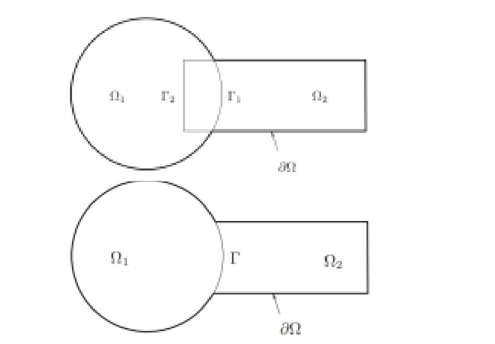
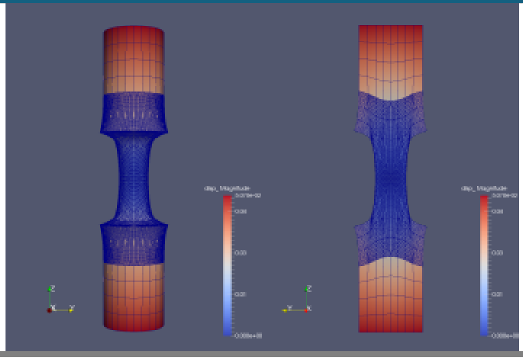
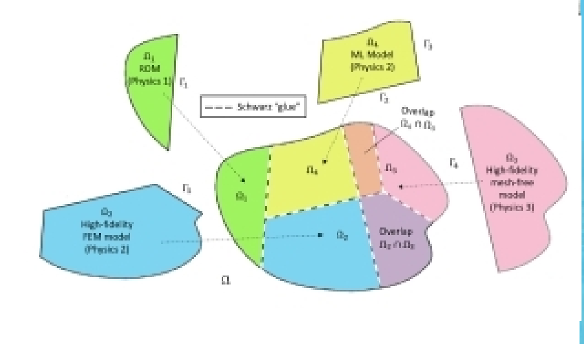
SAND2023-07537C

Sandia National Laboratories

Component-based coupling of conventional and data-driven models for predictive digital twins







Irina Tezaur[1], Joshua Barnett[1,2], Chris Wentland[1], Will Snyder[1,3], Alejandro Mota[1]

[1]Sandia National Laboratories, [2]Stanford University, [3]Virginia Tech University

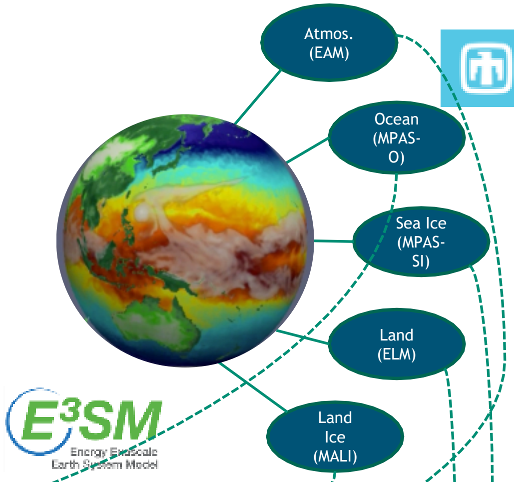
ICIAM 2023
Tokyo, Japan. August 20-25, 2023

SAND2023-XXXX

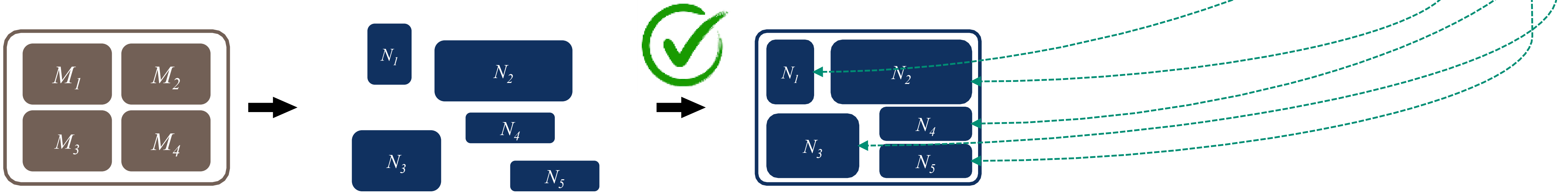
U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Motivation: multi-scale & multi-physics coupling



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



Complex System Model

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

Traditional Methods

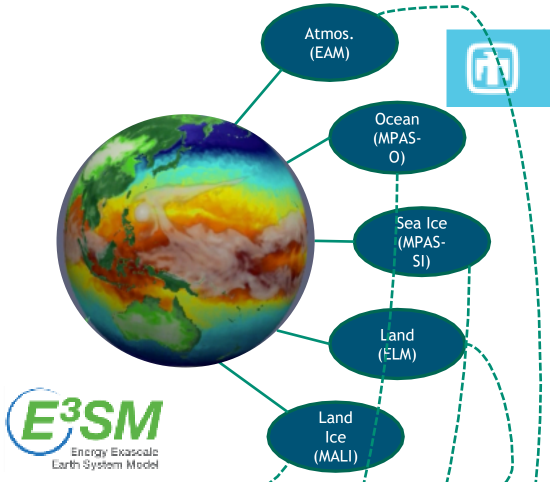
- Mesh-based (FE, FV, FD)
- Meshless (SPH, MLS)
- Implicit, explicit
- Eulerian, Lagrangian…

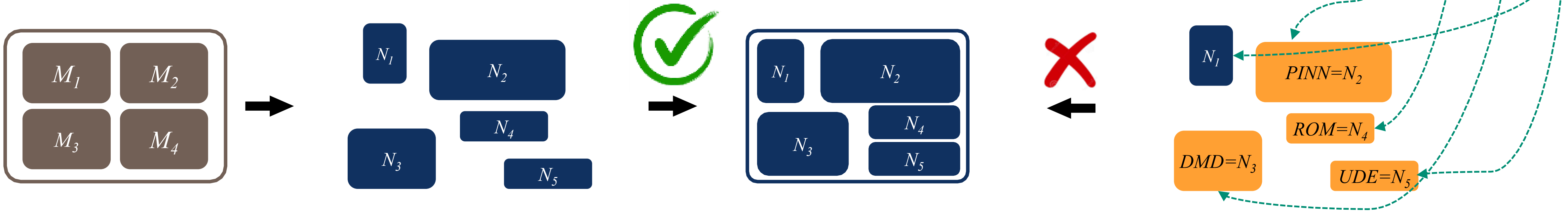
Coupled Numerical Model

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

Motivation: multi-scale & multi-physics coupling

There exist established **rigorous mathematical theories** for **coupling** multi-scale and multi-physics components based on **traditional discretization methods** ("Full Order Models" or FOMs).





Complex System Model

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

Traditional Methods

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

Coupled Numerical Model

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

Traditional + Data-Driven Methods

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

While there is currently a big push to integrate **data-driven methods** into modeling & simulation toolchains, existing algorithmic and software infrastructures are **ill-equipped** to handle **rigorous** plug-and-play integration of **non-traditional, data-driven models**!

Coupling Projects, Models and Methods

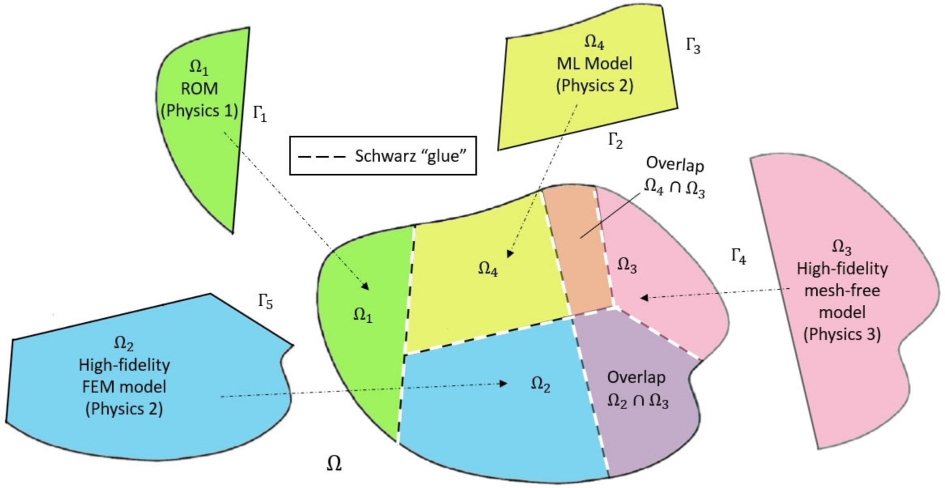
fHNM (flexible Heterogeneous Numerical Methods) & M2dt (Multi-faceted Mathematics for Predictive Digital Twins) projects: **discover** the mathematical principles that guide the **assembly** of **standard** and **data-driven numerical models** in stable, accurate and physically consistent ways, towards creating **predictive digital twins.**

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)



Coupling Projects, Models and Methods

fHNM (flexible Heterogeneous Numerical Methods) & M2dt (Multi-faceted Mathematics for Predictive Digital Twins) projects: discover the mathematical principles that guide the **assembly** of **standard** and **data-driven numerical models** in stable, accurate and physically consistent ways, towards creating **predictive digital twins.**

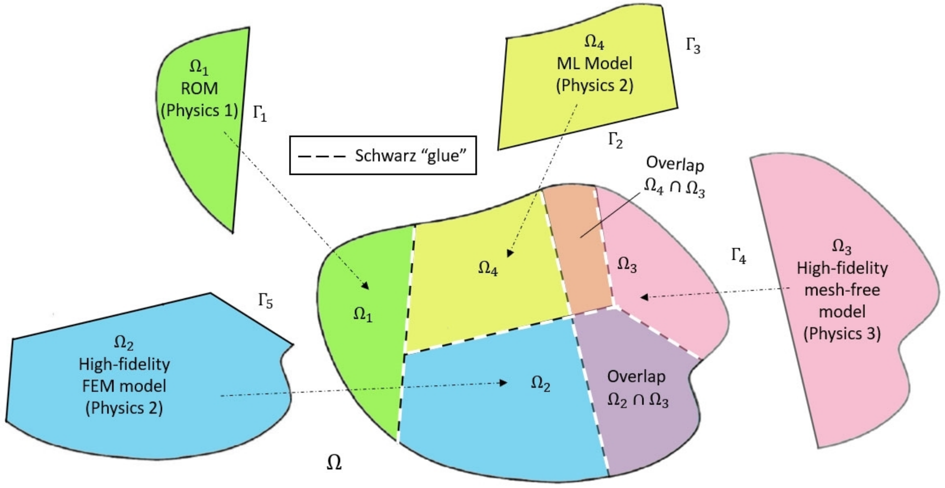
Data-driven models: to be "mixed-and-matched" with each other and first-principles models

- *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

This talk

Coupling methods:

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



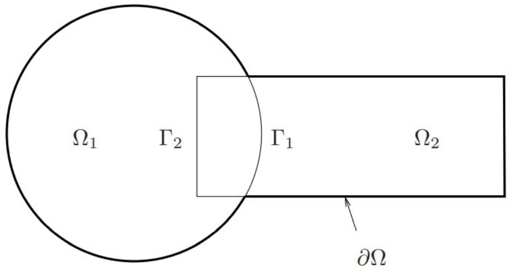
Outline

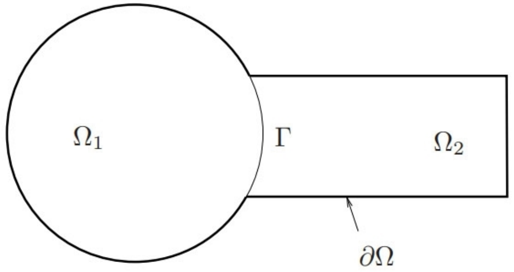
- The Schwarz Alternating Method for Domain Decomposition-Based Coupling

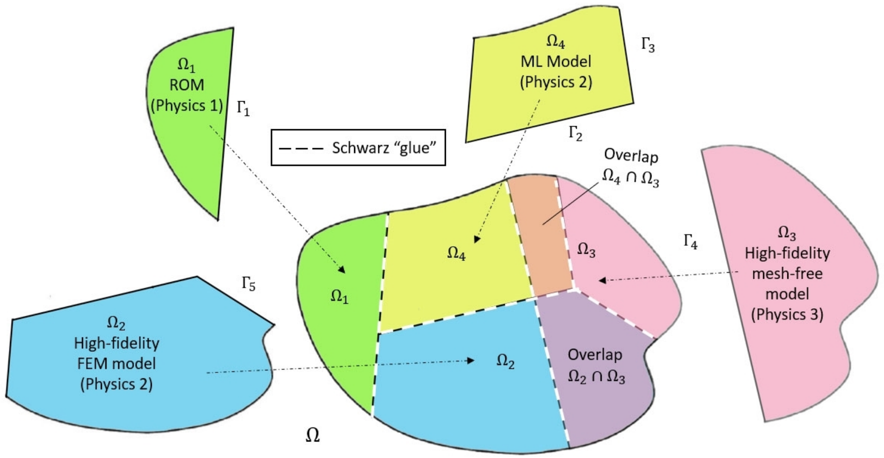
- Extension to FOM*-ROM# and ROM-ROM Coupling

- Numerical Examples
  - ➢ 1D Dynamic Wave Propagation in Hyperelastic Bar
  - ➢ 2D Burgers Equation

- Summary & Future Work







*Full-Order Model. #Reduced Order Model.

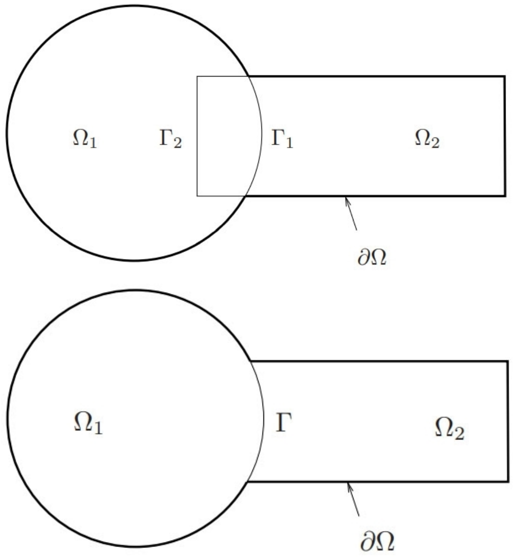
Outline

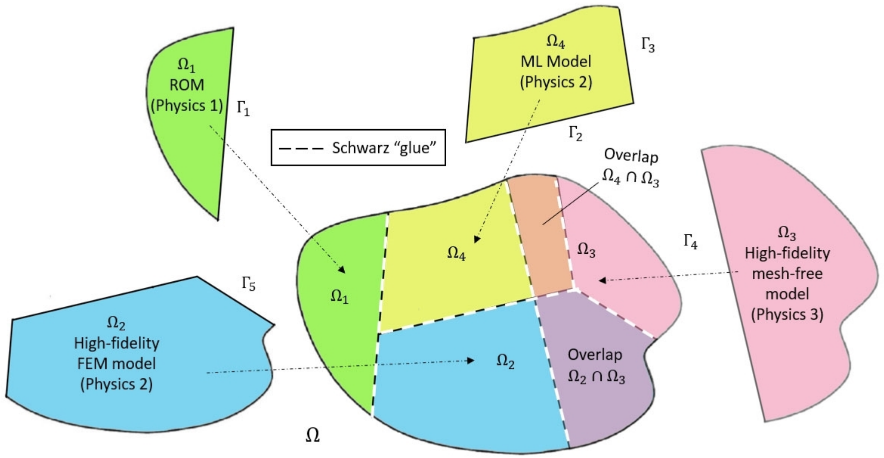
- **The Schwarz Alternating Method for Domain Decomposition-Based Coupling**

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

- Numerical Examples
  - ➢ 1D Dynamic Wave Propagation in Hyperelastic Bar
  - ➢ 2D Burgers Equation

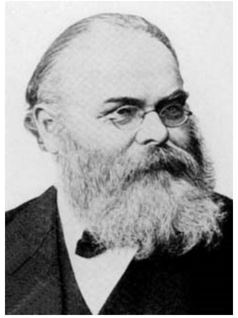
- Summary & Future Work





*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.

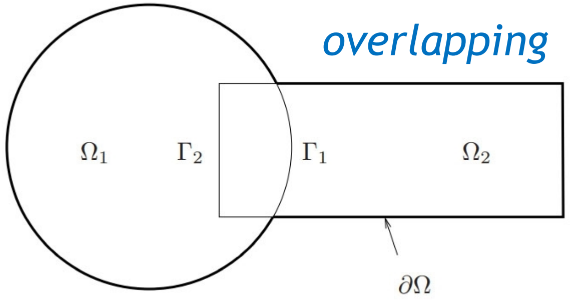
Basic Schwarz Algorithm

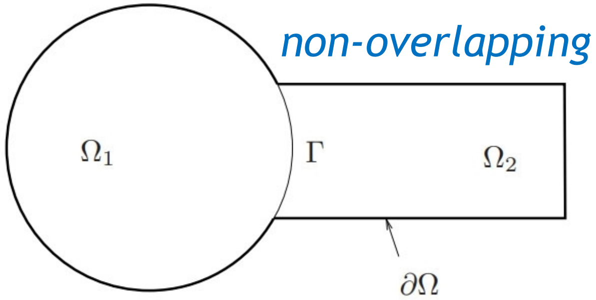
Initialize:

- 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.



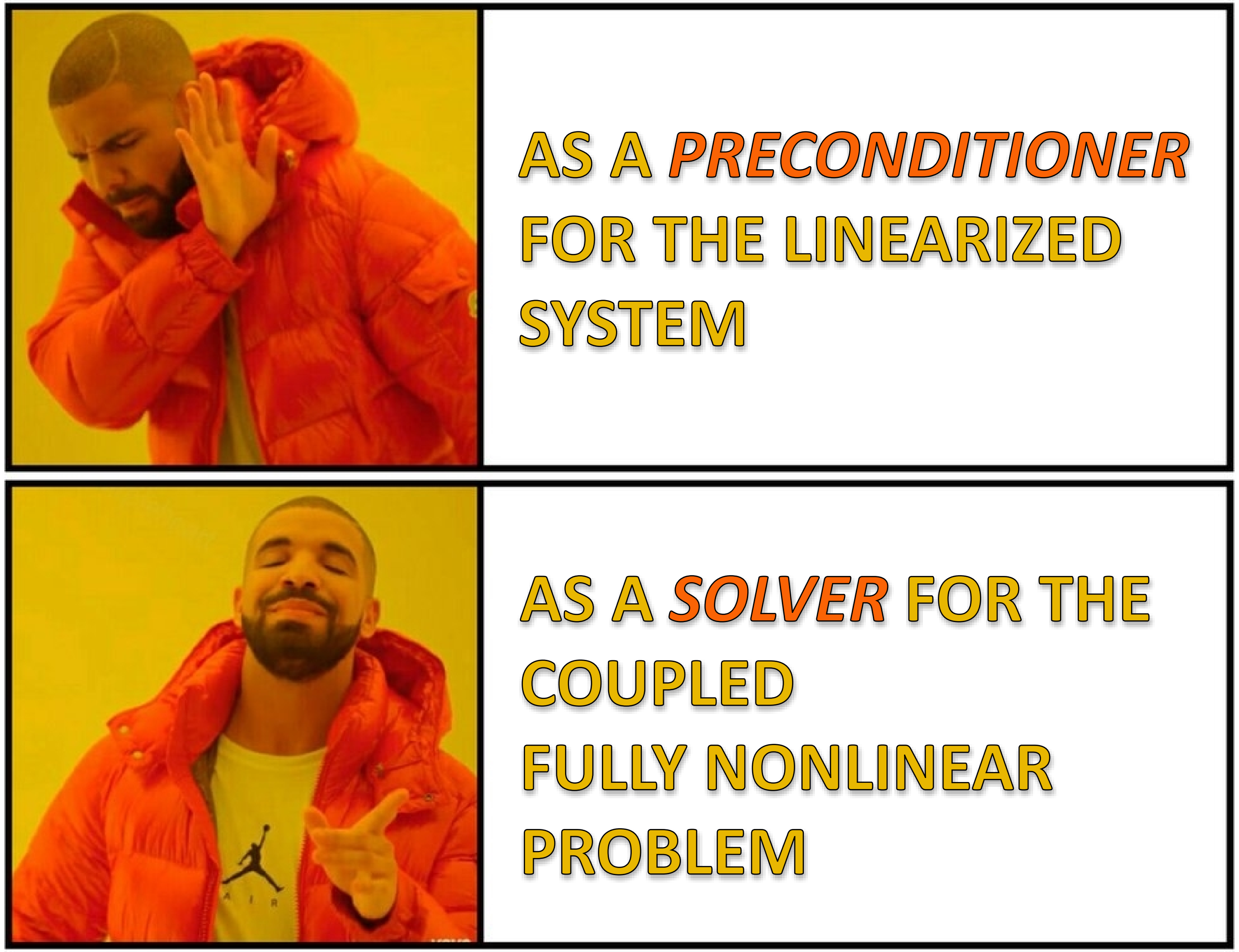


Overlapping Schwarz: convergent with all-Dirichlet transmission BCs[1] if $\Omega_1 \cap \Omega_2 \neq \emptyset$.

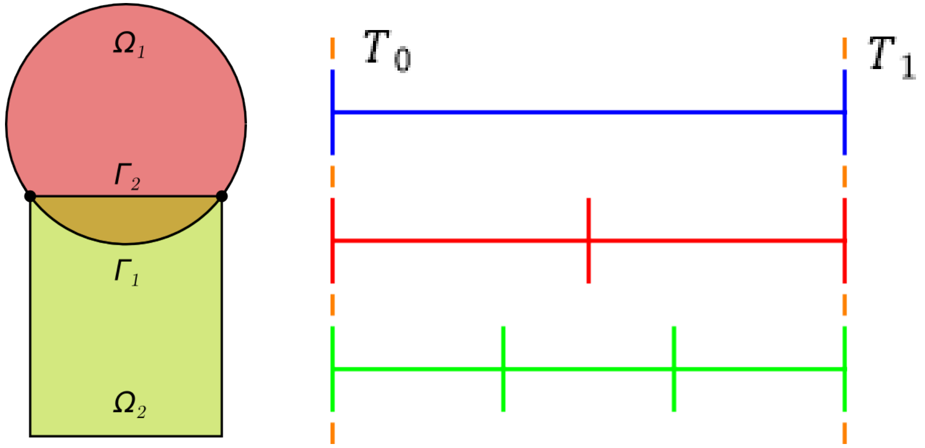
Non-overlapping Schwarz: convergent with Robin-Robin[2] or alternating Neumann-Dirichlet[3] transmission BCs.

[1]Schwarz, 1870; Lions, 1988. [2]Lions, 1990. [3]Zanolli *et al.*, 1987.

How We Use the Schwarz Alternating Method



Time-Advancement Within the Schwarz Framework



Controller time stepper

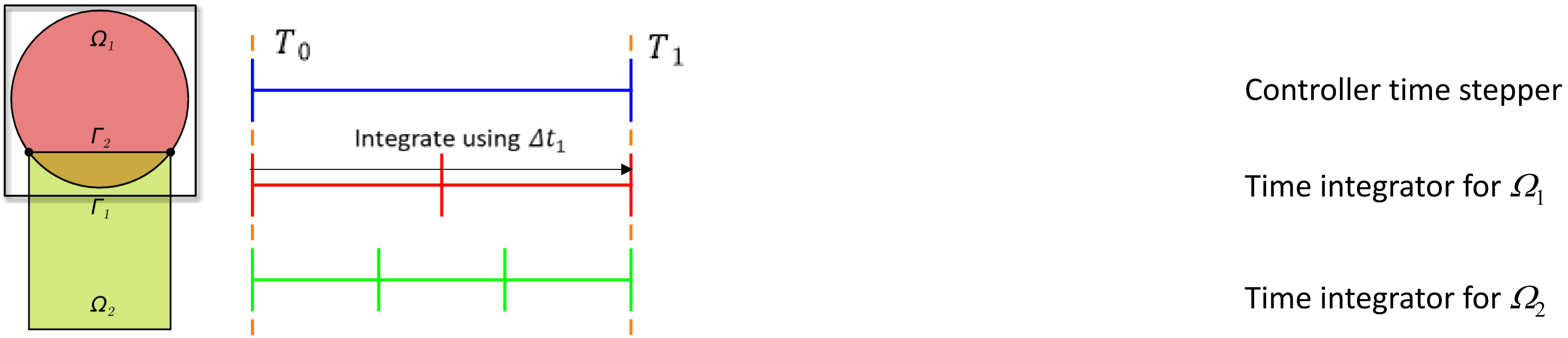
Time integrator for Ω_1

Time integrator for Ω_2

<u>***Step 0***</u>: Initialize $i = 0$ (controller time index).

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

Time-Advancement Within the Schwarz Framework



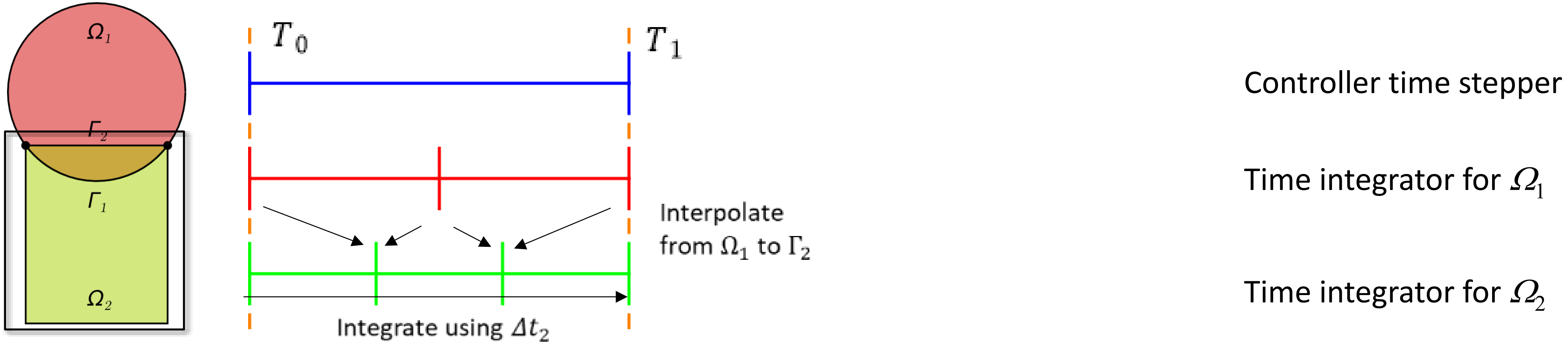
Step 0: Initialize $i = 0$ (controller time index).

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

Model PDE:

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

Time-Advancement Within the Schwarz Framework



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

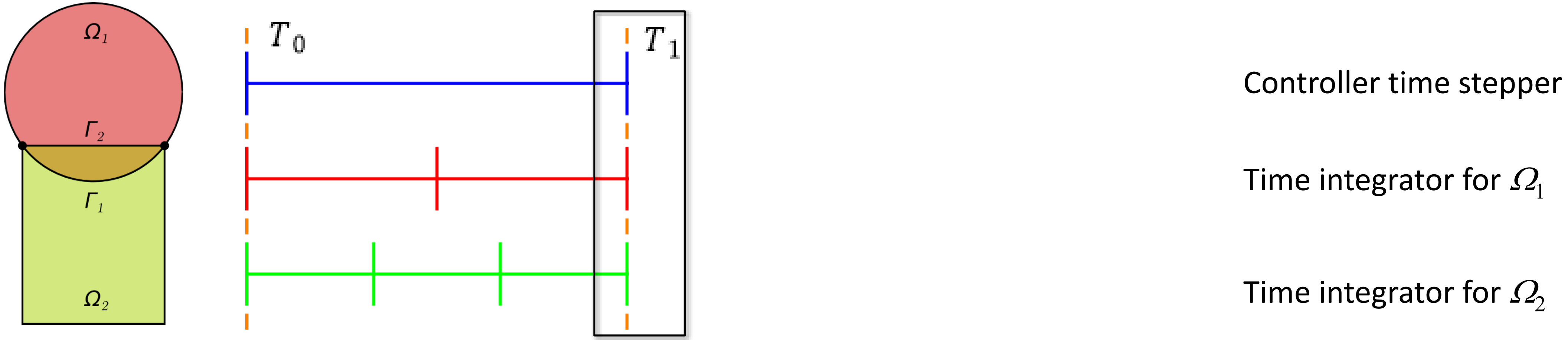
Step 1: Advance Ω_1 solution from time T_i to time T_{i+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ_1 at times $T_i + n\Delta t_1$.

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 $T_i + n\Delta t_2$.

Model PDE:

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

Time-Advancement Within the Schwarz Framework



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 $T_i + n\Delta t_1$.

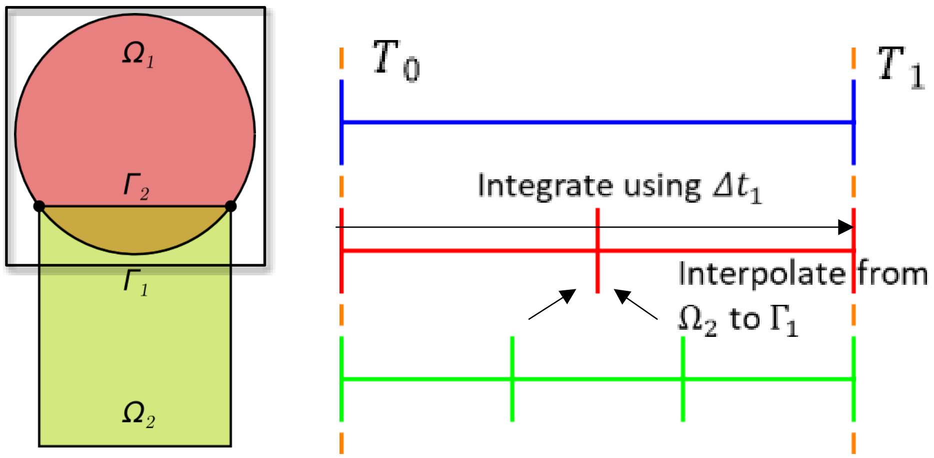
Step 2: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ_2 at times $T_i + n\Delta t_2$.

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

Model PDE:

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

Time-Advancement Within the Schwarz Framework



Controller time stepper

Time integrator for Ω_1

Time integrator for Ω_2

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

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

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 $T_i + n\Delta t_2$.

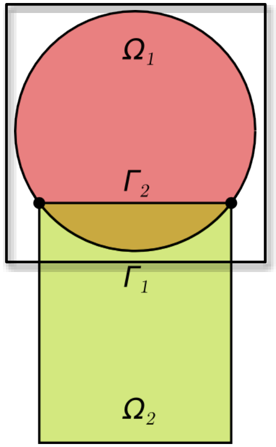
Step 3: Check for convergence at time T_{i+1}.

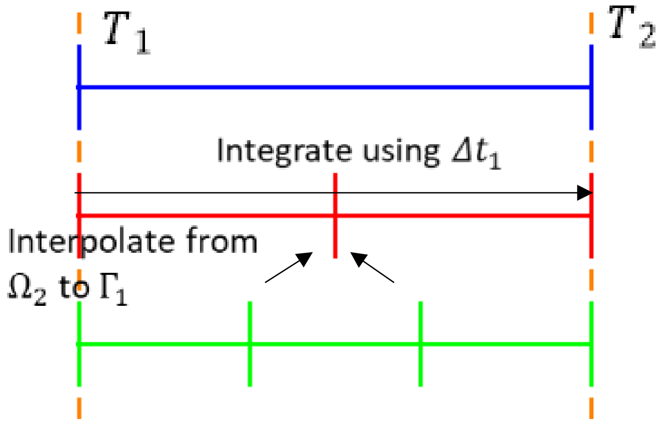
- If unconverged, return to Step 1.

Model PDE:

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

Time-Advancement Within the Schwarz Framework





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

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 $T_i + n\Delta t_2$.

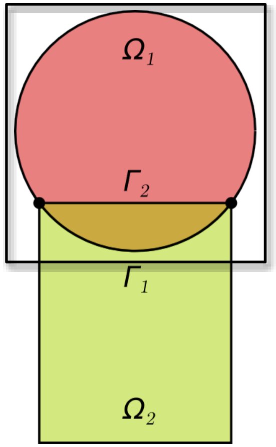
Step 3: Check for convergence at time T_{i+1}.

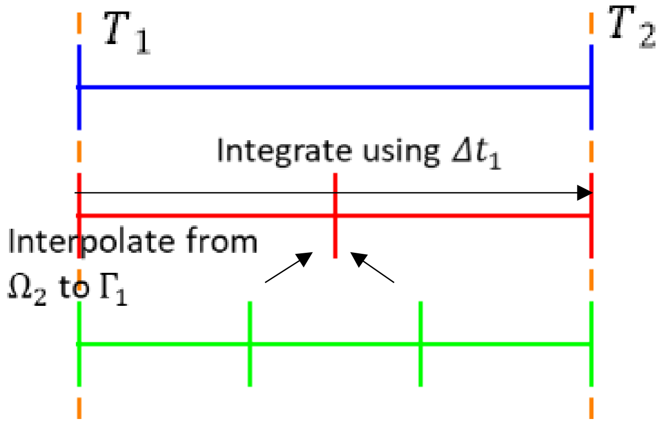
- If unconverged, return to Step 1.
- If converged, set $i = i + 1$ and return to Step 1.

Model PDE:

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

Time-Advancement Within the Schwarz Framework





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:

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

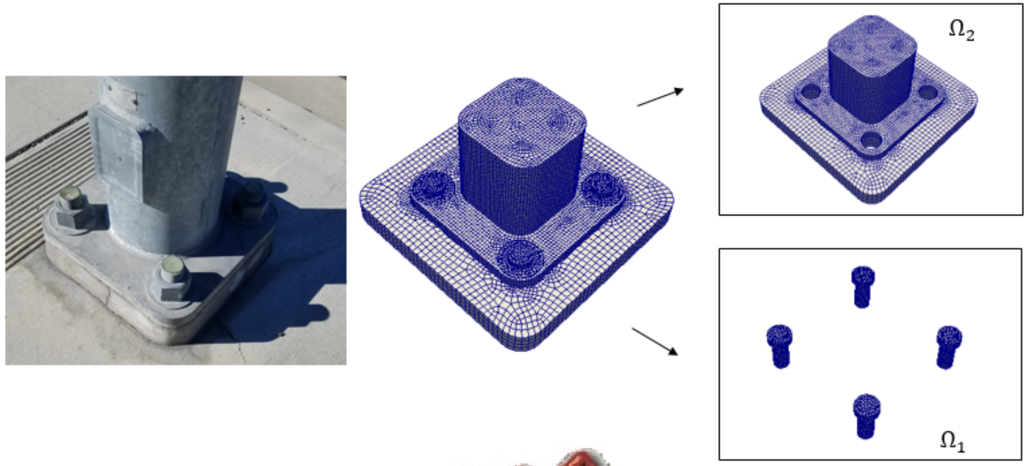
Schwarz for Multiscale FOM-FOM Coupling in Solid Mechanics[1]

- 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] SIERRA

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

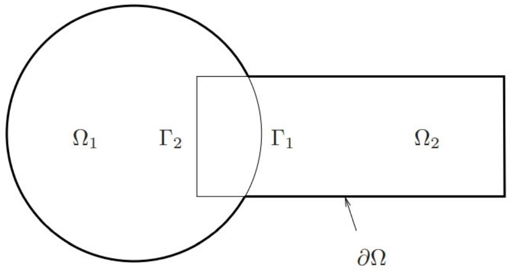
Outline

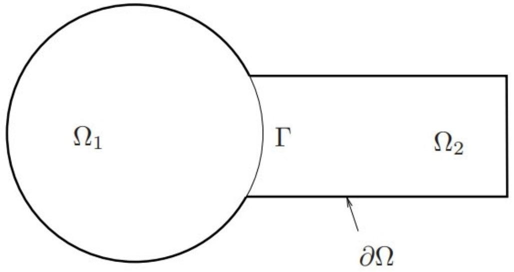
- The Schwarz Alternating Method for Domain Decomposition-Based Coupling

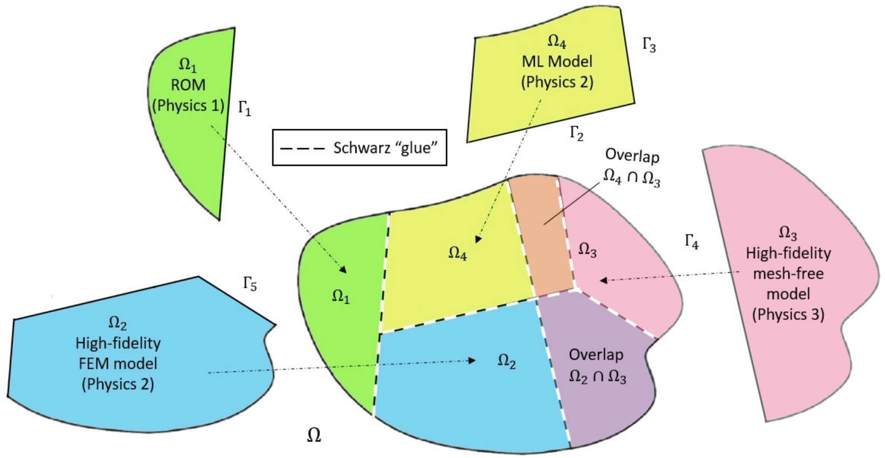
- **Extension to FOM*-ROM# and ROM-ROM Coupling**

- Numerical Examples
  - ➢ 1D Dynamic Wave Propagation in Hyperelastic Bar
  - ➢ 2D Burgers Equation

- Summary & Future Work





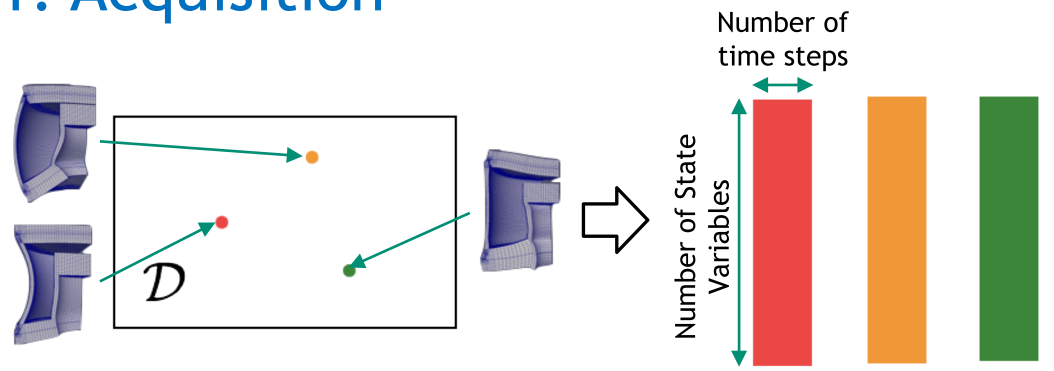


*Full-Order Model. #Reduced Order Model.

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

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

1. Acquisition

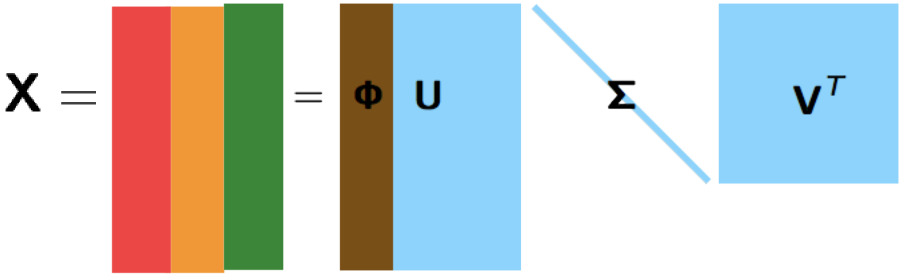


Solve ODE at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



ROM = projection-based Reduced Order Model

3. Projection-Based Reduction

Reduce the number of unknowns

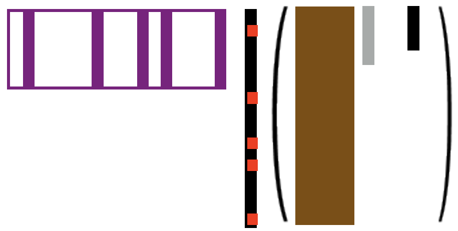
$\boldsymbol{u}(t) \approx \tilde{\boldsymbol{u}}(t) = \boldsymbol{\Phi}\hat{\boldsymbol{u}}(t)$

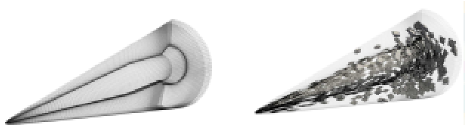
Perform Galerkin projection

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

Hyper-reduce nonlinear terms

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





Hyper-reduction/sample mesh

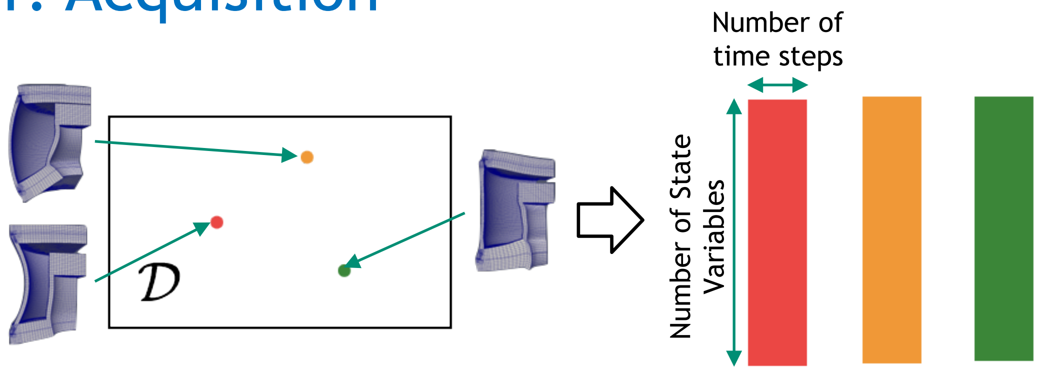
HROM = Hyper-reduced ROM

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

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

* Least-Squares Petrov-Galerkin

1. Acquisition

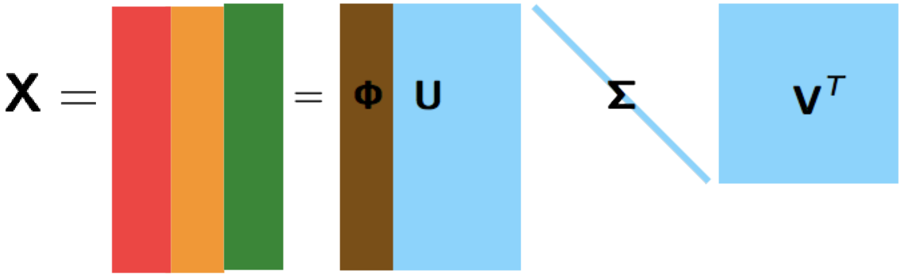


Solve ODE at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



3. Projection-Based Reduction

Choose ODE temporal discretization

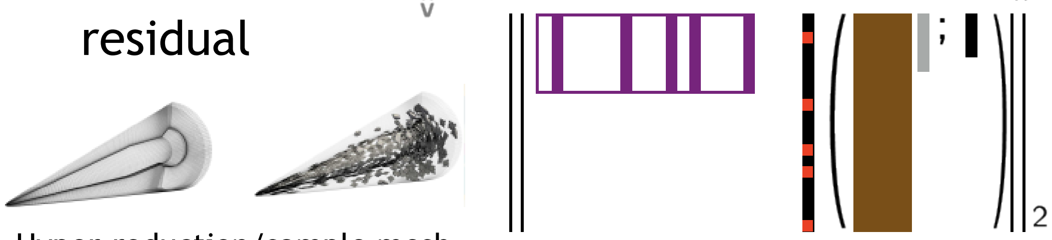
$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{f}(\boldsymbol{u}; t, \boldsymbol{\mu})$$
$$\Downarrow$$
$$\boldsymbol{r}^n(\boldsymbol{u}^n; \boldsymbol{\mu}) = 0, \ n = 1, \dots, T$$

Reduce the number of unknowns

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

Minimize residual

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



Hyper-reduction/sample mesh

ROM = projection-based Reduced Order Model

HROM = Hyper-reduced ROM

Schwarz Extensions to FOM-(H)ROM and (H)ROM-(H)ROM Couplings

Enforcement of Dirichlet boundary conditions (DBCs) in ROM at indices $\boldsymbol{i}_{\mathrm{Dir}}$

- Method I in [Gunzburger *et al*. 2007] is employed

$$\boldsymbol{u}(t) \approx \overline{\boldsymbol{u}} + \boldsymbol{\Phi}\widehat{\boldsymbol{u}}(t), \quad \boldsymbol{v}(t) \approx \overline{\boldsymbol{v}} + \boldsymbol{\Phi}\widehat{\boldsymbol{v}}(t), \quad \boldsymbol{a}(t) \approx \overline{\boldsymbol{a}} + \boldsymbol{\Phi}\widehat{\boldsymbol{a}}(t)$$

  - ➢ POD modes made to satisfy homogeneous DBCs: $\boldsymbol{\Phi}(\boldsymbol{i}_{\mathrm{Dir}}, :) = \boldsymbol{0}$
  - ➢ BCs imposed by modifying $\overline{\boldsymbol{u}}$, $\overline{\boldsymbol{v}}$, $\overline{\boldsymbol{a}}$: $\overline{\boldsymbol{u}}(\boldsymbol{i}_{\mathrm{Dir}}) \leftarrow \boldsymbol{\chi}_u$, $\overline{\boldsymbol{v}}(\boldsymbol{i}_{\mathrm{Dir}}) \leftarrow \boldsymbol{\chi}_v$, $\overline{\boldsymbol{a}}(\boldsymbol{i}_{\mathrm{Dir}}) \leftarrow \boldsymbol{\chi}_a$

Hyper-reduction considerations

- Boundary points must be included in sample mesh for DBC enforcement
- We employ the Energy-Conserving Sampling & Weighting Method (ECSW) [Farhat *et al*. 2015] → preserves Hamiltonian structure for solid mechanics problems

Choice of domain decomposition

- *Future work:* error indicator-based or reinforcement learning-based algorithms to determine "optimal" domain decomposition and ROM/FOM assignment

Snapshot collection and reduced basis construction

- POD results presented herein use snapshots obtained via FOM-FOM coupling on $\Omega = \cup_i \ \Omega_i$
- *Future work*: generate snapshots/bases separately in each Ω_i [Hoang *et al*. 2021, Smetana *et al*. 2022]

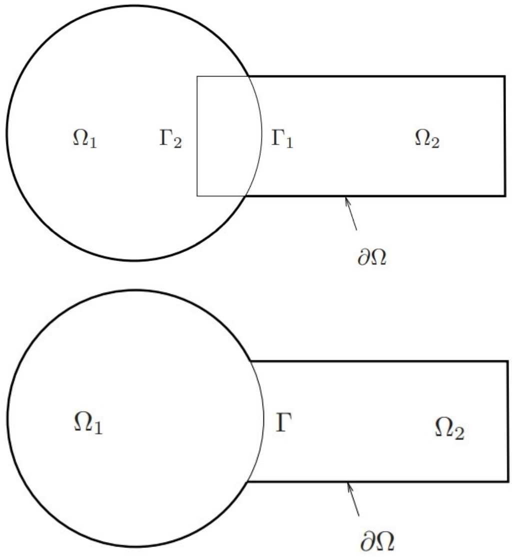
Outline

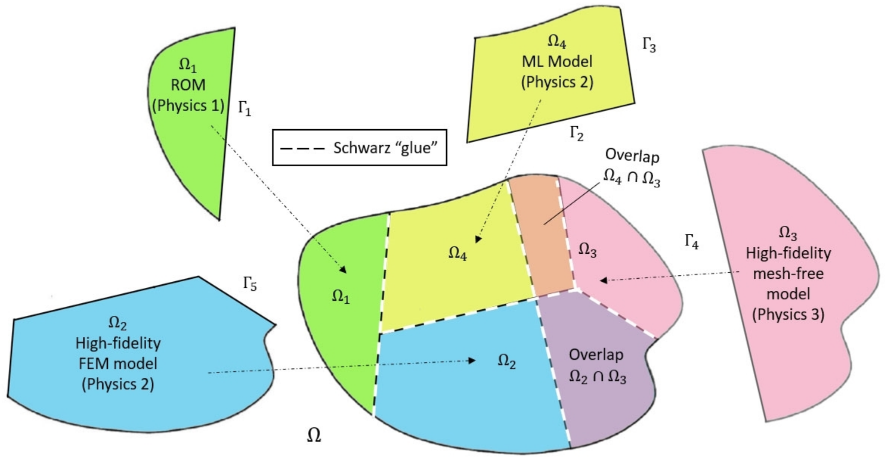
- The Schwarz Alternating Method for Domain Decomposition-Based Coupling

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

- **Numerical Examples**
  - ➢ **1D Dynamic Wave Propagation in Hyperelastic Bar**
  - ➢ 2D Burgers Equation

- Summary & Future Work





*Full-Order Model. #Reduced Order Model.

Numerical Example: 1D Dynamic Wave Propagation Problem

- ***1D beam*** geometry $\Omega = (0,1)$, clamped at both ends, with prescribed initial condition discretized using FEM + Newmark-β
- Simple problem but very ***stringent test*** for discretization/coupling methods, and ***difficult problem for ROMs***.
- Two ***constitutive models*** considered:
  - ➢ Linear elastic (problem has exact analytical solution)
  - ➢ Nonlinear hyperelastic Henky   ***This talk***

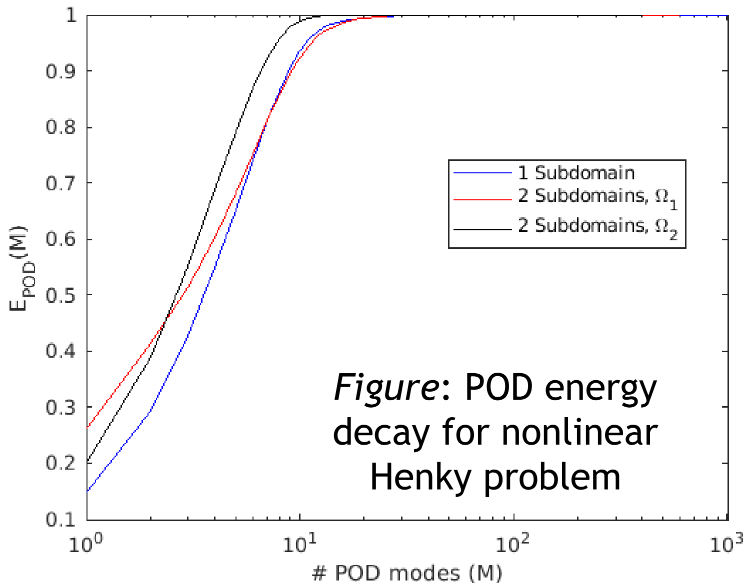


Figure: POD energy decay for nonlinear Henky problem

- ROMs results are ***reproductive*** and ***predictive***, and are based on the ***POD/Galerkin*** method, with POD calculated from FOM-FOM coupled model.
  - ➢ 50 POD modes capture ~100% snapshot energy for linear variant of this problem.
  - ➢ 536 POD modes capture ~100% snapshot energy for Henky variant of this problem.
- Hyper-reduced ROMs (HROMs) perform ***hyper-reduction*** using ECSW [Farhat *et al.*, 2015]
  - ➢ Ensures that ***Lagrangian structure*** of problem is preserved in HROM.
- ***Couplings tested:*** overlapping, non-overlapping, FOM-FOM, FOM-ROM, ROM-ROM, FOM-HROM, HROM-HROM, implicit-explicit, implicit-implicit, explicit-explicit.   ***This talk***

Numerical Example: 1D Dynamic Wave Propagation Problem

- **Two variants** of problem, with different initial conditions (ICs):
  - ➢ Symmetric Gaussian IC (top right)
  - ➢ Rounded Square IC (bottom right)

- **Non-overlapping domain decomposition (DD)** of $\Omega = \Omega_1 \cup \Omega_2$, where Ω_1 = [0, 0.6] and Ω_2 = [0.6, 1.0]
  - ➢ DD is based on heuristics: during time-interval considered ($0 \leq t \leq 1 \times 10^3$), sharper gradient forms in Ω_1, suggesting FOM or larger ROM is needed there.

- **Reproductive problem**:
  - ➢ Displacement snapshots collected using FOM-FOM non-overlapping coupling with **Symmetric Gaussian IC**
  - ➢ FOM-ROM, FOM-HROM, ROM-ROM and HROM-HROM run with **Symmetric Gaussian IC**

- **Predictive problem**:
  - ➢ Displacement snapshots collected using FOM-FOM non-overlapping coupling with **Symmetric Gaussian IC**
  - ➢ FOM-ROM, FOM-HROM, ROM-ROM and HROM-HROM run with **Rounded Square IC**

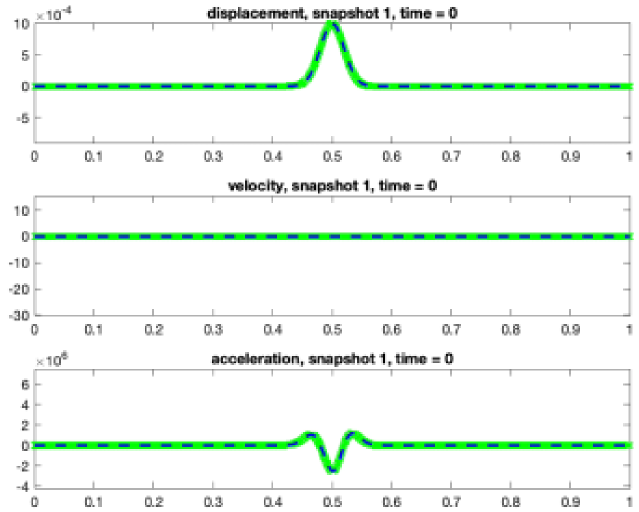
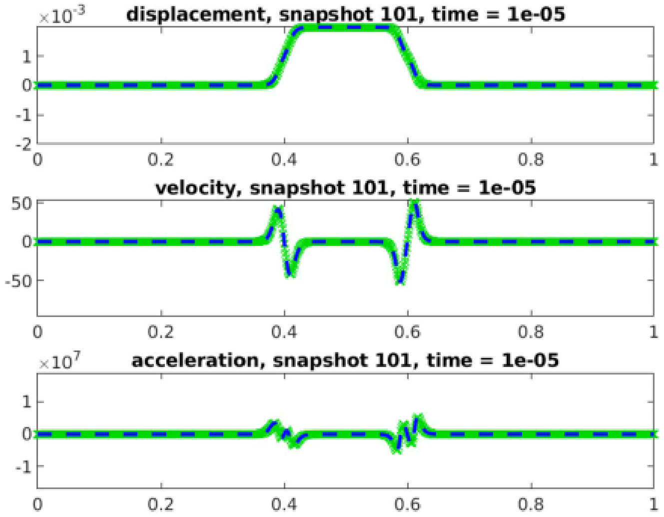
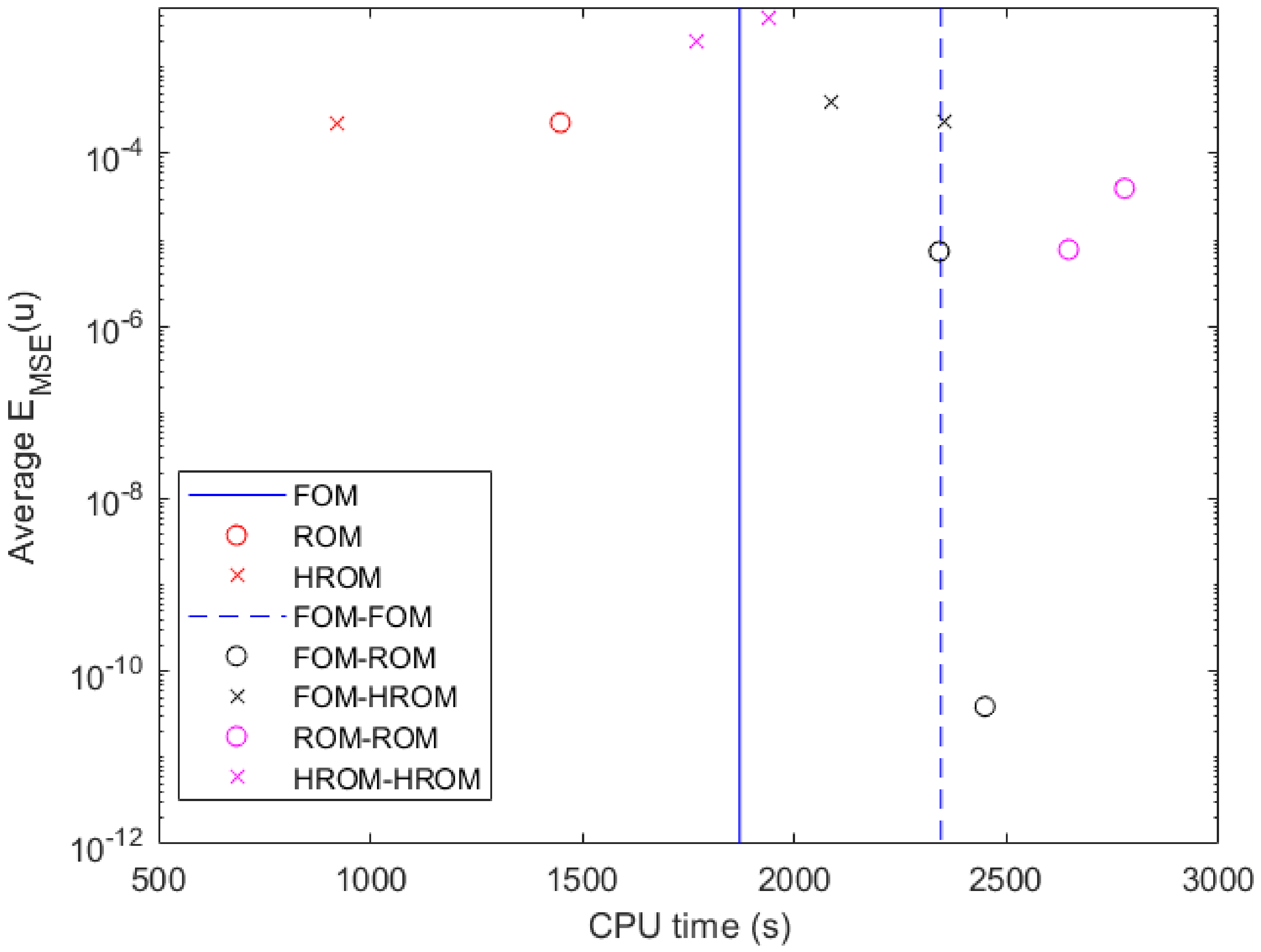


Figure above: Symmetric Gaussian IC problem solution
Figure below: Rounded Square IC problem solution



Numerical Example: Reproductive Problem Results



- **Single-domain** ROM and HROM are most **efficient**
- Couplings involving ROMs and HROMs enable one to achieve **smaller errors**
- Benefits of **hyper-reduction** are **limited** on **1D problem**
- **FOM-HROM** and **HROM-HROM** couplings **outperform** the **FOM-FOM** coupling in terms of CPU time by 12.5-32.6%

Numerical Example: Reproductive Problem Results

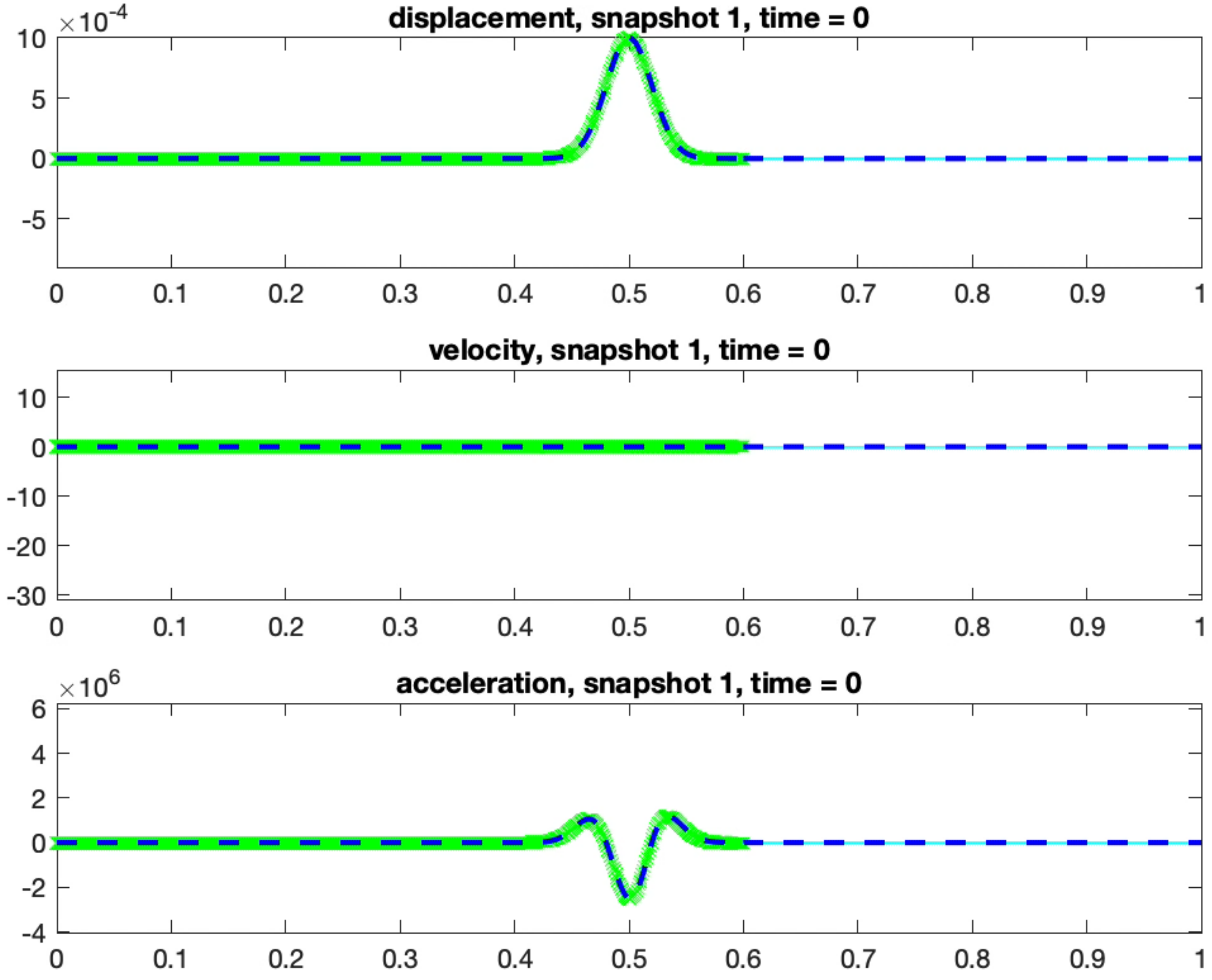
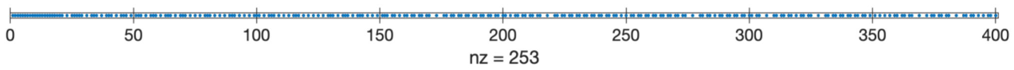


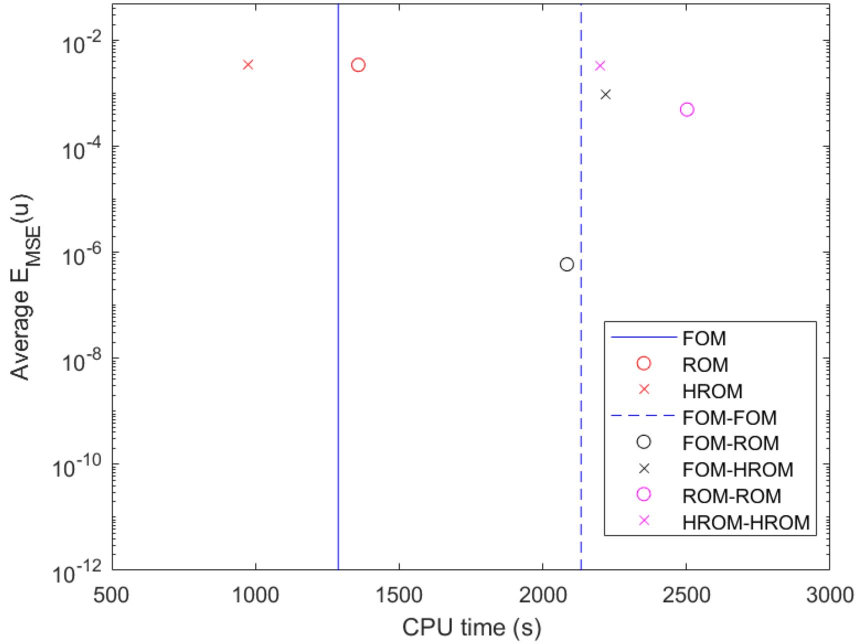
Figure left: FOM (green) – HROM (cyan) coupling compared with single-domain FOM solution (blue). HROM has 200 modes.

Figure below: ECSW algorithm samples 253/400 elements



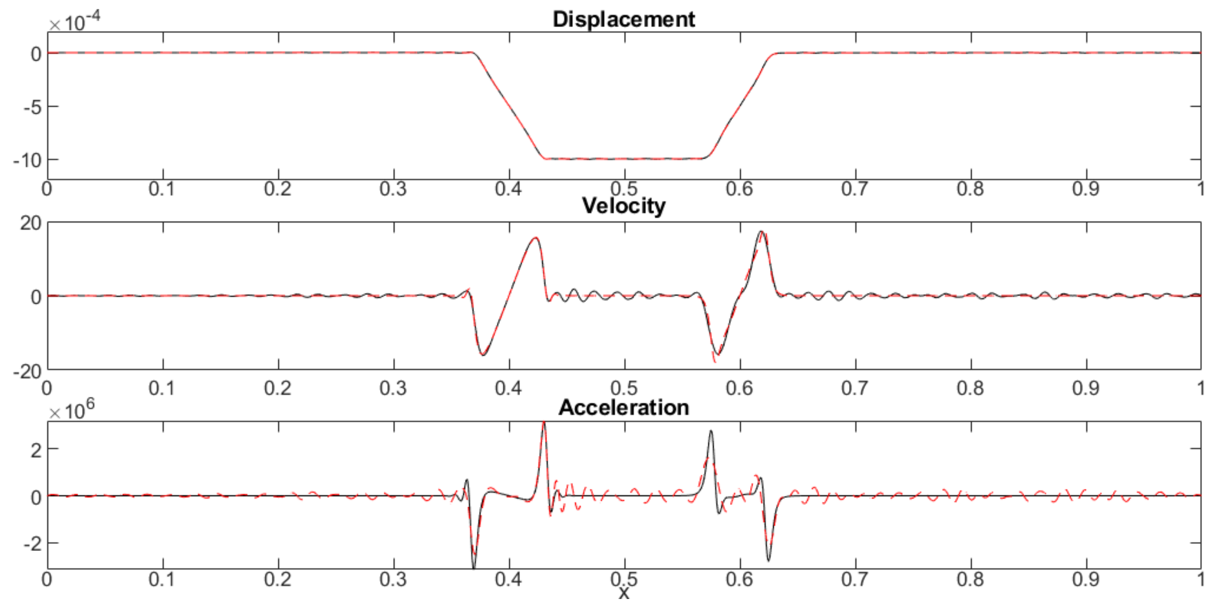
Numerical Example: Predictive Problem Results

Model	CPU time (s)	$N_{e,1}/N_{e,2}$	$\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{u}}_1)/\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{u}}_2)$	$\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{v}}_1)/\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{v}}_2)$	$\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{a}}_1)/\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{a}}_2)$	N_S
FOM	1.288×10^3	$-/-$	$-/-$	$-/-$	$-/-$	$-$
ROM	1.358×10^3	$-/-$	$3.451 \times 10^{-3}/-$	$6.750 \times 10^{-2}/-$	$3.021 \times 10^{-1}/-$	$-$
HROM	9.759×10^2	$614/-$	$3.463 \times 10^{-3}/-$	$6.750 \times 10^{-2}/-$	$3.021 \times 10^{-1}/-$	$-$
FOM-FOM	2.133×10^3	$-/-$	$-/-$	$-/-$	$-/-$	23,280
FOM-ROM	2.084×10^3	$-/-$	$1.907 \times 10^{-8}/$ 1.170×10^{-6}	$1.461 \times 10^{-6}/$ 9.882×10^{-5}	$3.973 \times 10^{-5}/$ 1.757×10^{-3}	23,288
FOM-HROM	2.219×10^3	$-/253$	1.967×10^{-4} 1.720×10^{-3}	4.986×10^{-3} 4.185×10^{-2}	2.768×10^{-2} 2.388×10^{-1}	29,700
ROM-ROM	2.502×10^3	$-/-$	$5.592 \times 10^{-4}/$ 4.346×10^{-4}	$1.575 \times 10^{-2}/$ 1.001×10^{-2}	$9.197 \times 10^{-2}/$ 5.304×10^{-2}	26,220
HROM-HROM	2.200×10^3	$405/253$	4.802×10^{-3} 1.960×10^{-3}	8.500×10^{-2} 4.630×10^{-2}	3.744×10^{-1} 2.580×10^{-1}	30,067

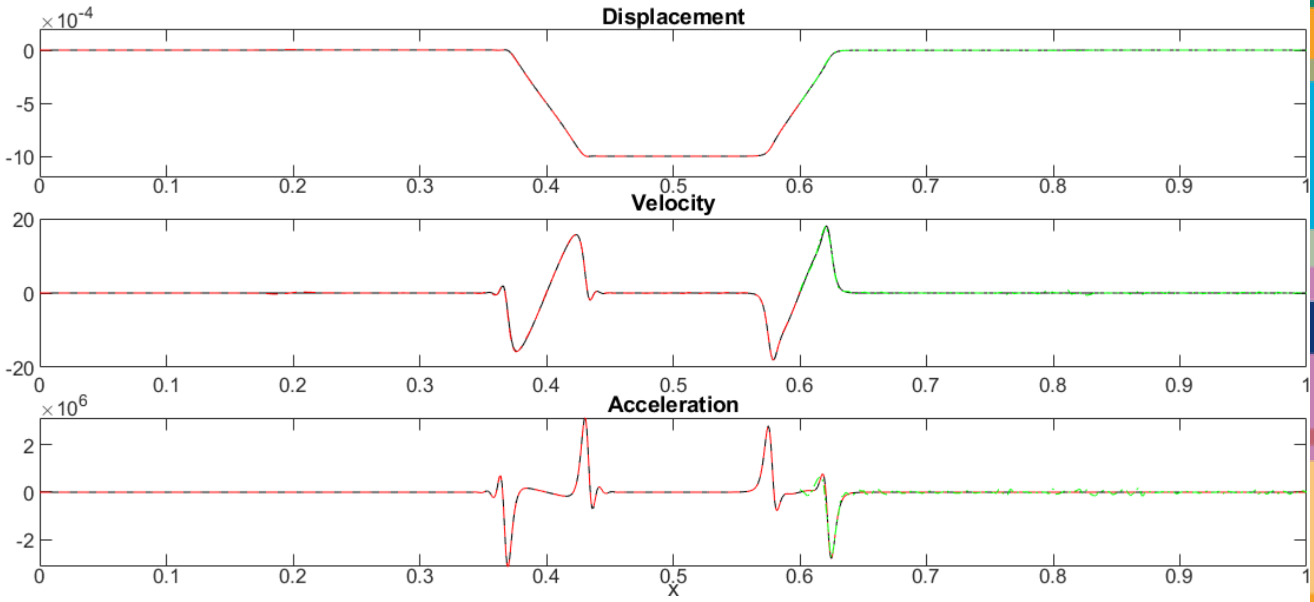


- Results indicate that **predictive accuracy/robustness** can be **improved** by **coupling** ROM or HROM to FOM
  - FOM-ROM coupling is **remarkably accurate**, achieving displacement error $O(1 \times 10^{-8})$
  - FOM-HROM and ROM-ROM couplings are **more accurate** than single-domain ROMs
  - HROM-HROM **on par** with single-domain HROM in terms of accuracy
- **Wall-clock times** of coupled models can be improved
  - FOM-HROM, ROM-ROM and HROM-HROM models are **slower** than FOM-FOM model as **more Schwarz iterations** required to achieve convergence
  - **Hyper-reduction** samples ~60% of total mesh points for this 1D traveling wave problem
    - Greater gains from hyper-reduction anticipated for 2D/3D problems

Numerical Example: Predictive Problem Results



Predictive single-domain ROM (M_1= 300) solution at final time

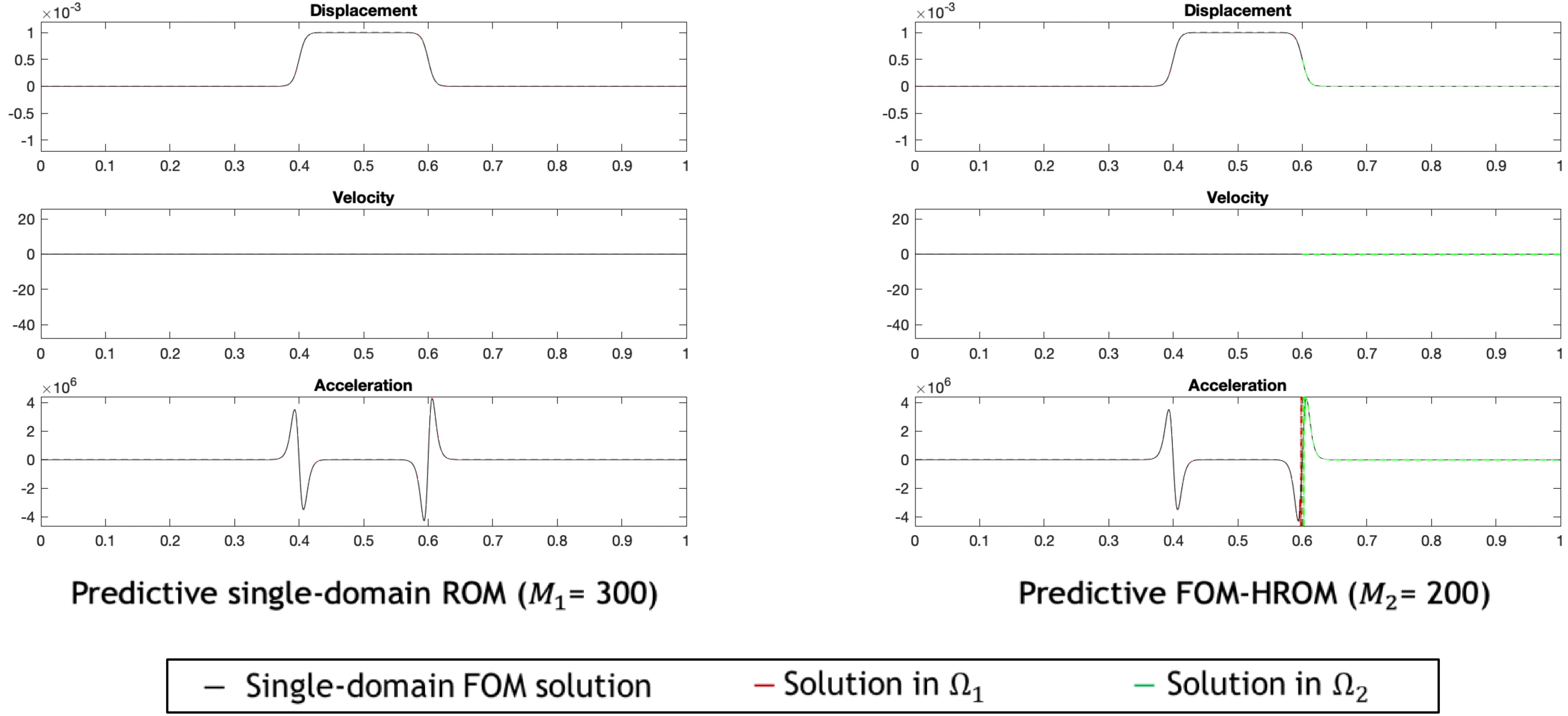


Predictive FOM-HROM (M_2= 200) solution at final time

— Single-domain FOM solution — Solution in Ω_1 — Solution in Ω_2

- Predictive **single-domain ROM** solution exhibits **spurious oscillations** in velocity and acceleration
- Predictive **FOM-HROM** solution is **smooth** and **oscillation-free**
  - ➢ Highlights coupling method's ability to improve ROM predictive accuracy

Numerical Example: Predictive Problem Results



Outline

- The Schwarz Alternating Method for Domain Decomposition-Based Coupling

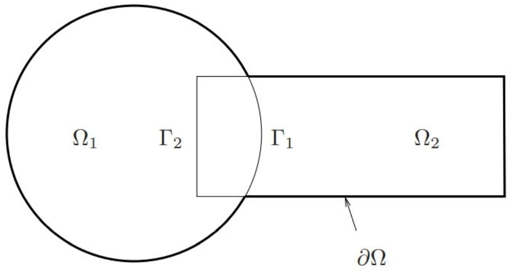
- Extension to FOM*-ROM# and ROM-ROM Coupling

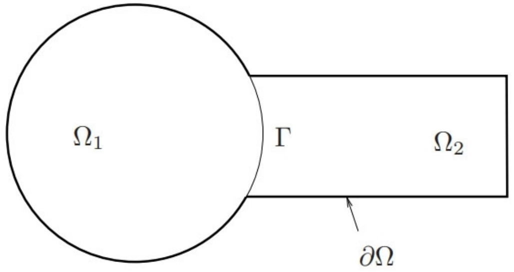
- **Numerical Examples**

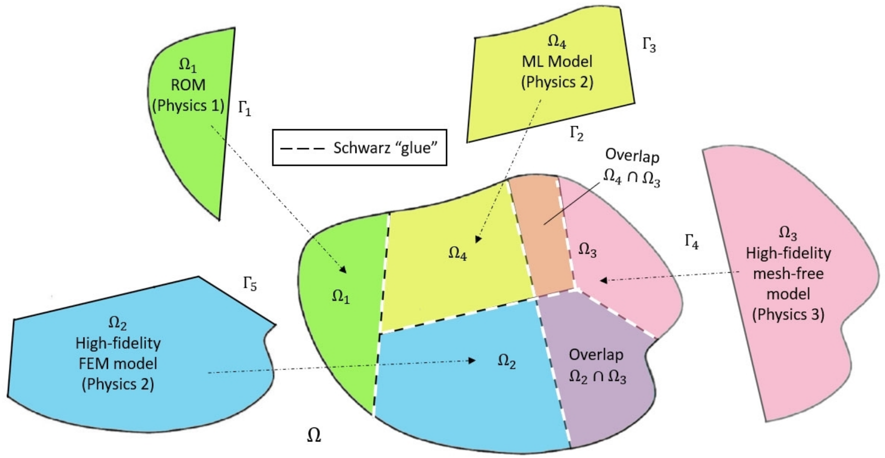
  - 1D Dynamic Wave Propagation in Hyperelastic Bar

  - **2D Burgers Equation**

- Summary & Future Work







*Full-Order Model. #Reduced Order Model.

Numerical Example: 2D Inviscid Burgers Problem

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

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

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

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

$$x,y \in [0,100],\ t \in [0,T_f]$$

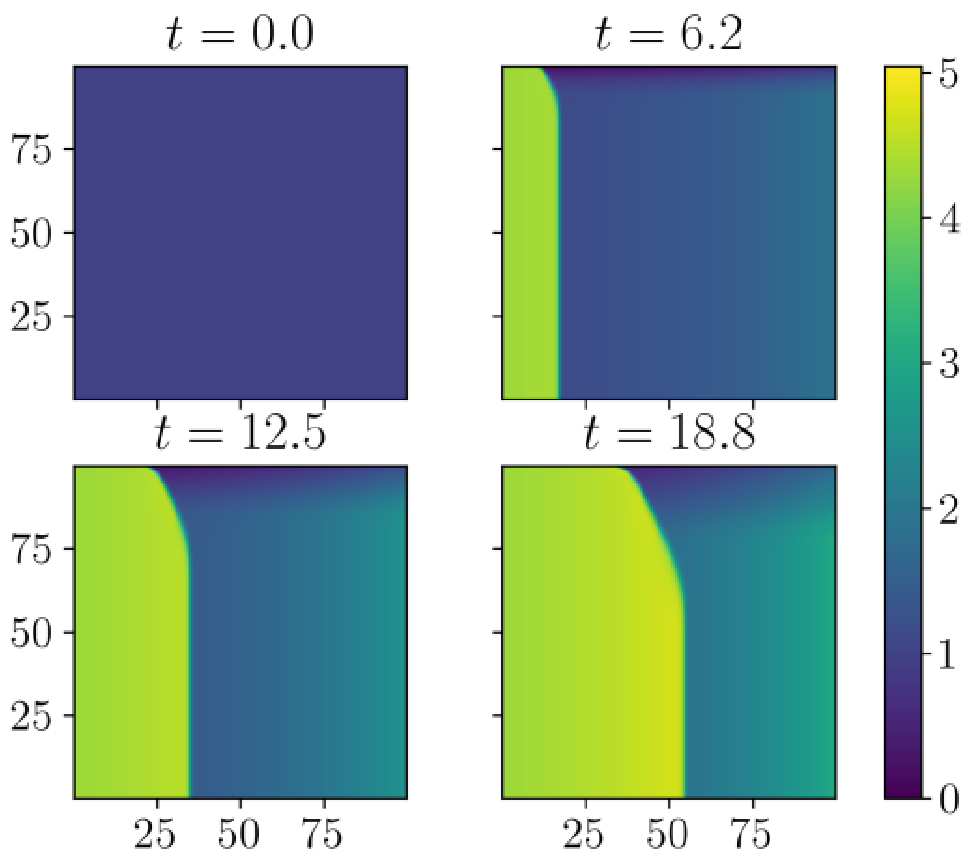
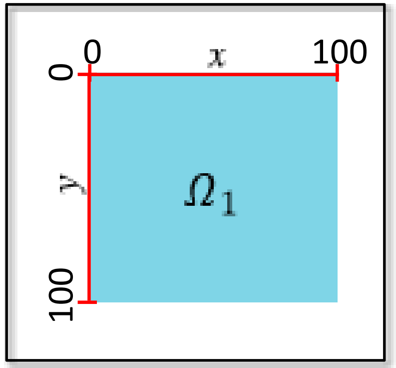


Figure above: solution of u component at various times

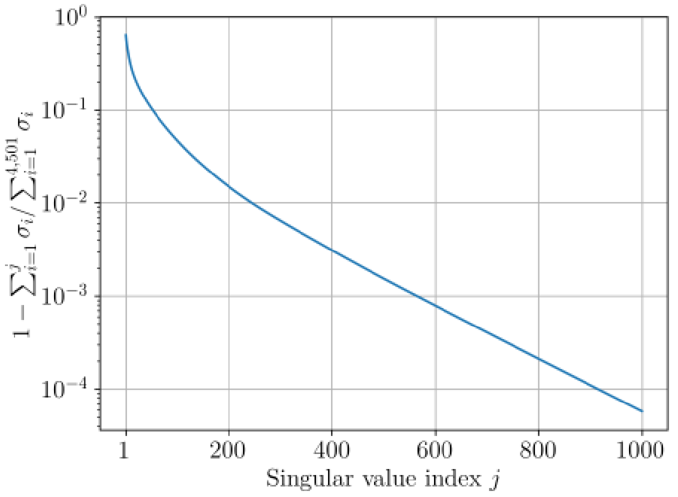


FOM discretization:

- Spatial discretization given by a **Godunov-type scheme** with $N = 250$ elements in each dimension
- Implicit temporal discretization: **trapezoidal method** with fixed $\Delta t = 0.05$; Choose $T_f = 25.0$

Numerical Example: 2D Inviscid Burgers Problem

- ***2D*** makes for a more appropriate testing of potential speedups from coupling subdomains to ROMs
- The **inviscid Burgers' equation** is a popular analog for fluid problems where shocks are possible, and is particularly difficult for conventional projection-based ROMs
- Two **parameters** considered:
  - ➢ Dirichlet BC parameterization μ_1
  - ➢ Source term parameterization μ_2



- ROMs results are ***predictive*** *and* are based on the ***Least-Squares Petrov-Galerkin (LSPG)*** method, with POD calculated from FOM coupling models.
  - ➢ Greater than 200 POD modes required to capture 99% snapshot energy for when sampling 9 $\boldsymbol{\mu} = [\mu_1, \mu_2]$ values
- Hyper-reduced ROMs (HROMs) perform ***hyper-reduction*** using ECSW [Farhat *et al.*, 2015]
- ***Couplings tested:*** overlapping, FOM-FOM, FOM-ROM, ROM-ROM, FOM-HROM, HROM-HROM, implicit-explicit, implicit-implicit, explicit-explicit.

This talk

Single Domain ROM

- **Spatial/temporal resolution:** $\Delta x_i = 0.4,\ \Delta y_i = 0.4,\ \Delta t_i = 0.05$
- **Uniform sampling** of $\mathcal{D} = [4.25, 5.50] \times [0.015, 0.03]$ by a 3×3 grid ⇒ 9 training parameter points characterized by $\Delta\mu_1 = 0.625$ and $\Delta\mu_2 = 0.0075$
- Queried but **unsampled parameter** point $\mu = [4.75, 0.02]$ with reduced dimension of $M = 95$
- **Reduced mesh** resulting from solving non-negative least squares problem formulate by ECSW gives $n_e = 5{,}689$ elements (9.1% of $N_e = 62{,}500$ elements).

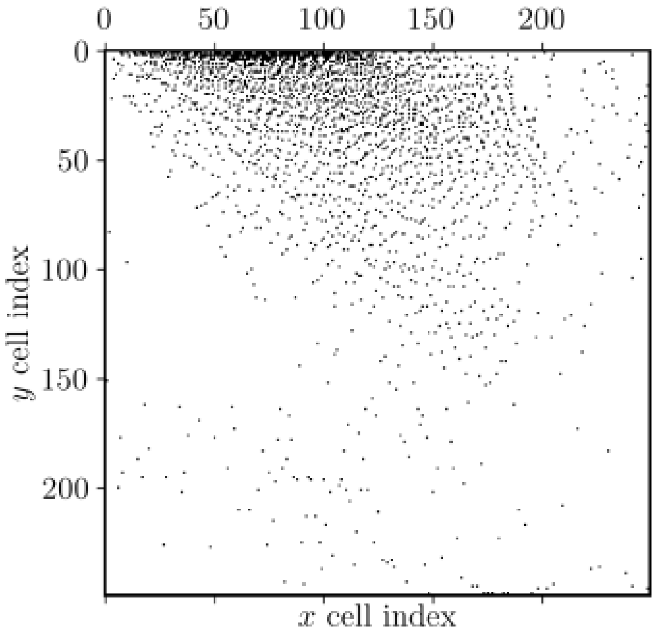


Figure above: Reduced mesh of single domain HROM

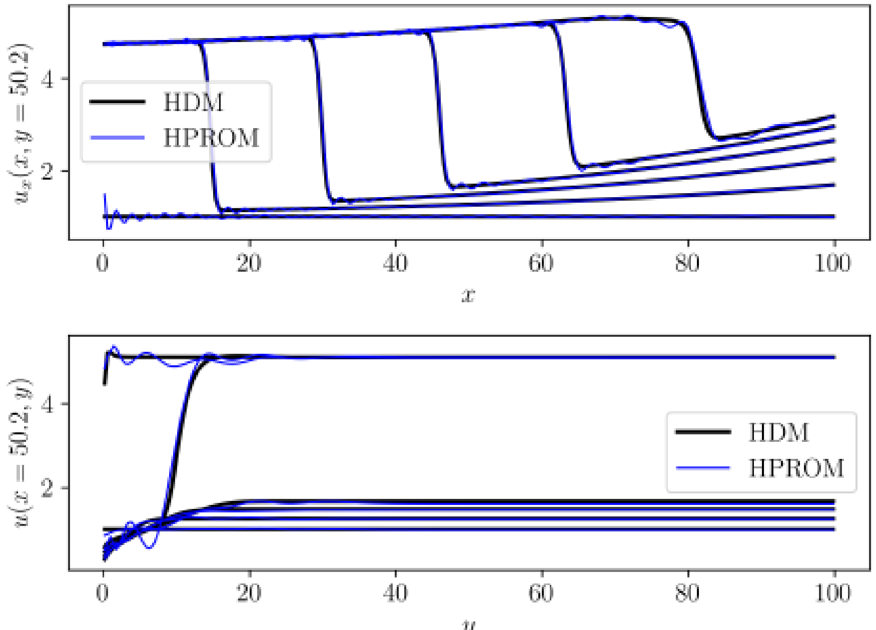
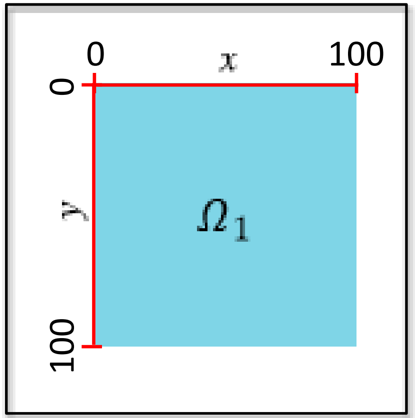


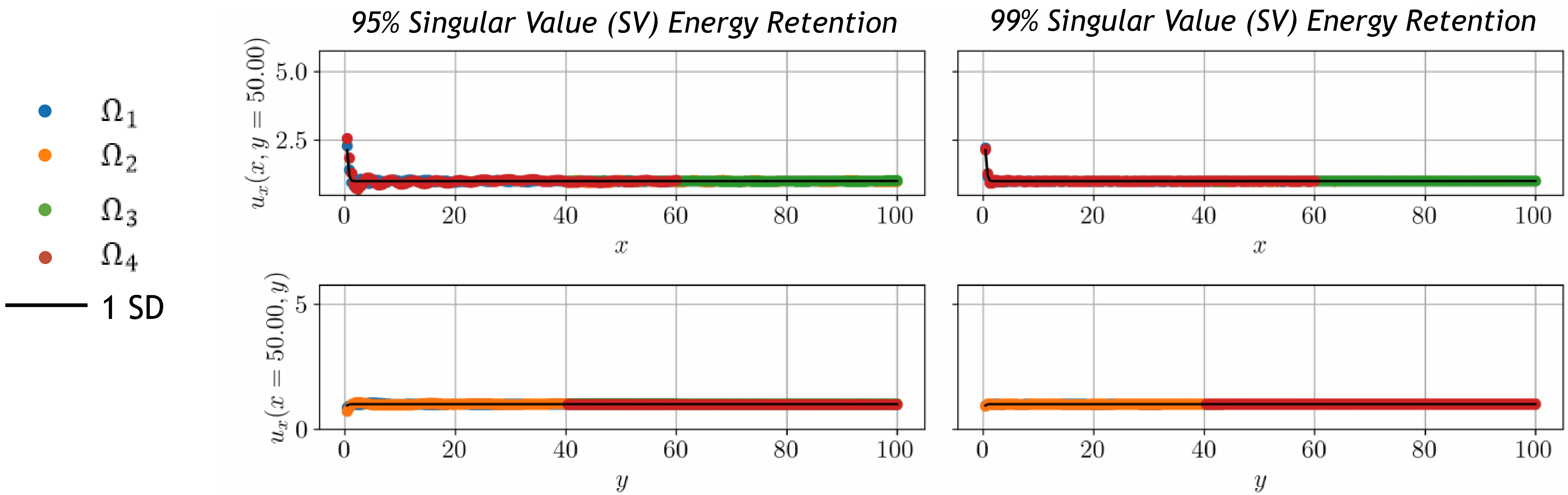
Figure above: HROM and FOM results at various time steps

% 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

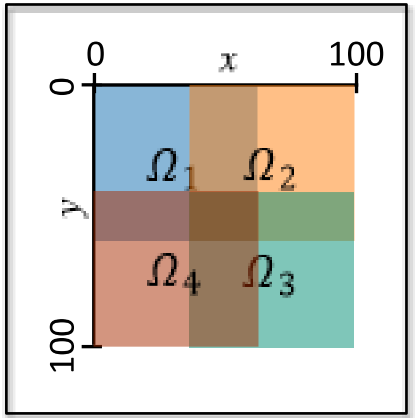


ROM-ROM-ROM-ROM Coupling

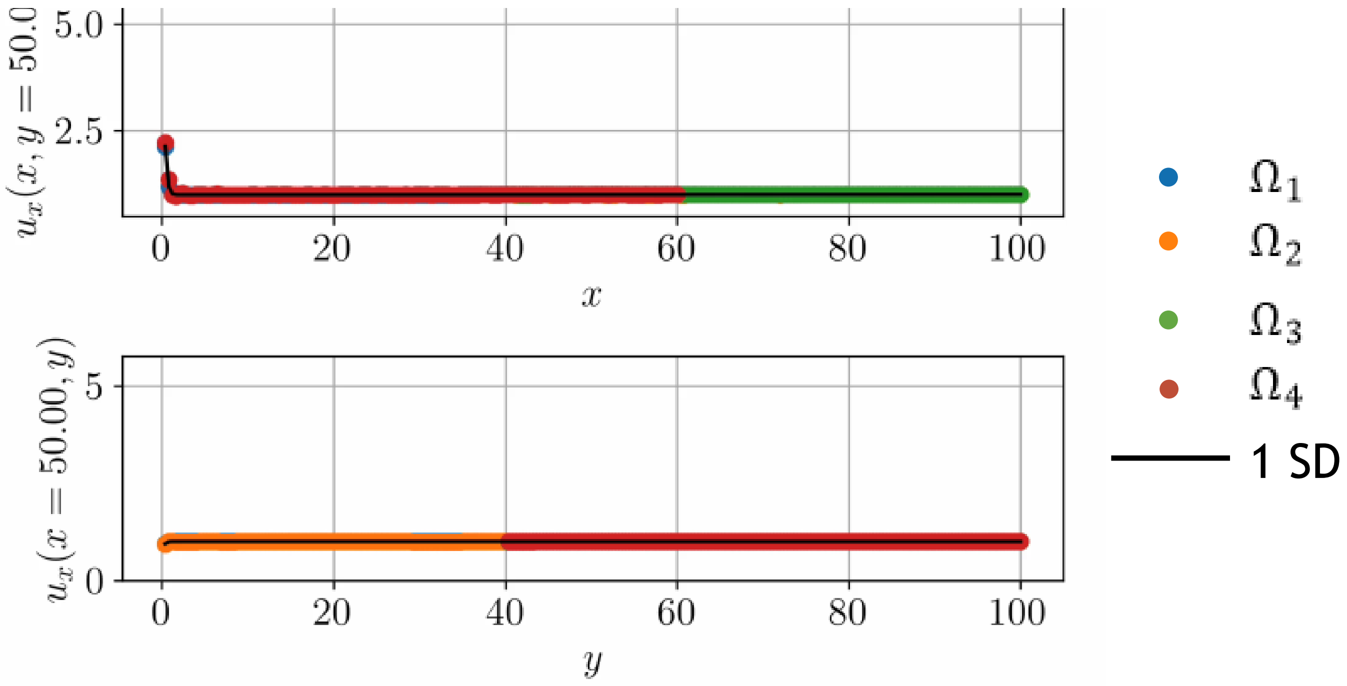


- Method converges in **only 3 Schwarz iterations** per controller time-step
- **Errors** $O(1\%)$ or less
- **1.47× speedup** over all-FOM coupling for 95% SV energy retention case

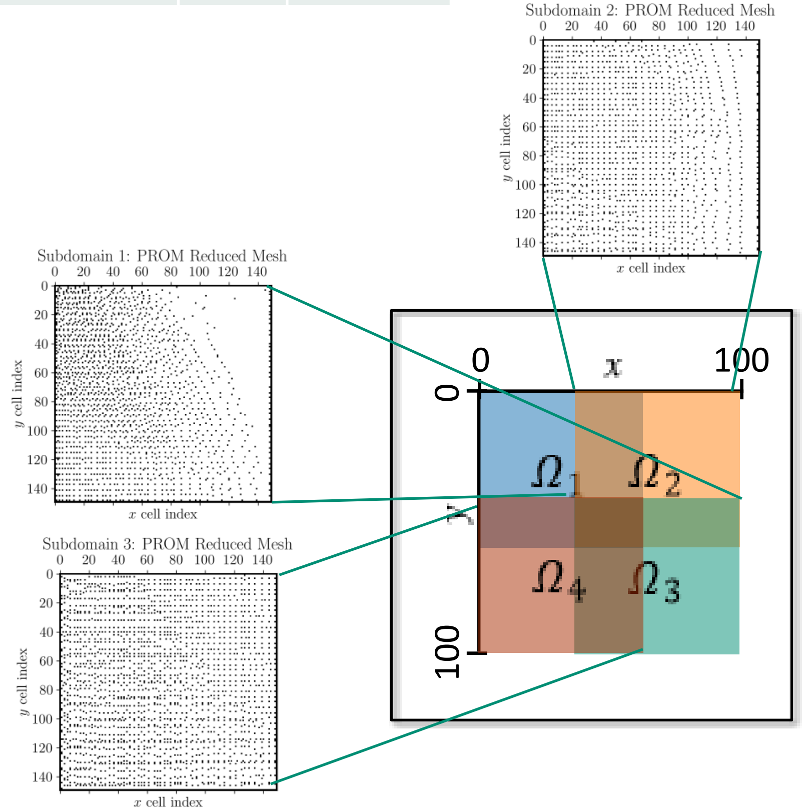
Subdomains	95% SV Energy			99% SV Energy		
	M	MSE (%)	CPU time (s)	M	MSE (%)	CPU time (s)
Ω_1	57	1.1	85	146	0.18	295
Ω_2	44	1.2	56	120	0.18	216
Ω_3	24	1.4	43	60	0.16	89
Ω_4	32	1.9	61	66	0.25	100
Total			**245**			**700**



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** and **additive Schwarz.**

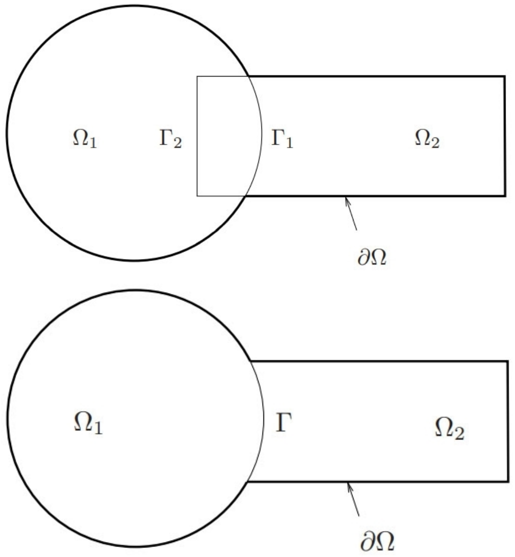
Outline

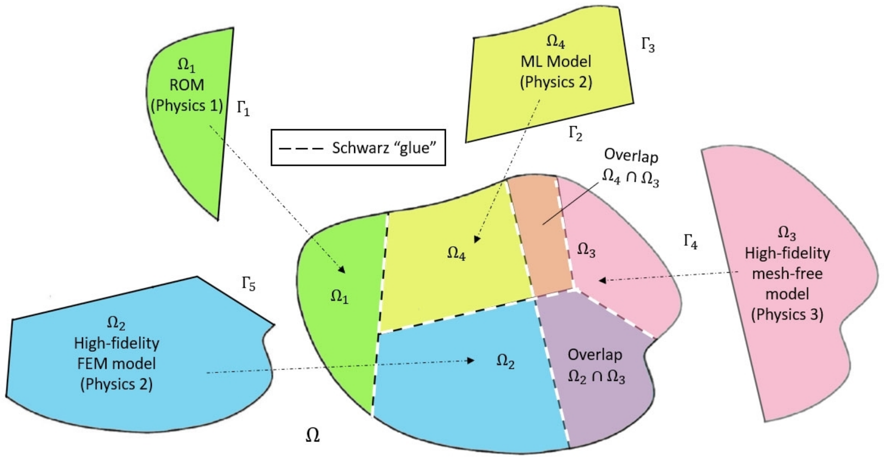
- The Schwarz Alternating Method for Domain Decomposition-Based Coupling

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

- Numerical Examples
  - ➢ 1D Dynamic Wave Propagation in Hyperelastic Bar
  - ➢ 2D Burgers Equation

- **Summary & Future Work**





*Full-Order Model. #Reduced Order Model.

Summary and Future Work

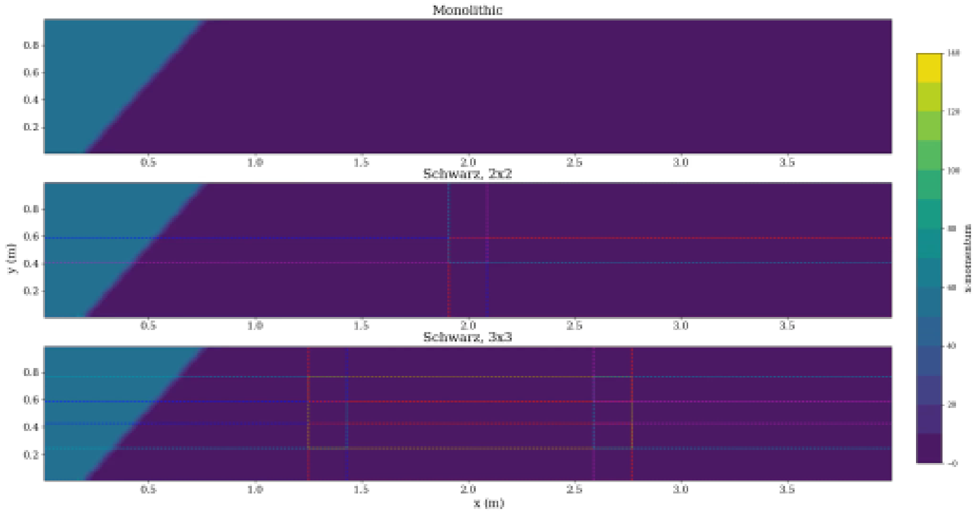
Summary:

- In a 1D solid mechanics and 2D hyperbolic PDE setting, Schwarz has been **demonstrated** for coupling of FOMs and (H)ROMs
- **Computational gains** can be achieved by coupling (H)ROMs

Ongoing & future work:

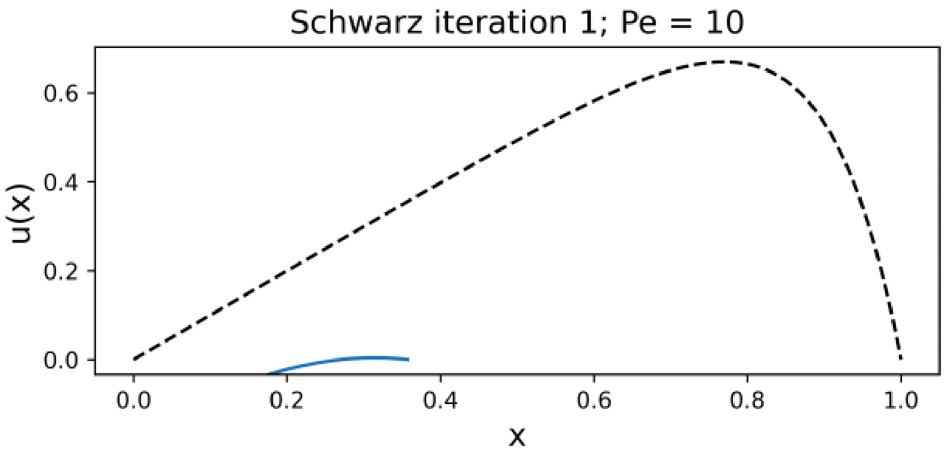
- Extension to **other applications** and **HPC codes** (e.g., compressible flow and Pressio demo-apps/Pressio)
- Improving method **efficiency** (e.g., **additive Schwarz**)
- Coupling **nonlinear approximation manifold methods**
- Dynamic **adaptation of domain** partitioning & "on-the-fly" **ROM-FOM switching** (reinforcement learning problem)
- **Learning** of **"optimal" transmission conditions** to ensure **structure preservation**
- Extension of Schwarz to coupling of **Physics Informed Neural Networks (PINNs)**

* https://https://pressio.github.io



Movie above: FOM-FOM coupling via Schwarz for 2D double Mach reflection Euler problem using pressio-demoapps*

Movie below: accelerating PINN training via PINN-PINN coupling using Schwarz



References

[1] A. Salinger, *et al*. "Albany: Using Agile Components to Develop a Flexible, Generic Multiphysics Analysis Code", *Int. J. Multiscale Comput. Engng*. 14(4) (2016) 415-438.

[2] H. Schwarz. “Über einen Grenzübergang durch alternierendes Verfahren”. In: Vierteljahrsschriftder Naturforschenden Gesellschaft in Zurich 15 (1870), pp. 272–286.

[3] S.L. Sobolev. “Schwarz’s Algorithm in Elasticity Theory”. In: Selected Works of S.L Sobolev. Volume I: equations of mathematical physics, computational mathematics and cubature formulats. Ed. By G.V. Demidenko and V.L. Vaskevich. New York: Springer, 2006.

[4] S. Mikhlin. “On the Schwarz algorithm”. In: Proceedings of the USSR Academy of Sciences 77 (1951), pp. 569–571.

[5] P.L. Lions. “On the Schwarz alternating method I.” In: 1988, First International Symposium on Domain Decomposition methods for Partial Differential Equations, SIAM, Philadelphia.

[6] SIERRA Solid Mechanics Team. Sierra/SM 4.48 User’s Guide. Tech. rep. SAND2018-2961. SNL Report, Oct. 2018.

[7] M. Gunzburger, J. Peterson, J. Shadid. “Reduced-order modeling of time-dependent PDEs with multiple parameters in the boundary data”. *CMAME* 196 (2007) 1030-1047.

[8] C. Hoang, Y. Choi, K. Carlberg. “Domain-decomposition least-squares Petrov–Galerkin (DD-LSPG) nonlinear model reduction”. *CMAME* 384 (2021) 113997.

[9] K. Smetana, T. Taddei. “Localized model reduction for nonlinear elliptic partial differential equations: localized training, partition of unity, and adaptive enrichment”, *ArXiV pre-print*, 2022.

[10] C. Farhat, T. Chapman, P. Avery. “Structure-preserving, stability & accuracy properties of the energy-conserving sampling and weighting method for the hyper reduction of nonlinear FE dynamic models”, *IJNME* 102 (2015) 1077-1110.

[11] M. Bergmann, A. Ferrero, A. Iollo, E. Lombardi, A. Scardigli, H. Telib. “A zonal Galerkin-free POD model for incompressible flows.” *JCP* 352 (2018) 301-325.

References (cont'd)

Green: GMM-based couplings
Blue: Schwarz-based couplings

[12] C. Sockwell, P. Bochev, K. Peterson, P. Kuberry. Interface Flux Recovery Framework for Constructing Partitioned Heterogeneous Time-Integration Methods. *Methods Numer. Meth. PDEs*, 2023 (in press).

[13] A. de Castro, P. Bochev, P. Kuberry, **I. Tezaur**. A synchronous partitioned scheme for coupled reduced order models based on separate reduced order bases for interior and interface nodes", *submitted to special issue of CMAME in honor of Tom Hughes' 80th birthday*.

[14] C. Sockwell, K. Peterson, P. Kuberry, P. Bochev, Interface Flux Recovery Framework for Constructing Partitioned Heterogeneous Time-Integration Methods, to appear.

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

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

[17] 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. *This talk*

Journal article on ROM-FOM/ROM-ROM coupling using Schwarz is in preparation.

Email: ikalash@sandia.gov
URL: www.sandia.gov/~ikalash

Team & Acknowledgments

Irina Tezaur

Joshua Barnett
Year-Round Intern

Alejandro Mota

Chris Wentland
Postdoc

Sandia National Laboratories

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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

Will Snyder
Summer Intern

Thank you! Questions?

Outline

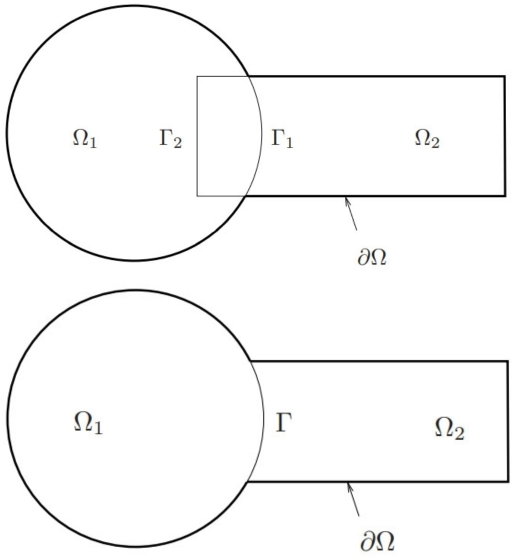
- The Schwarz Alternating Method for Domain Decomposition-Based Coupling

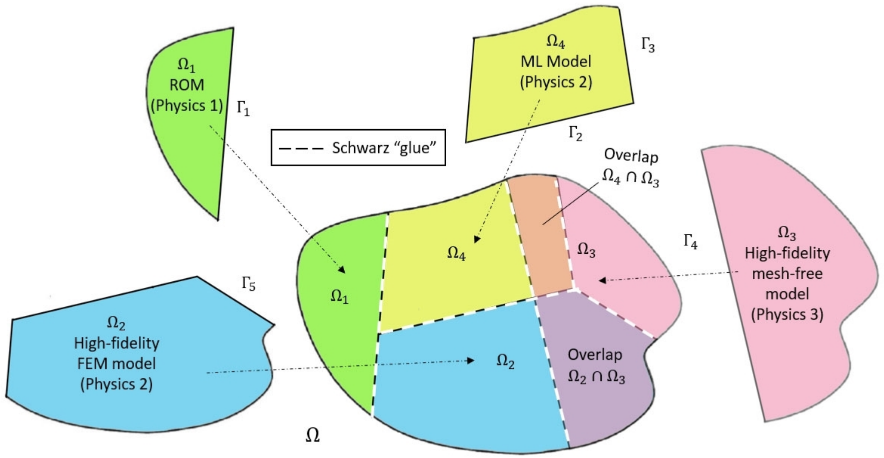
- Extension to FOM*-ROM# and ROM-ROM Coupling

- Numerical Examples
  - ➢ 1D Dynamic Wave Propagation in Hyperelastic Bar
  - ➢ 2D Burgers Equation

- Summary & Future Work

- **Bonus: PINN-PINN and PINN-FOM Coupling**

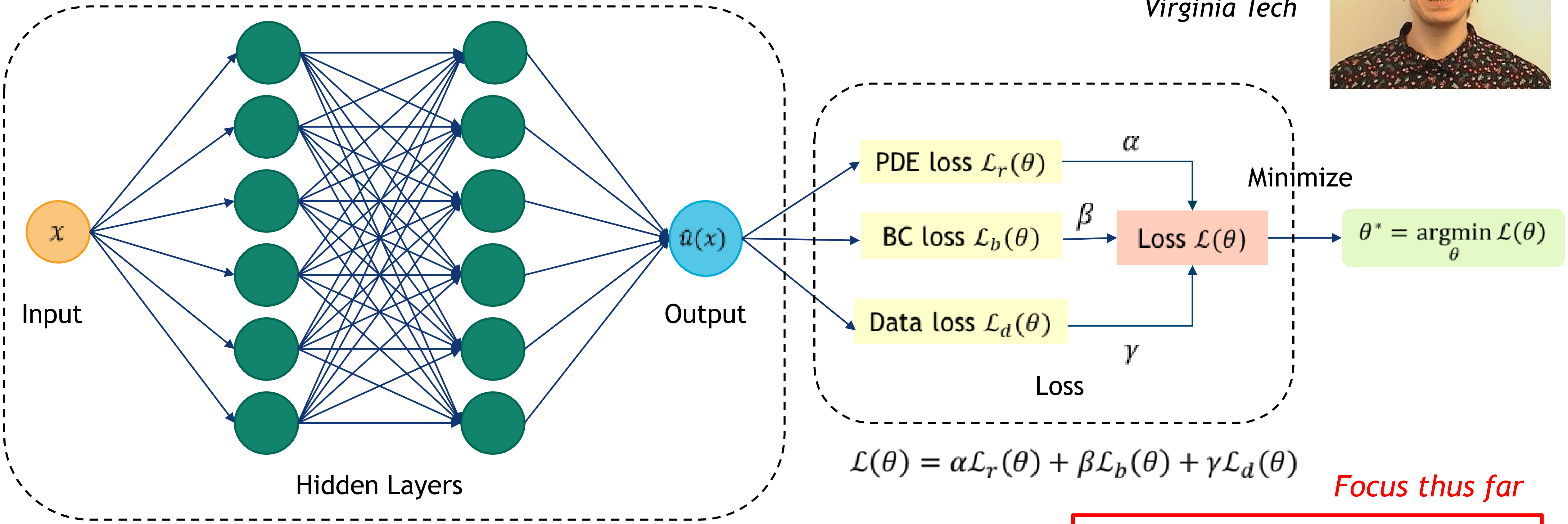




*Full-Order Model. #Reduced Order Model.

Bonus: PINN-PINN and PINN-FOM coupling

Will Snyder
Summer Intern
Virginia Tech



$$\mathcal{L}(\theta) = \alpha\mathcal{L}_r(\theta) + \beta\mathcal{L}_b(\theta) + \gamma\mathcal{L}_d(\theta)$$

Focus thus far

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

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

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

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

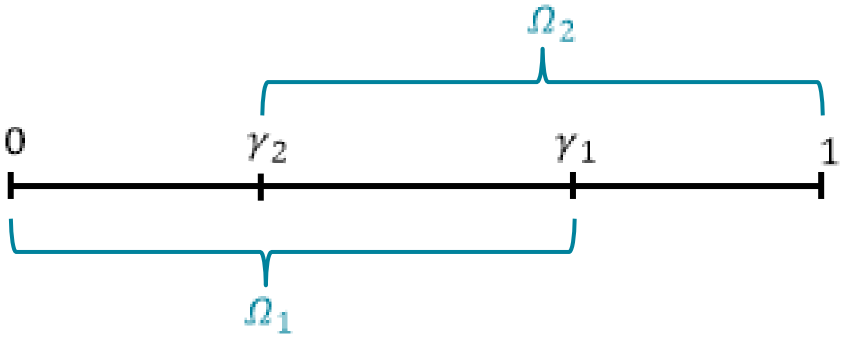
Bonus: PINN-PINN coupling

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

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

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

Can Schwarz help?



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

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

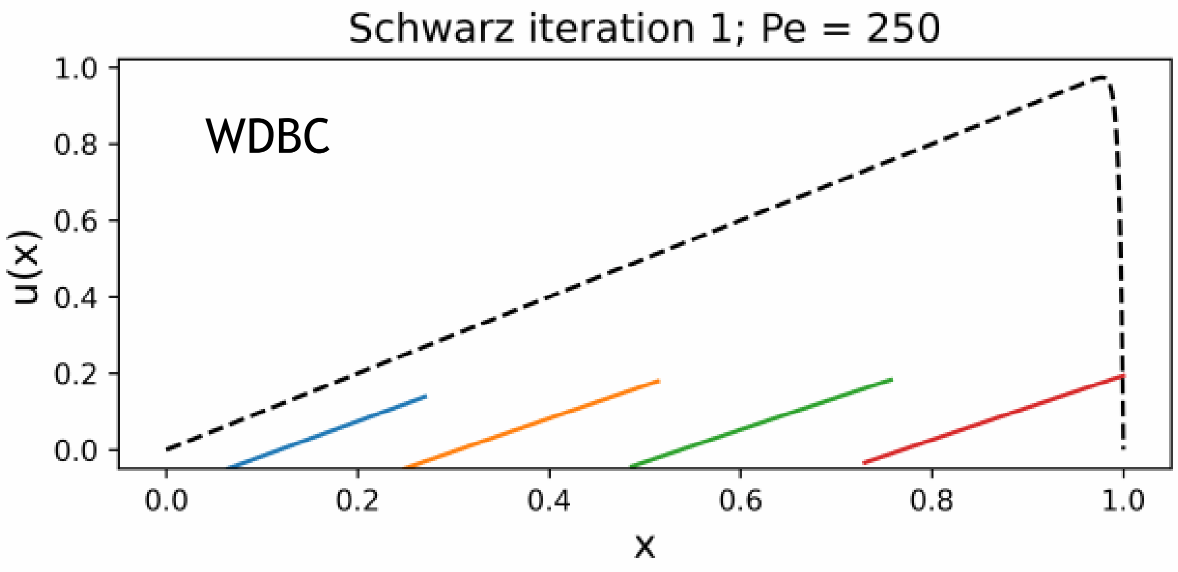
$$\mathcal{L}_{b,i}(\theta) = MSE\left(NN_{\Omega_i}(\partial\Omega,\theta)\right) + MSE\left(NN_{\Omega_i}(\gamma_i,\theta) - NN_{\Omega_j}(\gamma_i,\theta)\right)$$

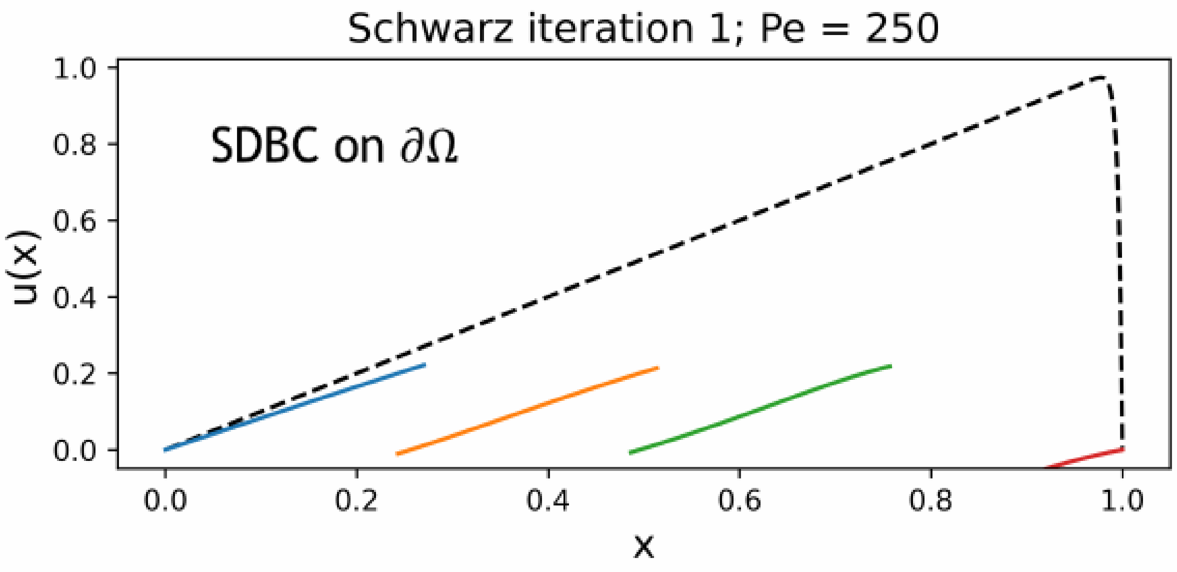
Schwarz PINN training algorithm:

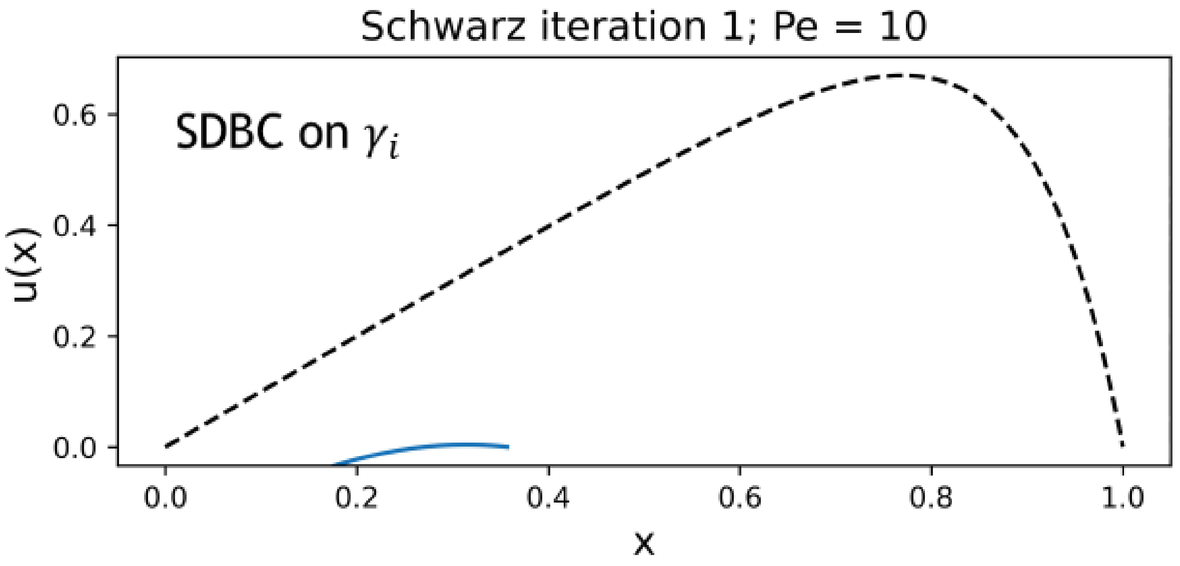
Loop over subdomains Ω_i until convergence of Schwarz method

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

Bonus: PINN-PINN coupling

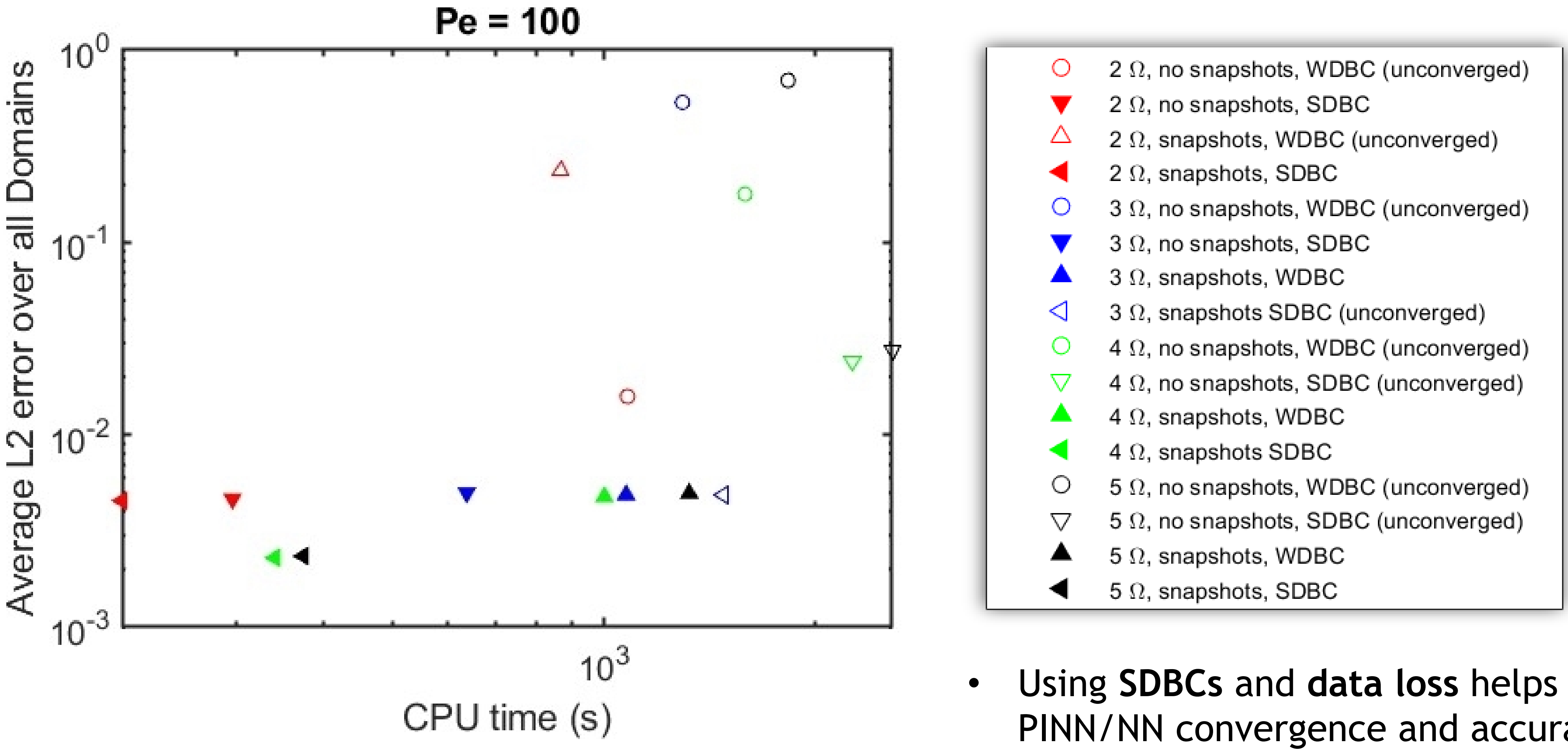






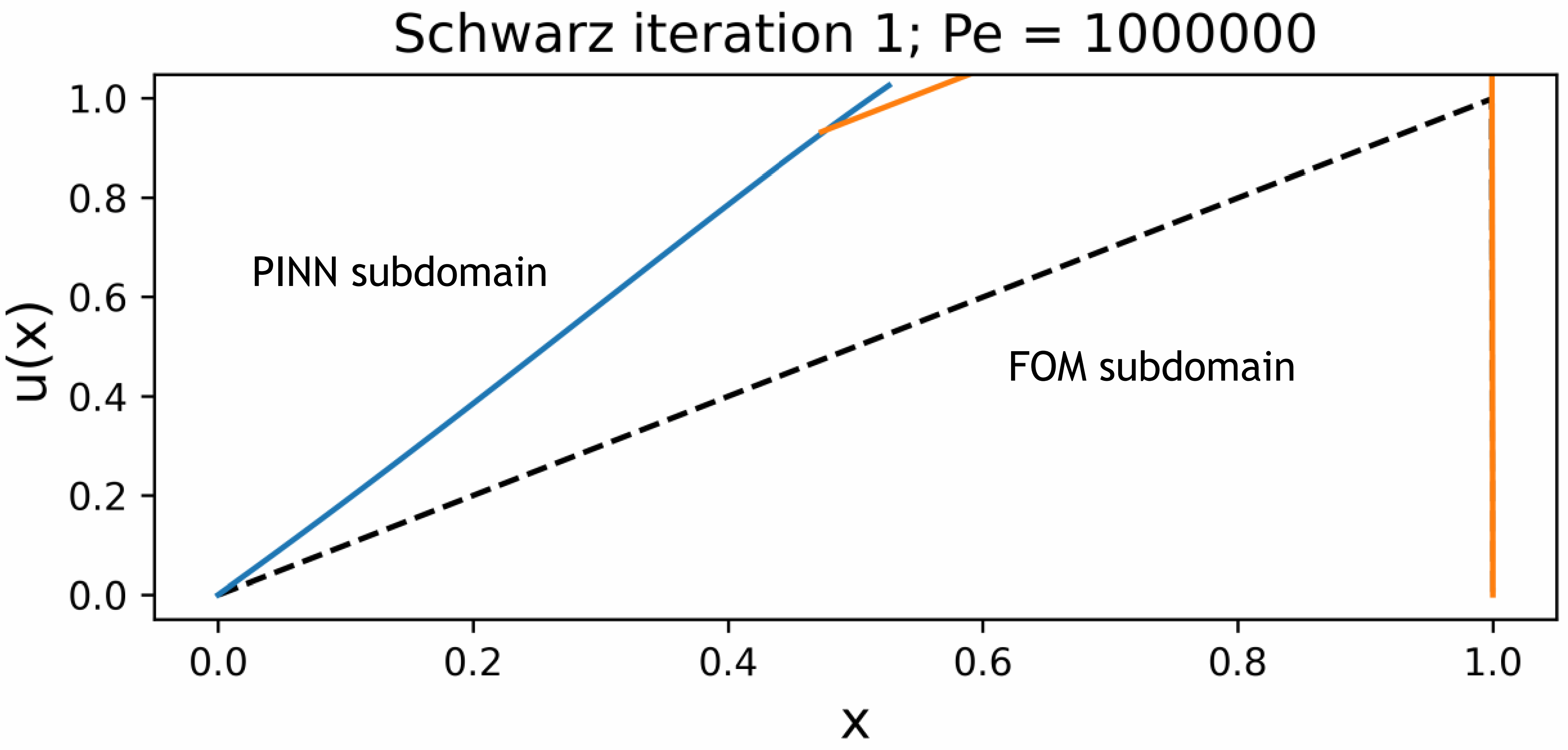
- How **Dirichlet boundary conditions** are handled has a large impact on PINN convergence
- Convergence not improved in general with **increasing overlap**
- Increasing **# subdomains** in general will increase CPU time

Bonus: PINN-PINN coupling



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

Bonus: PINN-FOM coupling



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

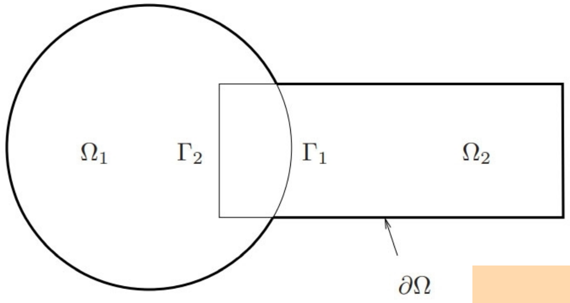
Start of Backup Slides

Spatial Coupling via 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]

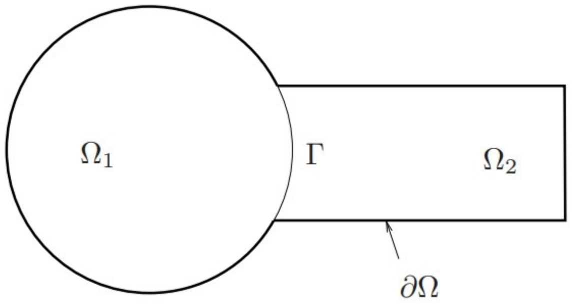
<u>This talk</u>: sequential subdomain solves (***multiplicative Schwarz***). Parallel subdomain solves (***additive Schwarz***) also possible.

Non-overlapping Domain Decomposition

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

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

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



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

Numerical Example: 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

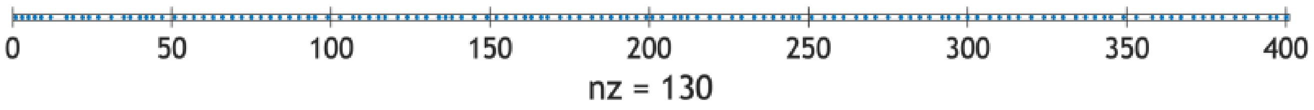


Figure left: sample sample mesh for 1D wave propagation problem

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)

Numerical Example: Reproductive Problem Results

Model	M_1/M_2	$N_{e,1}/N_{e,2}$	CPU time (s)	$\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{u}}_1)/\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{u}}_2)$	$\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{v}}_1)/\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{v}}_2)$	$\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{a}}_1)/\mathcal{E}_{\text{MSE}}(\tilde{\boldsymbol{a}}_2)$	N_S
FOM	$-/-$	$-/-$	1.871×10^3	$-/-$	$-/-$	$-/-$	$-$
ROM	$60/-$	$-/-$	1.398×10^3	$1.659 \times 10^{-2}/-$	1.037×10^{-1}	$4.681 \times 10^{-1}/-$	$-$
HROM	$60/-$	$155/-$	5.878×10^2	$1.730 \times 10^{-2}/-$	$1.063 \times 10^{-1}/-$	$4.741 \times 10^{-1}/-$	$-$
ROM	$200/-$	$-/-$	1.448×10^3	$2.287 \times 10^{-4}/-$	$4.038 \times 10^{-3}/-$	$4.542 \times 10^{-2}/-$	$-$
HROM	$200/-$	$428/-$	9.229×10^2	$8.396 \times 10^{-4}/-$	$8.947 \times 10^{-3}/-$	$7.462 \times 10^{-2}/-$	$-$
FOM-FOM	$-/-$	$-/-$	2.345×10^3	$-$	$-$	$-$	24,630
FOM-ROM	$-/80$	$-/-$	2.341×10^3	$2.171 \times 10^{-6}/1.253 \times 10^{-5}$	$3.884 \times 10^{-5}/2.401 \times 10^{-4}$	$2.982 \times 10^{-4}/2.805 \times 10^{-3}$	25,227
FOM-HROM	$-/80$	$-/130$	2.085×10^3	$2.022 \times 10^{-4}/5.734 \times 10^{-4}$	$1.723e \times 10^{-3}/5.776 \times 10^{-3}$	$7.421 \times 10^{-3}/3.791 \times 10^{-2}$	29,678
FOM-ROM	$-/200$	$-/-$	2.449×10^3	$4.754 \times 10^{-12}/7.357 \times 10^{-11}$	$1.835 \times 10^{-10}/4.027 \times 10^{-9}$	$5.550 \times 10^{-9}/1.401 \times 10^{-7}$	24,630
FOM-HROM	$-/200$	$-/252$	2.352×10^3	$1.421 \times 10^{-5}/4.563 \times 10^{-4}$	$1.724 \times 10^{-4}/2.243 \times 10^{-3}$	$9.567 \times 10^{-4}/1.364 \times 10^{-2}$	27,156
ROM-ROM	$200/80$	$-/-$	2.778×10^3	$4.861 \times 10^{-5}/3.093 \times 10^{-5}$	$1.219 \times 10^{-3}/4.177 \times 10^{-4}$	$1.586 \times 10^{-2}/3.936 \times 10^{-3}$	27,810
HROM-HROM	$200/80$	$315/130$	1.769×10^3	$3.410 \times 10^{-3}/6.662 \times 10^{-4}$	$4.110 \times 10^{-2}/6.432 \times 10^{-3}$	$2.485 \times 10^{-1}/4.307 \times 10^{-2}$	29,860
ROM-ROM	$300/80$	$-/-$	2.646×10^3	$2.580 \times 10^{-6}/1.292 \times 10^{-5}$	$6.226 \times 10^{-5}/2.483 \times 10^{-4}$	9.470×10^{-4} 2.906×10^{-3}	25,059
HROM-HROM	$300/80$	$405/130$	1.938×10^3	6.960×10^{-3} 7.230×10^{-4}	6.328×10^{-2} 7.403×10^{-3}	3.137×10^{-1} 4.960×10^{-2}	29,896

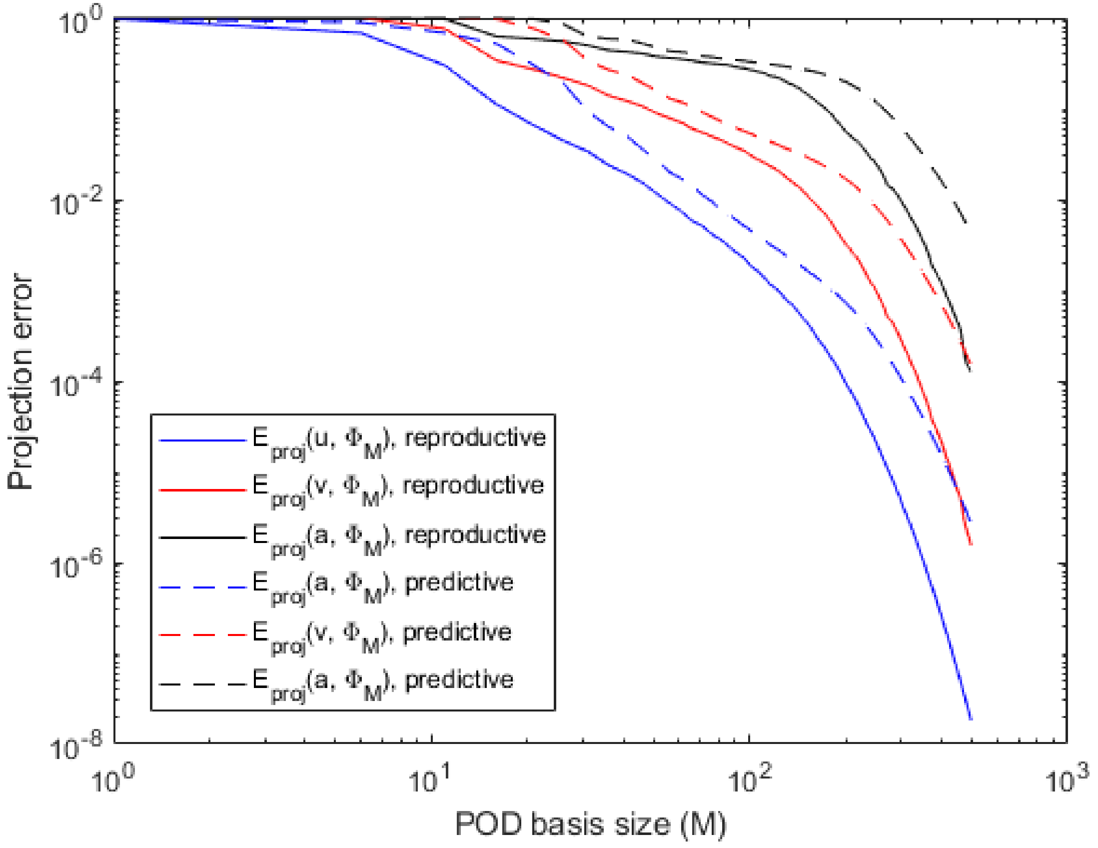
Green shading highlights most competitive coupled models

- All coupled models evaluated converged on average in <3 **Schwarz iterations** per time-step
- Larger FOM-ROM coupling has **same total # Schwarz iters** (N_S) as FOM-FOM coupling
- Other couplings require more Schwarz iters than FOM-FOM coupling to converge
  - ➢ **More Schwarz iters** required when coupling **less accurate models**
  - ➢ Larger 300/80 mode ROM-ROM takes less wall-clock time than smaller 200/80 mode ROM-ROM
- **FOM-HROM** and **HROM-HROM** couplings **outperform** the **FOM-FOM** coupling in terms of CPU time by 12.5-32.6%
- All couplings involving ROMs/HROMs are **at least as accurate** as single-domain ROMs/HROMs

Numerical Example: Predictive Problem Results

- Start by calculating **projection error** for reproductive and predictive version of the Rounded Square IC problem:

$$\mathcal{E}_{\text{proj}}(\boldsymbol{u}, \boldsymbol{\Phi}_M) := \frac{||\boldsymbol{u} - \boldsymbol{\Phi}_M(\boldsymbol{\Phi}_M^T\boldsymbol{\Phi}_M)^{-1}\boldsymbol{\Phi}_M^T\boldsymbol{u}||_2}{||\boldsymbol{u}||_2}$$



- Projection error suggests **predictive ROM** can achieve **accuracy** and **convergence** with **basis refinement**

- **O(100) modes** are needed to achieve sufficiently accurate ROM
  - ➢ Larger ROMs containing O(100) modes considered in our coupling experiments: M_1= 300, M_2= 200

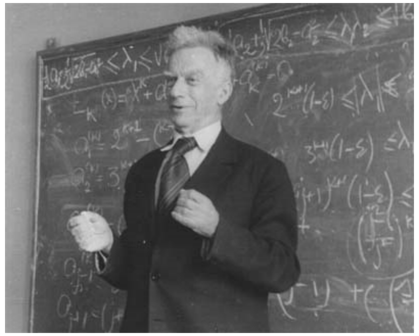
Theoretical Foundation

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

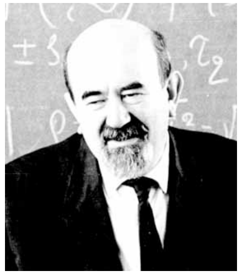
- S.L. Sobolev (1936): posed Schwarz method for ***linear elasticity*** in variational form and ***proved method's convergence*** by proposing a convergent sequence of energy functionals.
- S.G. Mikhlin (1951): ***proved convergence*** of Schwarz method for general linear elliptic PDEs.
- P.-L. Lions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

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

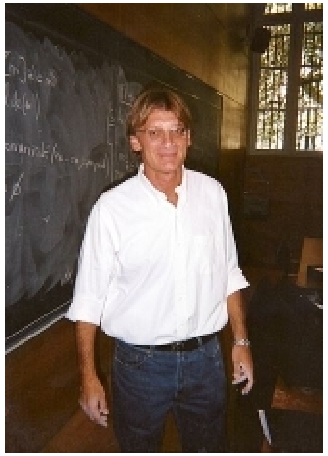
$$\nabla\cdot\boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



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.

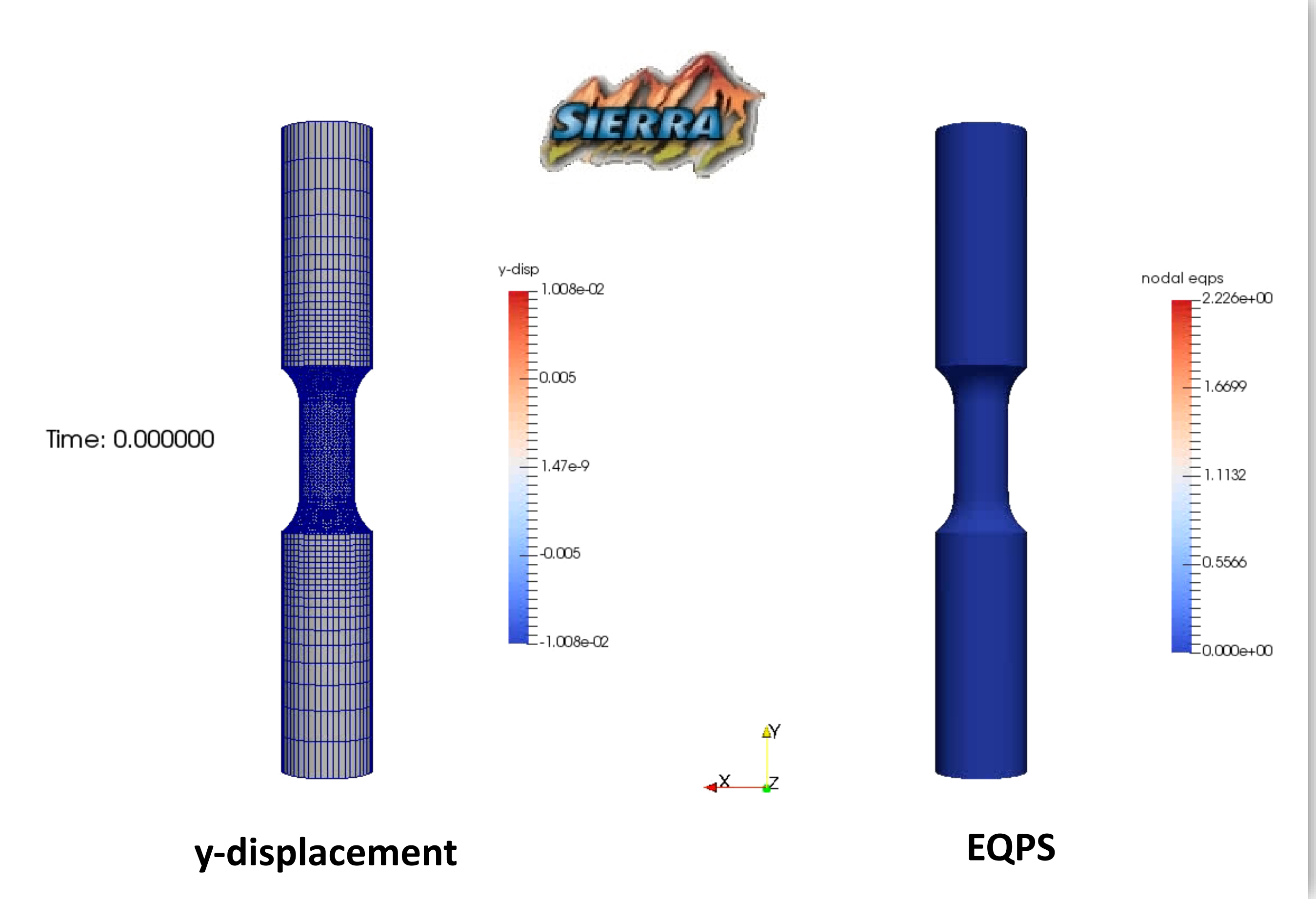
Schwarz Alternating Method for Dynamic Multiscale Coupling: Theory

- 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.

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



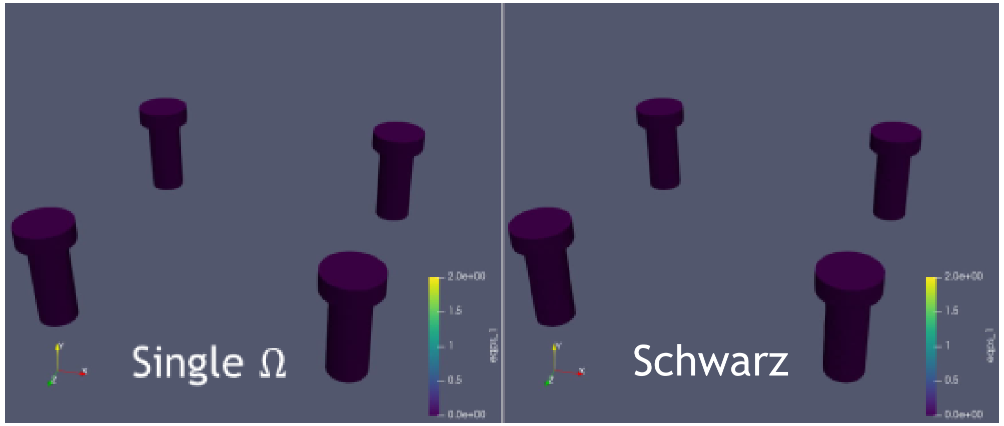


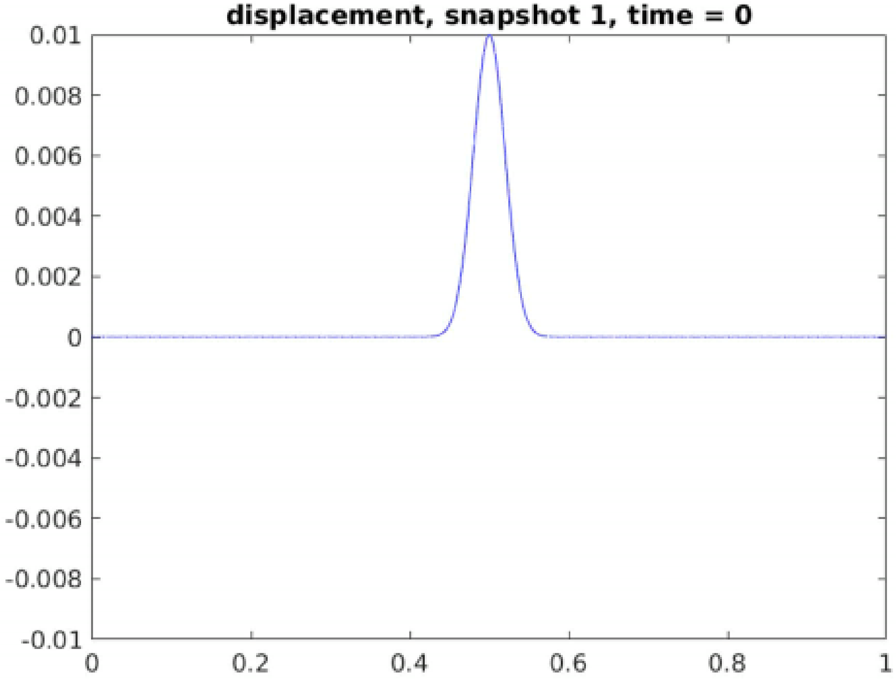
Figure above: tension specimen simulation coupling composite TET10 elements with HEX elements in Sierra/SM.

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

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

Numerical Example: Linear Elastic Wave Propagation Problem

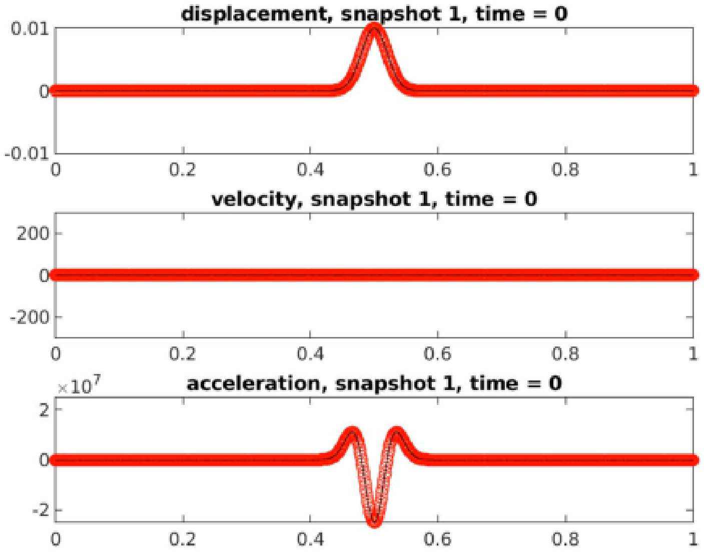
- Linear elastic ***clamped beam*** with Gaussian initial condition.
- Simple problem with analytical exact solution but very ***stringent test*** for discretization/coupling methods.
- ***Couplings tested:*** FOM-FOM, FOM-ROM, ROM-ROM, implicit-explicit, implicit-implicit, explicit-explicit.
- ROMs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

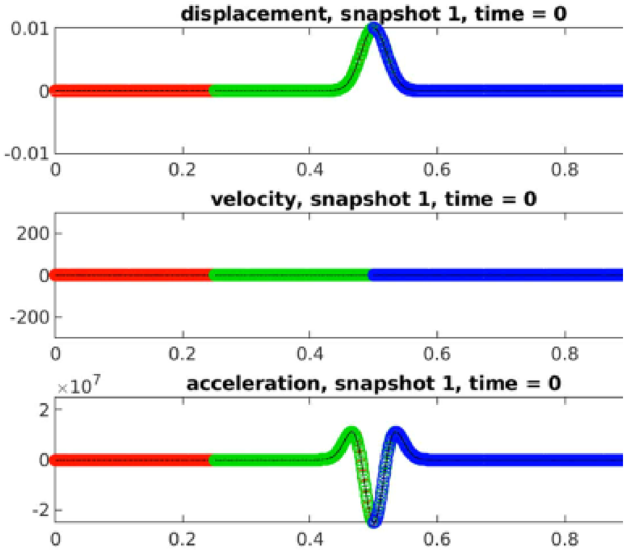


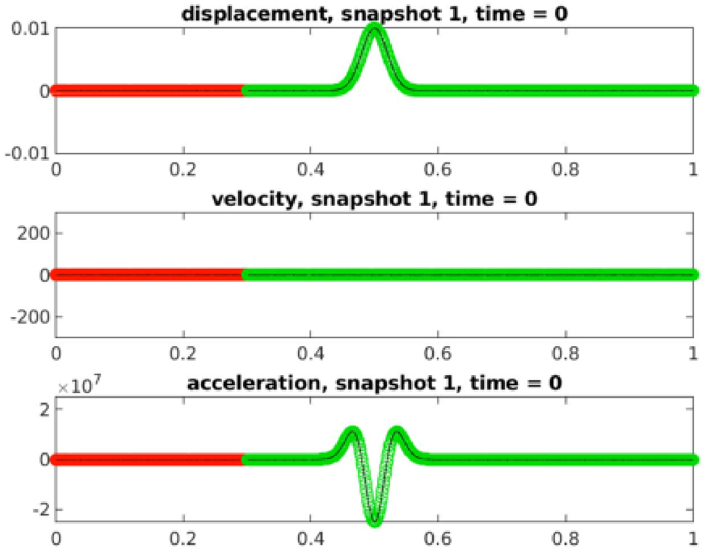
Above: 3D rendering of clamped beam with Gaussian initial condition. *Right:* Initial condition (blue) and final solution (red). Wave profile is negative of initial profile at time T = 1.0e-3.

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

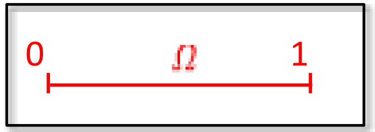
Coupling delivers accurate solution if each subdomain model is reasonably accurate, can couple different discretizations with different Δx, Δt and basis sizes.



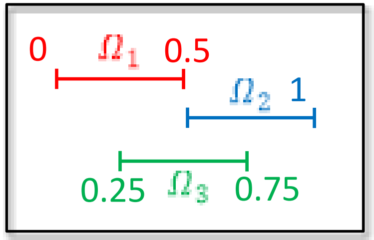




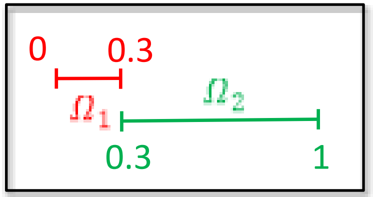
Single Domain FOM



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

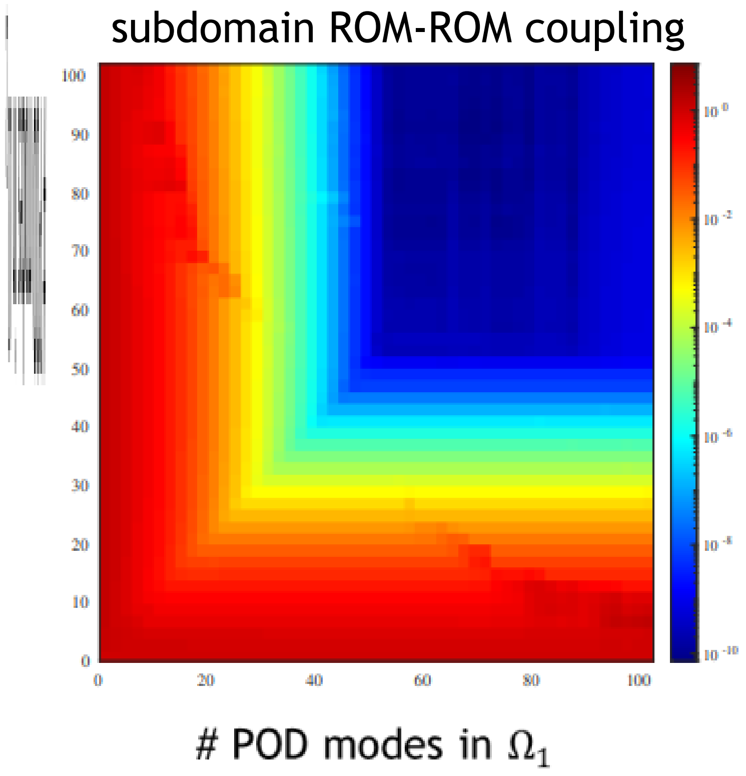
[1]Implicit 40 mode POD ROM, Δt =1e-6, Δx =1.25e-3
[2]Implicit FOM, Δt =1e-6, Δx =8.33e-4
[3]Explicit 50 mode POD ROM, Δt =1e-7, Δx =1e-3
[4]Implicit FOM, Δt =2.25e-7, Δx =1e-6
[5]Explicit 50 mode POD ROM, Δt =2.25e-7, Δx =1e-6

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

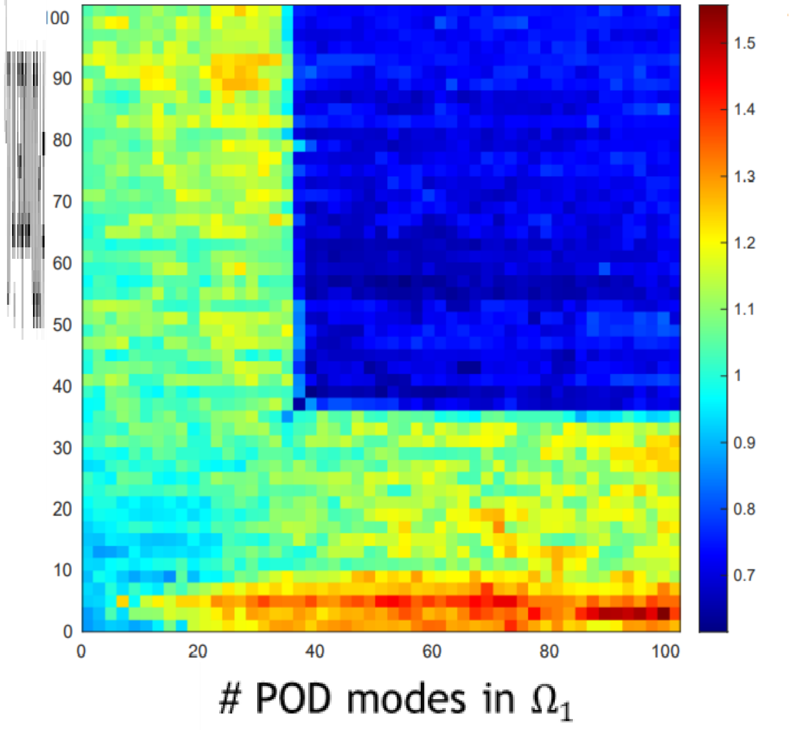
Linear Elastic Wave Propagation Problem: ROM-ROM Couplings

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

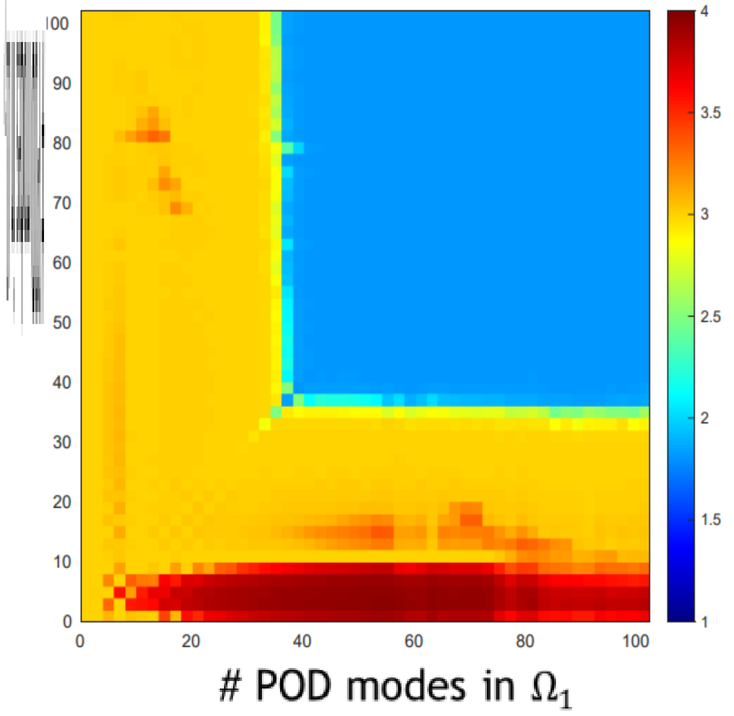
MSE in displacement for 2 subdomain ROM-ROM coupling



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



Average # Schwarz iterations for 2 subdomain ROM-ROM coupling



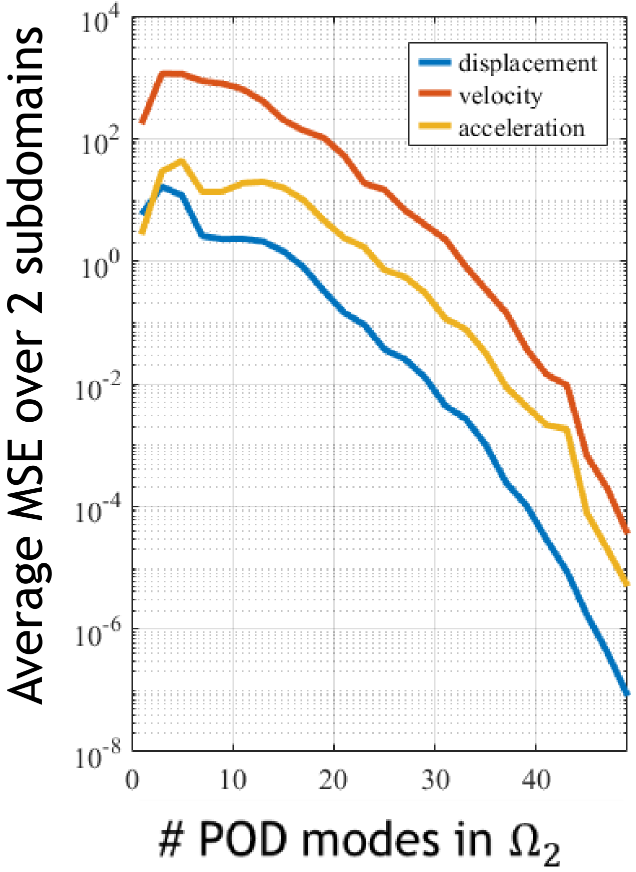
- **Smaller ROMs** are **not** the **fastest**: less accurate & require more Schwarz iterations to converge.
- All couplings converge in $\leq$ **4 Schwarz iterations** on average (FOM-FOM coupling requires average of 2.4 Schwarz iterations).

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

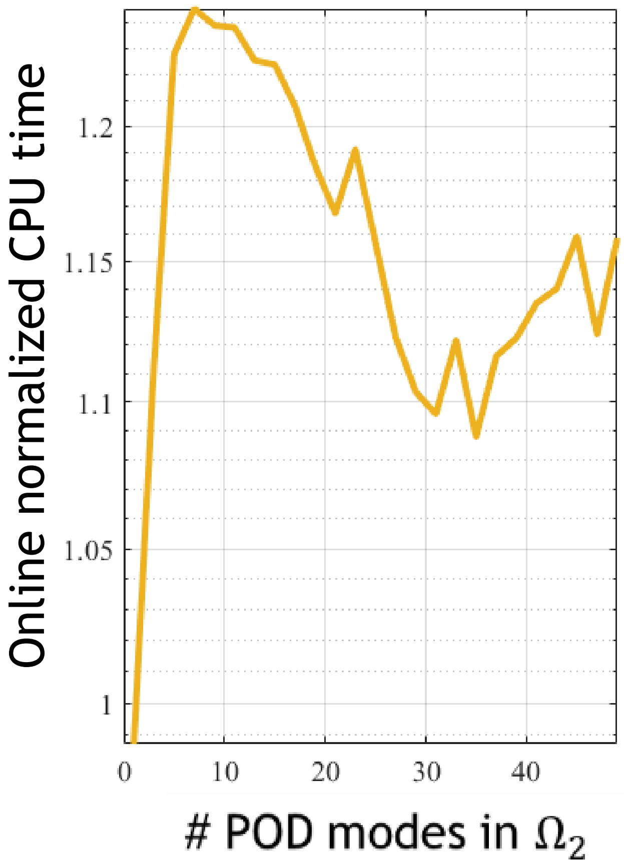
Linear Elastic Wave Propagation Problem: FOM-ROM Couplings

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.

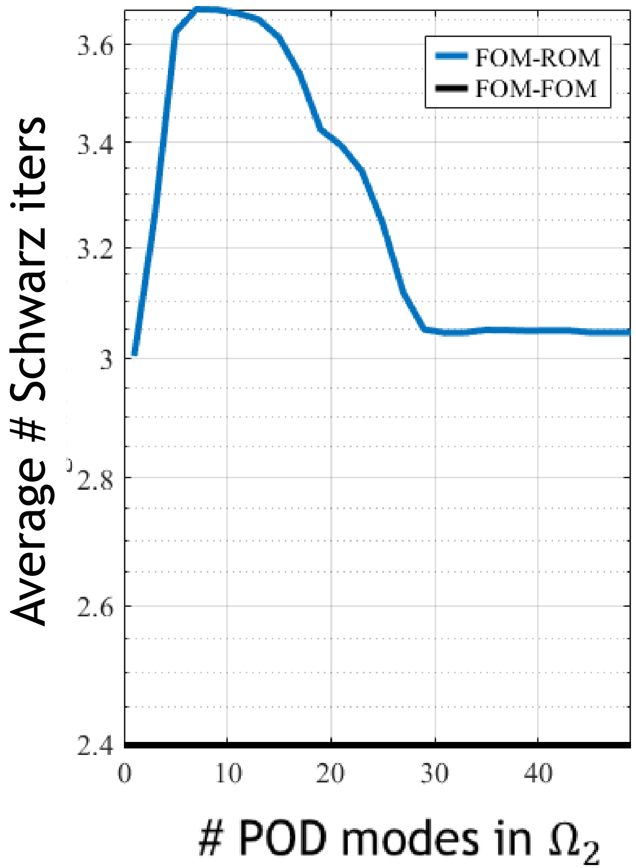
MSE for 2 subdomain FOM-ROM coupling



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



Average # Schwarz iterations for 2 subdomain couplings

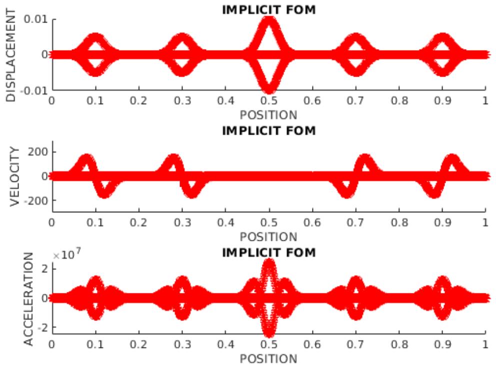


***WIP:* understanding & improving FOM-ROM coupling performance.**

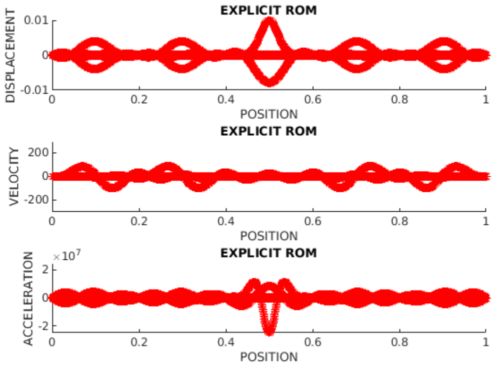
Overlapping implicit-implicit coupling with $\Omega_1 = [0, 0.75]$, $\Omega_2 = [0.25, 1]$

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

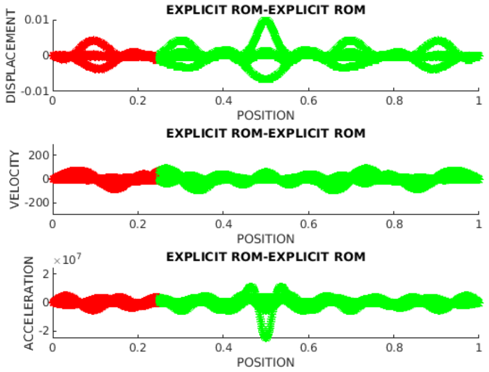
Inaccurate model + accurate model ≠ accurate model.



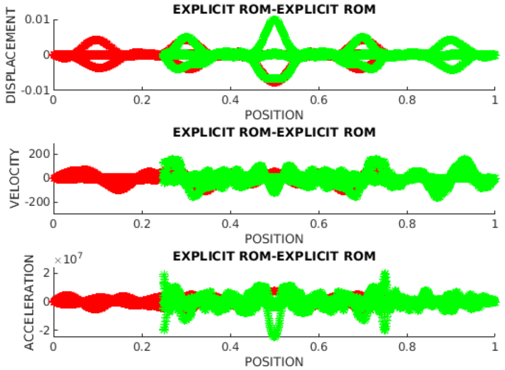
Single Domain, FOM (truth)



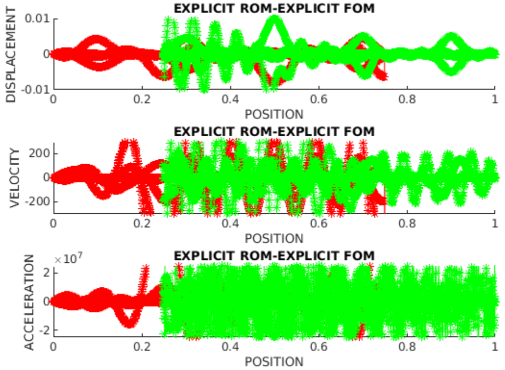
Single Domain, 10 mode POD



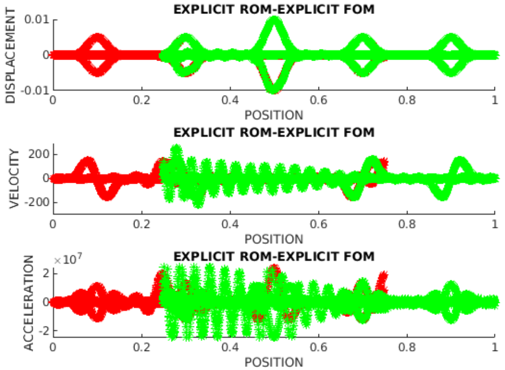
10 mode POD – 10 mode POD



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

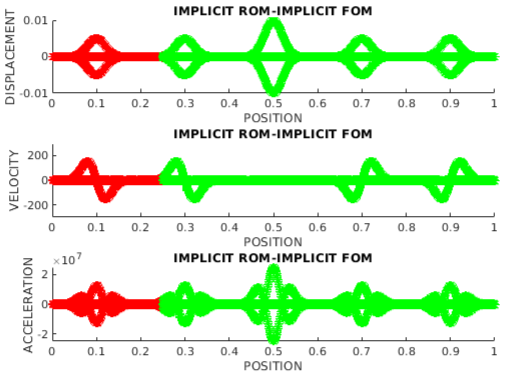
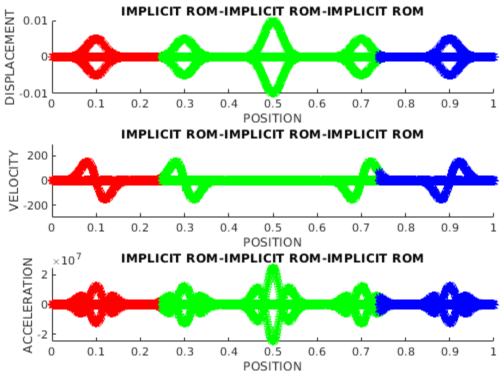


Figure above: $\Omega_1 = [0, 0.3]$, $\Omega_2 = [0.25, 1]$, 20 mode POD - FOM

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

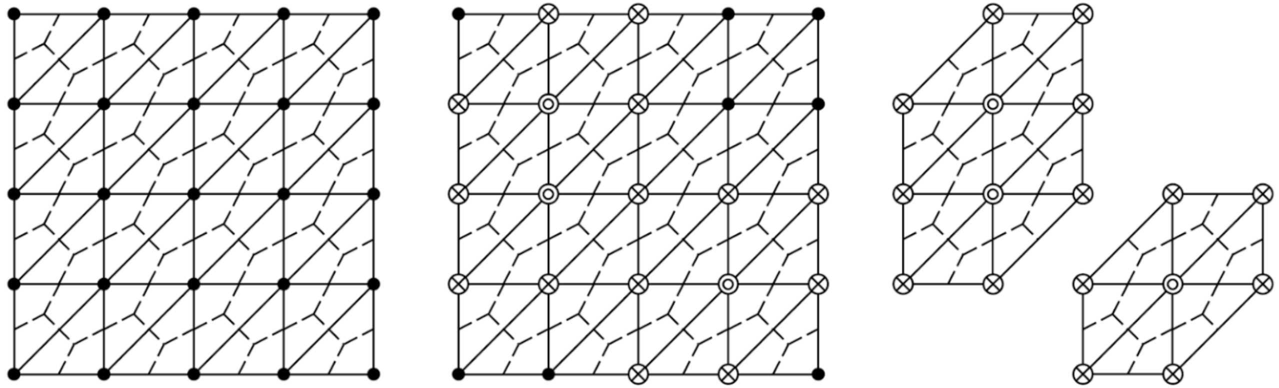


Energy-Conserving Sampling and Weighting (ECSW)

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

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

- $L_e \in \{0,1\}^{d_e\times N}$ 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:**

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

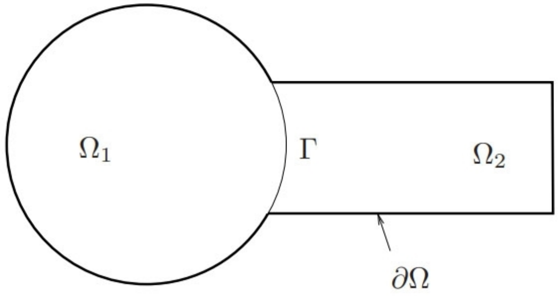
- Solve the above optimization problem using a **non-negative least squares solver** with an **early termination condition** to **promote sparsity** of the vector ξ

Numerical Example: 1D Dynamic Wave Propagation Problem

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

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

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



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

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

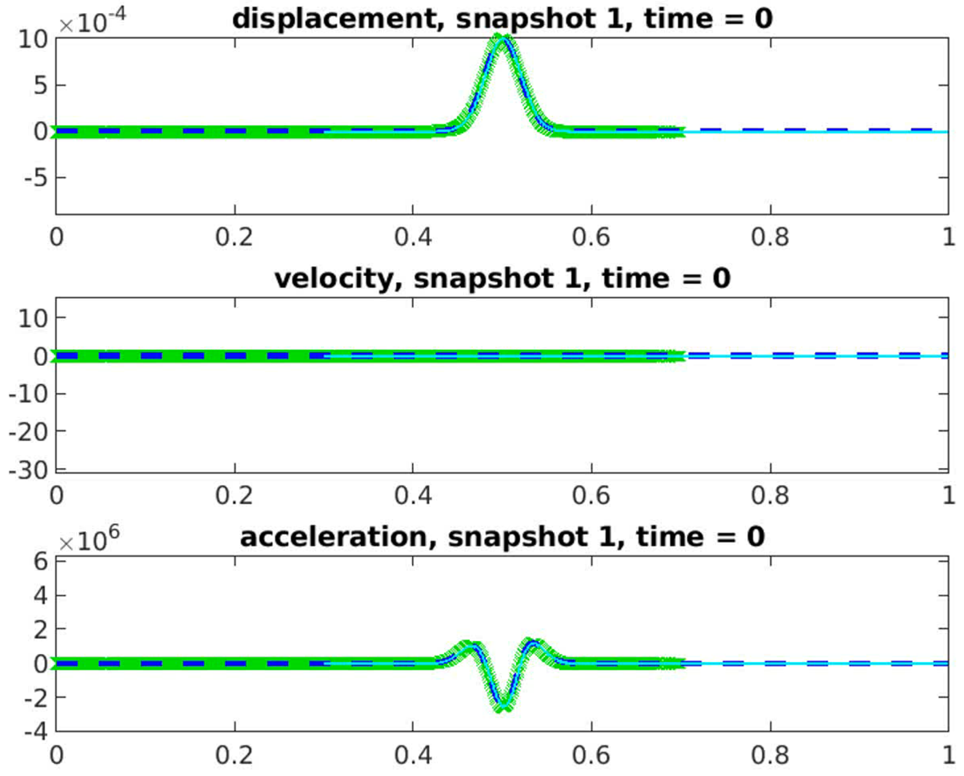
- All reproductive cases run on the **same RHEL8 machine** and all predictive cases run on the **same RHEL7 machine**, in MATLAB

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

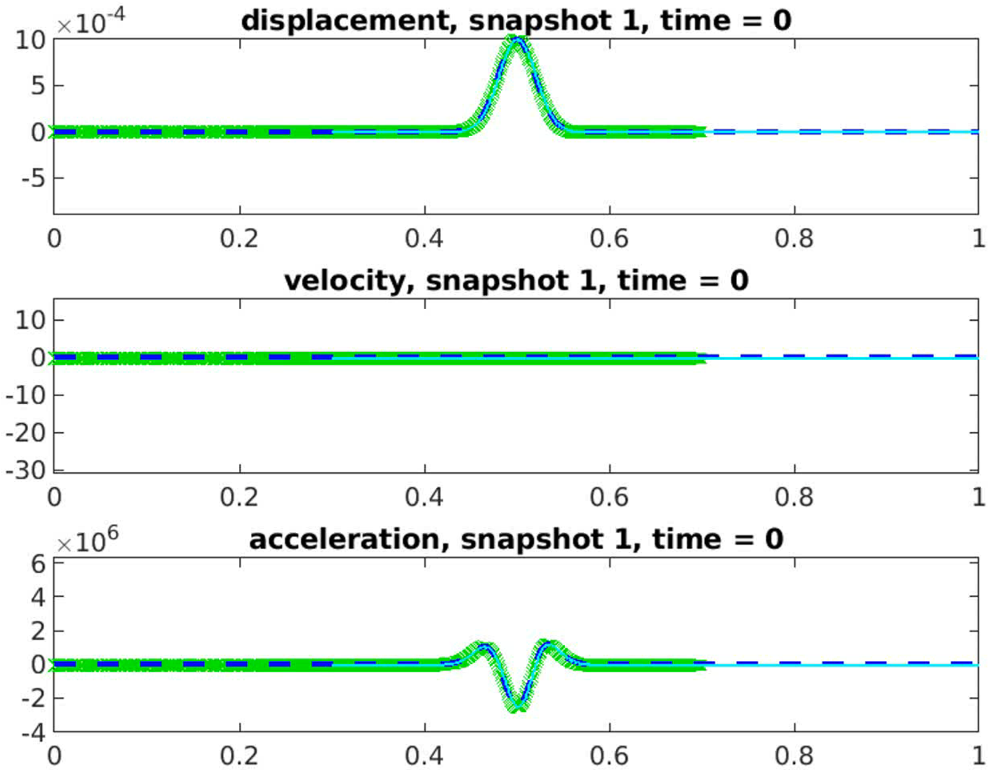
$$\varepsilon_{MSE}(\tilde{\boldsymbol{u}}_i) := \frac{\sqrt{\sum_{n=1}^{S} ||\tilde{\boldsymbol{u}}_i^n - \boldsymbol{u}_i^n||_2^2}}{\sqrt{\sum_{n=1}^{S} ||\boldsymbol{u}_i^n||_2^2}}$$

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.

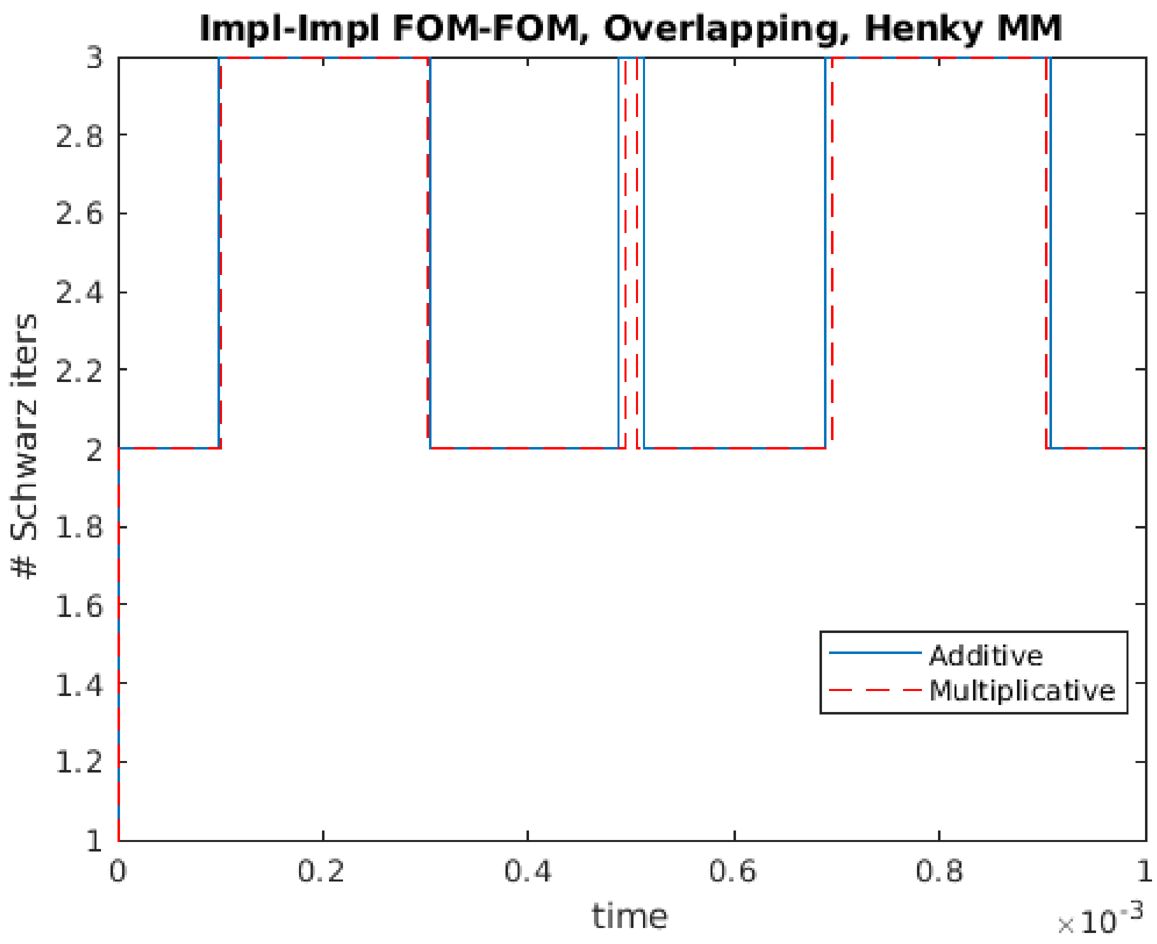


Multiplicative Schwarz



Additive Schwarz

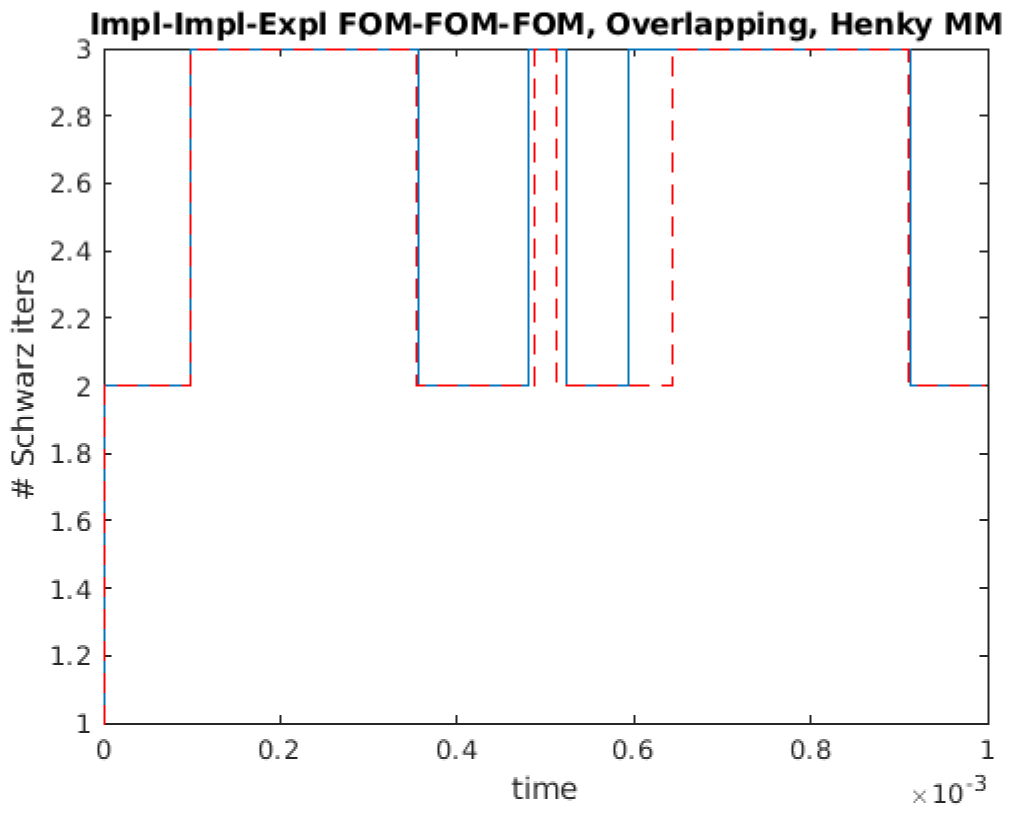
Overlapping Coupling, Nonlinear Henky MM, 2 Subdomains



- $\Omega = [0, 0.7] \cup [0.3, 1]$, 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

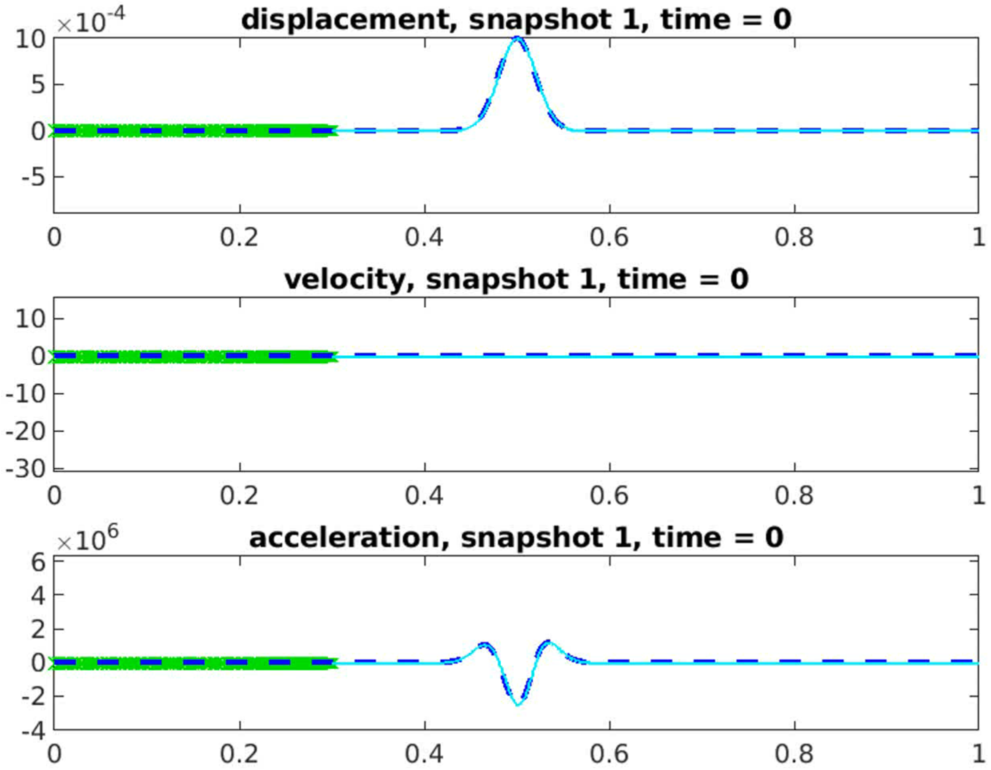


- $\Omega = [0, 0.3] \cup [0.25, 0.75] \cup [0.7, 1]$, implicit-implicit-explicit FOM-FOM-FOM coupling, dt = 1e-7, dx = 0.001.
- Solutions agree effectively to machine precision in mean square (MS) sense.
- Additive Schwarz has slightly more Schwarz iterations but is slightly faster than multiplicative.

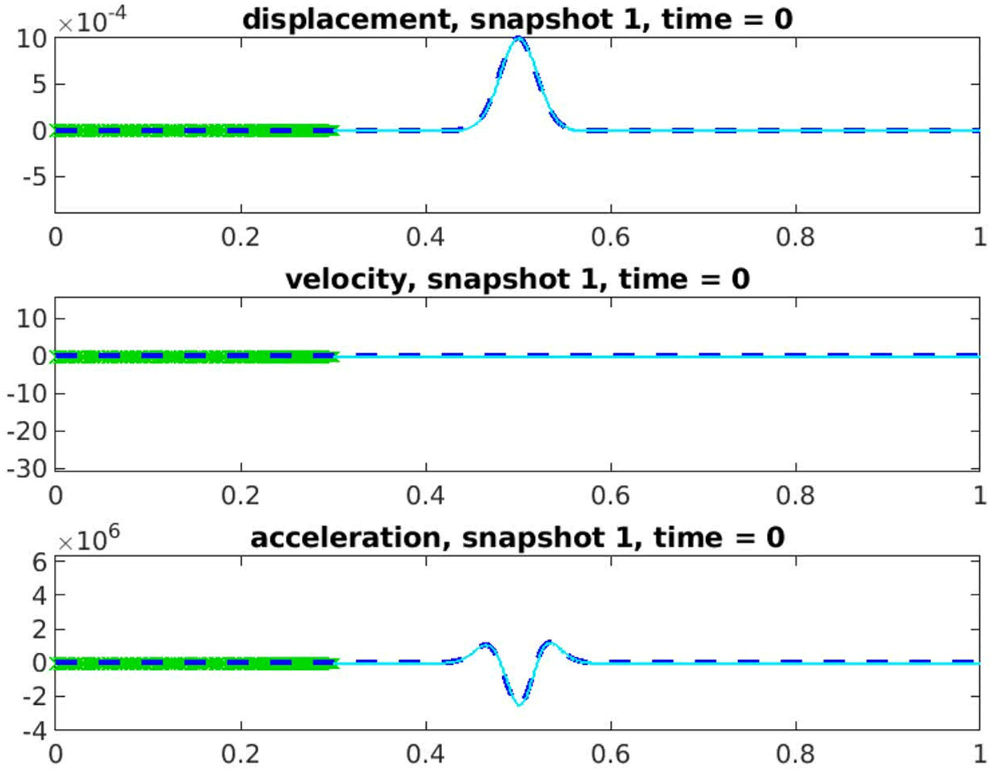
	Additive	Multiplicative
Total # Schwarz iters	26231	25459
CPU time	1.89e3s	2.05e3s
MS difference in disp	5.3052e-13/9.3724e-13/6.1911e-13	
MS difference in velo	7.2166e-12/2.2937e-11/2.4975e-11	
MS difference in acce	2.8962e-10/1.1042e-09/1.6994e-09	

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.

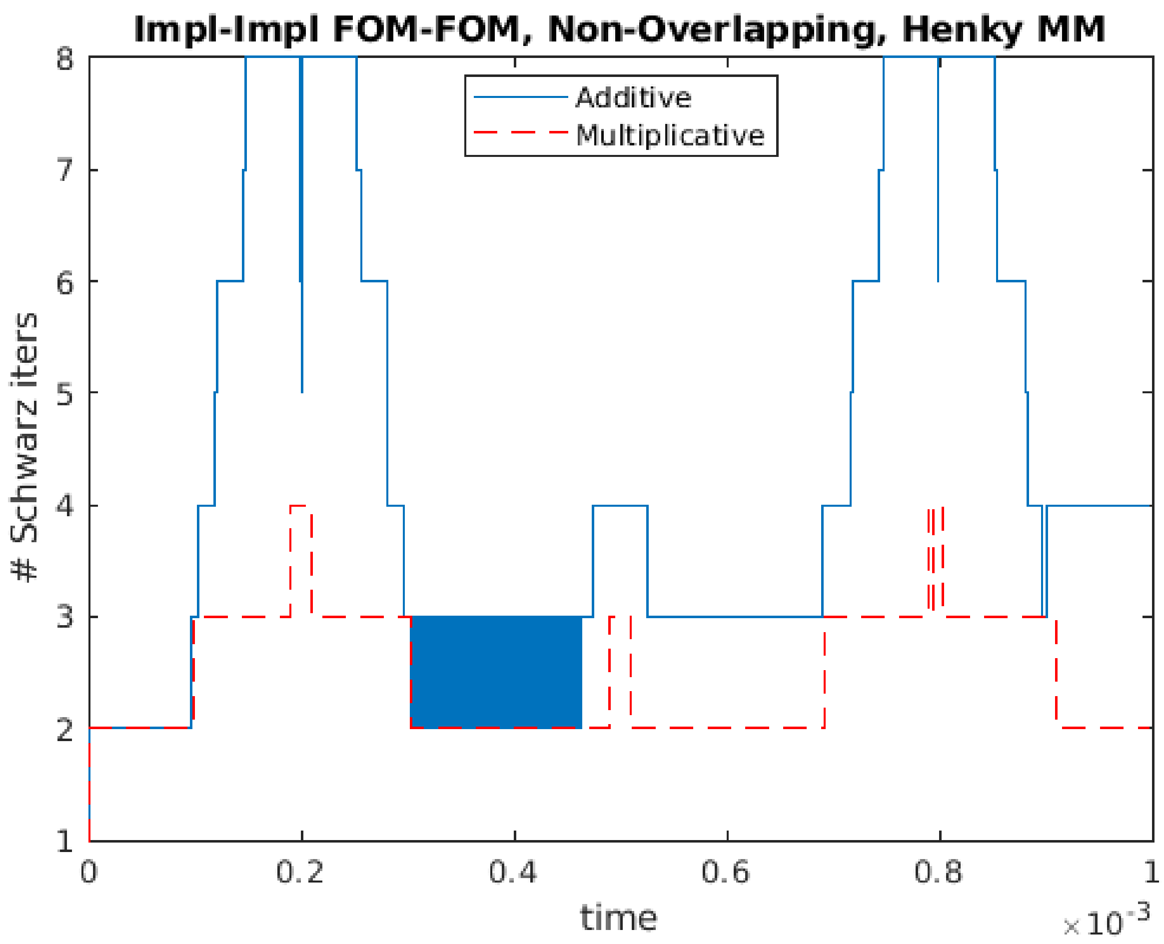


Multiplicative Schwarz



Additive Schwarz

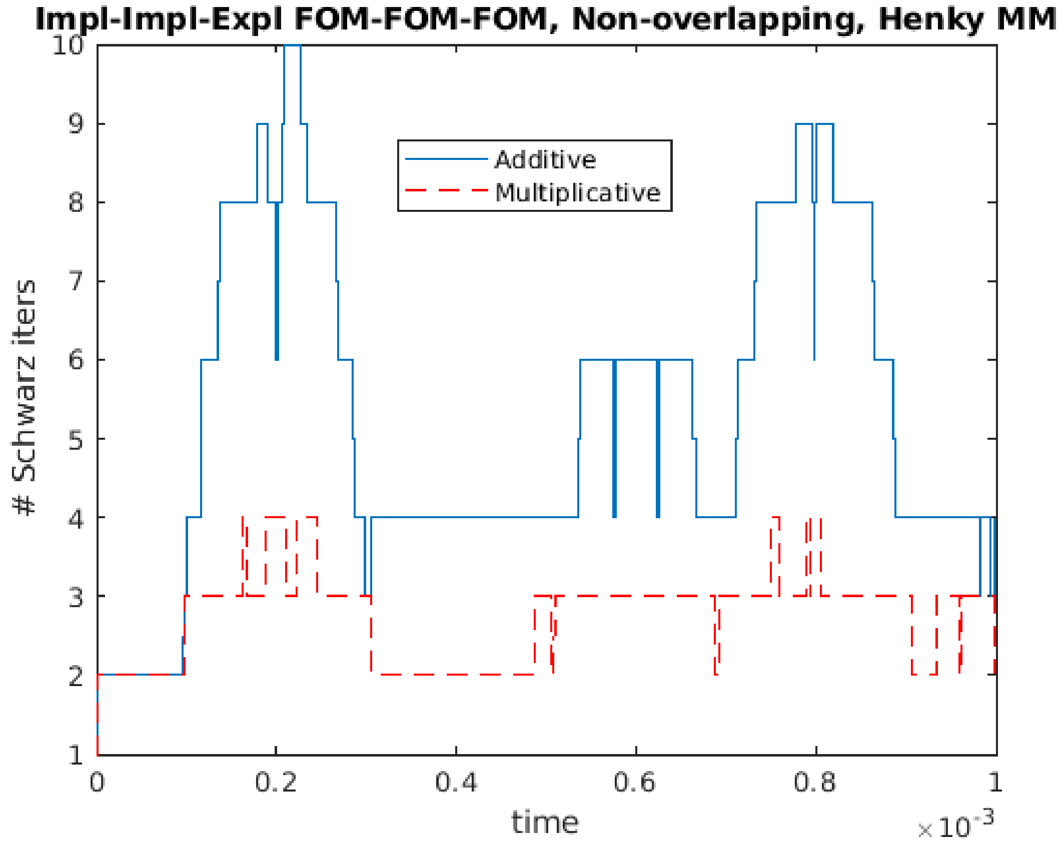
Non-overlapping Coupling, Nonlinear Henky MM, 2 Subdomains



- $\Omega = [0, 0.3] \cup [0.3, 1]$, 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	

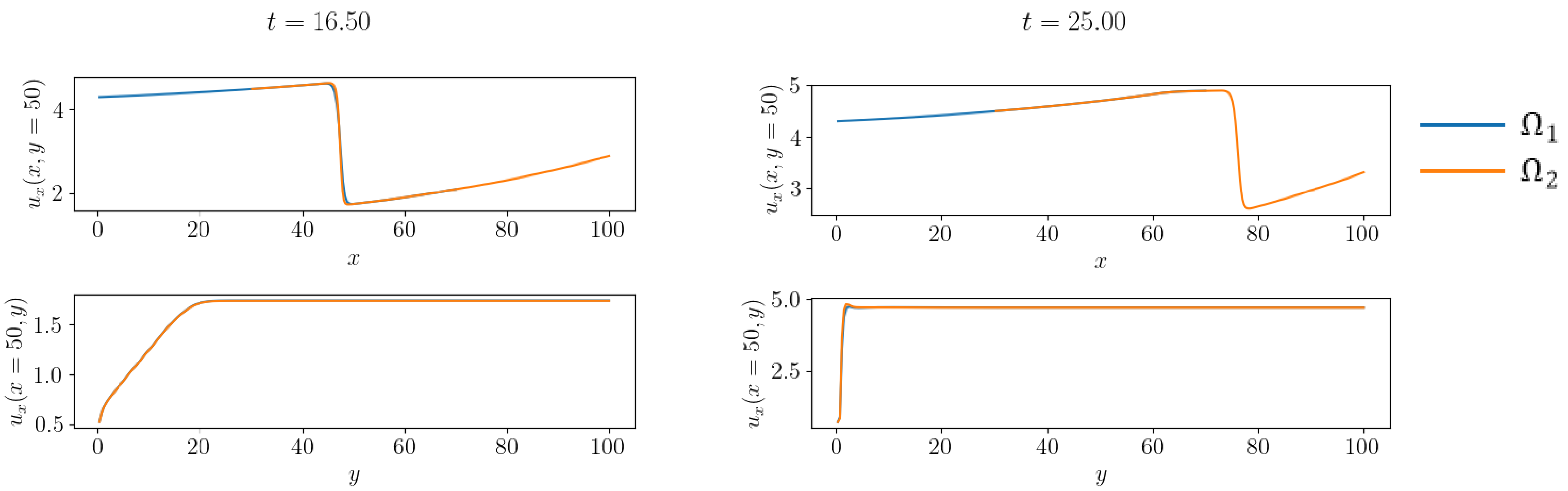
Non-overlapping Coupling, Nonlinear Henky MM, 3 Subdomains



- $\Omega = [0, 0.3] \cup [0.3, 0.7] \cup [0.7, 1]$, 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.

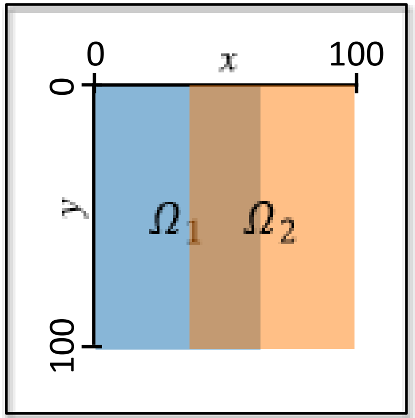
	Additive	Multiplicative
Total # Schwarz iters	53413	27509
CPU time	5.91e3s	2.87e3s
MS difference in disp	2.8036e-05/3.1142e-05/ 8.8395e-06	
MS difference in velo	1.4077e-05/1.2104e-05/6.5771e-06	
MS difference in acce	8.7885e-05/3.2707e-05/1.3778e-05	

FOM-FOM Coupling: Differing Resolution



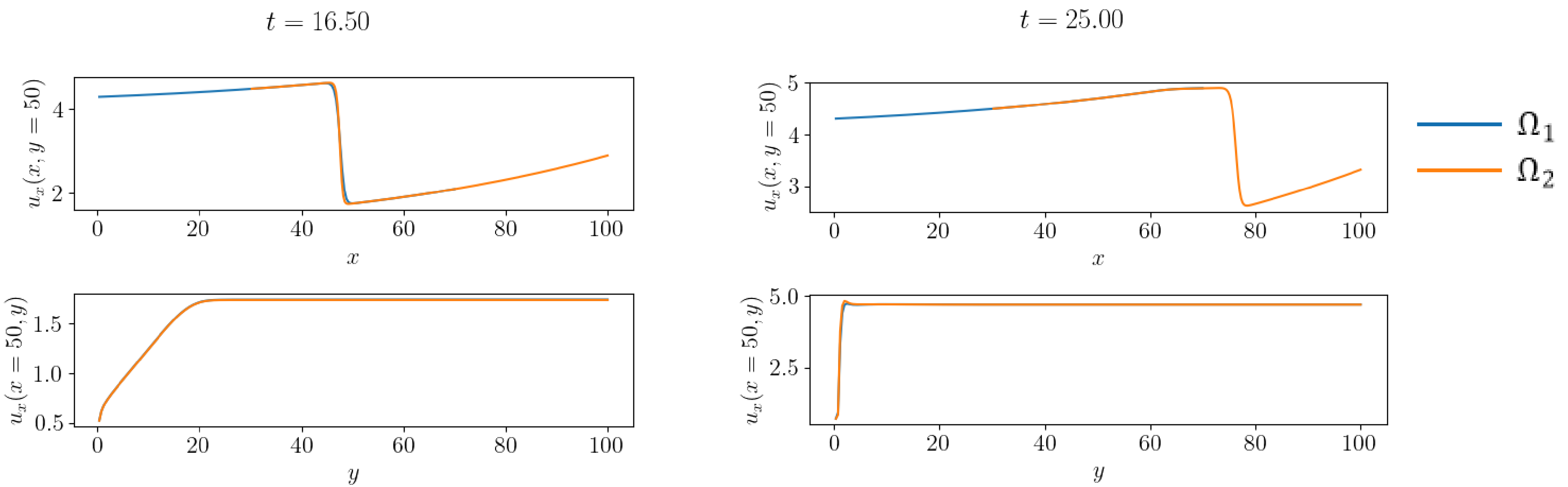
Figures above: Two-subdomain explicit-explicit overlapping coupling in x-axis [0, 70] U [30, 100] where $\mu = [4.3, 0.021]$, $\Delta t = 0.005$, $\Delta x_1 = 0.4, \Delta x_2 = 0.3$

- Figures show the mid-plane slice of the solution for u_x at various times
- The right subdomain is a finer mesh, and the difference in how the shock is resolved can be seen
- $\Omega_1 \rightarrow \Omega_2$ ordering gives 2 Schwarz iterations per global time step
- $\Omega_2 \rightarrow \Omega_1$ ordering gives 3 Schwarz iterations per global time step

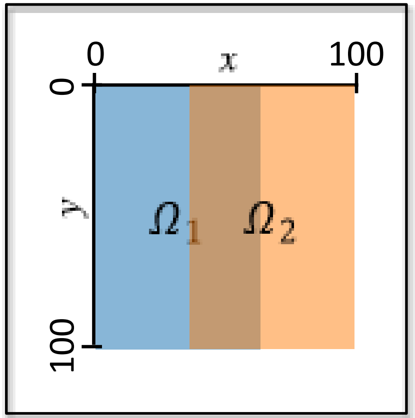


Order can be important!

FOM-FOM Coupling: Differing time integrators and Δt

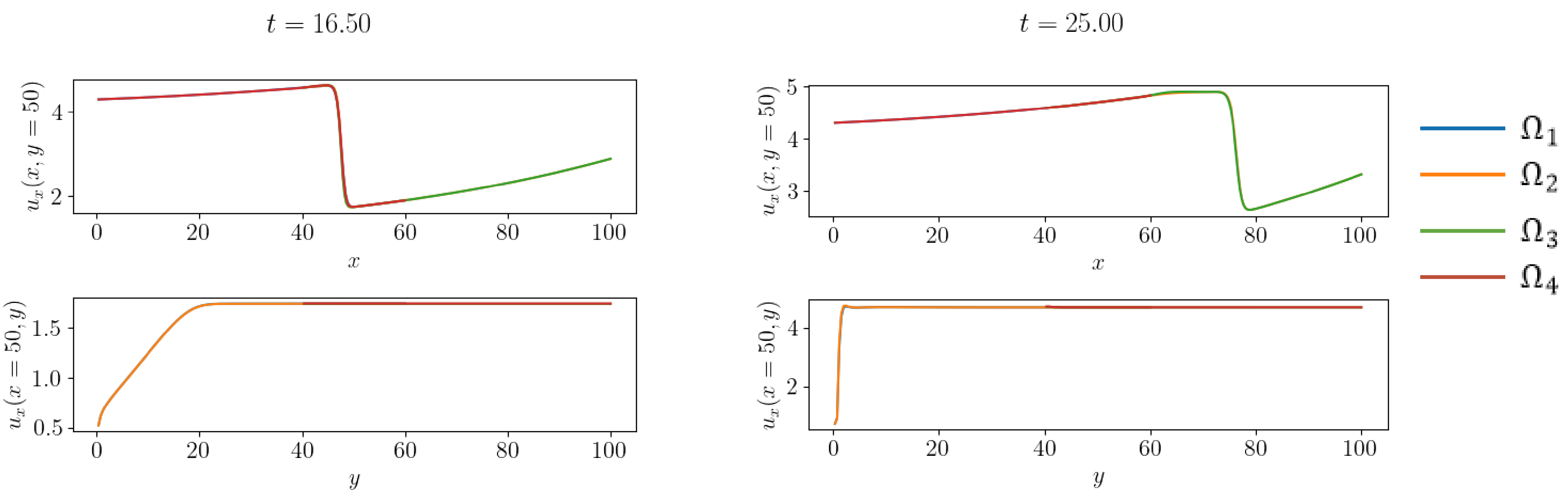


Figures above: Two-subdomain implicit-explicit overlapping coupling in x-axis [0, 70] U [30, 100], $\mu = [4.3, 0.021]$, $\Delta t_1 = 0.05$, $\Delta t_2 = 0.005$, $\Delta x_1 = 0.4, \Delta x_2 = 0.3$

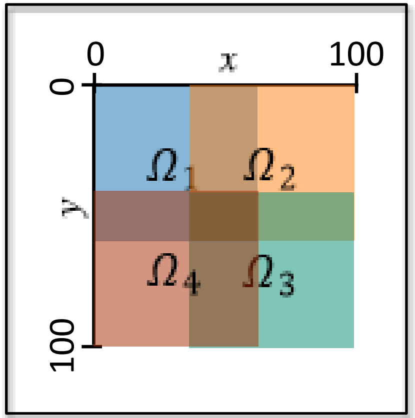


- Introducing a different time stepper in Ω_1 has not introduced artifacts and produces visually identical solution
- Choosing $\Omega_1 \rightarrow \Omega_2$ still only requires 2 Schwarz iterations per global time step

FOM-FOM Coupling: >2 Subdomains



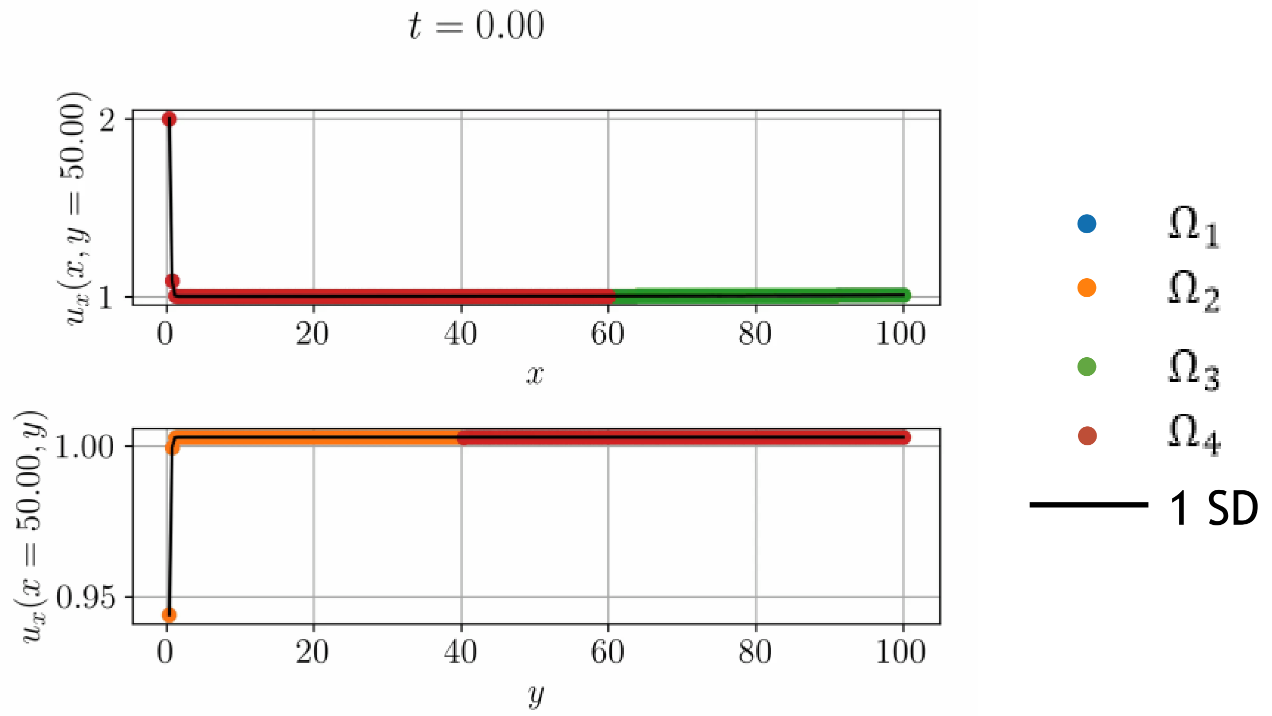
Figures above: Four-subdomain implicit-explicit-implicit-explicit overlapping coupling in x-axis [0, 60] U [40, 100] and y-axis [0,60] U [40, 100], $\mu = [4.3, 0.021]$,
$\Delta t_1 = \Delta t_3 = 0.05,\ \Delta t_2 = \Delta t_4 = 0.005,\ \Delta x_1 = \Delta x_4 = 0.4, \Delta x_2 = \Delta x_3 = 0.3$



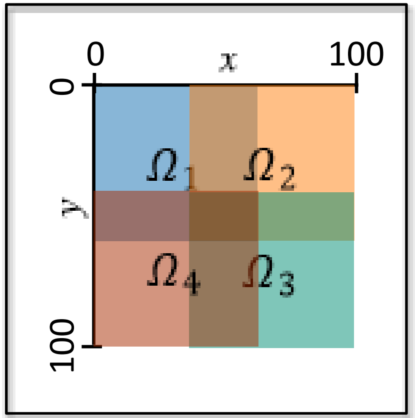
- Despite a heterogeneous mixture of different subdomains coupled in multiple dimensions with different solvers, resolutions, etc. the solution is still consistent
- Choosing $\Omega_1 \rightarrow \Omega_2 \rightarrow \Omega_3 \rightarrow \Omega_4$ requires 3 Schwarz iterations per global time step

FOM-FOM Coupling: >2 Subdomains

Subdomain	Wall Clock Time (s)	Total (s)
Monolithic	124	124
Ω_1	75	300
Ω_2	62	
Ω_3	62	
Ω_4	77	

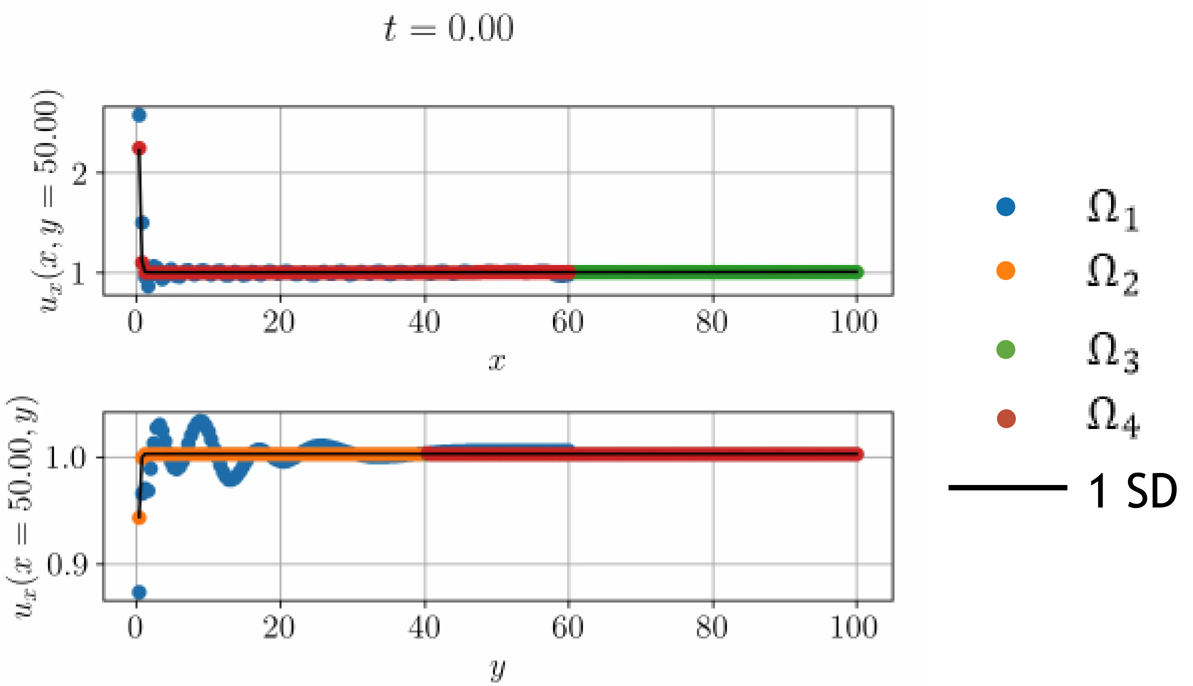


Figures above: Four-subdomain implicit-implicit-implicit-implicit overlapping coupling in x-axis [0, 60] U [40, 100] and y-axis [0,60] U [40, 100], $\mu = [4.3, 0.021]$, $\Delta t = 0.05,\ \Delta x_1 = \Delta x_4 = 0.4, \Delta x_2 = \Delta x_3 = 0.3$

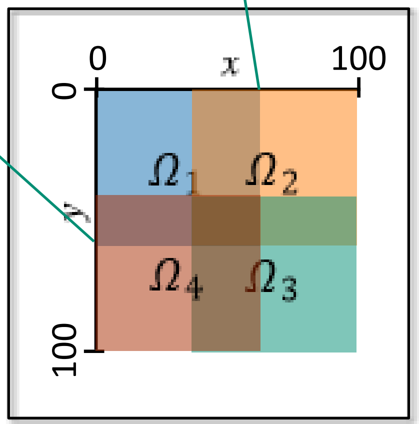


- Despite a heterogeneous mixture of different subdomains coupled in multiple dimensions with different solvers, resolutions, etc. the solution is still consistent
- Choosing $\Omega_1 \to \Omega_2 \to \Omega_3 \to \Omega_4$ requires 3 Schwarz iterations per global time step

HROM-FOM-FOM-FOM Coupling



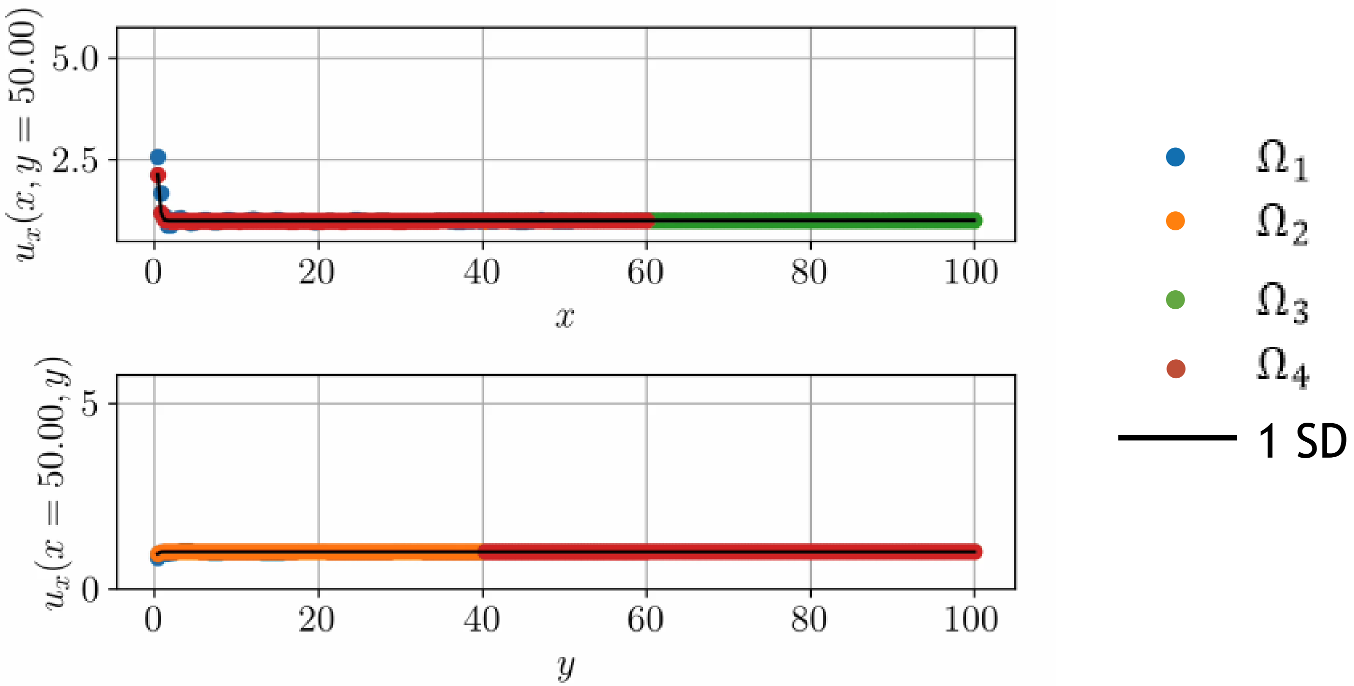
n_e= 4,346 (19% of N_e)

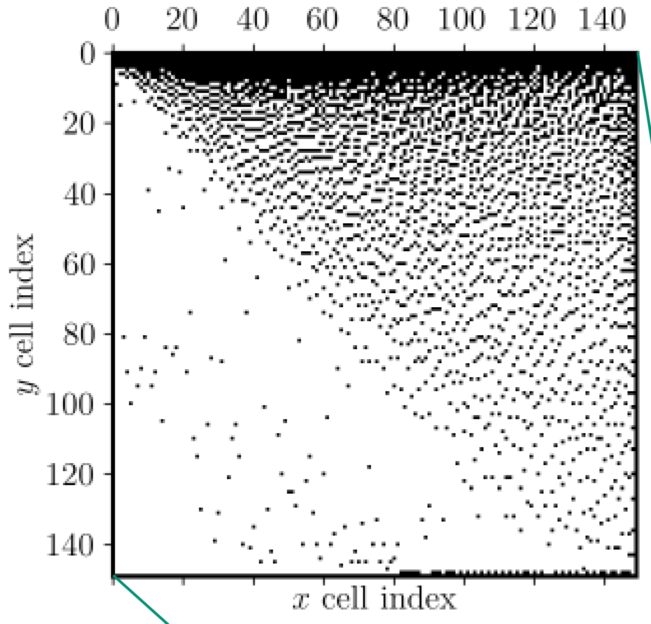


Domain	M	MSE (%)	HROM-FOM-FOM-FOM Wall Clock Time (s)	FOM-FOM-FOM-FOM Wall Clock Time (s)	Speedup
Ω_1	76	1.5	30	68	2.3
Total	–	–	276	300	1.1

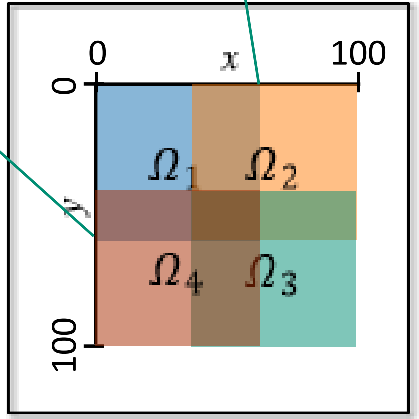
- We have **computational gain** even when choosing the "worst" subdomain for HROM
- No speedup over single-domain FOM (wall clock time = $124\ s$)
  - ➢ **Mitigation:** additive Schwarz, which admits more parallelism

HROM-FOM-FOM-FOM Coupling





$n_e = 4{,}346$ (19% of N_e)



- HROM is in Ω_1 and retains **95% of snapshot energy** $\Rightarrow$ 57 modes
  - HROM assignment is "**worst-case-scenario**"
- **Reduced mesh** trained only using a single parameter instance of $\boldsymbol{\mu} = [4.25, 0.0225]$
- Method converges in **3 Schwarz iterations** per controller time-step.
- Some **spurious oscillations** in first/last time steps due to **under-resolved solution**

Spurious oscillations *do not* impact Schwarz coupling.

Summary

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

- We have developed an **iterative** coupling formulation based on the **Schwarz alternating method** and an **overlapping** or **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
- 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)

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 (not shown)

- **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**

Ongoing & Future Work

- Extension/prototyping on more multi-D (2D/3D compressible flow[1], 2D/3D solid mechanics[2]) and multi-physics problems (FSI, Air-Sea coupling)
- Implementation/testing of **additive Schwarz variant**, which admits more parallelism
- **Analysis** of method's convergence for ROM-FOM and ROM-ROM couplings
- **Learning** of **"optimal" transmission conditions** to ensure **structure preservation**
- Extension of coupling methods to coupling of **Physics Informed Neural Networks (PINNs)** (WIP)
- Exploration of **connections** between **iterative Schwarz** and **optimization-based coupling** [Iollo *et al.*, 2022]
- Development of **smart domain decomposition approaches** based on error indicators, to determine optimal placement of ROM and FOM in a computational domain (including **on-the-fly ROM-FOM switching**)
- Extension of couplings to POD modes built from snapshots on **independently-simulated subdomains**
- **Journal article** currently in preparation.

[1] https://github.com/ Pressio/pressio-demoapps
[2] https://github.com/lxmota/norma