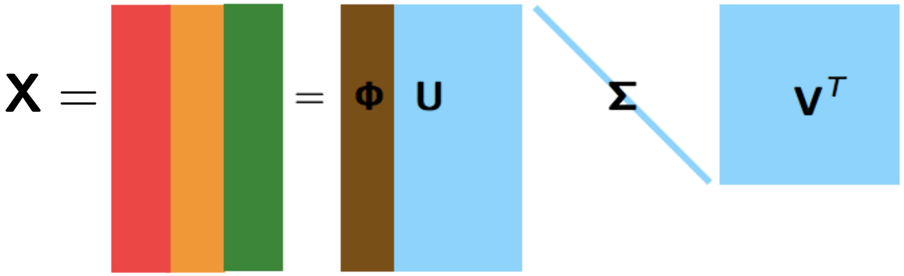


Solve ODE at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



ROM = projection-based Reduced Order Model

3. Projection-Based Reduction

Reduce the number of unknowns

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

Perform Galerkin projection

$\boldsymbol{\Phi}^T\boldsymbol{M}\boldsymbol{\Phi}\frac{d\hat{\boldsymbol{u}}}{dt} + \boldsymbol{\Phi}^T\boldsymbol{K}\boldsymbol{\Phi}\hat{\boldsymbol{u}} = \boldsymbol{\Phi}^T\boldsymbol{f}$

Hyper-reduce nonlinear terms

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

Hyper-reduction/sample mesh

HROM = Hyper-reduced ROM

ROM-ROM Coupling: Full Subdomain Bases & Full LM Spaces

- Collect **snapshots** using suitable monolithic FOM solve for equation (1) and **subtract DBC data** on $\Gamma_1 \cup \Gamma_2$
- **Partition** modified snapshots into **subdomain snapshot matrices** $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ on Ω_1 and Ω_2, respectively
- Calculate **"full" subdomain POD bases** $\boldsymbol{\Phi}_1$ and $\boldsymbol{\Phi}_2$ of dimensions M_1 and M_2 from SVD of $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$
- **Approximate** the solution as a **linear combination** of the POD modes in each subdomain:

$$\boldsymbol{c}_1(t) \approx \tilde{\boldsymbol{c}}_1(t) := \bar{\boldsymbol{c}}_1 + \boldsymbol{\Phi}_1 \hat{\boldsymbol{c}}_1(t), \qquad \boldsymbol{c}_2(t) \approx \tilde{\boldsymbol{c}}_2(t) := \bar{\boldsymbol{c}}_2 + \boldsymbol{\Phi}_2 \hat{\boldsymbol{c}}_2(t) \qquad (5)$$

- Substitute (5) into (2) and **project** (3) onto POD modes to obtain system of the form:

$$\begin{pmatrix} \widetilde{\boldsymbol{M}}_1 & \boldsymbol{0} & \widetilde{\boldsymbol{G}}_1^T \\ \boldsymbol{0} & \widetilde{\boldsymbol{M}}_2 & -\widetilde{\boldsymbol{G}}_2^T \\ \widetilde{\boldsymbol{G}}_1 & -\widetilde{\boldsymbol{G}}_2 & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \dot{\hat{\boldsymbol{c}}}_1 \\ \dot{\hat{\boldsymbol{c}}}_2 \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \boldsymbol{s}_1 \\ \boldsymbol{s}_2 \\ \boldsymbol{0} \end{pmatrix} \qquad \text{where } \widetilde{\boldsymbol{M}}_i := \boldsymbol{\Phi}_i^T \boldsymbol{M}_i \boldsymbol{\Phi}_i,\ \widetilde{\boldsymbol{G}}_i := \boldsymbol{G}_i \boldsymbol{\Phi}_i, \quad \boldsymbol{s}_i := \boldsymbol{\Phi}_i^T \boldsymbol{f}_i - \boldsymbol{\Phi}_i^T \boldsymbol{K}_i \boldsymbol{\Phi}_i \hat{\boldsymbol{c}}_i - \boldsymbol{\Phi}_i^T \boldsymbol{K}_i \bar{\boldsymbol{c}}_i - \boldsymbol{\Phi}_i^T \boldsymbol{M}_i \dot{\bar{\boldsymbol{c}}}_i \qquad (6)$$

Online ROM-ROM IVR Solution Algorithm with Full Subdomain Bases & LM Spaces: at each time step t^n

- ➢ Use $\hat{\boldsymbol{c}}_1^n$ and $\hat{\boldsymbol{c}}_2^n$ to compute updated RHS $\boldsymbol{s}_1^n$ and $\boldsymbol{s}_2^n$
- ➢ Solve the Schur complement system for $\boldsymbol{\lambda}^n$:

$$(\widetilde{\boldsymbol{G}}_1 \widetilde{\boldsymbol{M}}_1^{-1} \widetilde{\boldsymbol{G}}_1^T + \widetilde{\boldsymbol{G}}_2 \widetilde{\boldsymbol{M}}_2^{-1} \widetilde{\boldsymbol{G}}_2^T) \boldsymbol{\lambda}^n = \widetilde{\boldsymbol{G}}_1 \widetilde{\boldsymbol{M}}_1^{-1} \boldsymbol{s}_1^n - \widetilde{\boldsymbol{G}}_2 \widetilde{\boldsymbol{M}}_2^{-1} \boldsymbol{s}_2^n$$

- ➢ Advance the following systems forward in time: $\widetilde{\boldsymbol{M}}_1 \dot{\hat{\boldsymbol{c}}}_1^n = \boldsymbol{s}_1^n - \widetilde{\boldsymbol{G}}_1 \boldsymbol{\lambda}^n$ and $\widetilde{\boldsymbol{M}}_2 \dot{\hat{\boldsymbol{c}}}_2^n = \boldsymbol{s}_2^n + \widetilde{\boldsymbol{G}}_2 \boldsymbol{\lambda}^n$

ROM-ROM Coupling: What Could Go Wrong?

A provably non-singular dual Schur complement requires:

1. ***Symmetric positive-definite projected mass matrices*** $\widetilde{M}_i$

2. ***Projected constraint matrix*** $\left(\widetilde{G}_1, \widetilde{G}_2\right)^T$ ***must have full column rank***

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Volume 417, Part B, 15 December 2023, 116398

Explicit synchronous partitioned scheme for coupled reduced order models based on composite reduced bases ☆

Amy de Castro [a b], Pavel Bochev [b], Paul Kuberry [b], Irina Tezaur [c]

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   - ☹ Not guaranteed for "full" LM space, taken as trace of underlying FEM discretization space

ROM-ROM Coupling: What Could Go Wrong?

A provably non-singular dual Schur complement requires:

1. ***Symmetric positive-definite projected mass matrices*** $\widetilde{\boldsymbol{M}}_i$
   - ☹ Not guaranteed *a priori* with full subdomain bases $\boldsymbol{\Phi}_1$ and $\boldsymbol{\Phi}_2$
   - ☺ Remedied by creating separate **“split” reduced bases** $\boldsymbol{\Phi}_{i,\Gamma}$ and $\boldsymbol{\Phi}_{i,0}$, for interface and interior DOFs
     - ➢ Columns of each basis matrix will have full column rank

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2. ***Projected constraint matrix*** $\left(\widetilde{\boldsymbol{G}}_1, \widetilde{\boldsymbol{G}}_2\right)^{\boldsymbol{T}}$ ***must have full column rank***
   - ☹ Not guaranteed for “full” LM space, taken as trace of underlying FEM discretization space
   - ☺ Remedied by **reducing LM space** to ensure satisfaction of discrete *inf-sup* condition for (6)
     - ➢ Reduce size of LM space to size $N_{R,\Gamma} < N_{R,1\Gamma} + N_{R,2\Gamma}$, where $N_{R,i\Gamma}$ = # POD modes in $\boldsymbol{\Phi}_{i,\Gamma}$
     - ➢ For now, approximate $\boldsymbol{\lambda} \approx \boldsymbol{\Phi}_{\text{LM}}\hat{\boldsymbol{\lambda}}$ where $\boldsymbol{\Phi}_{\text{LM}} = \boldsymbol{\Phi}_{i,\Gamma}$ for $i = 1,2$, so that $N_{R,\Gamma} = N_{R,i\Gamma}$

ROM-ROM Coupling: Split Bases & Reduced LM Spaces

- Consider two **separate expansions** for **interface** and **interior DOFs** for $i = 1{,}2$:

$$\boldsymbol{c}_{i,0}(t) \approx \tilde{\boldsymbol{c}}_{i,0}(t) := \bar{\boldsymbol{c}}_{i,0} + \boldsymbol{\Phi}_{i,0}\hat{\boldsymbol{c}}_{i,0}(t), \quad \boldsymbol{c}_{i,\Gamma}(t) \approx \tilde{\boldsymbol{c}}_{i,\Gamma}(t) := \bar{\boldsymbol{c}}_{i,\Gamma} + \boldsymbol{\Phi}_{i,\Gamma}\hat{\boldsymbol{c}}_{i,\Gamma}(t)$$

- Substituting above expansions into (2) and projecting equations onto reduced bases gives system of the form:

Reduced LM space also helps **prevent over-constraining** for **full subdomain basis** implementation.

$$\begin{pmatrix} \widetilde{\boldsymbol{M}}_{1,\Gamma} & \widetilde{\boldsymbol{M}}_{1,\Gamma 0} & \boldsymbol{0} & \boldsymbol{0} & \widetilde{\boldsymbol{G}}_1^T \\ \widetilde{\boldsymbol{M}}_{1,0\Gamma} & \widetilde{\boldsymbol{M}}_{1,0} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \widetilde{\boldsymbol{M}}_{2,\Gamma} & \widetilde{\boldsymbol{M}}_{2,\Gamma 0} & -\widetilde{\boldsymbol{G}}_2^T \\ \boldsymbol{0} & \boldsymbol{0} & \widetilde{\boldsymbol{M}}_{2,0\Gamma} & \widetilde{\boldsymbol{M}}_{2,0} & \boldsymbol{0} \\ \widetilde{\boldsymbol{G}}_1 & \boldsymbol{0} & -\widetilde{\boldsymbol{G}}_2 & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \dot{\hat{\boldsymbol{c}}}_{1,\Gamma} \\ \dot{\hat{\boldsymbol{c}}}_{1,0} \\ \dot{\hat{\boldsymbol{c}}}_{2,\Gamma} \\ \dot{\hat{\boldsymbol{c}}}_{1,0} \\ \hat{\boldsymbol{\lambda}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{s}_{1,\Gamma} \\ \boldsymbol{s}_{1,0} \\ \boldsymbol{s}_{2,\Gamma} \\ \boldsymbol{s}_{2,0} \\ \boldsymbol{0} \end{pmatrix}$$

Split basis + reduced LM space guarantees ROM-ROM coupling has **non-singular dual Schur complement***.

Online ROM-ROM IVR Solution Algorithm with Split Bases & Reduced LM Spaces: at each time step t^n

- ➢ Use $\hat{\boldsymbol{c}}_{i,0}^n$ and $\hat{\boldsymbol{c}}_{i,\Gamma}^n$ to compute updated RHS $\boldsymbol{s}_{i,0}^n$ and $\boldsymbol{s}_{i,\Gamma}^n$ for $i = 1{,}2$.
- Define $\widetilde{\boldsymbol{M}}_{i,jk} := \boldsymbol{\Phi}_{i,j}^T \boldsymbol{M}_{i,jk} \boldsymbol{\Phi}_{i,k}$, $\widetilde{\boldsymbol{G}}_i := \boldsymbol{\Phi}_{\mathrm{LM}}^T \boldsymbol{G}_i \boldsymbol{\Phi}_{i,\Gamma}$, $\widetilde{\boldsymbol{P}}_i := \widetilde{\boldsymbol{M}}_{i,\Gamma} - \widetilde{\boldsymbol{M}}_{i,\Gamma 0} \boldsymbol{M}_{i,0}^{-1} \widetilde{\boldsymbol{M}}_{i,\Gamma 0}$ for $\{j,k\} \in \{0,\Gamma\}$ and solve:

$$\left(\widetilde{\boldsymbol{G}}_1 \widetilde{\boldsymbol{P}}_1^{-1} \widetilde{\boldsymbol{G}}_1^T + \widetilde{\boldsymbol{G}}_2 \widetilde{\boldsymbol{P}}_2^{-1} \widetilde{\boldsymbol{G}}_2^T\right)\hat{\boldsymbol{\lambda}}^n = \widetilde{\boldsymbol{G}}_1 \widetilde{\boldsymbol{P}}_1^{-1}\left(\boldsymbol{s}_{1,\Gamma}^n - \widetilde{\boldsymbol{M}}_{1,\Gamma 0} \boldsymbol{M}_{1,0}^{-1} \boldsymbol{s}_{1,0}^n\right) - \widetilde{\boldsymbol{G}}_2 \widetilde{\boldsymbol{P}}_2^{-1}\left(\boldsymbol{s}_{2,\Gamma}^n - \widetilde{\boldsymbol{M}}_{2,\Gamma 0} \boldsymbol{M}_{2,0}^{-1} \boldsymbol{s}_{2,0}^n\right)$$

- ➢ Advance the following systems forward in time:

$$\begin{pmatrix} \widetilde{\boldsymbol{M}}_{i,\Gamma} & \widetilde{\boldsymbol{M}}_{i,\Gamma 0} \\ \widetilde{\boldsymbol{M}}_{i,\Gamma 0} & \widetilde{\boldsymbol{M}}_{i,\Gamma} \end{pmatrix} \begin{pmatrix} \dot{\hat{\boldsymbol{c}}}_{i,\Gamma}^n \\ \dot{\hat{\boldsymbol{c}}}_{i,0}^n \end{pmatrix} = \begin{pmatrix} \boldsymbol{s}_{i,\Gamma}^n + (-1)^i \widetilde{\boldsymbol{G}}_i^T \hat{\boldsymbol{\lambda}}^n \\ \boldsymbol{s}_{i,0}^n \end{pmatrix}$$

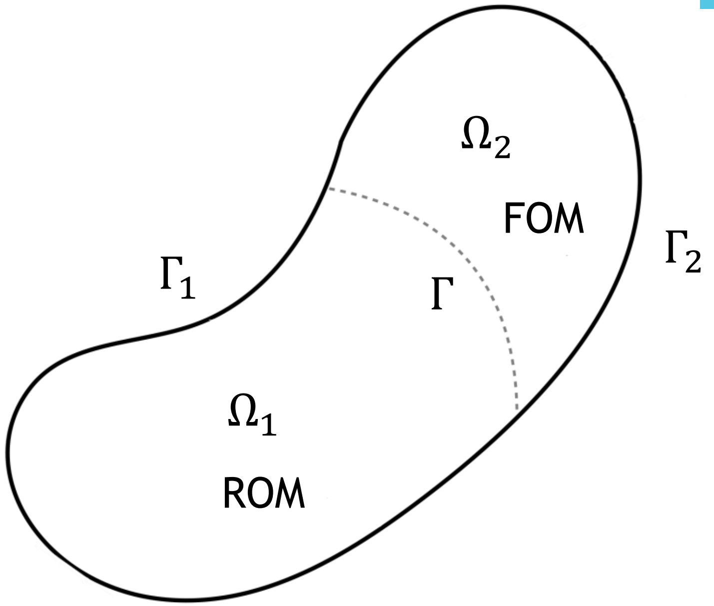
* See [de Castro *et al.*, 2023]

Extension to ROM-FOM Coupling

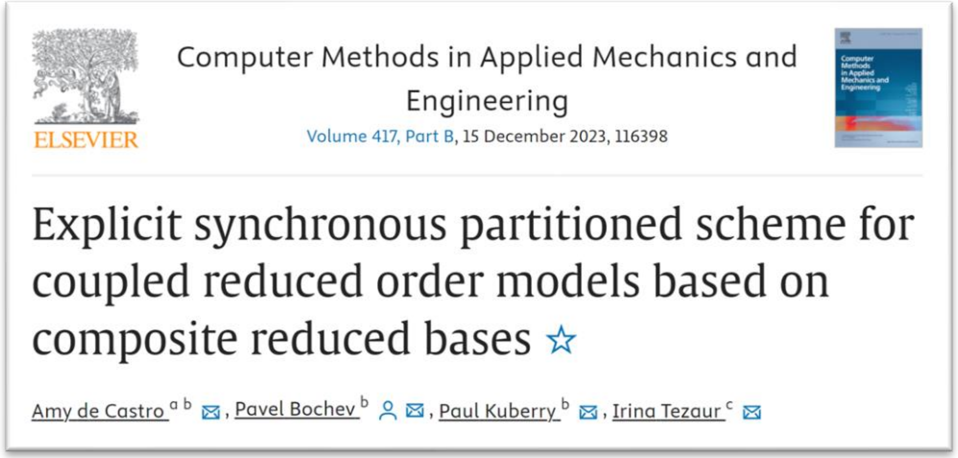
- Assume WLOG ROM is in Ω_1 and FOM is in Ω_2, so that **Schur complement** takes the form:

$$\widehat{\boldsymbol{S}} := \widehat{\boldsymbol{G}}_1 \widetilde{\boldsymbol{M}}_1^{-1} \widehat{\boldsymbol{G}}_1^T + \widehat{\boldsymbol{G}}_2 \boldsymbol{M}_2^{-1} \widehat{\boldsymbol{G}}_2^T$$

- There are **multiple choices** for LM space that guarantee an **s.p.d. Schur complement** and ***inf-sup* stability**:
  - ➢ May use **full LM (fLM) space**, defined as trace of FE space on Ω_1
  - ➢ May use **reduced LM (rLM) space**, as in ROM-ROM coupling



- Proven using a **variational** (rather than discrete) approach in [de Castro *et al.*, 2023]:


Computer Methods in Applied Mechanics and Engineering
Volume 417, Part B, 15 December 2023, 116398

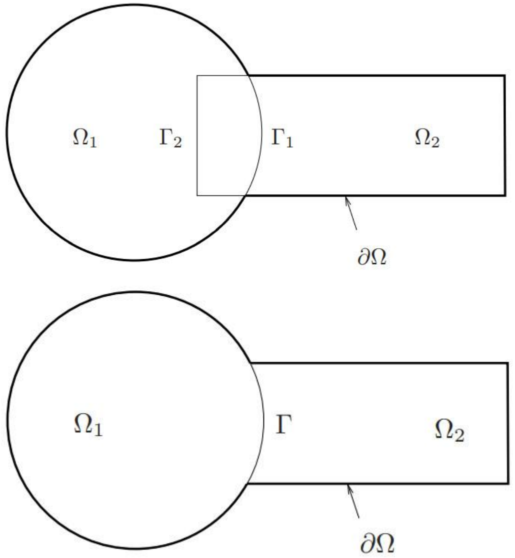
Explicit synchronous partitioned scheme for coupled reduced order models based on composite reduced bases ☆

Amy de Castro [a b], Pavel Bochev [b], Paul Kuberry [b], Irina Tezaur [c]

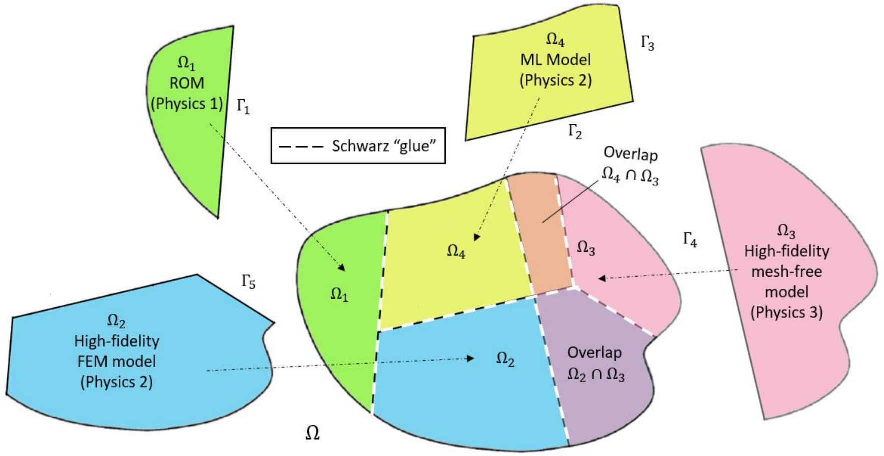
Formulations yield **provably non-singular Schur complements**, independent of **mesh size** or **reduced basis dimension**.

Outline

1. The Alternating Schwarz Method for FOM*-ROM# and ROM-ROM Coupling
   - Method Formulation
   - ROM Construction and Implementation
   - Numerical Examples



2. **A Lagrange Multiplier-based Partitioned Scheme for FOM-ROM and ROM-ROM Coupling**
   - Method Formulation
   - ROM Construction and Implementation
   - **Numerical Examples**
3. Summary and Future Work



*Full-Order Model. #Reduced Order Model.

Model Problem: 2D High Peclet Transmission Problem

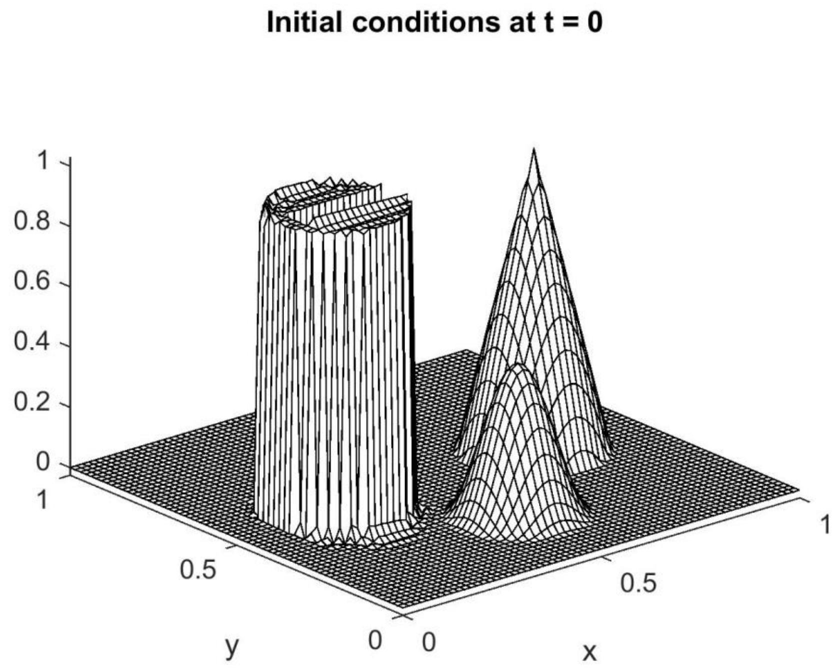
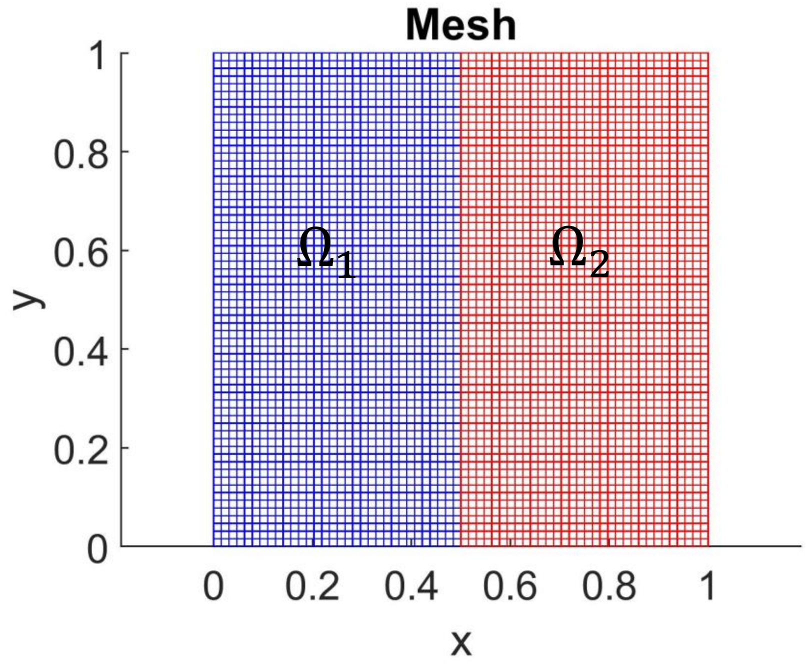


Figure left: initial condition.
Figure right: mesh and DD.



Problem setup:

- $\Omega = (0,1)^2$, DD into 2 subdomains (top right)
- **Homogeneous source** and **homogeneous Dirichlet** boundary conditions
- Cone, cylinder and smooth hump **initial condition**
- **Rotating advection field** $(0.5 - y, x - 0.5)$ for one full rotation
- **Viscosity** κ_i can **vary** across subdomains: $\kappa_1 \neq \kappa_2$

FOM discretization:

- Spatial discretization given by **finite element method** with $N = 64$ elements in each dimension
- IMEX Crank-Nicholson discretization in time (treating LM explicitly) with fixed $\Delta t = 6.734 \times 10^{-3}$ for $\kappa_i < 10^{-2}$ and $\Delta t = 9.156 \times 10^{-4}$ for $\kappa_i = 10^{-2}$

POD/Galerkin ROM Setup

- **Prediction across $\boldsymbol{\kappa_i}$**: training parameters $\kappa_1 = \kappa_2 = 10^{-2}$ and $\kappa_1 = \kappa_2 = 10^{-8}$, testing parameters $\kappa_1 = 10^{-5}$, $\kappa_2 = 10^{-4}$
- Snapshots collected by **restricting** single-domain solution to Ω_i
- $M_1 = 23$, $M_2 = 19$ interior modes and 5 interface modes capture **99% of snapshot energy**
- **Full LM (fLM) space** has dimension of 63 (# nodes on Γ) .
- **Reduced LM (rLM) space** has dimension:

$$N_{R,i\Gamma} = \min\left\{\frac{1}{4}N_{R,i0}, 63\right\}$$

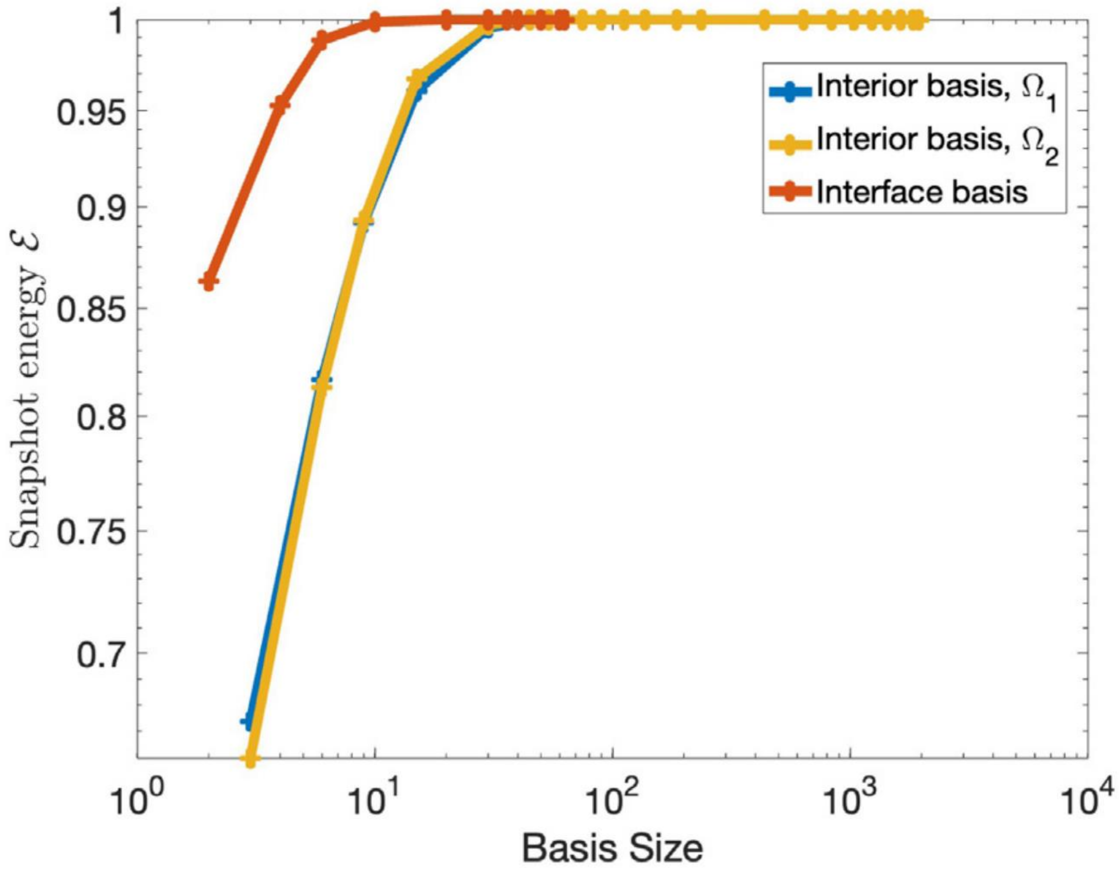
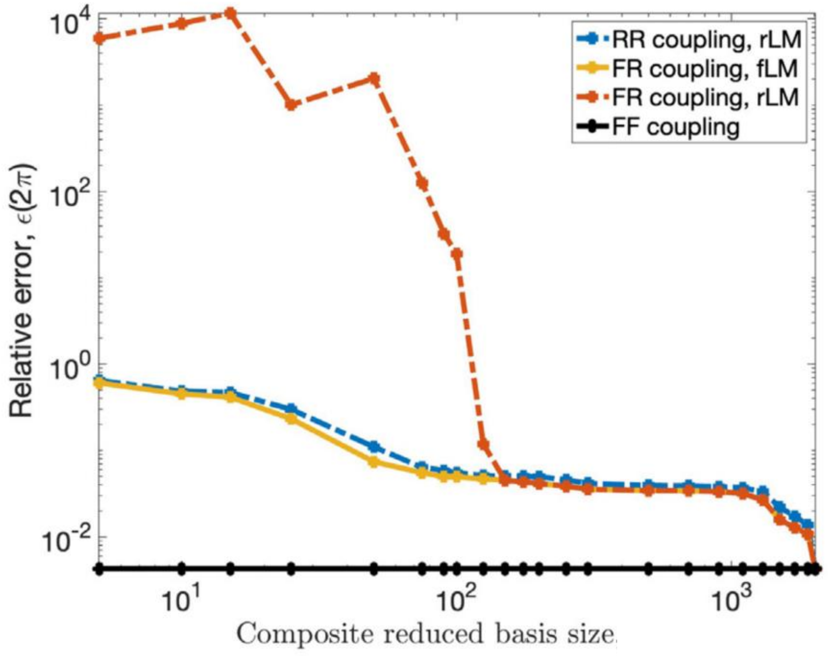
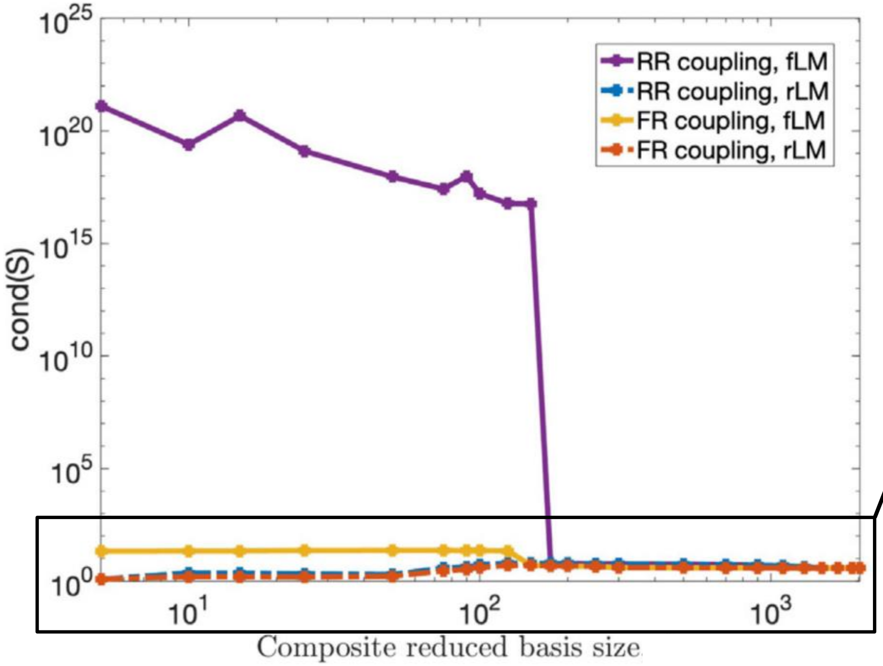
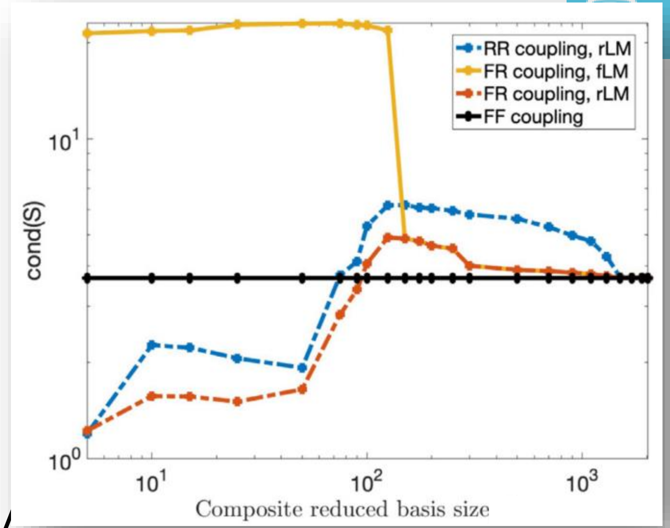


Figure above: snapshot energies as a function of the basis sizes.

Relative Errors and Condition Numbers





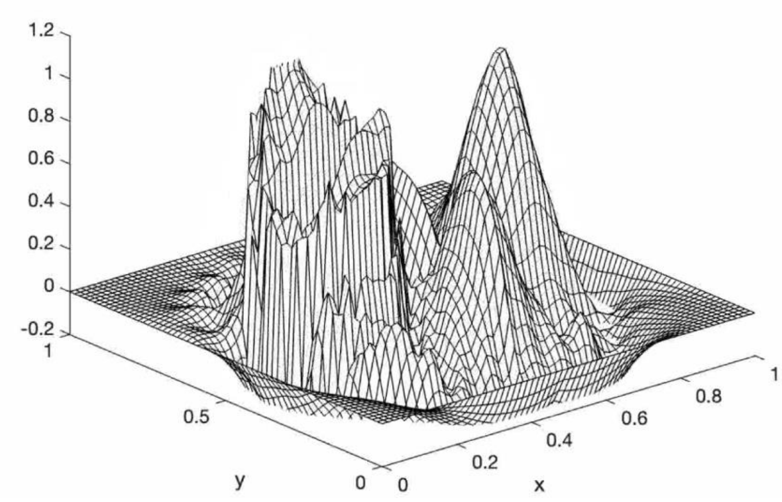


RR = ROM-ROM
FR = FOM-ROM
FF = FOM-FOM
fLM = full LM space
rLM = reduced LM space

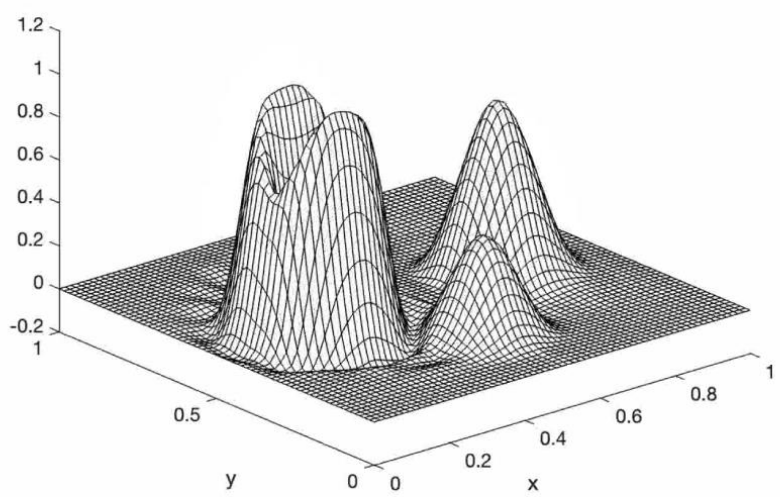
Figure above left: relative errors at final time 2π w.r.t. single-domain FOM solution.
Figure above right: Schur complement condition numbers for RR, FR and FF couplings.

- All stable couplings **converge** with basis refinement
- FR-rLM formulation has **much larger errors** for small basis sizes (left figure)
- Using **rLM space** improves **condition number** (right figures)
- **Condition** number of stable couplings with rLM is O(1) **independent** of the **reduced basis size**

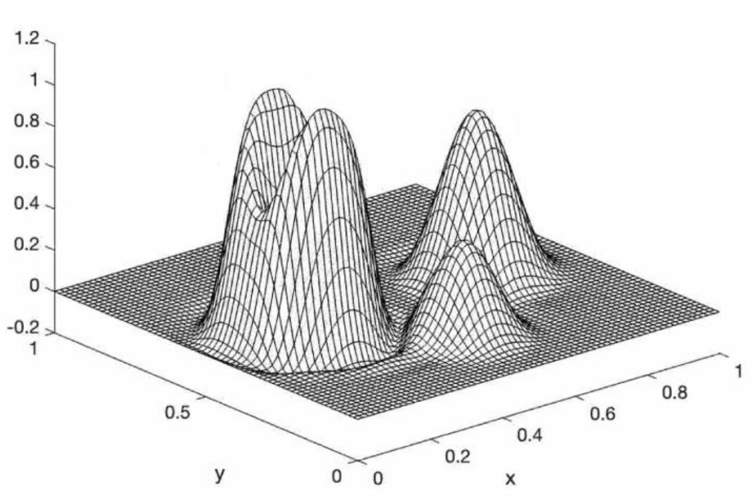
Comparison of Solutions at Final Time



Naïve ROM-ROM coupling with fLM Lagrange multiplier space



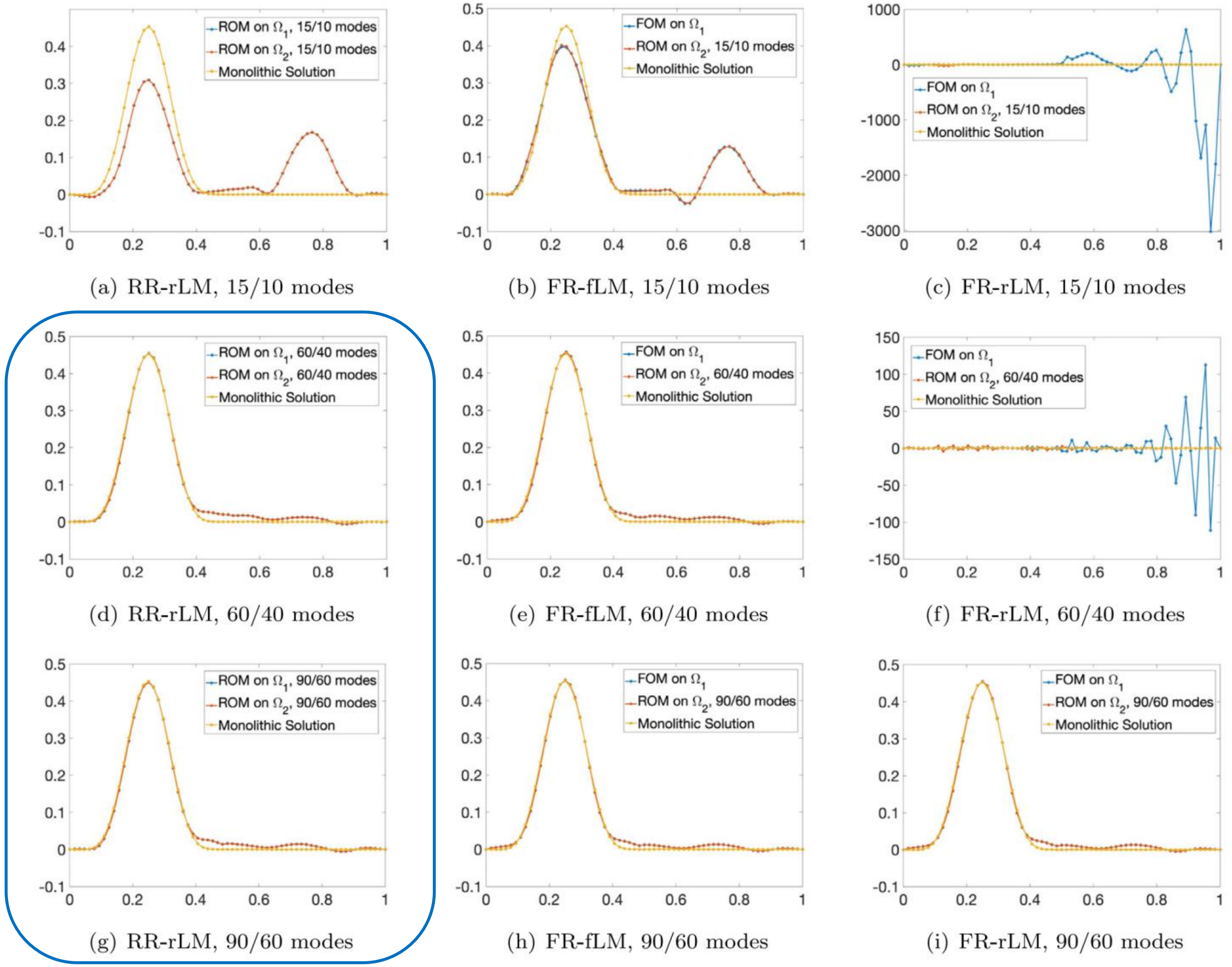
Provably-stable ROM-ROM coupling with rLM Lagrange multiplier space



FOM-FOM coupling

Provably-stable ROM-ROM (and FOM-ROM) formulations deliver **artifact-free** solutions unlike naïve (unstable) coupling formulations!

Comparison of Interface States at Final Time



(a) RR-rLM, 15/10 modes (b) FR-fLM, 15/10 modes (c) FR-rLM, 15/10 modes

(d) RR-rLM, 60/40 modes (e) FR-fLM, 60/40 modes (f) FR-rLM, 60/40 modes

(g) RR-rLM, 90/60 modes (h) FR-fLM, 90/60 modes (i) FR-rLM, 90/60 modes

The label "m/n modes" corresponds to m **interior** and n **interface** modes.

- All formulations **converge** to monolithic solution with basis **refinement**
- **Oscillations** in **FR-rLM** formulations with "small" basis sizes are due to accumulation of interface errors during time-integration caused by the **approximate enforcement** of the coupling condition

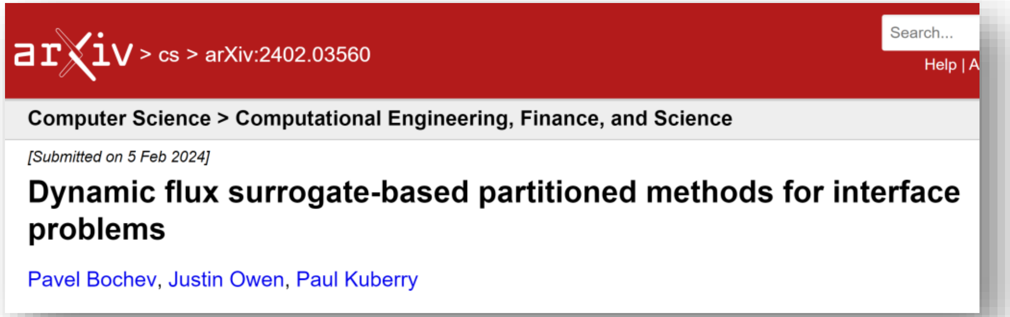
Model	CPU time (s)
Monolithic FOM	90.79
FOM-FOM	105.89
ROM-ROM, rLM, 90/60 modes	45.57
ROM-ROM, rLM, 60/40 modes	25.36
ROM-ROM, rLM, 15/10 modes	10.19

Accurate ROM-ROM couplings offer 1.99-3.58× speedup w.r.t. monolithic FOM!

Ongoing Work: Approximation of Interface Flux with Data-Driven Surrogates

- Bottleneck in GMM-based coupling approach is solving the Schur system given by $\boldsymbol{S} := \boldsymbol{G}_1 \boldsymbol{M}_1^{-1} \boldsymbol{G}_1^T + \boldsymbol{G}_2 \boldsymbol{M}_2^{-1} \boldsymbol{G}_2^T$, especially when coupling involves FOMs

Key idea: use data-driven techniques to create **efficient surrogates** that approximate the dynamics of the **interface flux**, to avoid **expensive Schur complement** solves in GMM.



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Computer Science > Computational Engineering, Finance, and Science

[Submitted on 5 Feb 2024]

Dynamic flux surrogate-based partitioned methods for interface problems

Pavel Bochev, Justin Owen, Paul Kuberry

We consider two different **surrogates** $\boldsymbol{\lambda} = \mathcal{F}(\boldsymbol{y})$ for the **interface flux** dynamics (to replace (4)) using similar states $\boldsymbol{y}$:

- ***DMD surrogate***: $\boldsymbol{y}_{k+1} = A\boldsymbol{y}_k$
- ***nODE surrogate***: $\frac{d\boldsymbol{y}}{dt} = f(t, \boldsymbol{y}, u; \theta) =$ feed-forward NN

- **Training data** consists of both the flux ($\boldsymbol{\lambda}_{k-1}$) and patches of the states near the interface
- DMD or nODE trained to **learn** the **mapping** from $\boldsymbol{y}_{k-1} := \left(\boldsymbol{\lambda}_{k-1}, \boldsymbol{u}_{1,k}(\delta_1), \boldsymbol{u}_{2,k}(\delta_2)\right)^T$ to $\boldsymbol{y}_k$
- Preliminary results indicate that the **new DMD approach** is **more accurate** than lumped mass GMM approach and around **20× times cheaper** than a consistent mass GMM approach (Figure 11)

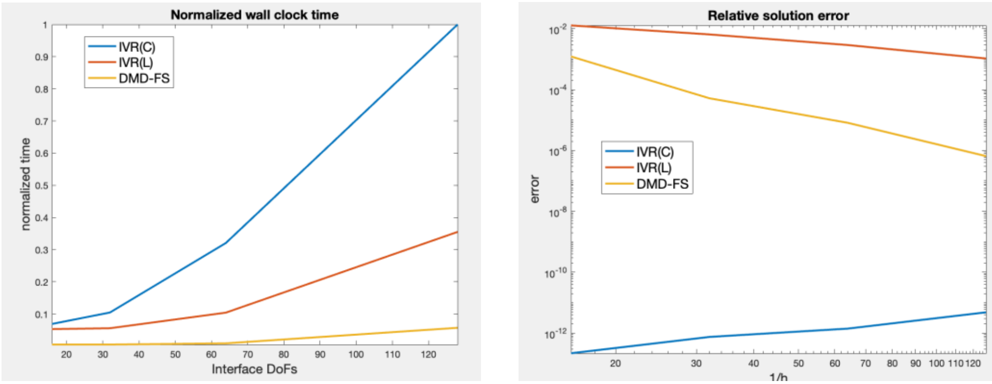

Figure above: CPU times (left) and relative errors (right) for GMM method with consistent mass (IVR(C)), lumped mass (IVR(L)) and a DMD surrogate (DMD-FS)

Outline

1. The Alternating Schwarz Method for FOM*-ROM# and ROM-ROM Coupling
   - Method Formulation
   - ROM Construction and Implementation
   - Numerical Examples

2. A Lagrange Multiplier-based Partitioned Scheme for FOM-ROM and ROM-ROM Coupling
   - Method Formulation
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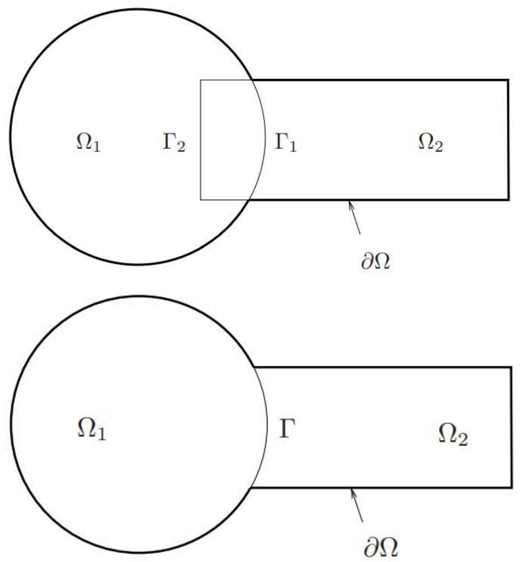
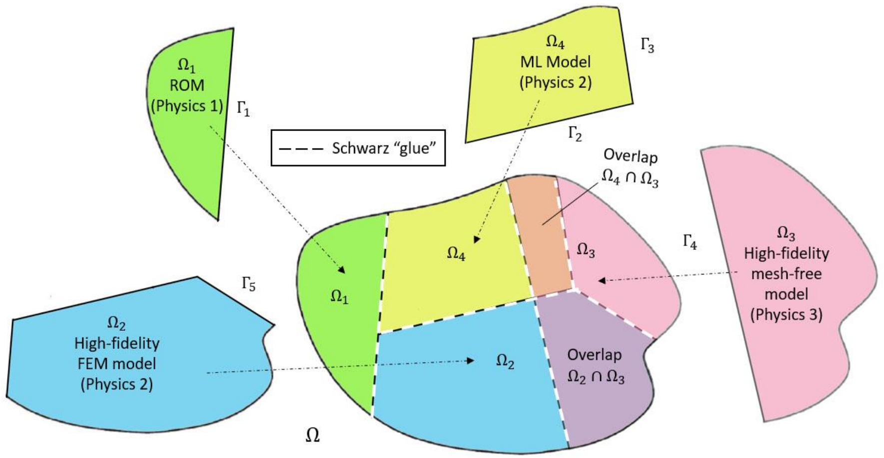
   - Numerical Examples

3. **Summary and Future Work**





*Full-Order Model. #Reduced Order Model.

Summary

- **Two domain decomposition-based methods** for coupling projection-based ROMs with each other and with conventional full order models have been proposed
  - ➢ An **iterative** coupling formulation based on the **Schwarz alternating method** and an **overlapping** or **non-overlapping DD**
  - ➢ A **Lagrange multiplier-based** single-pass **(non-iterative)** partitioned **scheme** based on **non-overlapping DD**
- Numerical results show **promise** in using the proposed methods to create **heterogeneous coupled models** comprised of arbitrary combinations of **ROMs** and/or **FOMs**
  - ➢ Coupled models can be **computationally efficient** w.r.t analogous FOM-FOM couplings
  - ➢ Coupling introduces **no numerical artifacts** into the solution

Opinion: *hybrid FOM-ROM models are the future!*

- FOM-ROM and ROM-ROM have potential to **improve** the **predictive viability** of projection-based ROMs, by enabling the **spatial localization of ROMs** (via DD) and the **online integration of high-fidelity information** into these models (via FOM coupling)

Ongoing & Future Work

Alternating Schwarz-based Coupling

- Complete study involving **Euler Riemann problem** with **moving shocks**
- **Journal article** in preparation
- **Rigorous analysis** of why Dirichlet-Dirichlet BC "work" when employing non-overlapping Schwarz with discretizations that employ ghost cells
- Extension to coupling of **non-intrusive ROMs** (dynamic mode decomposition or DMD, operator inference or OpInf, neural networks or NNs)
  - ➢ With Ian Moore (summer intern starting May 2024, from Virginia Tech)

Lagrange Multiplier-Based Partitioned Coupling

- Extension to **nonlinear** problems with hyper-reduction
- Alternate constructions for **reduced Lagrange multiplier space** (e.g., from snapshots of fluxes)
- DMD or nODE **flux surrogates** to reduce computational cost of Schur complement interface problem

General

- **Numerical comparison** of alternating Schwarz and LM-based partitioned coupling methods
- Development of **smart domain decomposition approaches**, to determine optimal placement of ROM and FOM in a computational domain (including **on-the-fly ROM-FOM switching**)
- Development of "**bottom-up**" subdomain ROMs that are trained separately
- Application to **other problems**, including **multi-physics problems,** and Sandia **production** applications

Team & Acknowledgments

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Sandia National Laboratories

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Pavel Bochev

Amy De Castro

Paul Kuberry

U.S. DEPARTMENT OF ENERGY | Office of Science

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

References

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URL: www.sandia.gov/~ikalash

[1] K. Peterson, P. Bochev, P. Kuberry, "Explicit synchronous partitioned algorithms for interface problems based on Lagrange multipliers", *Comput. Math. with Appl.*, 78 (2019), pp. 459–482.
[2] A. Mota, **I. Tezaur**, C. Alleman. "The Schwarz Alternating Method in Solid Mechanics", *Comput. Meth. Appl. Mech. Engng*. 319 (2017), 19-51.
[3] A. Mota, **I. Tezaur**, G. Phlipot. "The Schwarz Alternating Method for Dynamic Solid Mechanics", *Comput. Meth. Appl. Mech. Engng.* 121 (21) (2022) 5036-5071.
[4] J.M. Connors, K. Sockwell, "A Multirate Discontinuous-Galerkin-in-Time Framework for Interface-Coupled Problems", *SIAM Journal on Numerical Analysis*, 5(60), 2373-2404, 2022.
[5] K. Sockwell, P. Bochev, K. Peterson, P. Kuberry. "Interface flux recovery framework for constructing partitioned heterogeneous time-integration methods", *Numer. Meth. For PDEs* 39(5) 3572-3595, 2023.
[6] 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, 2023. https://arxiv.org/abs/2210.12551
[7] A. de Castro, P. Kuberry, **I. Tezaur**, P. Bochev. "A Novel Partitioned Approach for Reduced Order Model – Finite Element Model (ROM-FEM) and ROM-ROM Coupling", in *Proceedings of the ASCE Earth and Space 18th Biennial International Conference*, 475-489, 2023.
[8] A. de Castro, P. Bochev, P. Kuberry, **I. Tezaur**. "Explicit synchronous partitioned scheme for coupled reduced order models based on composite reduced bases", *Comput. Meth. Appl. Mech. Engng*. 417B 116398, 2023.
[9] 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
[10] P. Bochev, J. Owen, P. Kuberry. "Dynamic flux surrogate-based partitioned methods for interface problems", ArXiv pre-print, 2024. https://arxiv.org/abs/2402.03560
[11] E. Hawkins, P. Bochev, P. Kuberry. "An optimization-based approach for coupling projection-based reduced order models", *Computer Science Research Institute Summer Proceedings 2023*, S. Seritan and B. Reuter, eds., Technical report SAND2023-13916R, Sandia National Laboratories, 2023, pp. 63-70.

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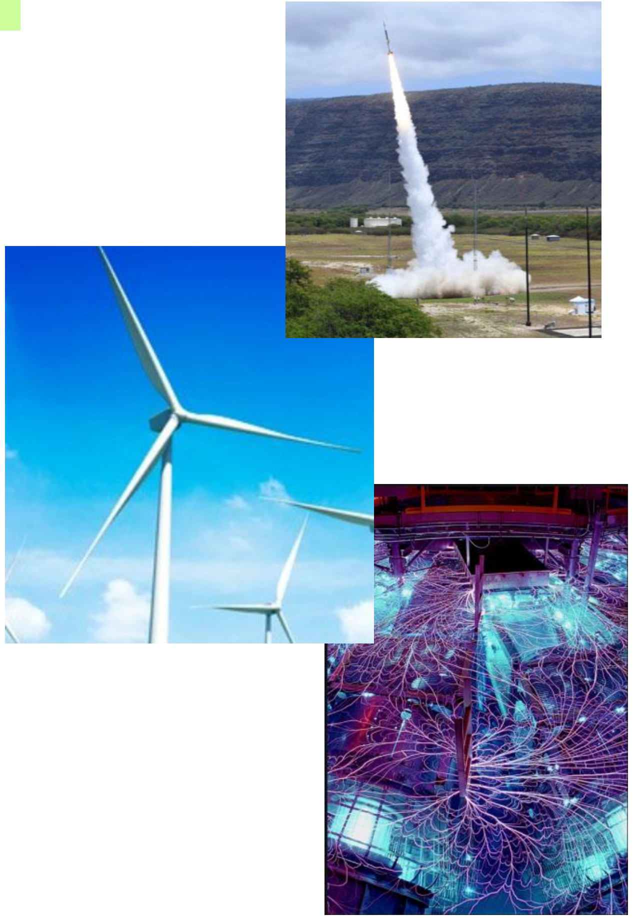


- Sandia is a **multidisciplinary** national lab and Federally Funded Research & Development Center (FFRDC).
- Contractor for U.S. DOE's National Nuclear Security Administration (**NNSA**).
- **Two main sites**: Albuquerque, NM and Livermore, CA

Careers at Sandia National Labs

Students: please consider Sandia and other national labs as a potential employer for summer internships and when you graduate!

- Sandia is a ***great*** place to work!
  - Very ***collaborative*** environment
  - Lots of ***interesting*** problems that require ***fundamental research*** in applied math/computational science and impact ***mission-critical applications***.
  - Great ***work/life balance***.

- ***Opportunities*** at/with Sandia:
  - Interns (summer, year-round)
  - Post docs
  - Several prestigious post doctoral fellowships (von Neumann, Truman, Hruby, Collis)
  - Staff

Please see: www.sandia.gov/careers for info about current opportunities.

Start of Backup Slides

Model Problem 3: 2D Euler Equations Riemann Problem

Pressio

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

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

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: $p_1 \in [1.125, 1.375, 1.625, 1.875]$

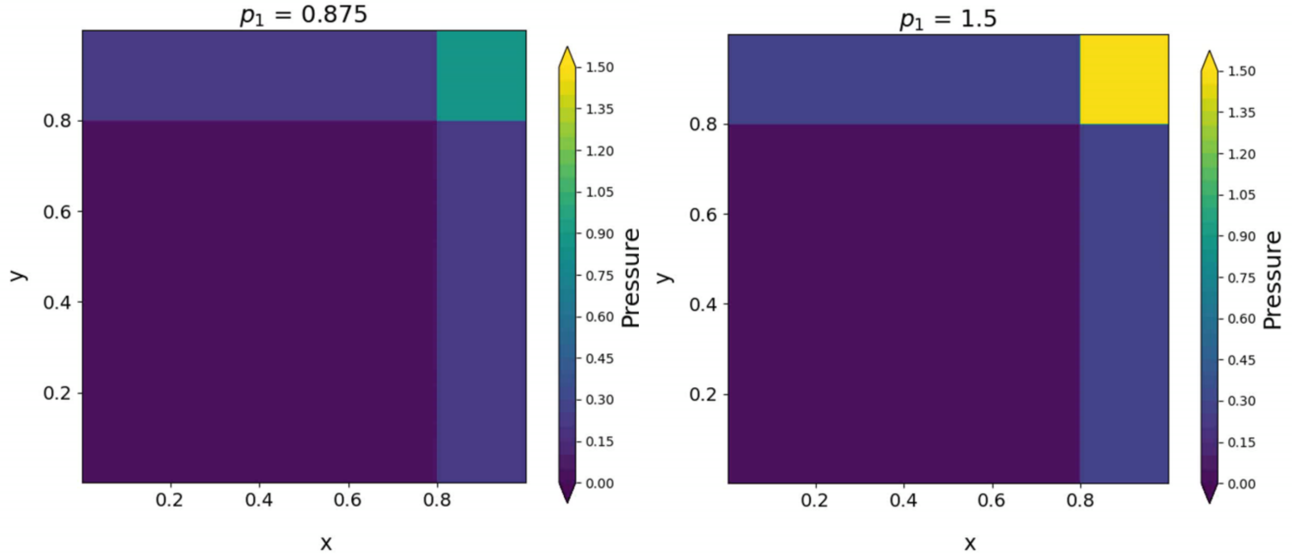


Figure above: FOM solutions to Euler Riemann problem for $p_1 = 0.875$ (left) and $p_1 = 1.5$ (right).

Preliminary results (WIP)

FOM discretization:

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

*Schulz-Rinne, 1993.

Schwarz Coupling Details

Choice of domain decomposition

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

Snapshot collection and reduced basis construction

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

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

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

Choice of hyper-reduction

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

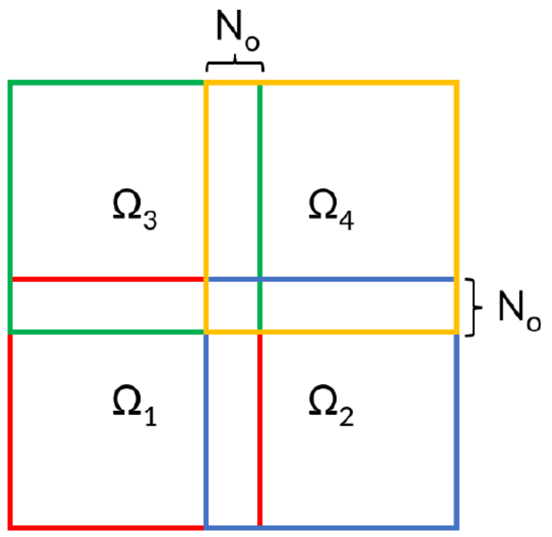


Figure above: DD of Ω into 4 subdomains

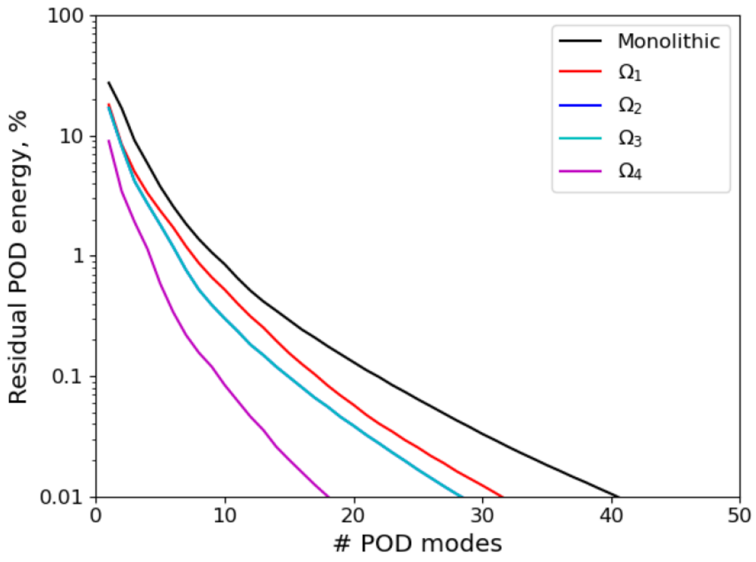
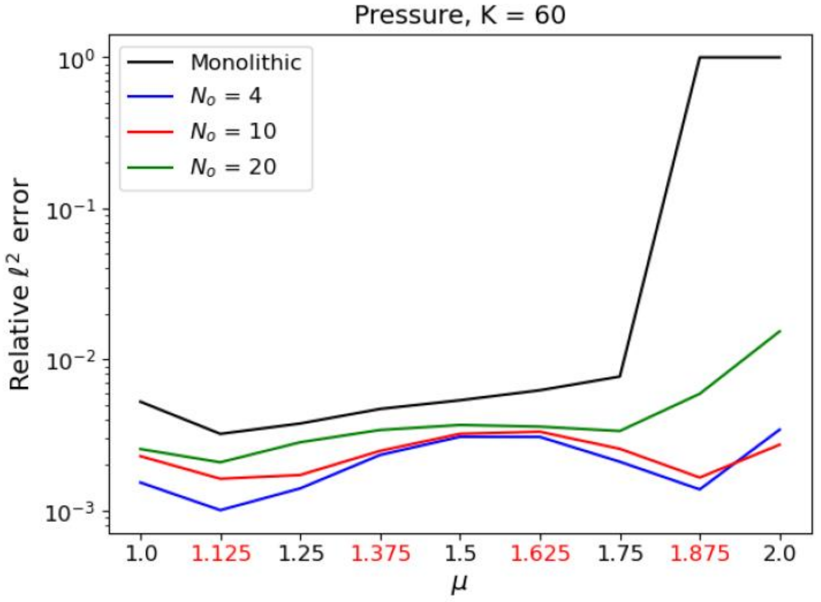


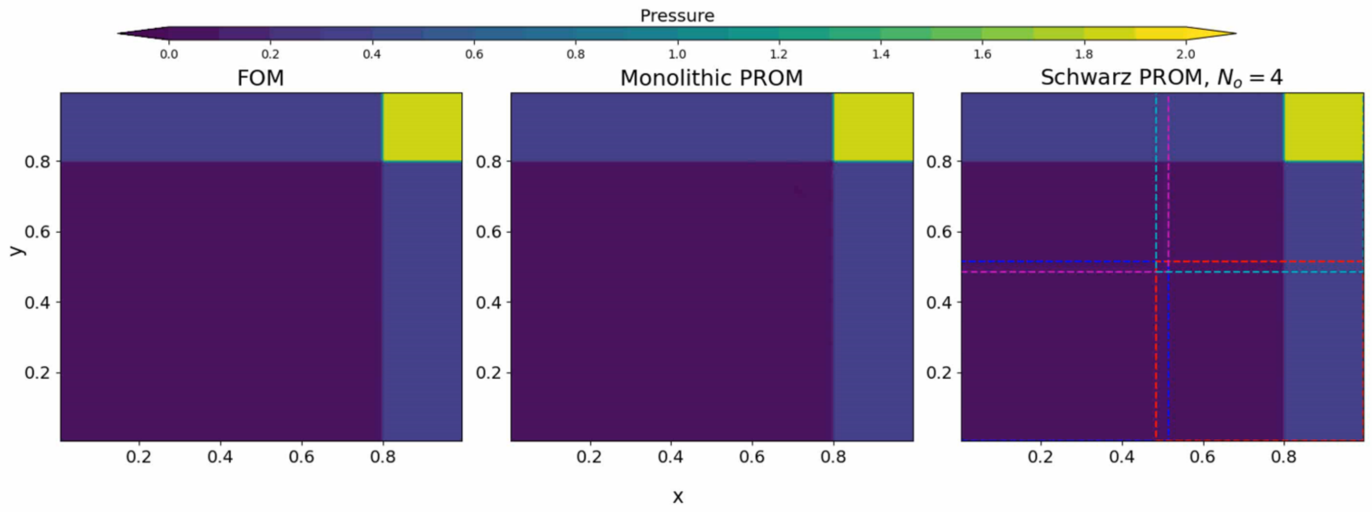
Figure above: Slow decay of POD energy for Euler problem

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

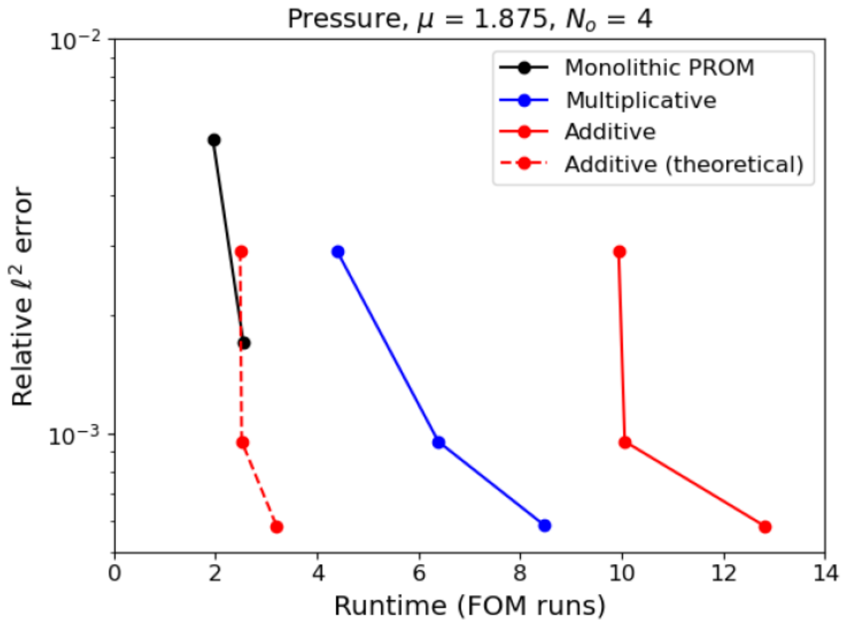
Model Problem 3: All-ROM Coupling + Overlapping Schwarz

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



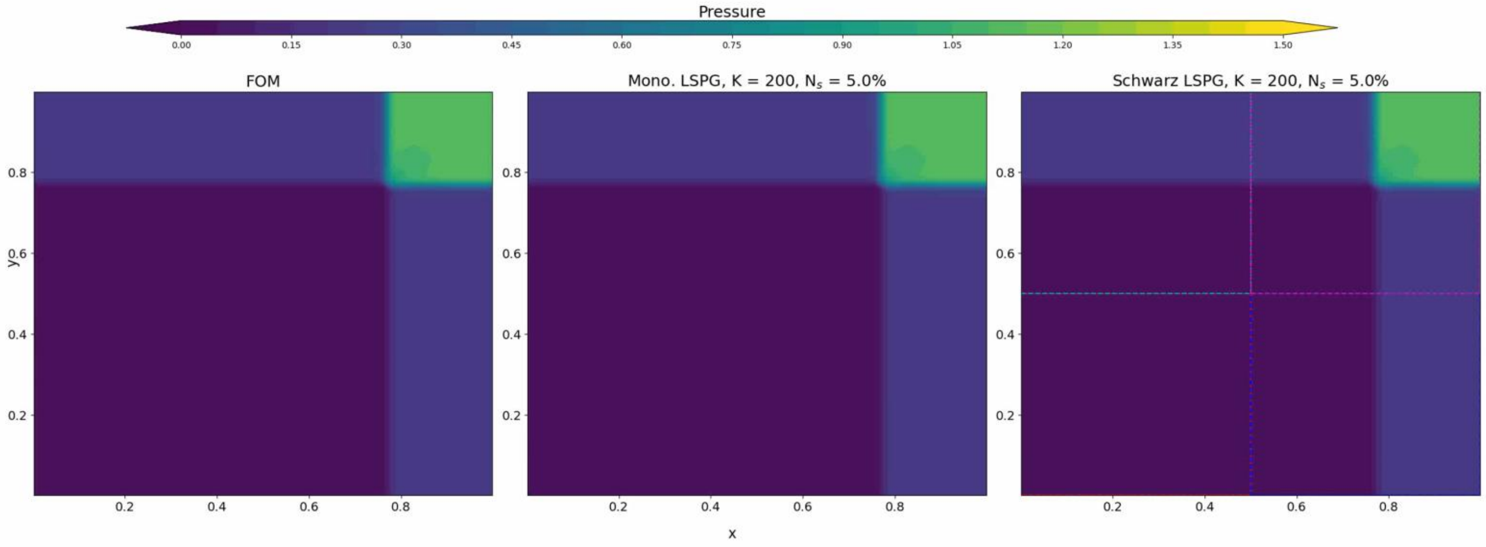


Movie above: FOM (left), $K = 50$ monolithic ROM (middle), and $K = 50$ overlapping Schwarz ROM with $N_o = 4$ (left) for $p_1 = 1.875$.



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

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



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

Preliminary results (WIP)

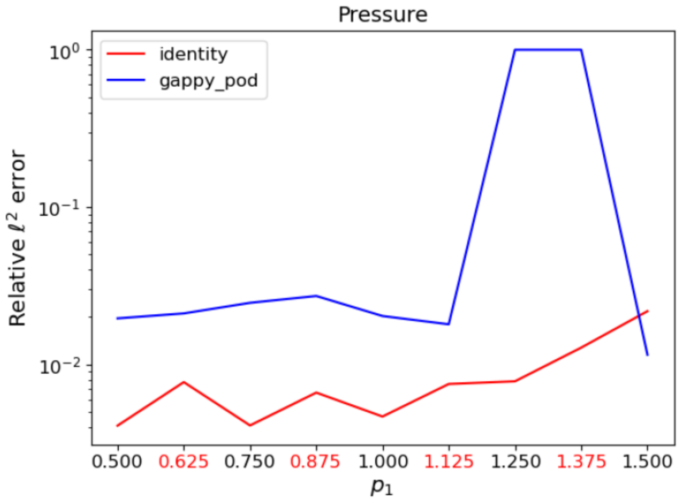


Figure above: collocation and gappy POD relative errors for K=200, 1% sampling rate.

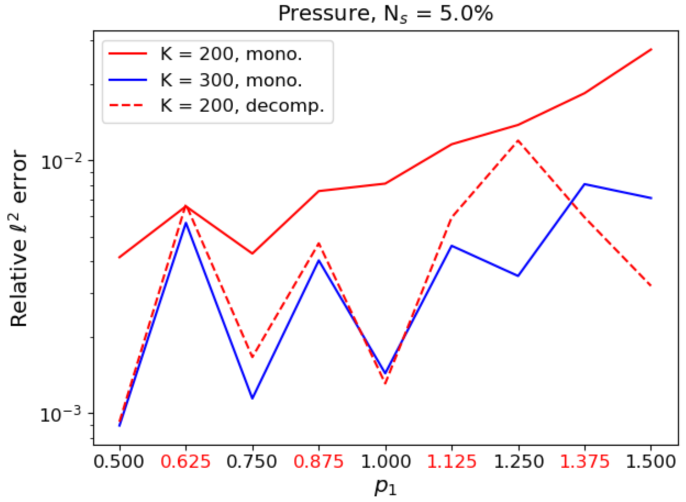


Figure above: monolithic vs. decomposed HROM errors with 5% sampling rate no overlap.

Other Ongoing Work: Optimization-Based Coupling (OBC)

Key Idea: introduce **control** as the shared Neumann BC on the interface Γ satisfying the continuity of flux, and form a **loss function that**, when minimized, will enforce the **continuity of states**.

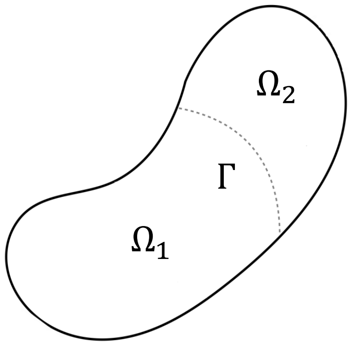
- In each time-step, find $(u_1^n, u_2^n, g^n) \in X_1^n \times X_2^n \times L^2(\Gamma)$ that **minimizes**

$$J_\delta(u_1^n, u_2^n, g^n) := \frac{1}{2}||u_1^n - u_2^n||_\Gamma^2 + \frac{1}{2}\delta||g^n||_\Gamma^2$$

subject to

$$\frac{1}{\Delta t}\left(u_i^n - u_i^{n-1}, v\right) + (\sigma_i(u_i^n), \nabla v) = (f_i^n, v) + (-1)^i (g^n, v)_\Gamma,\ \forall v \in V_i,\ \ i = 1{,}2$$

The **control** g^n is common to both subdomains, **implicitly** enforcing **continuity of flux**



- We **relax** the constrained optimization problem with a Lagrange multiplier μ_i
- Past related work extended [Gunzburger, 1999; Gunzburger, 2000; Kuberry, 2013] to **ROM-ROM** and **ROM-FOM coupling**
- **Accurate results** for **ROM-ROM coupling** when using **FEM adjoints**
- **Linear patch tests pass** to the tolerance of the penalty parameter δ
- Ongoing work investigating **alternative snapshot matrices** onto which the adjoint equations are projected to enable using **fewer modes**

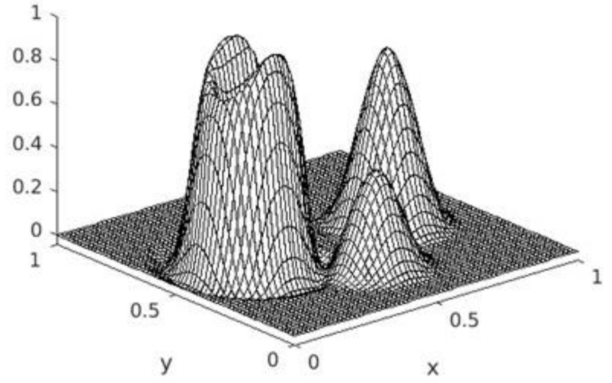


Figure above: ROM-ROM coupling at final timestep.

Comparison of Methods

Alternating Schwarz-based Coupling Method

- Can do **FOM-FOM**, **FOM-ROM**, **ROM-ROM** coupling
- **Overlapping** or **non-overlapping** DD
- **Iterative** formulation (less intrusive but likely requires more CPU time)

- Can couple **different mesh resolutions** and **element types**
- Can use **different time-integrators** with **different time-steps** in different subdomains
- **No interface bases** required

- **Sequential subdomain solves** in multiplicative Schwarz variant
  - ➢ **Parallel** subdomain solves possible with **additive Schwarz** variant

- **Extensible** in **straightforward** way to **PINN/DMD** data-driven model

Lagrange Multiplier-Based Partitioned Coupling Method

- Can do **FOM-FOM**, **FOM-ROM**, **ROM-ROM** coupling
- **Non-overlapping** DD
- **Monolithic** formulation requiring hybrid formulation (more intrusive but more efficient)

- Can couple **different mesh resolutions** and **element types**
- Can use **different explicit time-integrators** with **different time-steps** in different subdomains
- Provably convergent variant requires **interface bases**
- **Parallel subdomain solves** if explicit or IMEX time-integrator is employed

- **Extensions** to **PINN/DMD** data-driven models are **not obvious**

Numerical Examples: 1D Dynamic Wave Propagation Problem

- **Basis sizes** M_1 and M_2 vary from 60 to 300
  - ➢ Larger ROM used in Ω_1, since solution has **steeper gradient** here
- For couplings involving FOM and ROM/HROM, **FOM** is placed in $\boldsymbol{\Omega_1}$, since solution has steeper gradient here
- **Non-negative least-squares optimization problem** for ECSW weights solved using MATLAB's lsqnonneg function with early termination criterion (solution step-size tolerance = 10^{-4})
  - ➢ Ensures all HROMs have **consistent termination criterion** w.r.t. MATLAB implementation
  - ➢ However, **relative error tolerance** of selected reduced elements will differ
    - ❖ Switching to termination criterion based on relative error is work in progress and expected to improve HROM results
  - ➢ Convergence tolerance determines **size of sample mesh** $N_{e,i}$
  - ➢ **Boundary points** must be in sample mesh for application of Schwarz BC

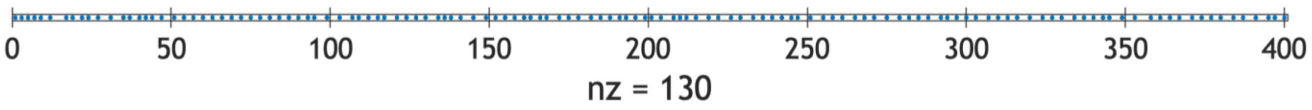


Figure left: sample sample mesh for 1D wave propagation problem

J. Barnett, I. Tezaur, A. Mota. "The Schwarz alternating method for the seamless coupling of nonlinear reduced order models and full order models", in Computer Science Research Institute Summer Proceedings 2022, S.K. Seritan and J.D. Smith, eds., Technical Report SAND2022-10280R, Sandia National Laboratories, 2022, pp. 31-55. (https://arxiv.org/abs/2210.12551)

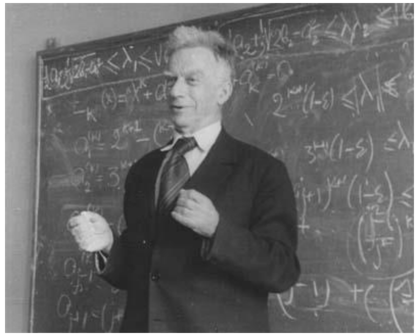
Theoretical Foundation

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

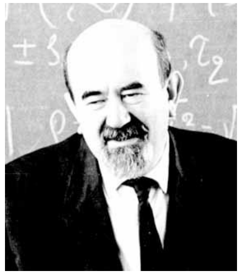
- **S.L. Sobolev (1936)**: posed Schwarz method for ***linear elasticity*** in variational form and ***proved method's convergence*** by proposing a convergent sequence of energy functionals.
- **S.G. Mikhlin (1951):** ***proved convergence*** of Schwarz method for general linear elliptic PDEs.
- **P.-L.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

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

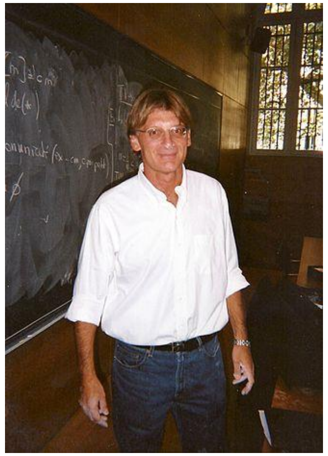
$$\nabla \cdot \boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



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

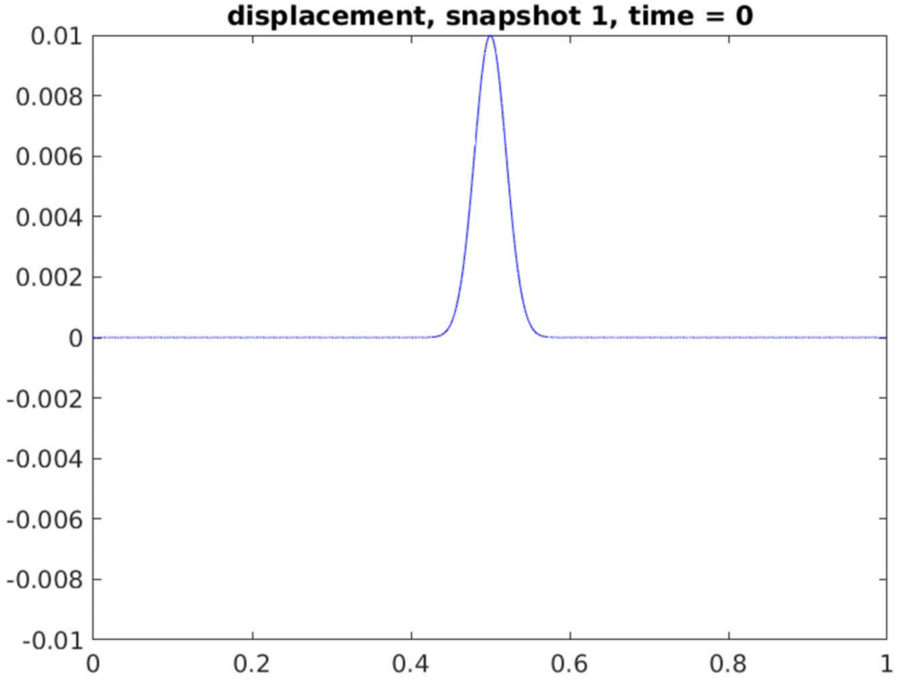
- Like for quasistatics, dynamic alternating Schwarz method converges provided each single-domain problem is ***well-posed*** and ***overlap region*** is ***non-empty***, under some ***conditions*** on Δt.
- ***Well-posedness*** for the dynamic problem requires that action functional $S[\boldsymbol{\varphi}] := \int_I \int_\Omega L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) dV dt$ 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.

Numerical Examples: Linear Elastic Wave Propagation Problem

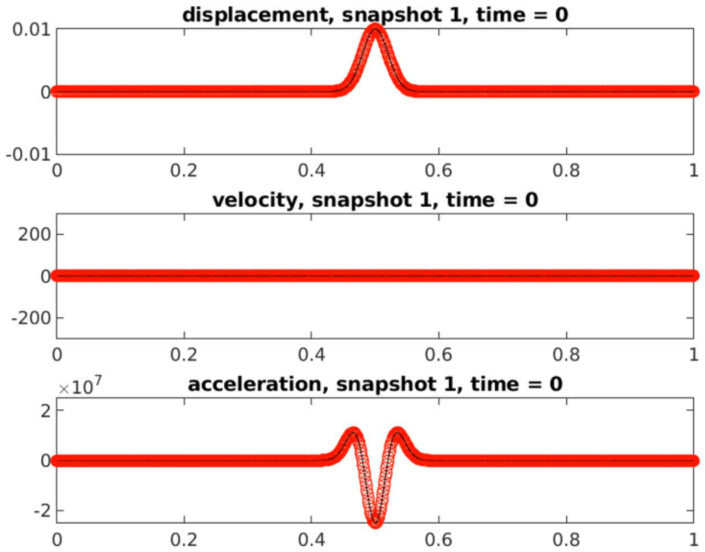
- Linear elastic ***clamped beam*** with Gaussian initial condition.
- Simple problem with analytical exact solution but very ***stringent test*** for discretization/coupling methods.
- ***Couplings tested:*** FOM-FOM, FOM-ROM, ROM-ROM, implicit-explicit, implicit-implicit, explicit-explicit.
- ROMs are ***reproductive*** and based on the ***POD/Galerkin*** method.
  - ➢ 50 POD modes capture ~100% snapshot energy



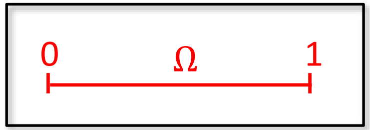
Above: 3D rendering of clamped beam with Gaussian initial condition. *Right*: Initial condition (blue) and final solution (red). Wave profile is negative of initial profile at time T = 1.0e-3.

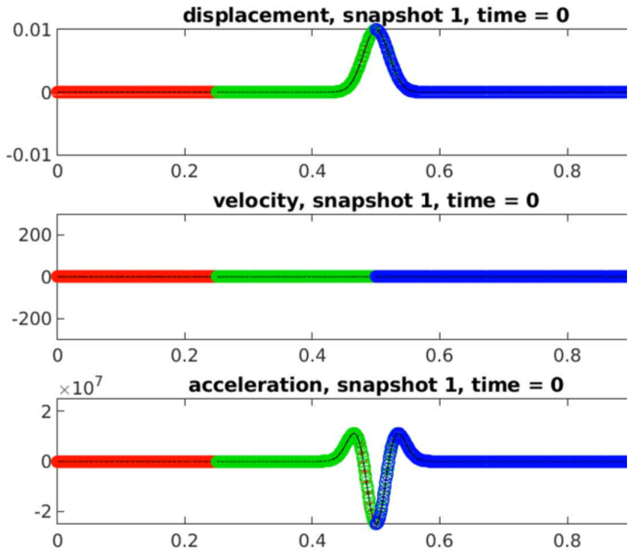
Linear Elastic Wave Propagation Problem: FOM-ROM and ROM-ROM Couplings

Coupling delivers accurate solution if each subdomain model is reasonably accurate, can couple different discretizations with different Δx, Δt and basis sizes.

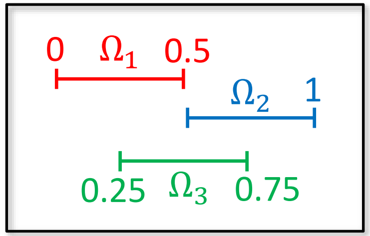


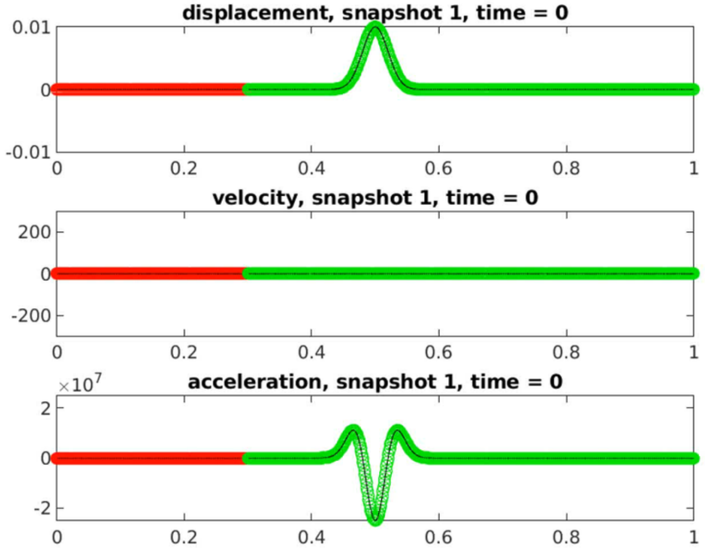
Single Domain FOM



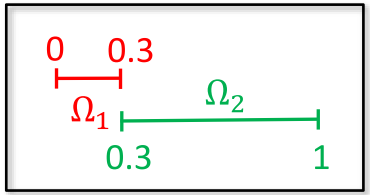


3 overlapping subdomain
ROM[1]-FOM[2]-ROM[3]





2 non-overlapping subdomain
FOM[4]-ROM[5] ($\theta = 1$)



[1]Implicit 40 mode POD ROM, Δt=1e-6, Δx=1.25e-3
[2]Implicit FOM, Δt =1e-6, Δx =8.33e-4
[3]Explicit 50 mode POD ROM, Δt =1e-7, Δx =1e-3

[5]Implicit FOM, Δt =2.25e-7, Δx =1e-6
[4]Explicit 50 mode POD ROM, Δt =2.25e-7, Δx =1e-6

Linear Elastic Wave Propagation Problem: FOM-ROM and ROM-ROM Couplings

Coupled models are reasonably accurate w.r.t. FOM-FOM coupled analogs and convergence with respect to basis refinement for FOM-ROM and ROM-ROM coupling is observed.

	disp MSE[6]	velo MSE	acce MSE
Overlapping ROM[1]-FOM[2]-ROM[3]	1.05e-4	1.40e-3	2.32e-2
Non-overlapping FOM[4]-ROM[5]	2.78e-5	2.20e-4	3.30e-3

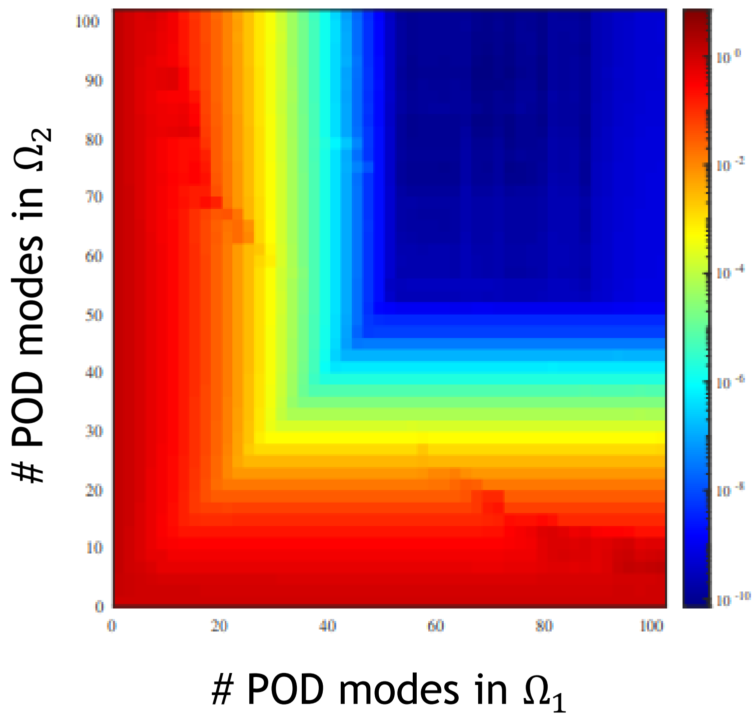
[1]Implicit 40 mode POD ROM, Δt =1e-6, Δx =1.25e-3
[2]Implicit FOM, Δt =1e-6, Δx =8.33e-4
[3]Explicit 50 mode POD ROM, Δt =1e-7, Δx =1e-3
[4]Implicit FOM, Δt =2.25e-7, Δx =1e-6
[5]Explicit 50 mode POD ROM, Δt =2.25e-7, Δx =1e-6

[6]MSE= $\text{mean squared error} = \sqrt{\sum_{n=1}^{N_t} \left\|\tilde{\boldsymbol{u}}^n(\boldsymbol{\mu}) - \boldsymbol{u}^n(\boldsymbol{\mu})\right\|_2^2} \Big/ \sqrt{\sum_{n=1}^{N_t} \left\|\boldsymbol{u}^n(\boldsymbol{\mu})\right\|_2^2}.$

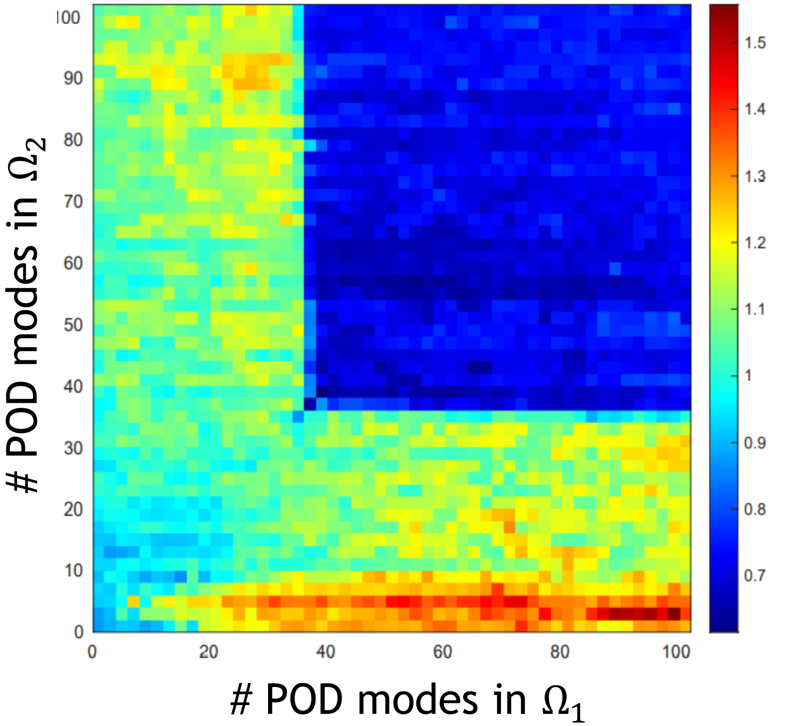
Linear Elastic Wave Propagation Problem: ROM-ROM Couplings

ROM-ROM coupling gives errors < O(1e-6) & speedups over FOM-FOM coupling for basis sizes > 40.

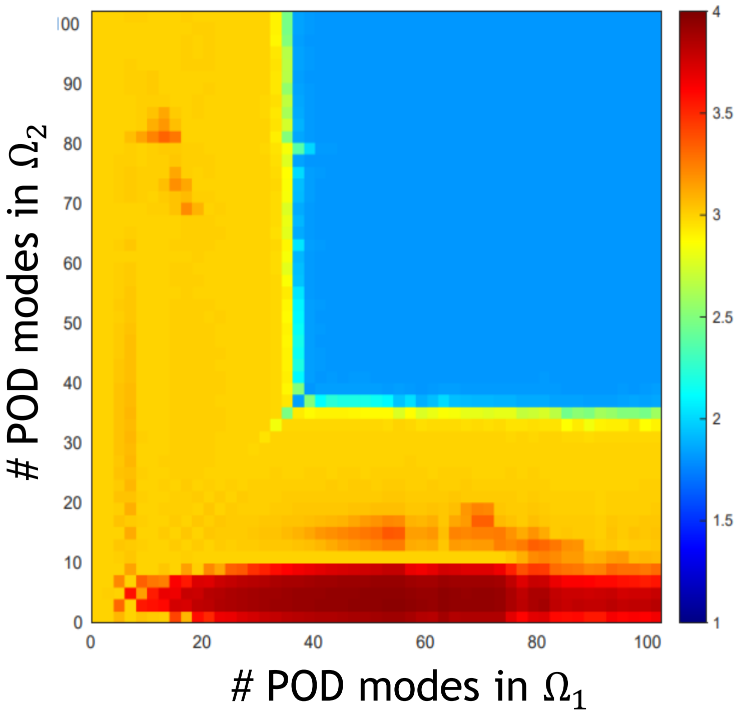
MSE in displacement for 2 subdomain ROM-ROM coupling



CPU times for 2 subdomain ROM-ROM coupling normalized by FOM-FOM CPU time



Average # Schwarz iterations for 2 subdomain ROM-ROM coupling



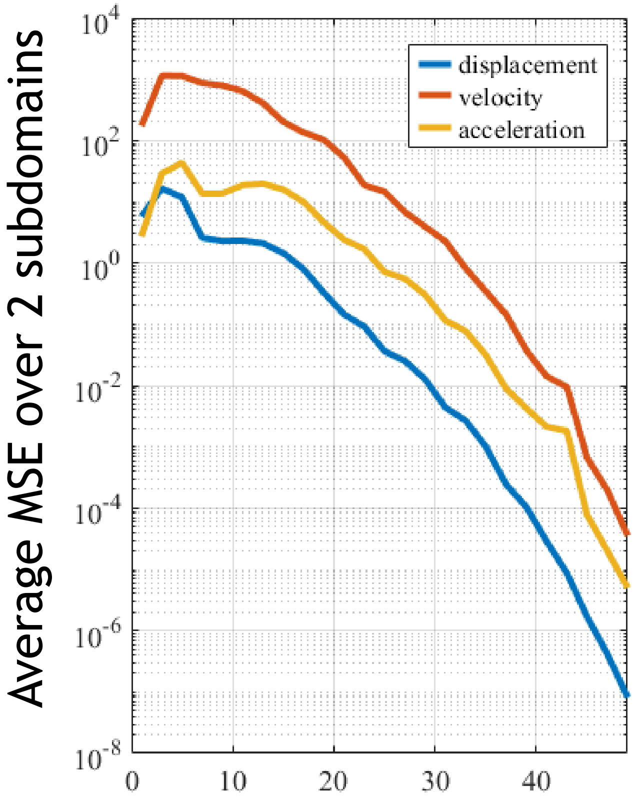
- **Smaller ROMs** are **not** the **fastest**: less accurate & require more Schwarz iterations to converge.
- All couplings converge in $\leq$ **4 Schwarz iterations** on average (FOM-FOM coupling requires average of 2.4 Schwarz iterations).

Overlapping implicit-implicit coupling with $\Omega_1 = [0, 0.75]$, $\Omega_2 = [0.25, 1]$

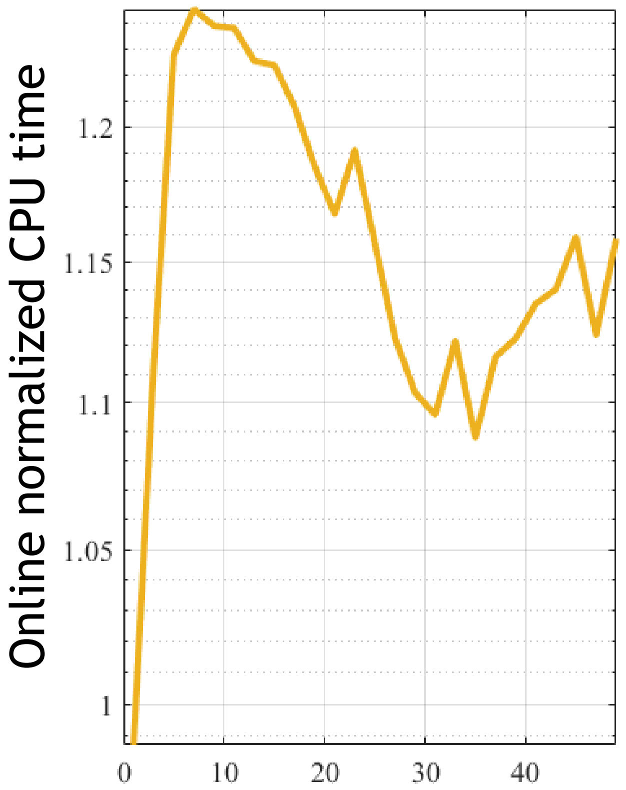
Linear Elastic Wave Propagation Problem: FOM-ROM Couplings

FOM-ROM coupling shows convergence with basis refinement. FOM-ROM couplings are 10-15% slower than comparable FOM-FOM coupling due to increased # Schwarz iterations.

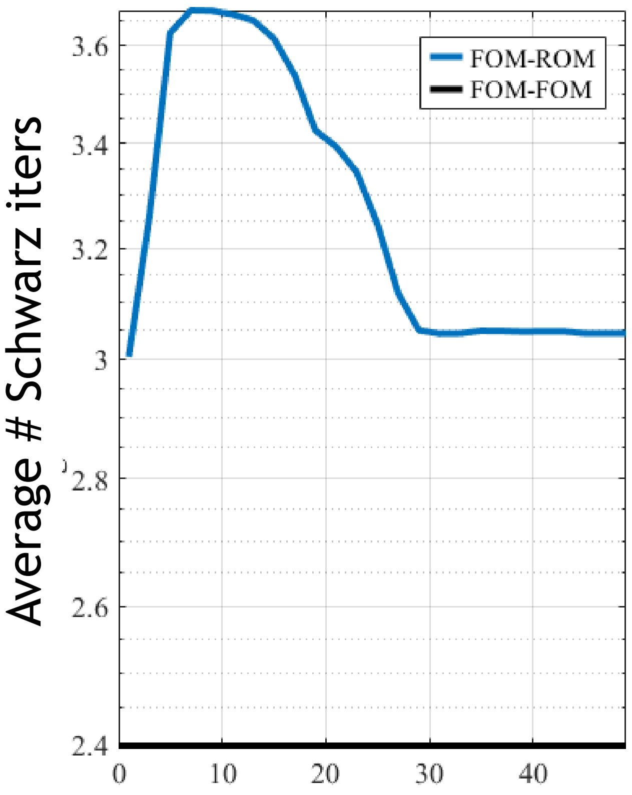
MSE for 2 subdomain FOM-ROM coupling



CPU times for 2 subdomain FOM-ROM coupling normalized by FOM-FOM CPU time



Average # Schwarz iterations for 2 subdomain couplings

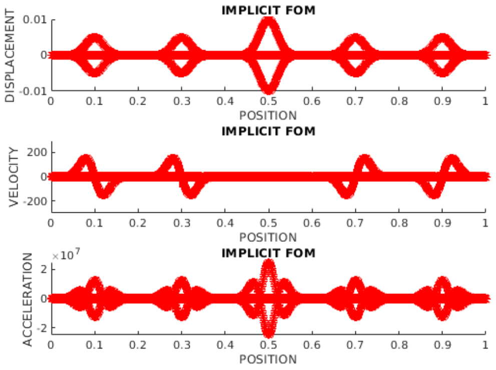


WIP: *understanding & improving FOM-ROM coupling performance.*

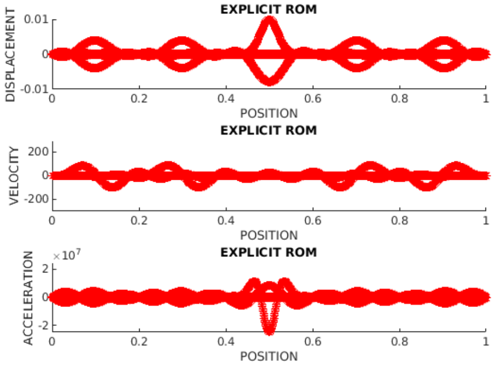
Overlapping implicit-implicit coupling with $\Omega_1 = [0, 0.75]$, $\Omega_2 = [0.25, 1]$

Linear Elastic Wave Propagation Problem: FOM-ROM and ROM-ROM Couplings

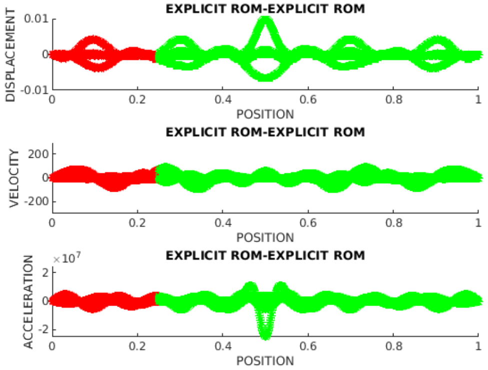
Inaccurate model + accurate model ≠ accurate model.



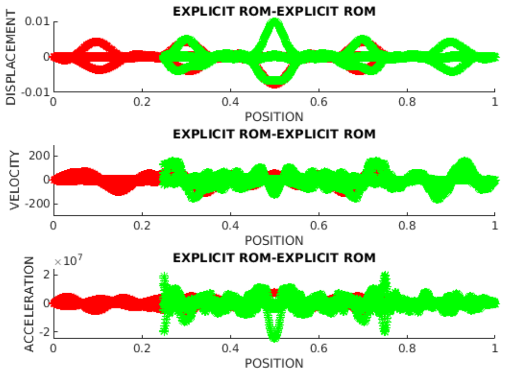
Single Domain, FOM (truth)



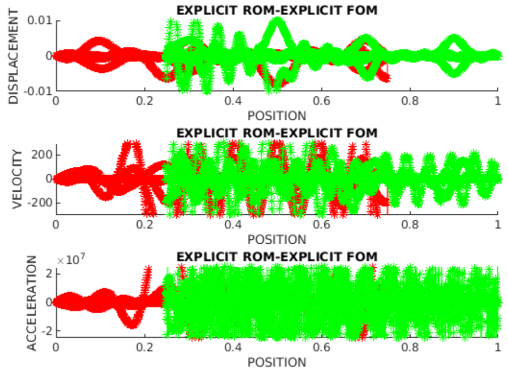
Single Domain, 10 mode POD



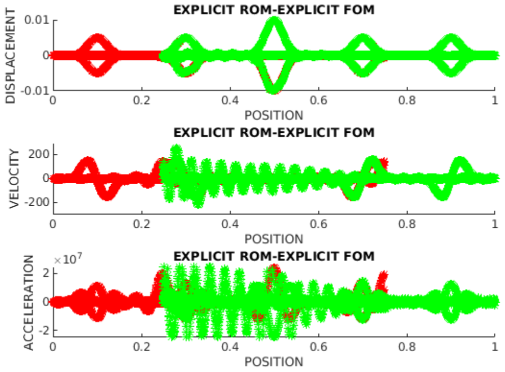
10 mode POD – 10 mode POD



10 mode POD – 50 mode POD



10 mode POD – FOM



20 mode POD - FOM

Figures above: $\Omega_1 = [0, 0.75]$, $\Omega_2 = [0.25, 1]$

Observation suggests need for **"smart" domain decomposition.**

Accuracy can be improved by "gluing" several smaller, spatially-local models

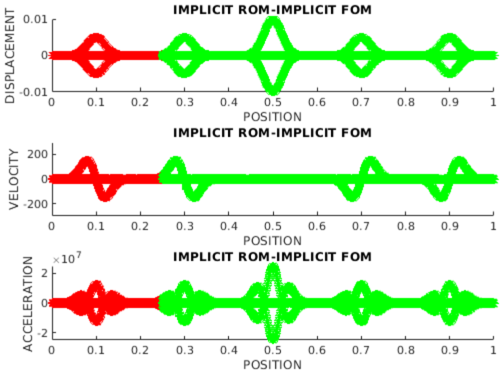
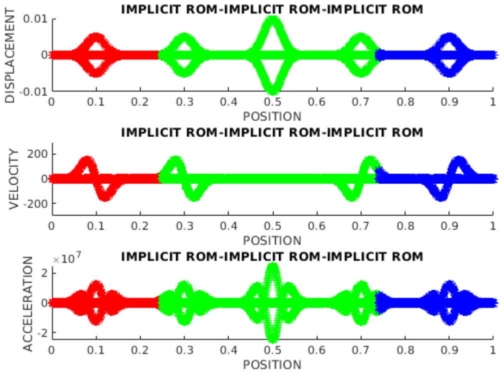


Figure above: $\Omega_1 = [0, 0.3]$, $\Omega_2 = [0.25, 1]$, 20 mode POD - FOM

Figure below: $\Omega_1 = [0, 0.26]$, $\Omega_2 = [0.25, 0.75]$, $\Omega_3 = [0.74, 1]$, 15 mode POD - 30 mode POD - 15 mode POD

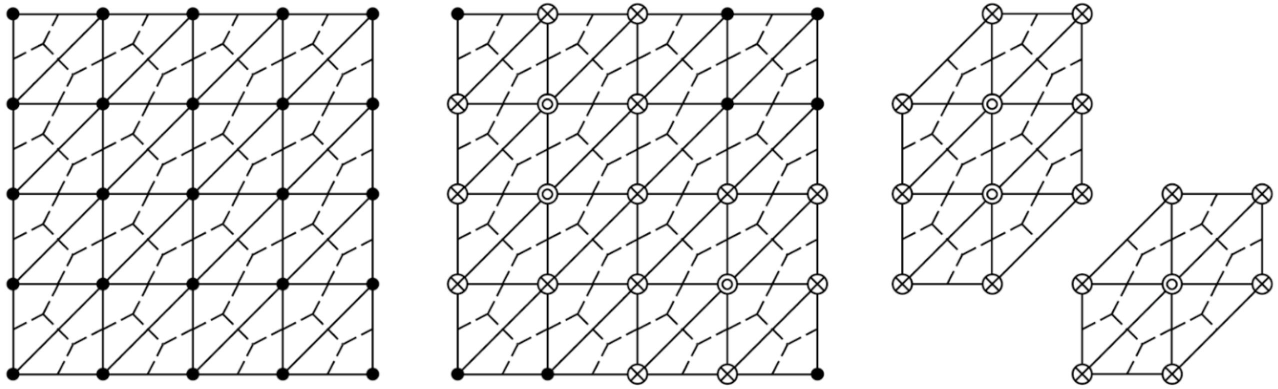


Energy-Conserving Sampling and Weighting (ECSW)

- **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**:

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

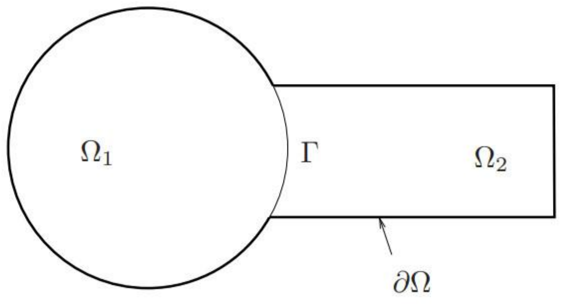
- Solve the above optimization problem using a **non-negative least squares solver** with an **early termination condition** to **promote sparsity** of the vector $\boldsymbol{\xi}$

Numerical Examples: 1D Dynamic Wave Propagation Problem

- Alternating **Dirichlet-Neumann** Schwarz BCs with **no relaxation** ($\theta = 1$) on Schwarz boundary Γ

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

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



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

θ	Min # Schwarz Iters	Max # Schwarz Iters	Total # Schwarz Iters
1.10	3	9	59,258
1.00	1	4	24,630
0.99	1	5	35,384
0.95	3	6	45,302
0.90	3	8	56,114

  - A **parameter sweep study** revealed $\theta = 0$ gave best performance (min # Schwarz iterations)

- All couplings were **implicit-implicit** with $\Delta t_1 = \Delta t_2 = \Delta T = 10^{-7}$ and $\Delta x_1 = \Delta x_2 = 10^{-3}$
  - Time-step and spatial resolution chosen to be small enough to resolve the propagating wave

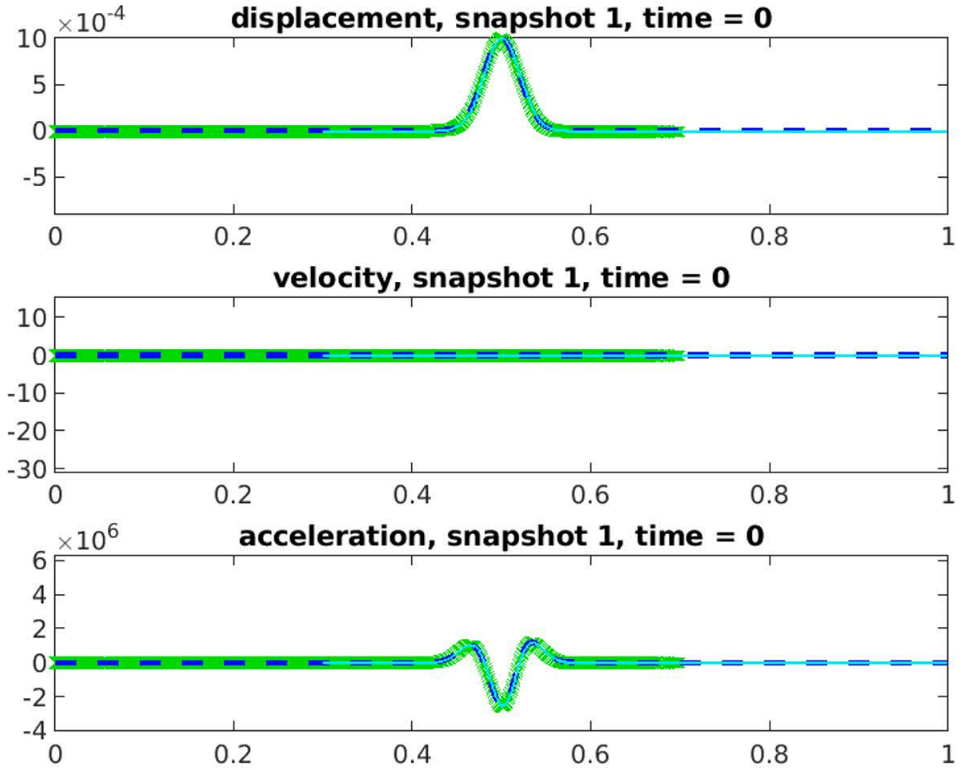
- All reproductive cases run on the **same RHEL8 machine** and all predictive cases run on the **same RHEL7 machine**, in MATLAB

- Model **accuracy** evaluated w.r.t. analogous FOM-FOM coupling using **mean square error (MSE)**:

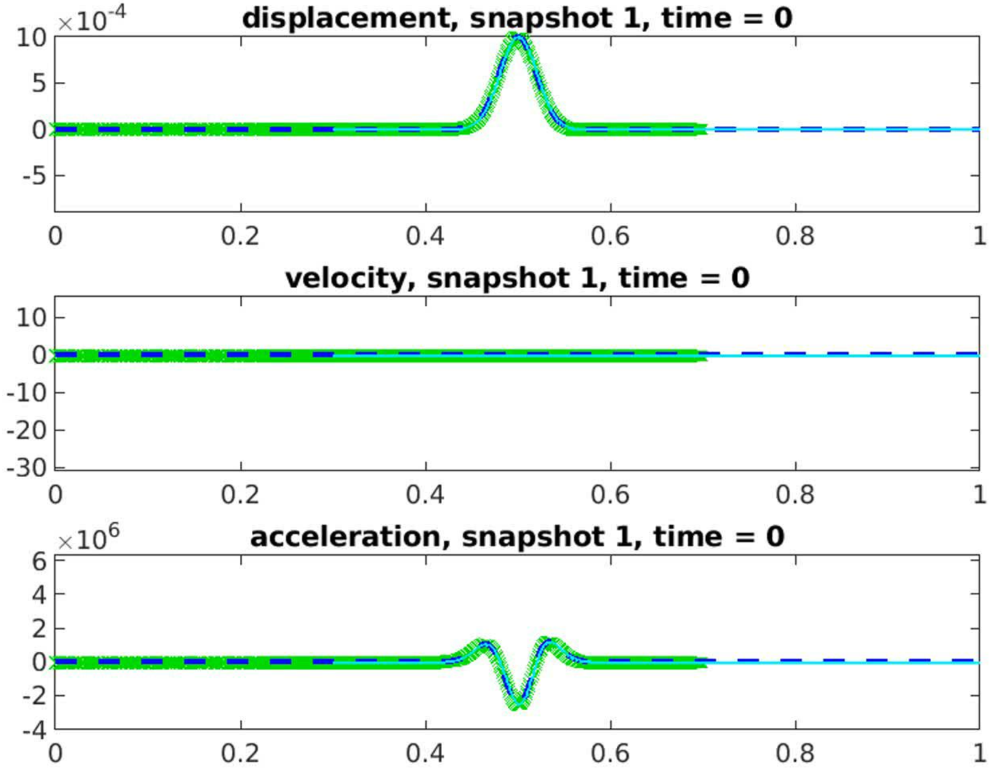
$$\varepsilon_{MSE}(\tilde{\boldsymbol{u}}_i) := \frac{\sqrt{\sum_{n=1}^{S} ||\tilde{\boldsymbol{u}}_i^n - \boldsymbol{u}_i^n||_2^2}}{\sqrt{\sum_{n=1}^{S} ||\boldsymbol{u}_i^n||_2^2}}$$

Overlapping Coupling, Nonlinear Henky MM, 2 Subdomains

- $\Omega = [0, 0.7] \cup [0.3, 1]$, implicit-implicit FOM-FOM coupling, dt = 1e-7, dx=1e-3.

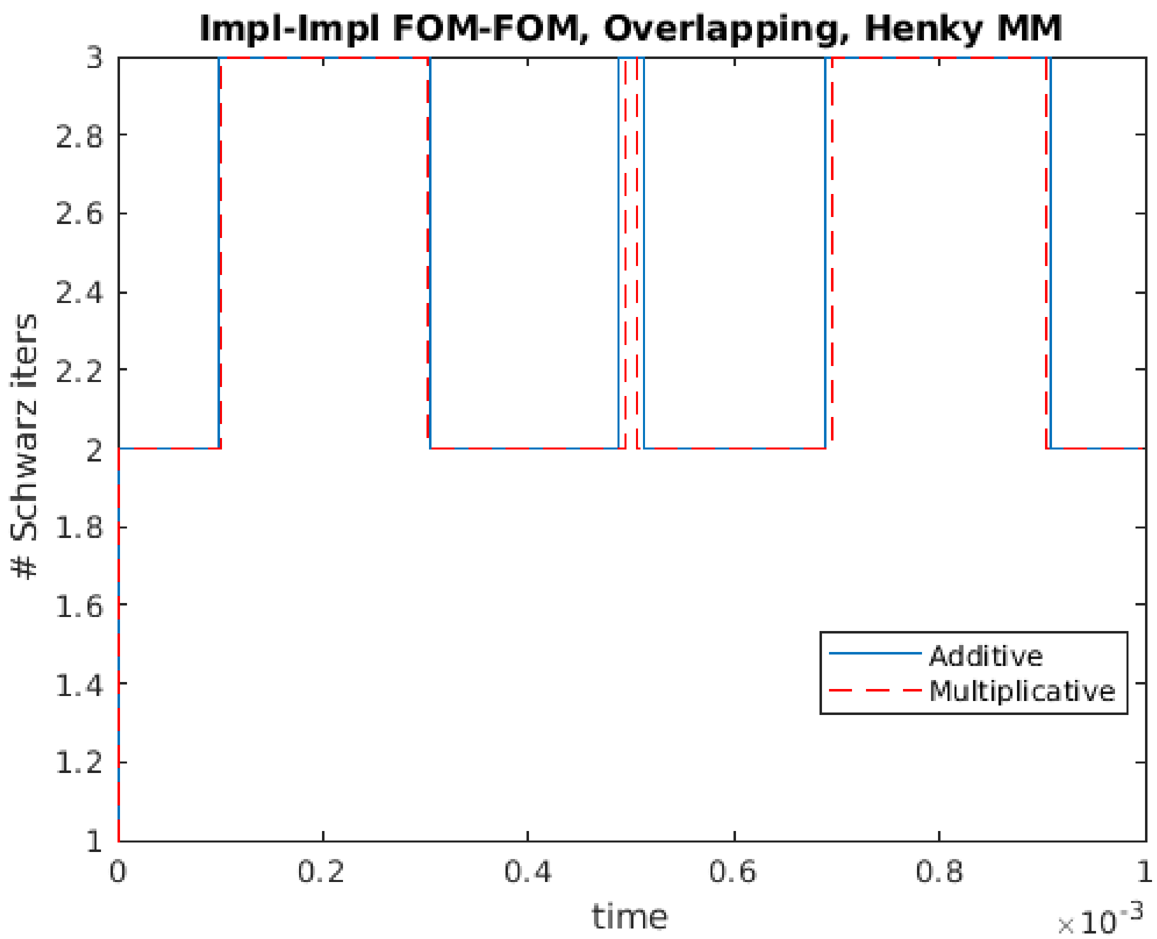


Multiplicative Schwarz



Additive Schwarz

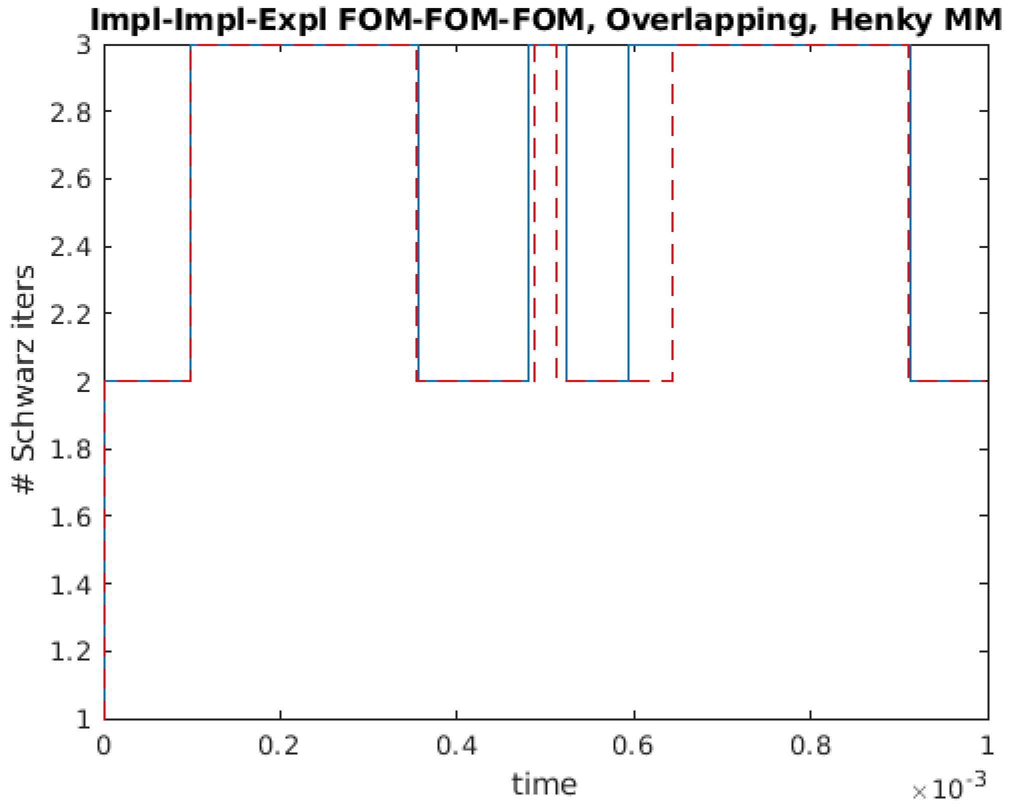
Overlapping Coupling, Nonlinear Henky MM, 2 Subdomains



- $\Omega = [0, 0.7] \cup [0.3, 1]$, implicit-implicit FOM-FOM coupling, dt = 1e-7, dx=1e-3.
- Additive Schwarz requires slightly more Schwarz iterations but is actually faster.
- Solutions agree effectively to machine precision in mean square (MS) sense.

	Additive	Multiplicative
Total # Schwarz iters	24495	24211
CPU time	2.03e3s	2.16e3
MS difference in disp	6.34e-13/6.12e-13	
MS difference in velo	1.35e-11/1.86e-11	
MS difference in acce	5.92e-10/1.07e-9	

Overlapping Coupling, Nonlinear Henky MM, 3 Subdomains

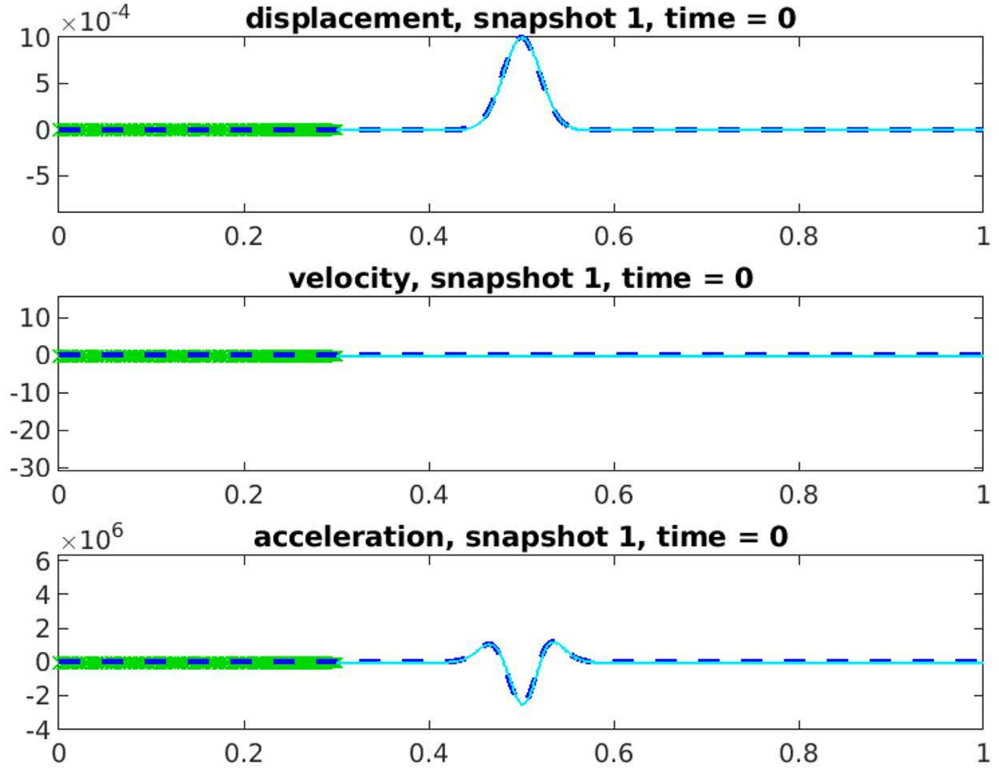


- $\Omega = [0, 0.3] \cup [0.25, 0.75] \cup [0.7, 1]$, implicit-implicit-explicit FOM-FOM-FOM coupling, dt = 1e-7, dx = 0.001.
- Solutions agree effectively to machine precision in mean square (MS) sense.
- Additive Schwarz has slightly more Schwarz iterations but is slightly faster than multiplicative.

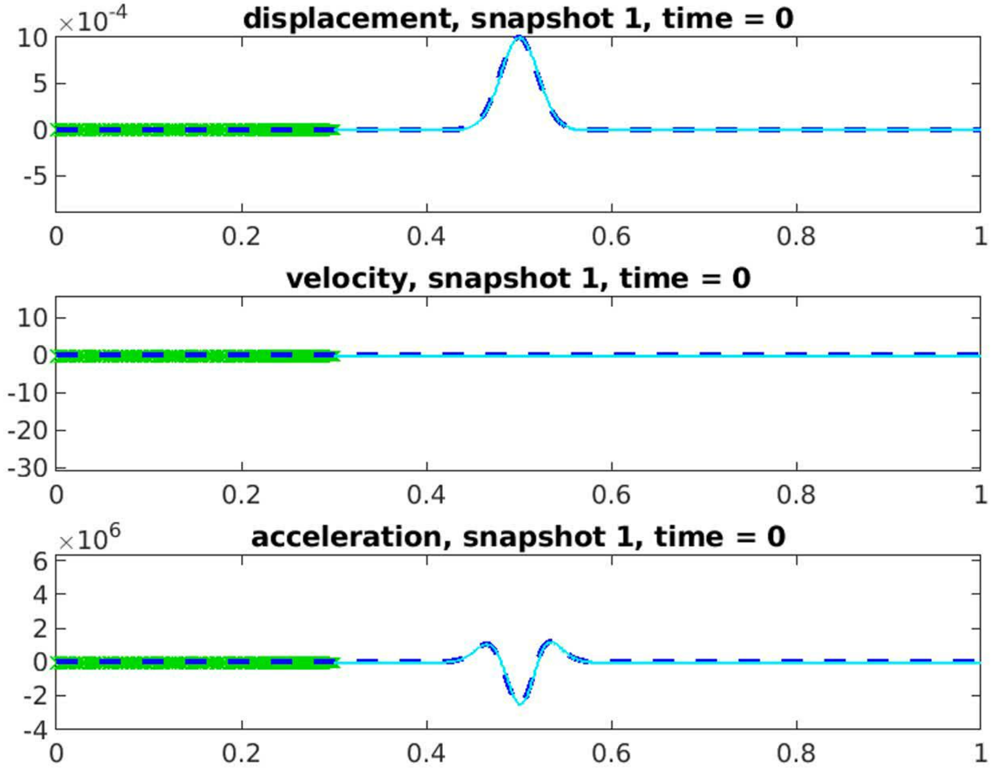
	Additive	Multiplicative
Total # Schwarz iters	26231	25459
CPU time	1.89e3s	2.05e3s
MS difference in disp	5.3052e-13/9.3724e-13/6.1911e-13	
MS difference in velo	7.2166e-12/2.2937e-11/2.4975e-11	
MS difference in acce	2.8962e-10/1.1042e-09/1.6994e-09	

Non-overlapping Coupling, Nonlinear Henky MM, 2 Subdomains

- $\Omega = [0, 0.3] \cup [0.3, 1]$, implicit-implicit FOM-FOM coupling, dt = 1e-7, dx = 1e-3.

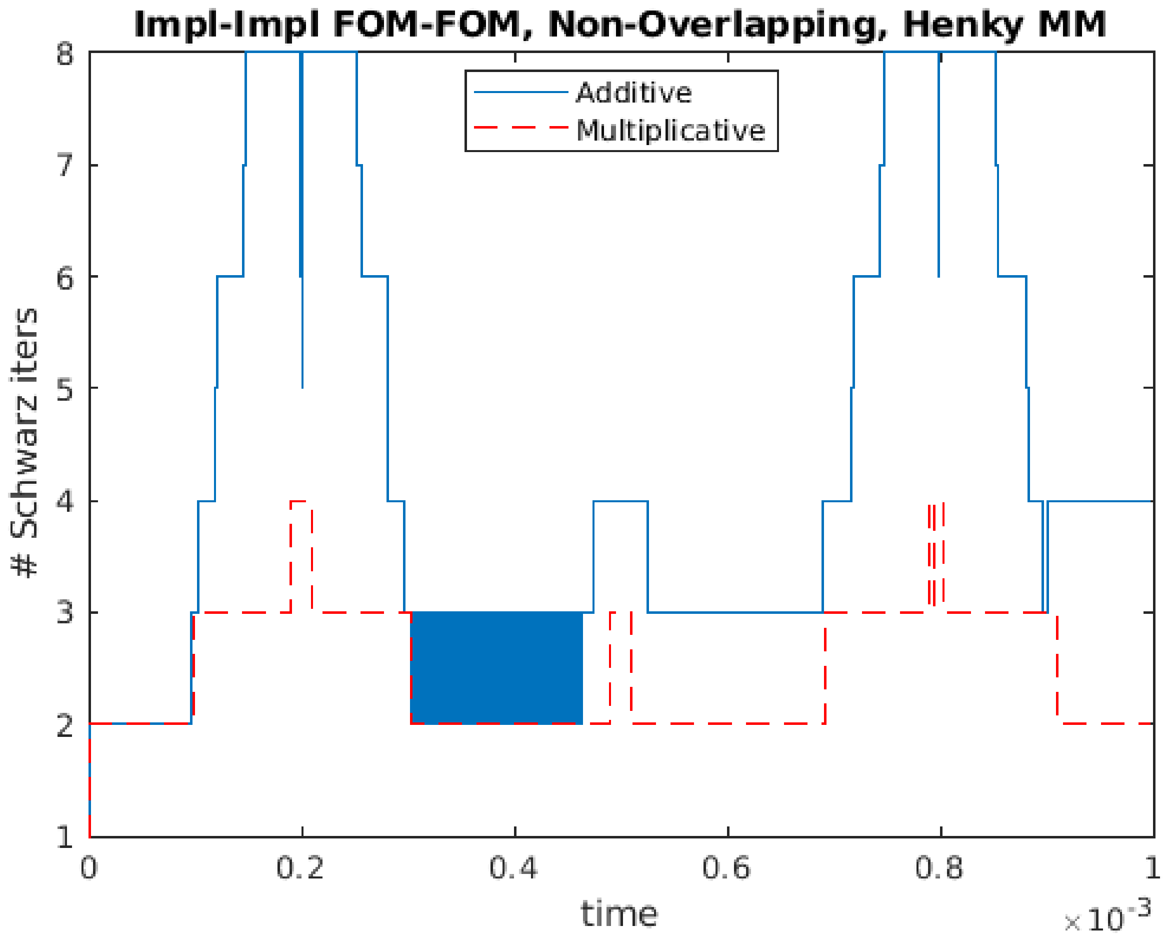


Multiplicative Schwarz



Additive Schwarz

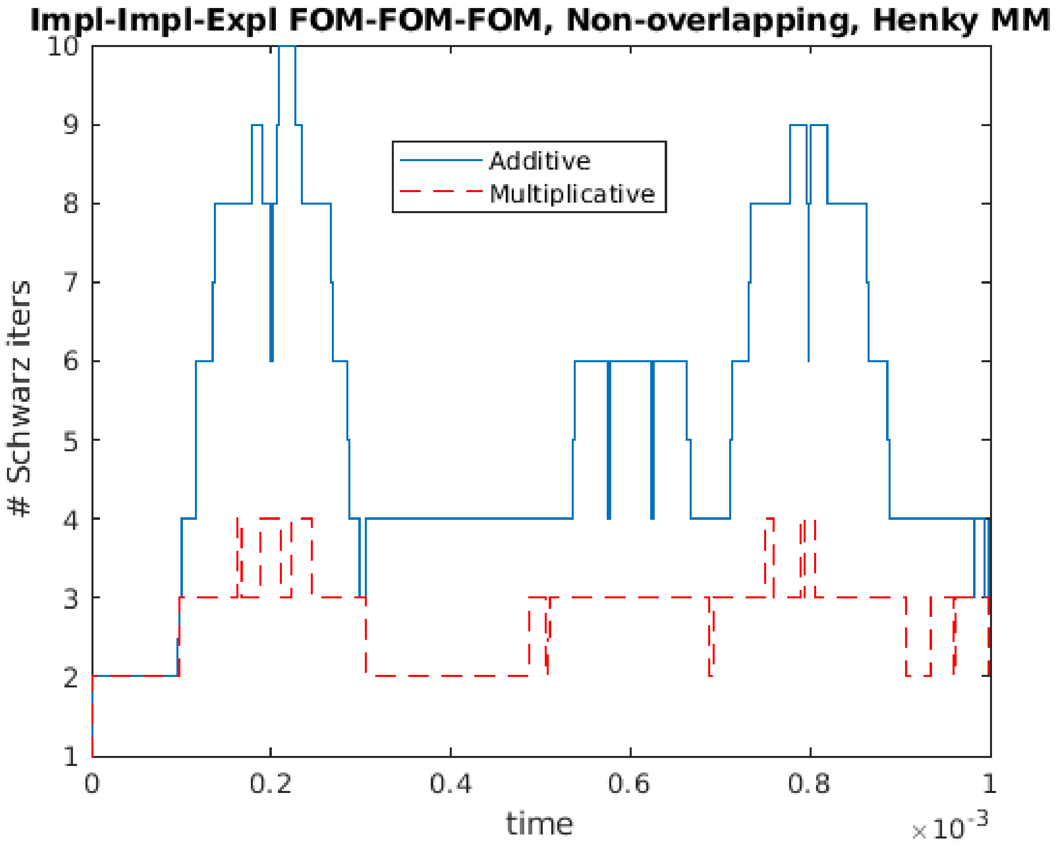
Non-overlapping Coupling, Nonlinear Henky MM, 2 Subdomains



- $\Omega = [0, 0.3] \cup [0.3, 1]$, implicit-implicit FOM-FOM coupling, dt = 1e-7, dx = 1e-3.
- Additive Schwarz requires 1.81x Schwarz iterations (and 1.9x CPU time) to converge. CPU time could be reduced through added parallelism of additive Schwarz.
  - ➢ Note blue square for additive Schwarz…
- Additive and multiplicative solutions differ in mean square (MS) sense by O(1e-5).

	Additive	Multiplicative
Total # Schwarz iters	44895	24744
CPU time	1.87e3s	982.5s
MS difference in disp	4.26e-5/2.74e-5	
MS difference in velo	1.02e-5/5.91e-6	
MS difference in acce	5.84e-5/1.21e-5	

Non-overlapping Coupling, Nonlinear Henky MM, 3 Subdomains



- $\Omega = [0, 0.3] \cup [0.3, 0.7] \cup [0.7, 1]$, implicit-implicit-explicit FOM-FOM-FOM coupling, dt = 1e-7, dx = 0.001.
- Additive Schwarz has about 1.94x number Schwarz iterations and is about 2.06x slower – similar to 2 subdomain variant of this problem. No "blue square".
  - ➢ Results suggest you could win with additive Schwarz if you parallelize and use enough domains.
- Additive/multiplicative solutions differ by O(1e-5), like for 2 subdomain variant of this problem.

	Additive	Multiplicative
Total # Schwarz iters	53413	27509
CPU time	5.91e3s	2.87e3s
MS difference in disp	2.8036e-05/3.1142e-05/ 8.8395e-06	
MS difference in velo	1.4077e-05/1.2104e-05/6.5771e-06	
MS difference in acce	8.7885e-05/3.2707e-05/1.3778e-05	