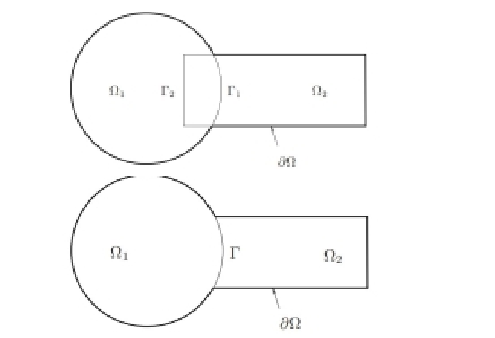
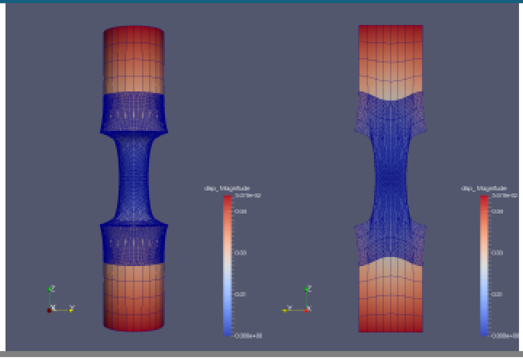
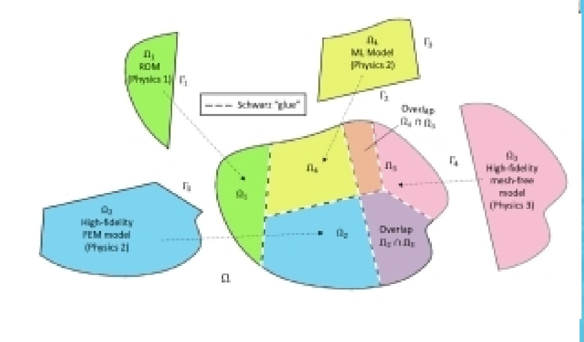
SAND2023-02528C

Application of the Schwarz alternating method for the coupling of nonlinear solid mechanics-based and fluids-based full order models to nonlinear reduced order models







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

[1]Sandia National Laboratories, [2]Stanford University

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SAND2023-02528C

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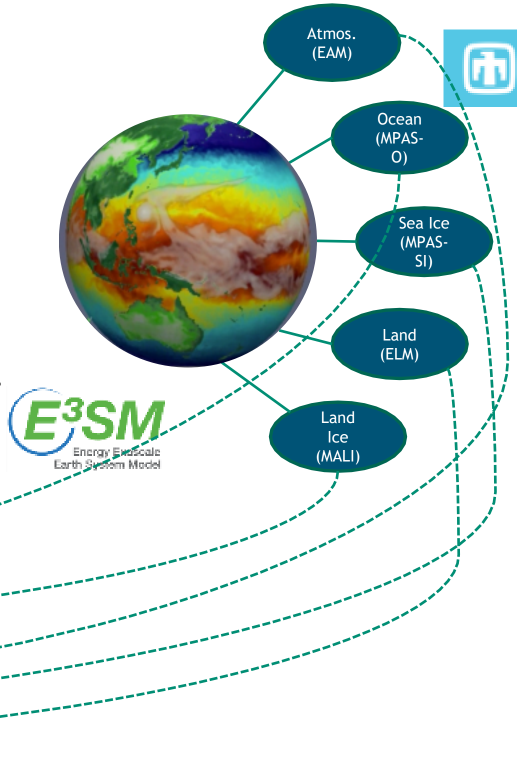
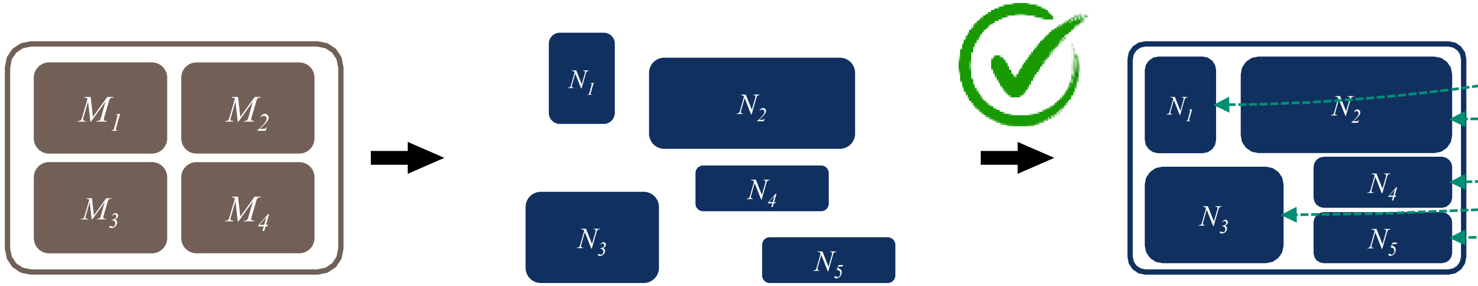
Motivation

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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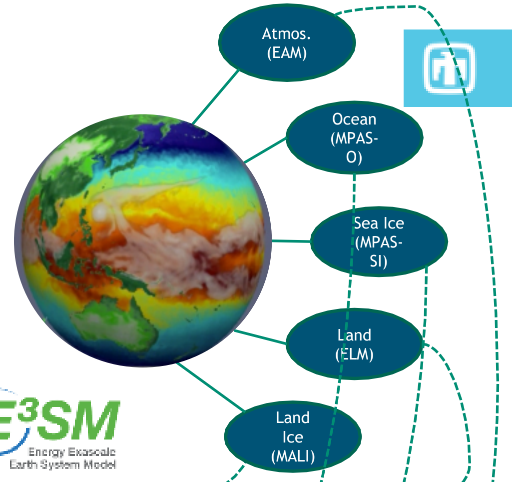

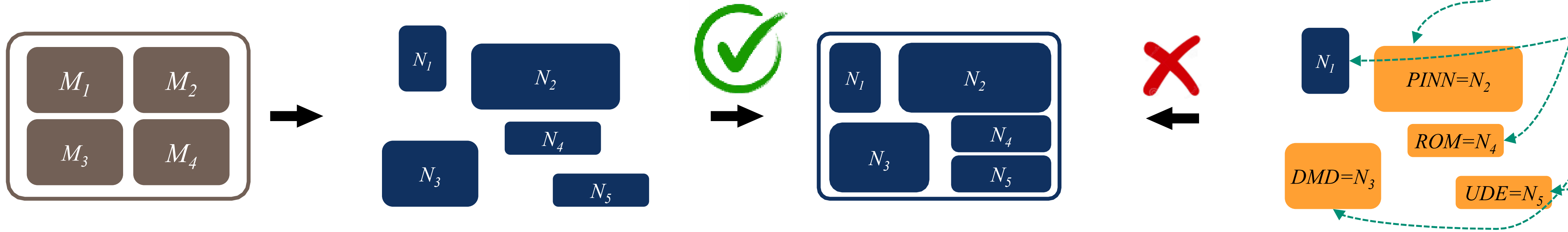

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Traditional + Data-Driven Methods

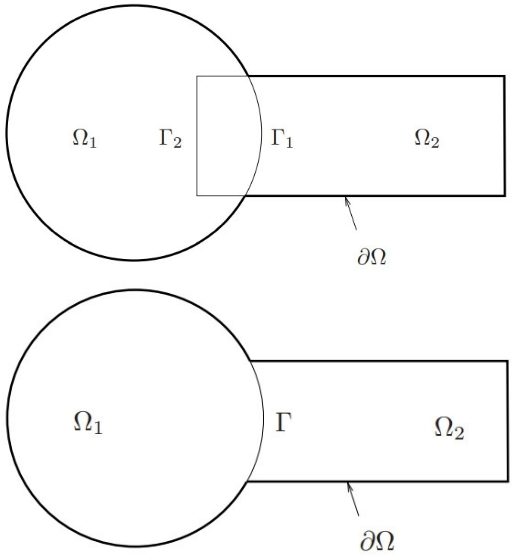
- PINNs
- Neural ODEs
- Projection-based ROMs, …

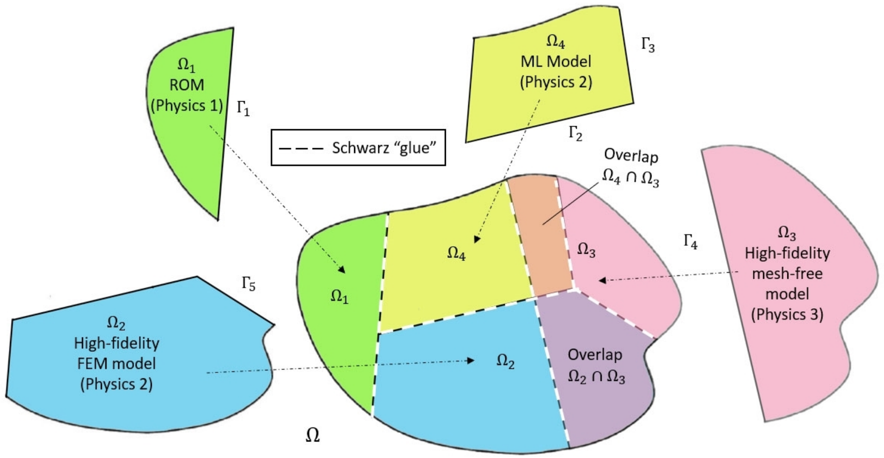
- There is currently a big push to integrate **data-driven methods** into modeling & simulation toolchains.

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

Outline

1. The Alternating Schwarz Method for FOM*-ROM# and ROM-ROM Coupling
    - Method Formulation
    - ROM Construction and Implementation
    - Numerical Example: Solid Mechanics
    - Numerical Example: Fluid Mechanics
2. Summary and Comparison of Methods
3. Future Work





*Full-Order Model. #Reduced Order Model.

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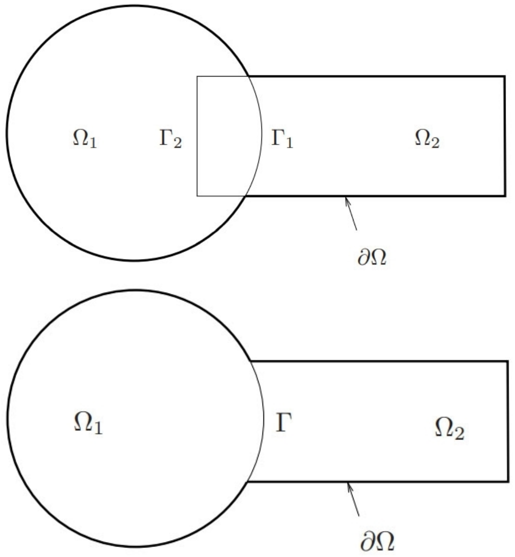

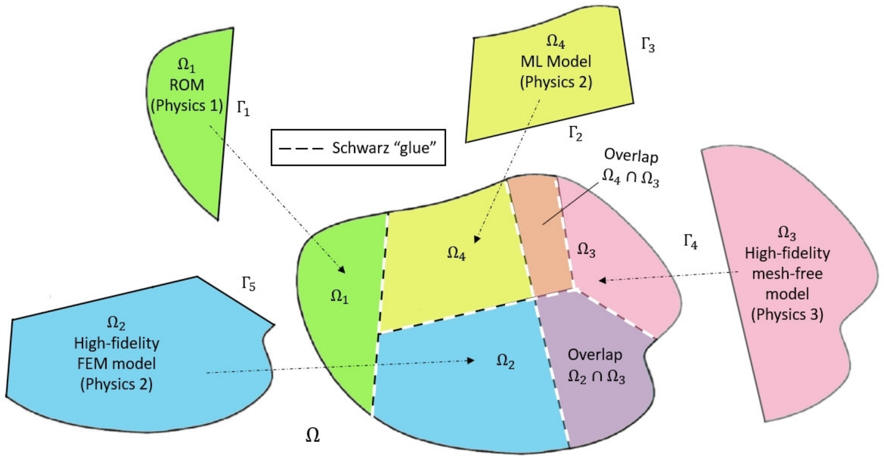

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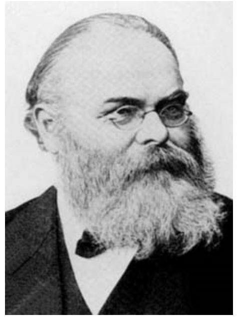
Schwarz Alternating Method for Domain Decomposition

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

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



H. Schwarz (1843–1921)

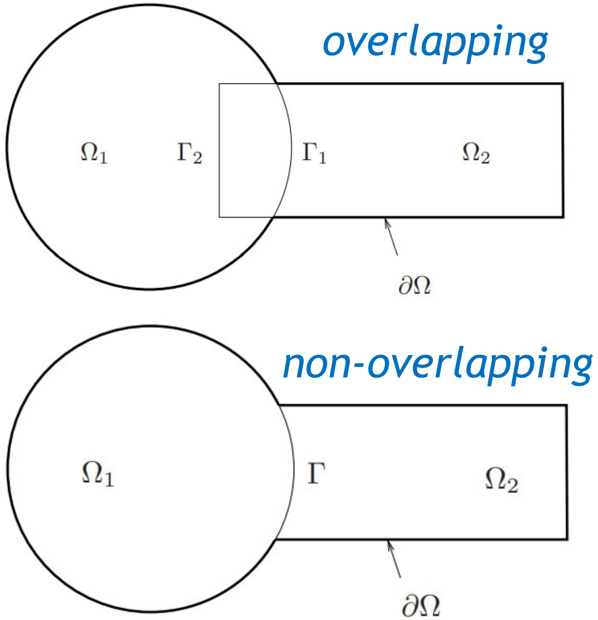
Basic Schwarz Algorithm

Initialize:

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

Iterate until convergence:

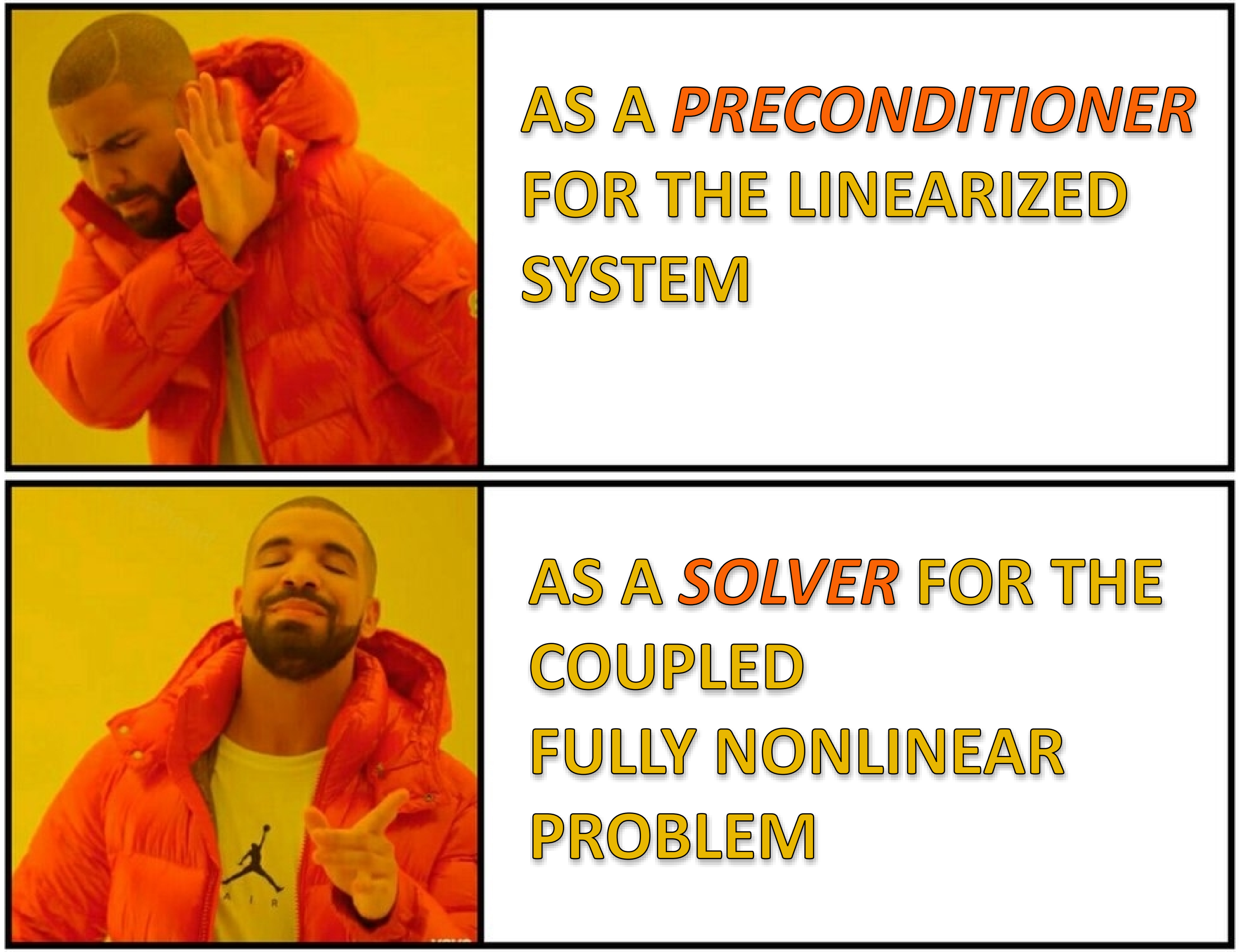
- Solve PDE by any method on Ω_2 w/ transmission BCs on Γ_2 based on values just obtained for Ω_1.
- Solve PDE by any method on Ω_1 w/ transmission BCs on Γ_1 based on values just obtained for Ω_2.



- 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

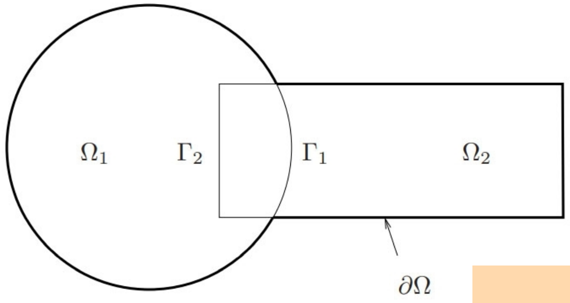


Spatial Coupling via Alternating Schwarz

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]

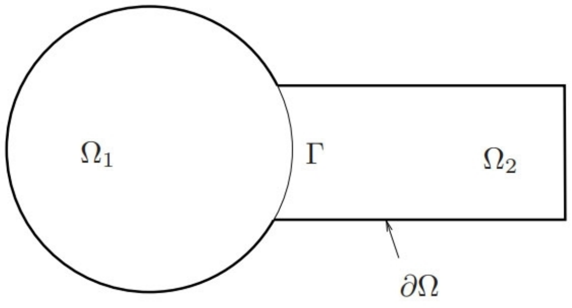
<u>This talk</u>: sequential subdomain solves (***multiplicative Schwarz***). Parallel subdomain solves (***additive Schwarz***) also possible.

Non-overlapping Domain Decomposition

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

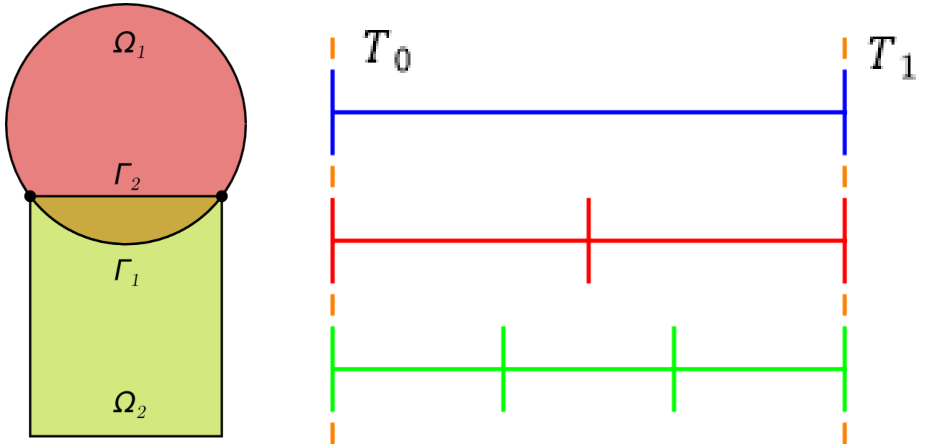
$$\begin{cases} N\left(\boldsymbol{u}_2^{(n+1)}\right) = f \text{ ,} & \text{in } \Omega_2 \\ \boldsymbol{u}_2^{(n+1)} = \boldsymbol{g}, & \text{on } \partial\Omega_2 \backslash \Gamma \\ \boldsymbol{\nabla u}_2^{(n+1)} \cdot \boldsymbol{n} = \boldsymbol{\nabla u}_1^{(n+1)} \cdot \boldsymbol{n}, & \text{on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

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



- 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)

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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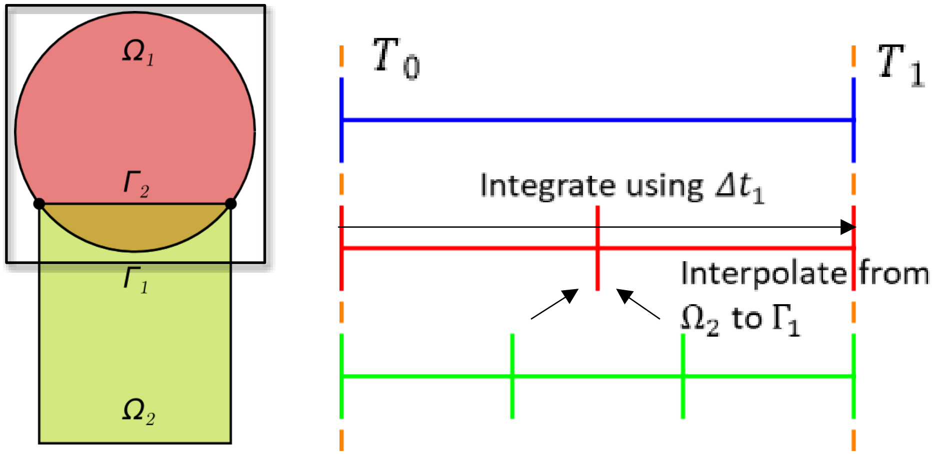

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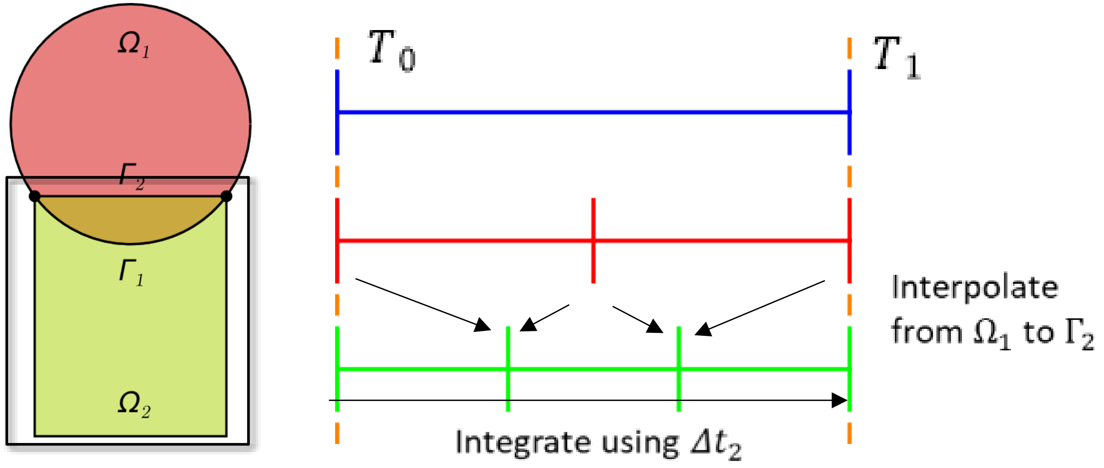

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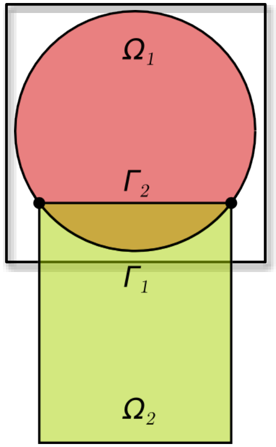

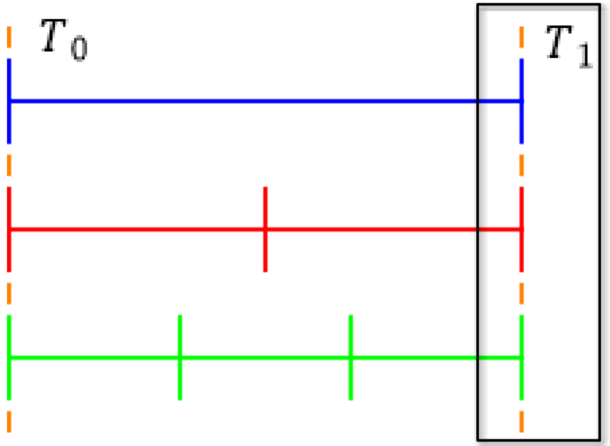

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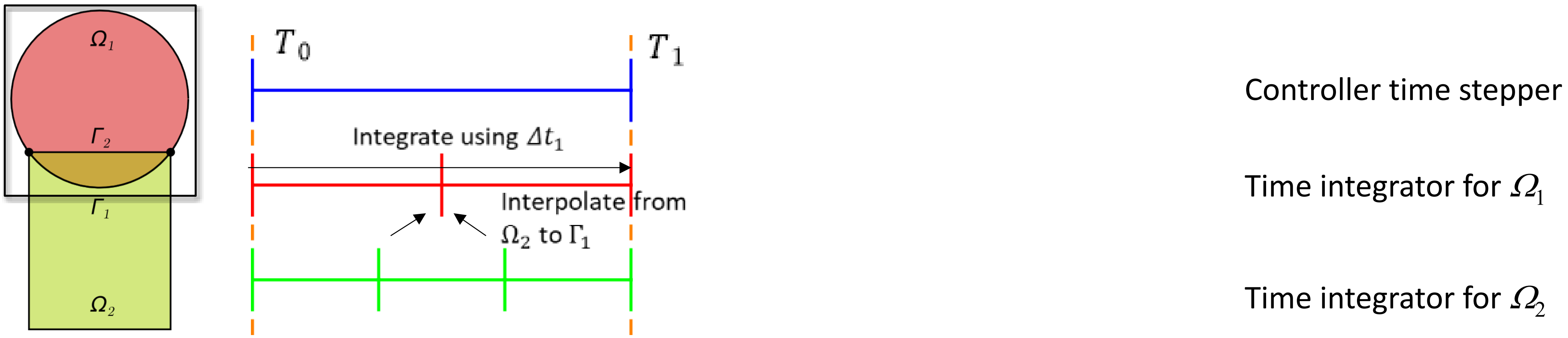

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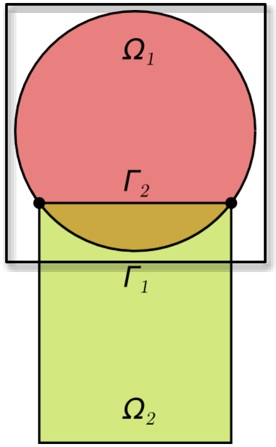

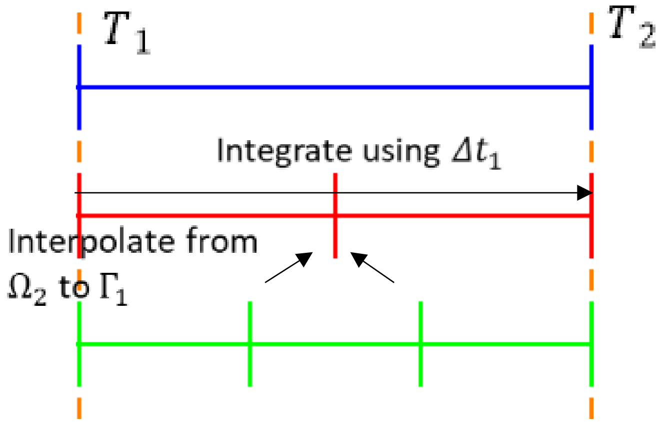

Can use ***different integrators*** with ***different time steps*** within each domain!

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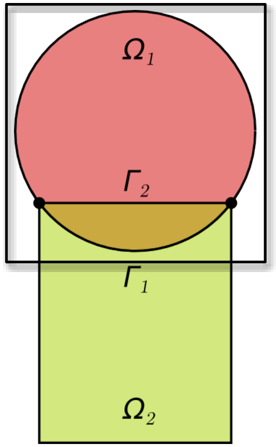

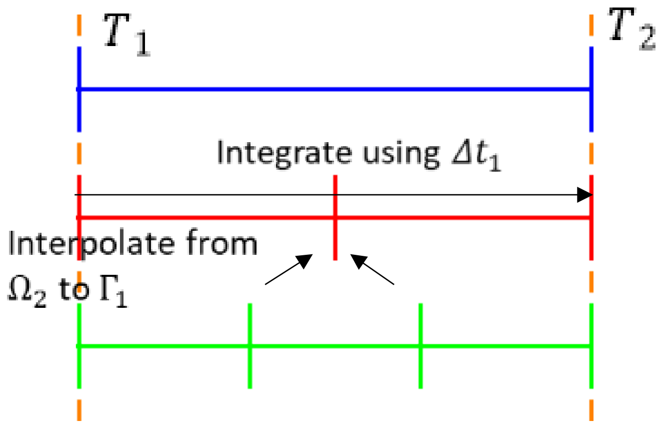

Time-stepping procedure is **equivalent** to doing Schwarz on **space-time domain** [Mota *et al.* 2022].

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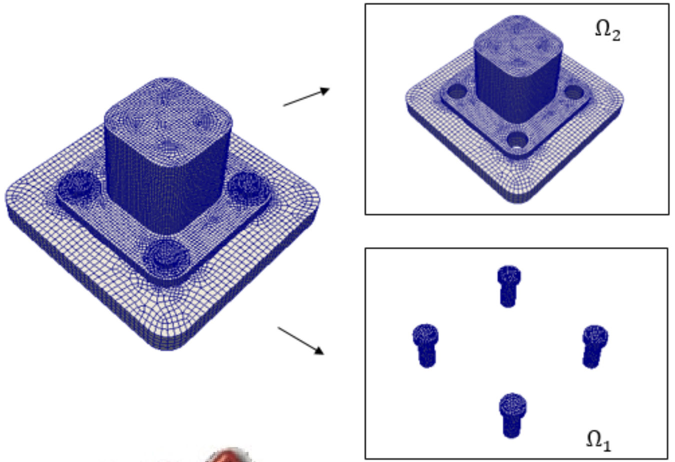
Schwarz for Multiscale FOM-FOM Coupling in Solid Mechanics[1]

- 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[2] SIERRA

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

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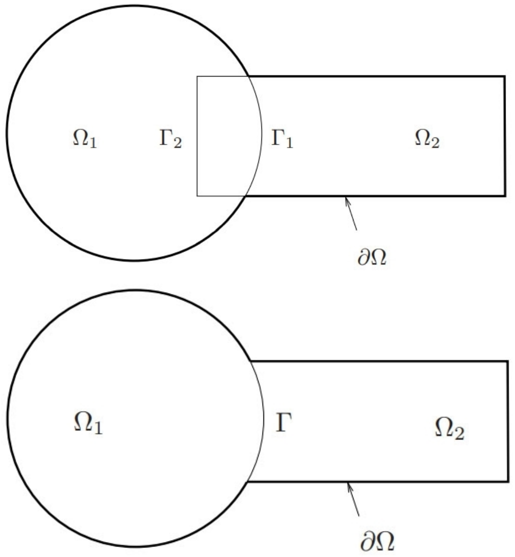

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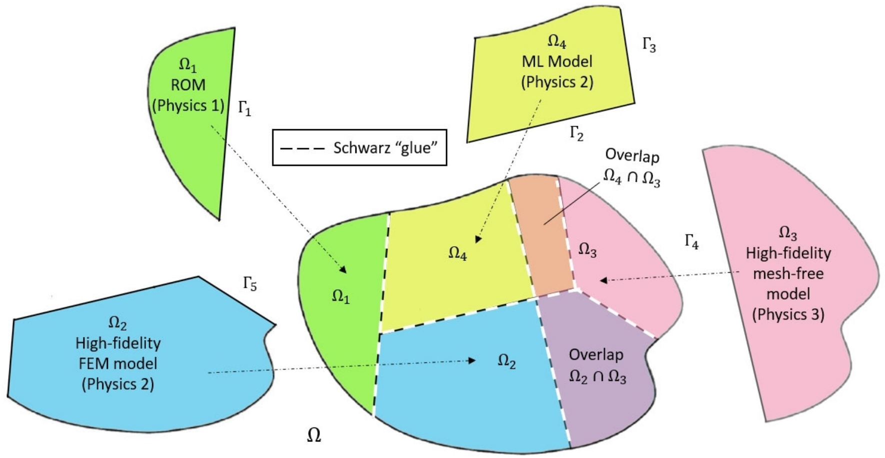
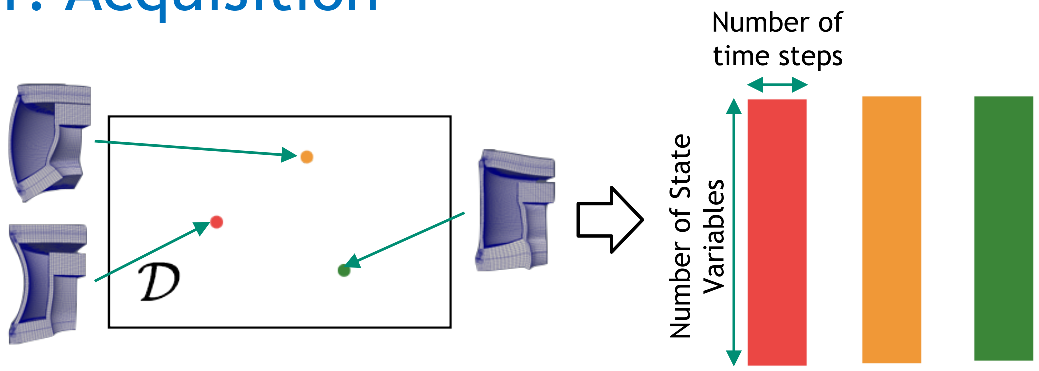


*Full-Order Model. #Reduced Order Model.

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

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

1. Acquisition

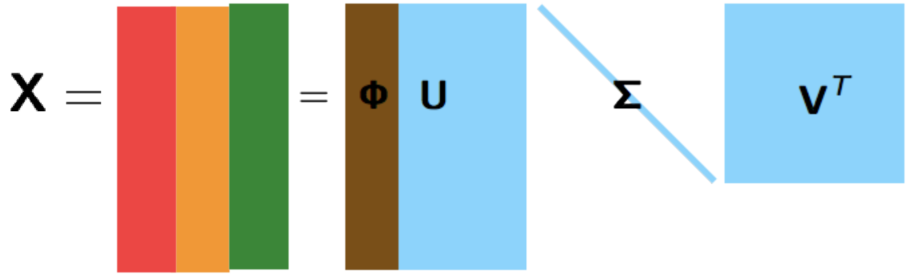


Solve ODE at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



ROM = projection-based Reduced Order Model

3. Projection-Based Reduction

Reduce the number of unknowns

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

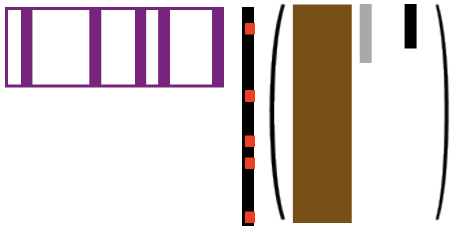
Perform Galerkin projection

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

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

Schwarz Extensions to FOM-ROM and ROM-ROM Couplings

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

- 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: $\boldsymbol{\Phi}(\boldsymbol{i}_{\text{Dir}},:) = \boldsymbol{0}$
  - ➢ BCs imposed by modifying $\overline{\boldsymbol{u}}, \overline{\boldsymbol{v}}, \overline{\boldsymbol{a}}$: $\overline{\boldsymbol{u}}(\boldsymbol{i}_{\text{Dir}}) \leftarrow \chi_u$, $\overline{\boldsymbol{v}}(\boldsymbol{i}_{\text{Dir}}) \leftarrow \chi_v$, $\overline{\boldsymbol{a}}(\boldsymbol{i}_{\text{Dir}}) \leftarrow \chi_a$

Choice of domain decomposition

- Error-based indicators that help decide in what region of the domain a ROM can be viable should drive domain decomposition [Bergmann *et al*. 2018] (future work)

Snapshot collection and reduced basis construction

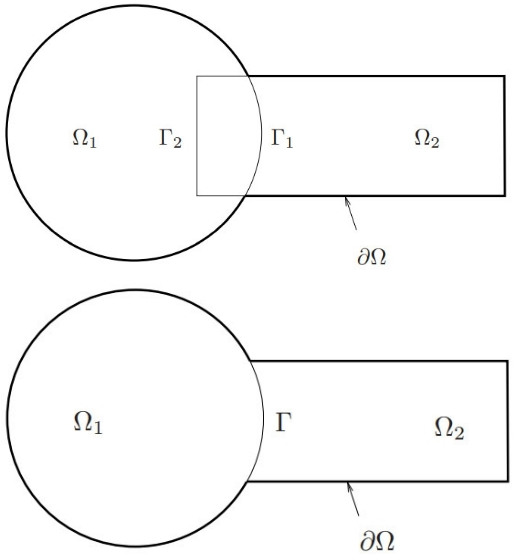
- POD results presented herein use snapshots obtained via FOM-FOM coupling on $\Omega = \cup_i \ \Omega_i$
- *Scenario I*: generate snapshots/bases separately in each Ω_i [Hoang *et al*. 2021, Smetana *et al*. 2022]

For nonlinear solid mechanics, hyper-reduction methods need to preserve Hamiltonian structure

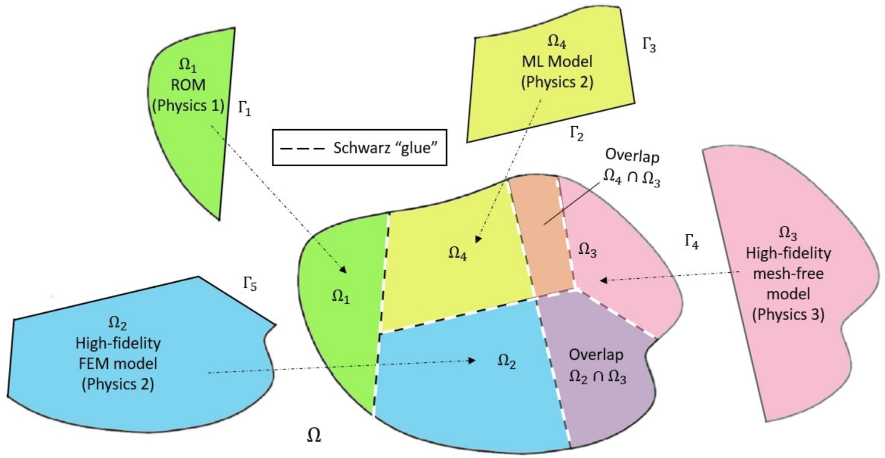
- We employ the Energy-Conserving Sampling & Weighting Method (ECSW) [Farhat *et al*. 2015]
- Boundary points must be included in sample mesh for DBC enforcement

Outline

1. **The Alternating Schwarz Method for FOM*-ROM# and ROM-ROM Coupling**
   - Method Formulation
   - ROM Construction and Implementation
   - **Numerical Example: Solid Mechanics**
   - Numerical Example: Fluid Mechanics



2. Summary and Comparison of Methods
3. 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.
- Two **constitutive models** considered:
  - Linear elastic (problem has exact analytical solution)
  - Nonlinear hyperelastic Henky *This talk*

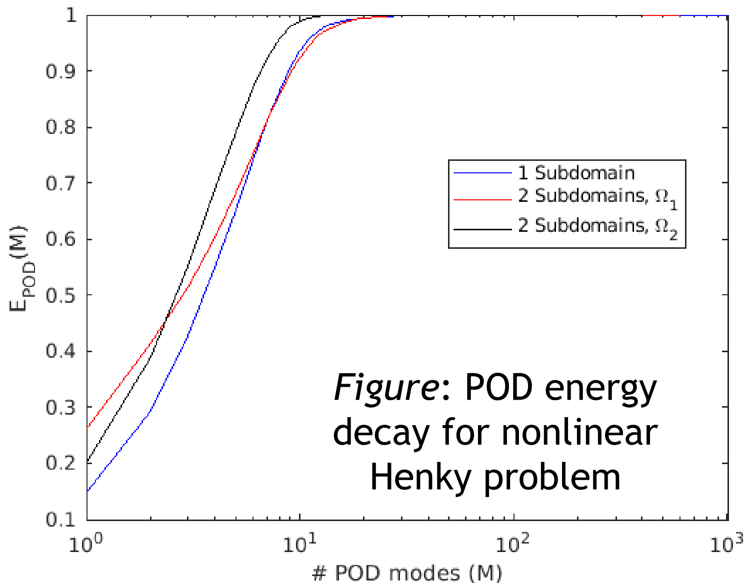


Figure: POD energy decay for nonlinear Henky problem

- 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**

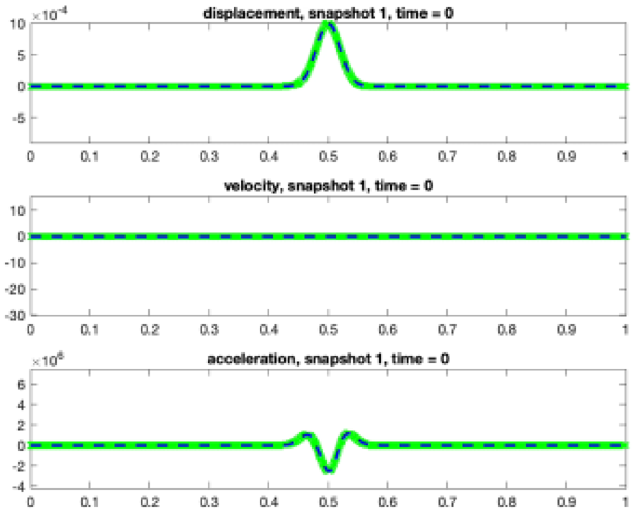
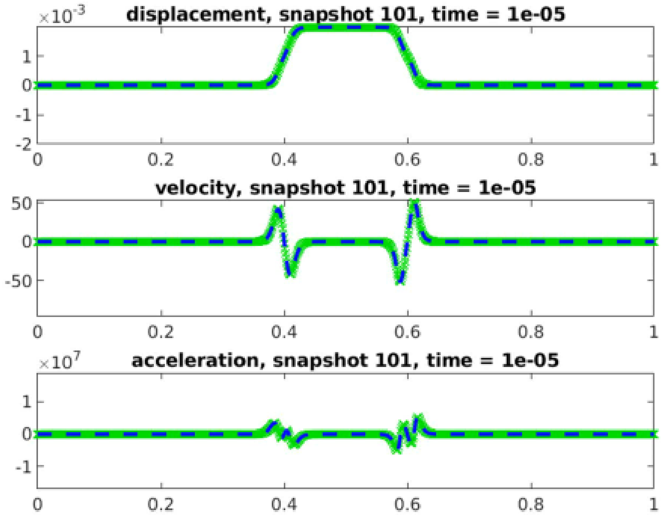


Figure above: Symmetric Gaussian IC problem solution
Figure below: Rounded Square IC problem solution



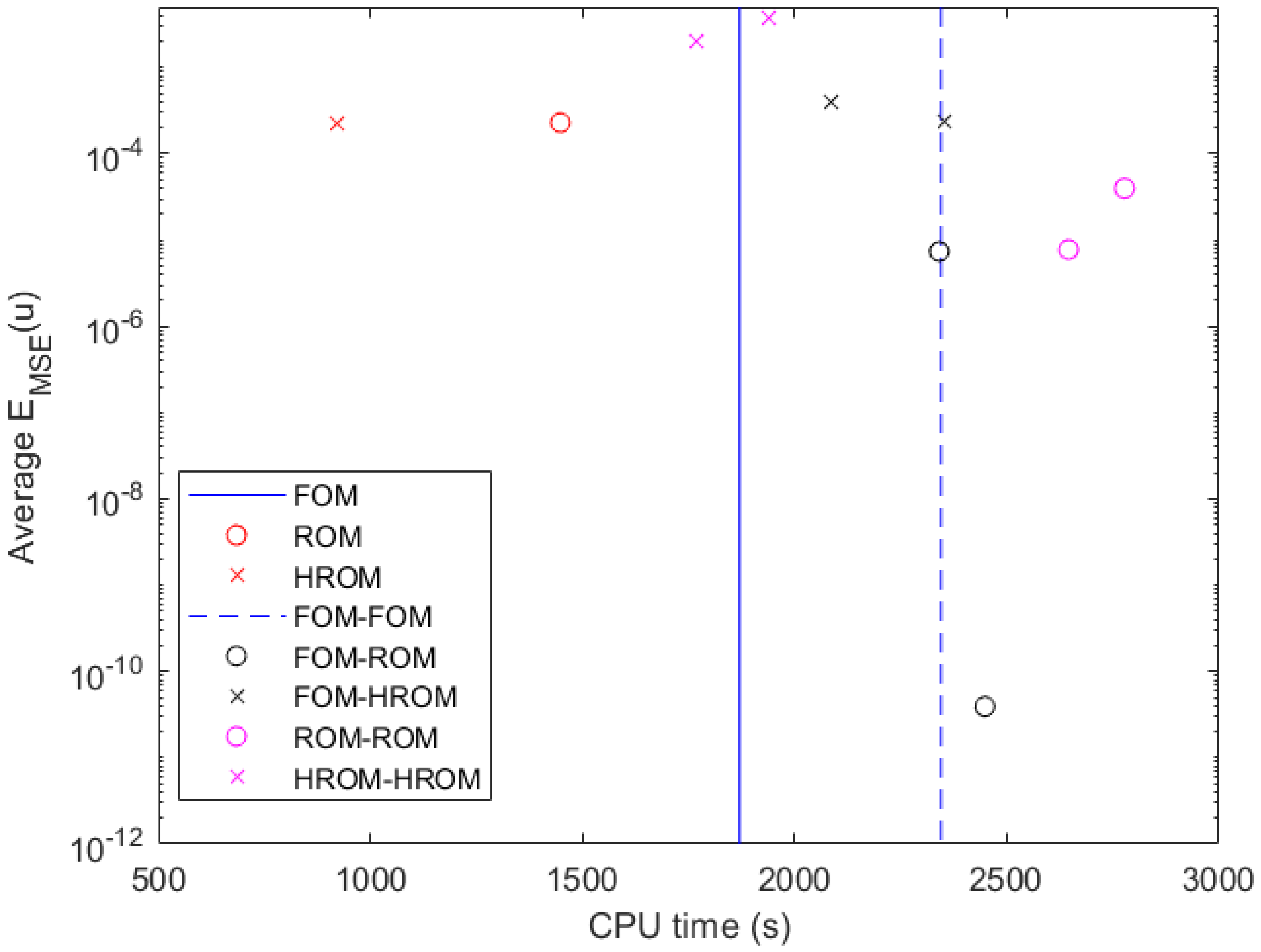
Numerical Example: Reproductive Problem Results

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	1.659×10^{-2}/–	1.037×10^{-1}	4.681×10^{-1}/–	–
HROM	60/–	155/–	5.878×10^2	1.730×10^{-2}/–	1.063×10^{-1}/–	4.741×10^{-1}/–	–
ROM	200/–	–/–	1.448×10^3	2.287×10^{-4}/–	4.038×10^{-3}/–	4.542×10^{-2}/–	–
HROM	200/–	428/–	9.229×10^2	8.396×10^{-4}/–	8.947×10^{-3}/–	7.462×10^{-2}/–	–
FOM-FOM	–/–	–/–	2.345×10^3	–	–	–	24,630
FOM-ROM	–/80	–/–	2.341×10^3	2.171×10^{-6}/ 1.253×10^{-5}	3.884×10^{-5}/ 2.401×10^{-4}	2.982×10^{-4}/ 2.805×10^{-3}	25,227
FOM-HROM	–/80	–/130	2.085×10^3	2.022×10^{-4}/ 5.734×10^{-4}	$1.723e \times 10^{-3}$/ 5.776×10^{-3}	7.421×10^{-3}/ 3.791×10^{-2}	29,678
FOM-ROM	–/200	–/–	2.449×10^3	4.754×10^{-12}/ 7.357×10^{-11}	1.835×10^{-10}/ 4.027×10^{-9}	5.550×10^{-9}/ 1.401×10^{-7}	24,630
FOM-HROM	–/200	–/252	2.352×10^3	1.421×10^{-5}/ 4.563×10^{-4}	1.724×10^{-4}/ 2.243×10^{-3}	9.567×10^{-4}/ 1.364×10^{-2}	27,156
ROM-ROM	200/80	–/–	2.778×10^3	4.861×10^{-5}/ 3.093×10^{-5}	1.219×10^{-3}/ 4.177×10^{-4}	1.586×10^{-2}/ 3.936×10^{-3}	27,810
HROM-HROM	200/80	315/130	1.769×10^3	3.410×10^{-3}/ 6.662×10^{-4}	4.110×10^{-2}/ 6.432×10^{-3}	2.485×10^{-1}/ 4.307×10^{-2}	29,860
ROM-ROM	300/80	–/–	2.646×10^3	2.580×10^{-6}/ 1.292×10^{-5}	6.226×10^{-5}/ 2.483×10^{-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: 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**

Numerical Example: Reproductive Problem Results

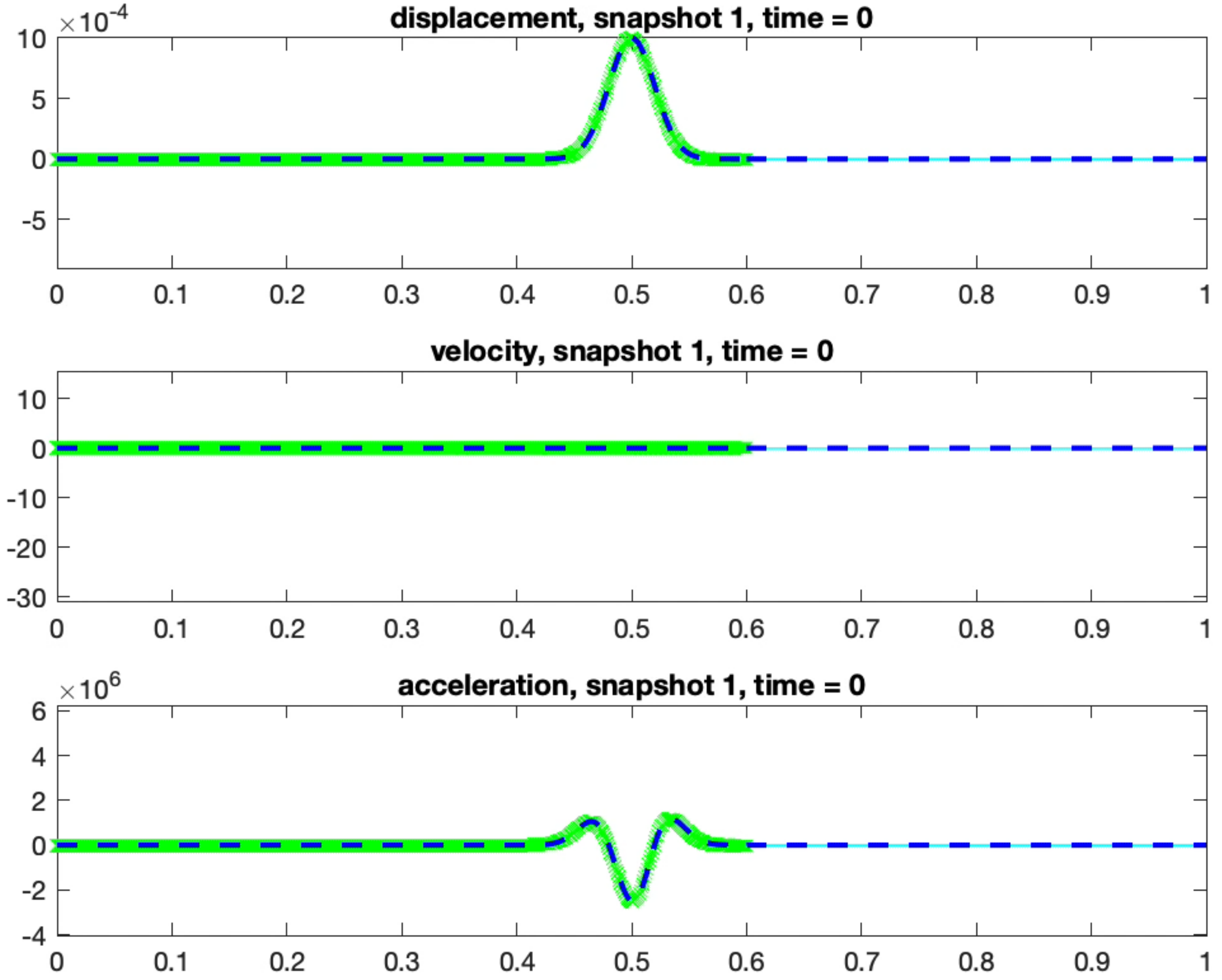
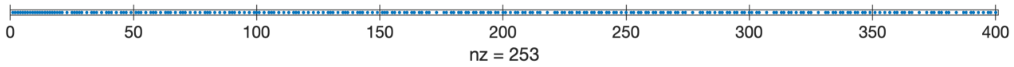


Figure left: FOM (green) – HROM (cyan) coupling compared with single-domain FOM solution (blue). HROM has 200 modes.

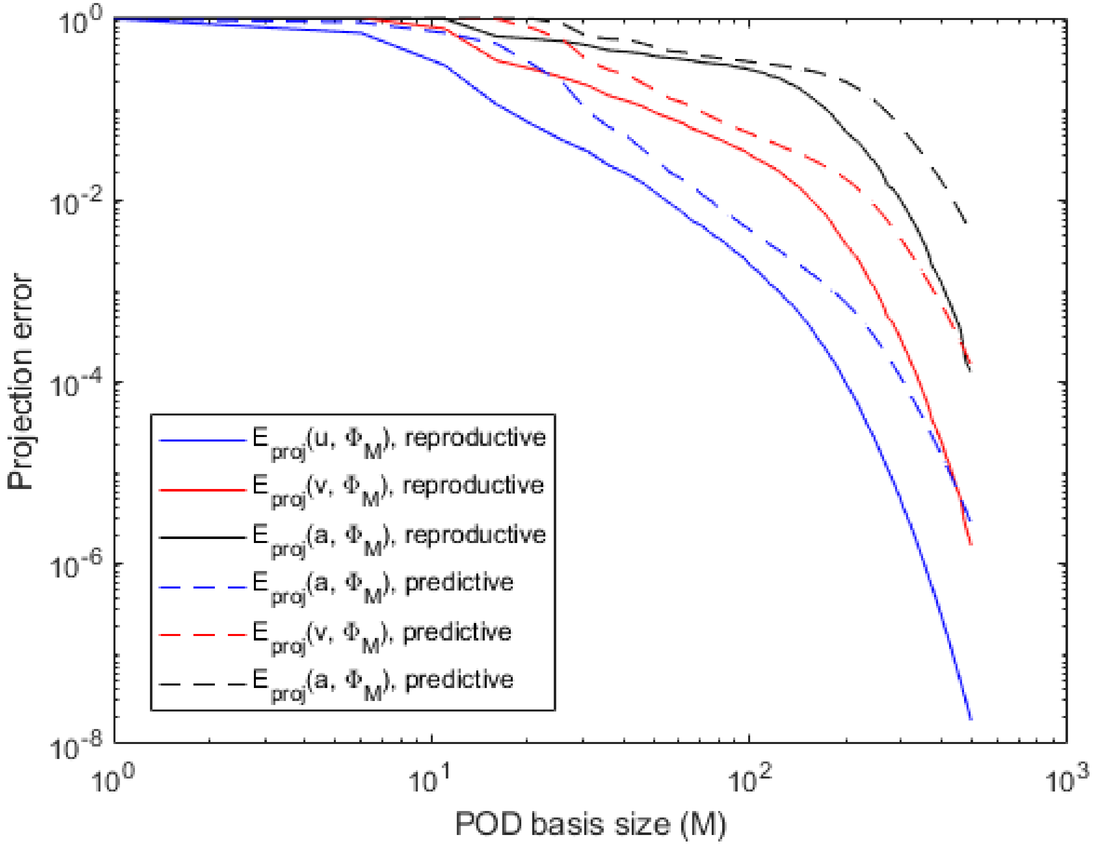
Figure below: ECSW algorithm samples 253/400 elements



Numerical Example: Predictive Problem Results

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

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

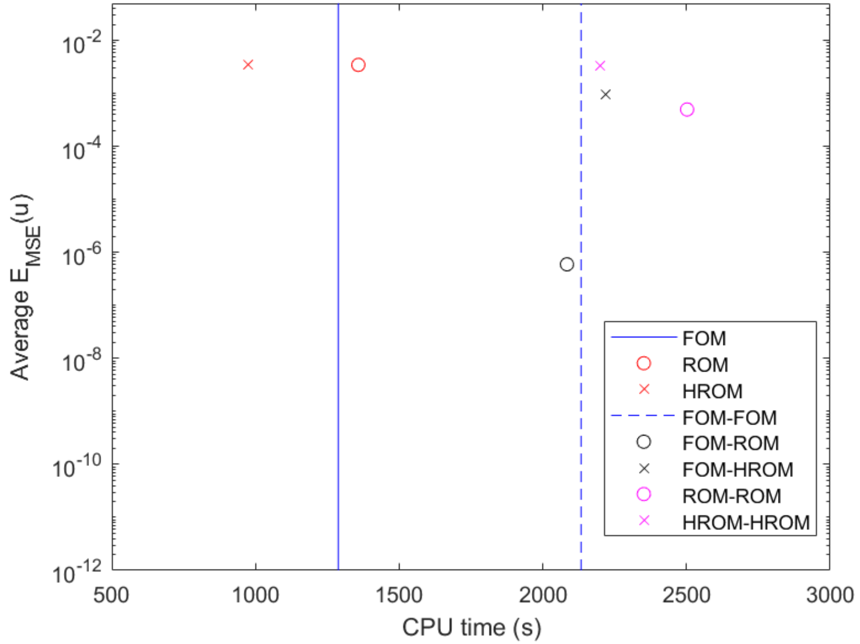


- Projection error suggests **predictive ROM** can achieve **accuracy** and **convergence** with **basis refinement**

- **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

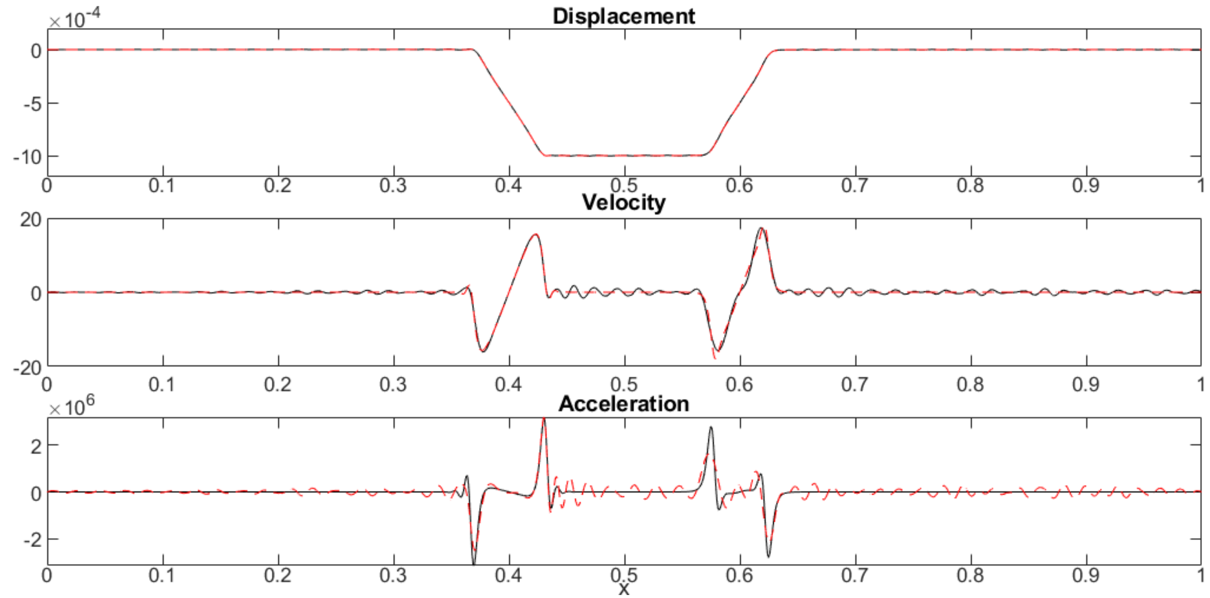
Numerical Example: Predictive Problem Results

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

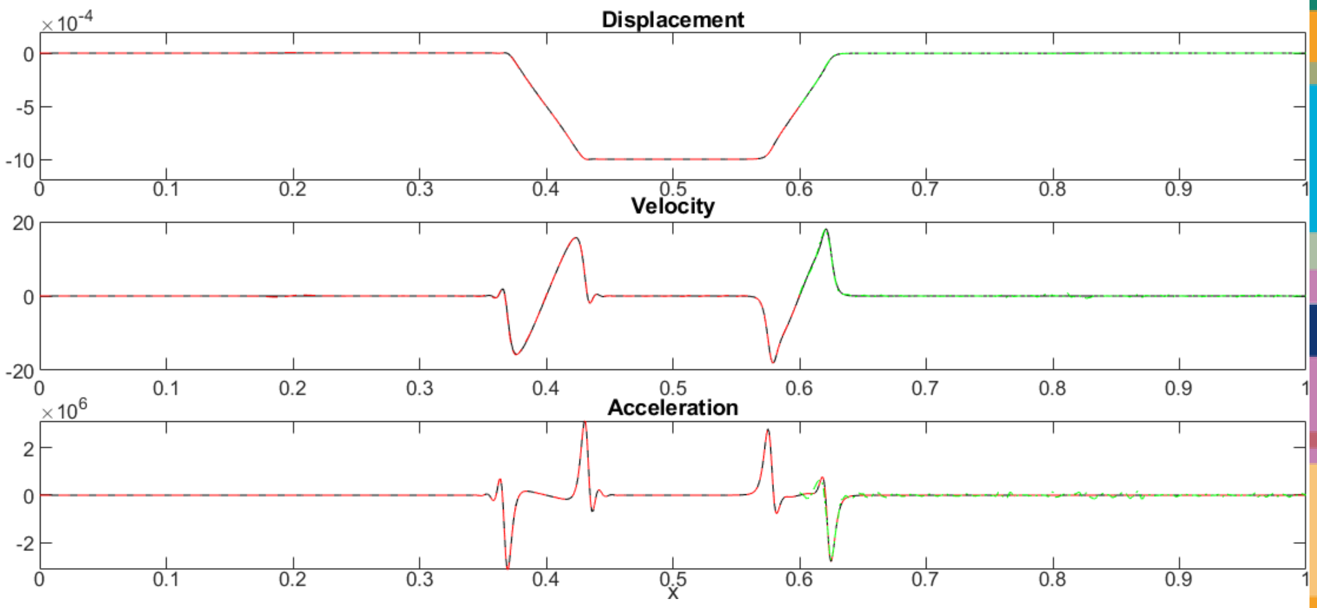


- Results indicate that **predictive accuracy/robustness** can be **improved** by **coupling** ROM or HROM to FOM
  - FOM-ROM coupling is **remarkably accurate**, achieving displacement error $O(1 \times 10^{-8})$
  - FOM-HROM and ROM-ROM couplings are **more accurate** than single-domain ROMs
  - HROM-HROM **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

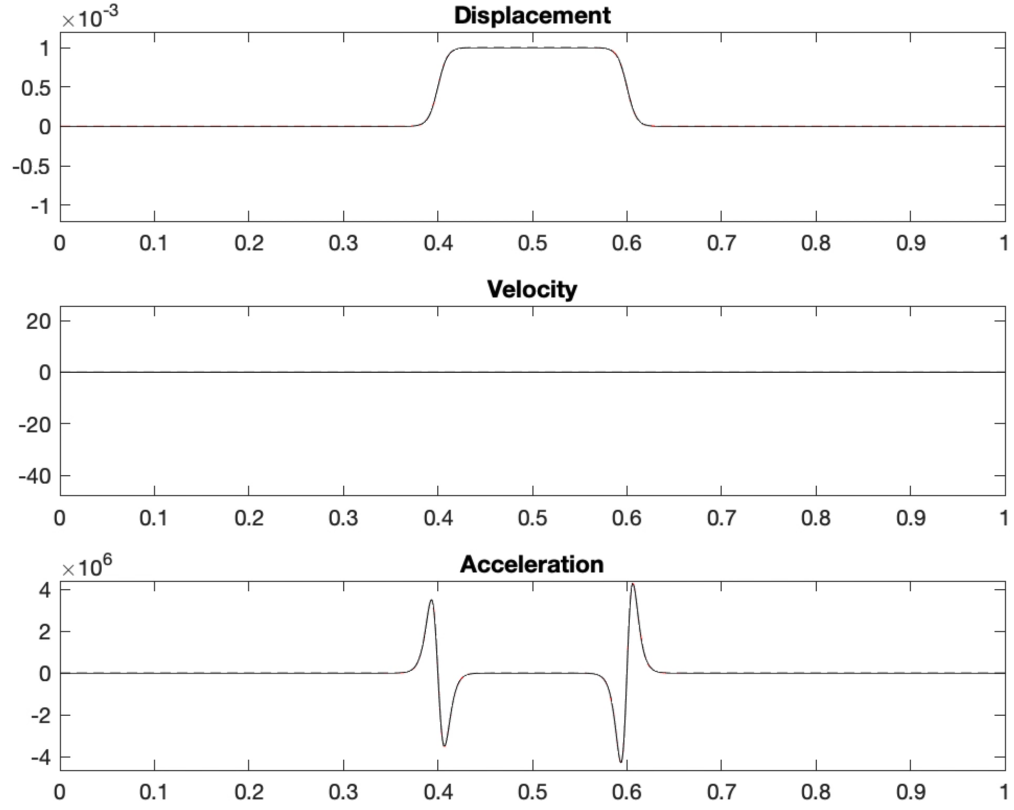


Predictive FOM-HROM (M_2= 200) solution at final time

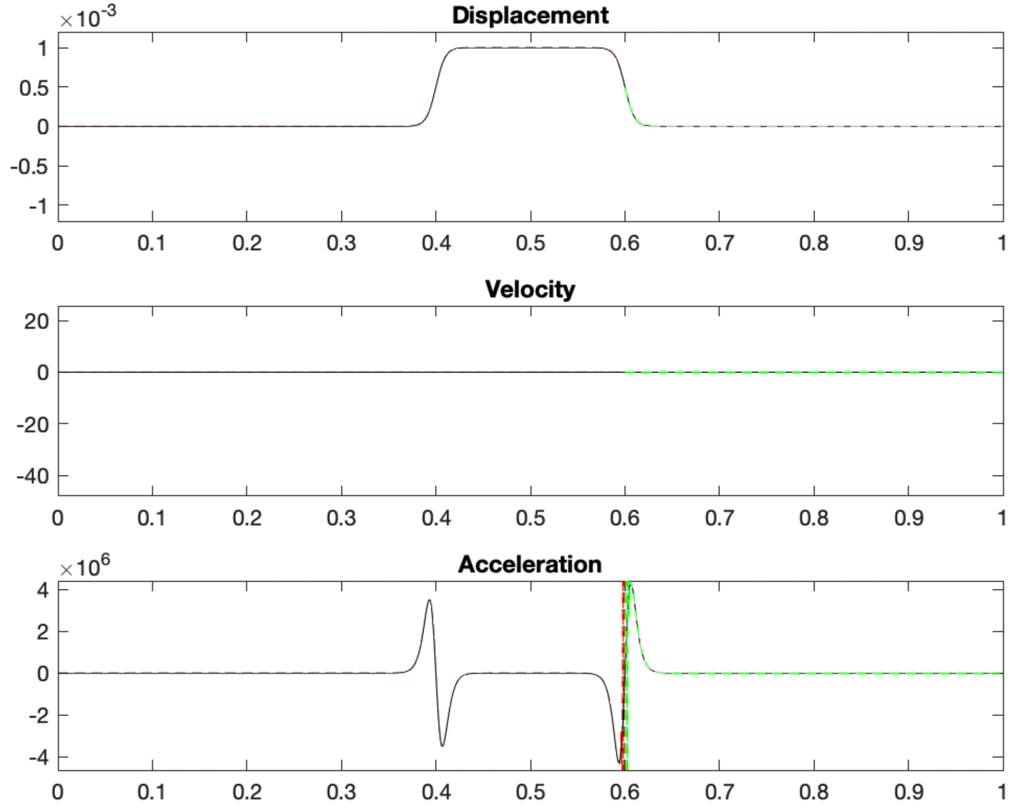
— Single-domain FOM solution — Solution in Ω_1 — Solution in Ω_2

- 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



Predictive single-domain ROM (M_1= 300)



Predictive FOM-HROM (M_2= 200)

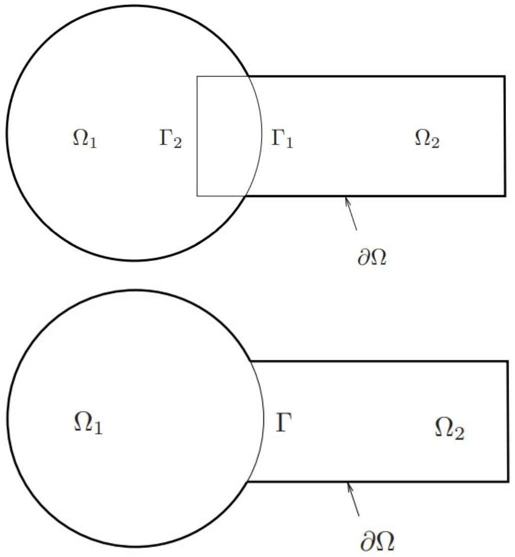
— Single-domain FOM solution — Solution in Ω_1 — Solution in Ω_2

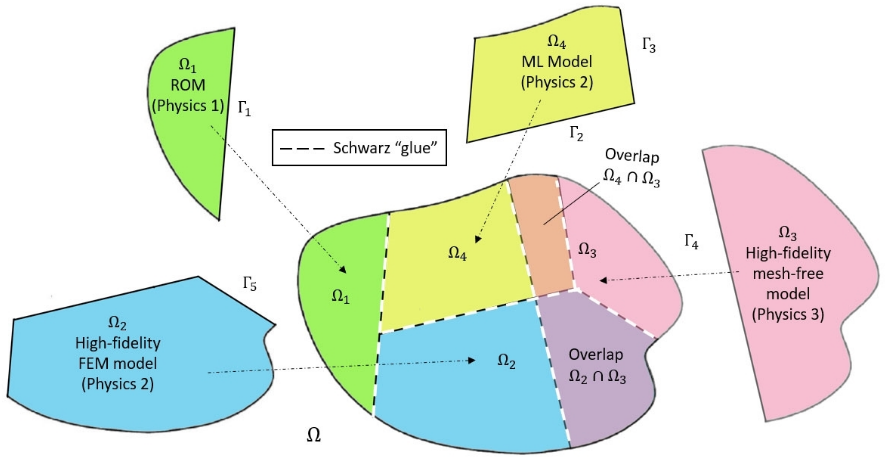
Outline

1. **The Alternating Schwarz Method for FOM*-ROM# and ROM-ROM Coupling**
   - Method Formulation
   - ROM Construction and Implementation
   - Numerical Example: Solid Mechanics
   - **Numerical Example: Fluid Mechanics**

2. Summary and Comparison of Methods

3. Future Work





*Full-Order Model. #Reduced Order Model.

Numerical Example: 2D Inviscid Burgers Problem

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

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

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

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

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

- Spatial discretization given by a **Godunov-type scheme** with N = 250 elements in each dimension
- Temporal discretization given by the **trapezoidal method** with fixed $\Delta t = 0.05$ where $T_f = 25.0$ for a total of 500 time steps
- Following coupled subdomains will occupy the same geometric footprint as the FOM with different solvers, resolution, and subdomain decomposition

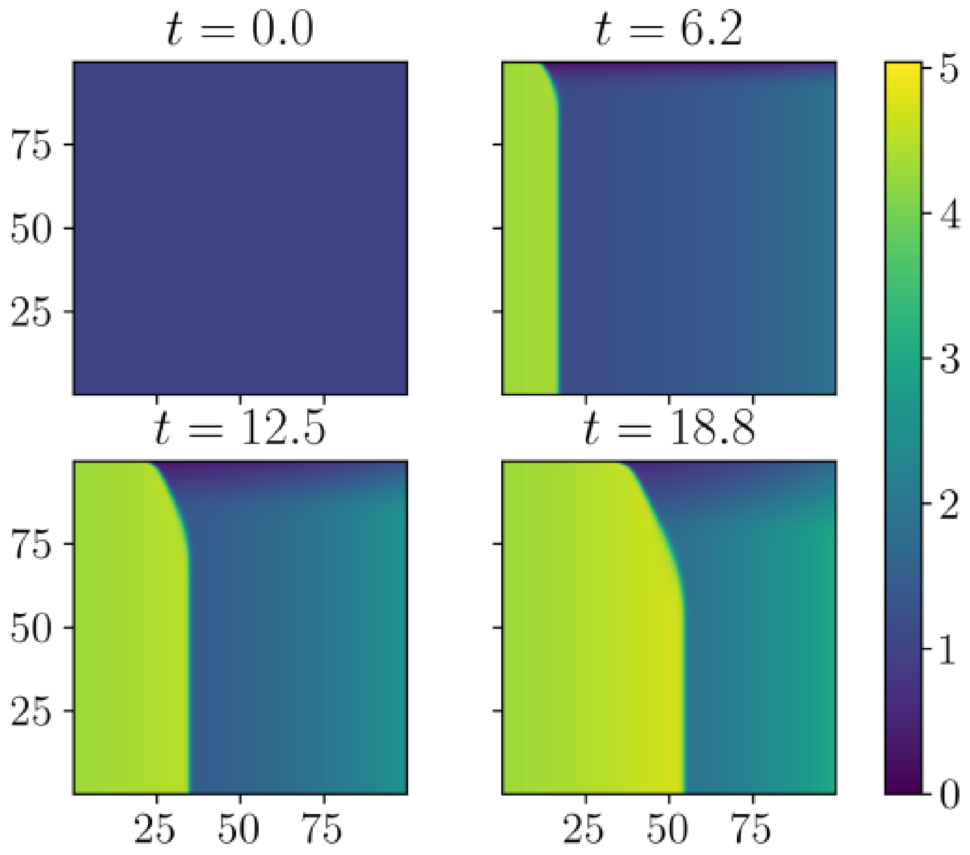
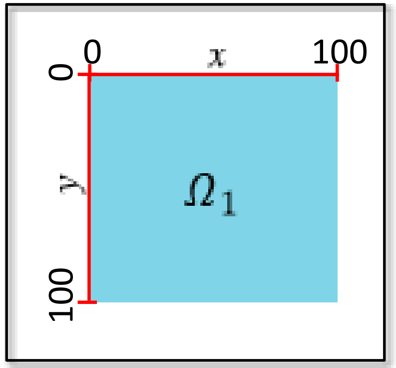
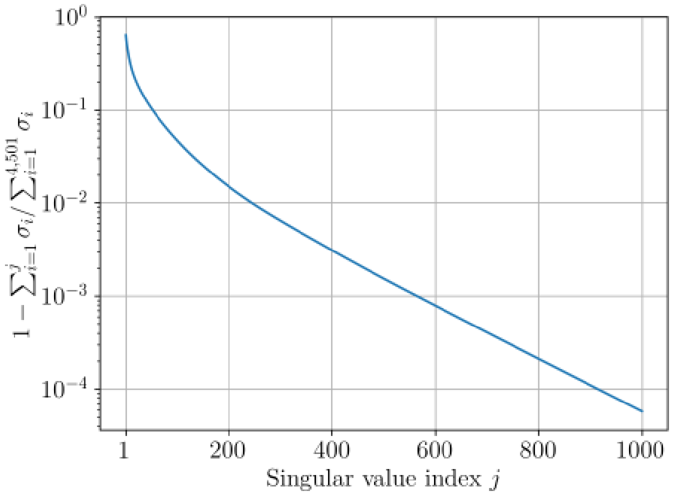


Figure above: solution of u component at various times



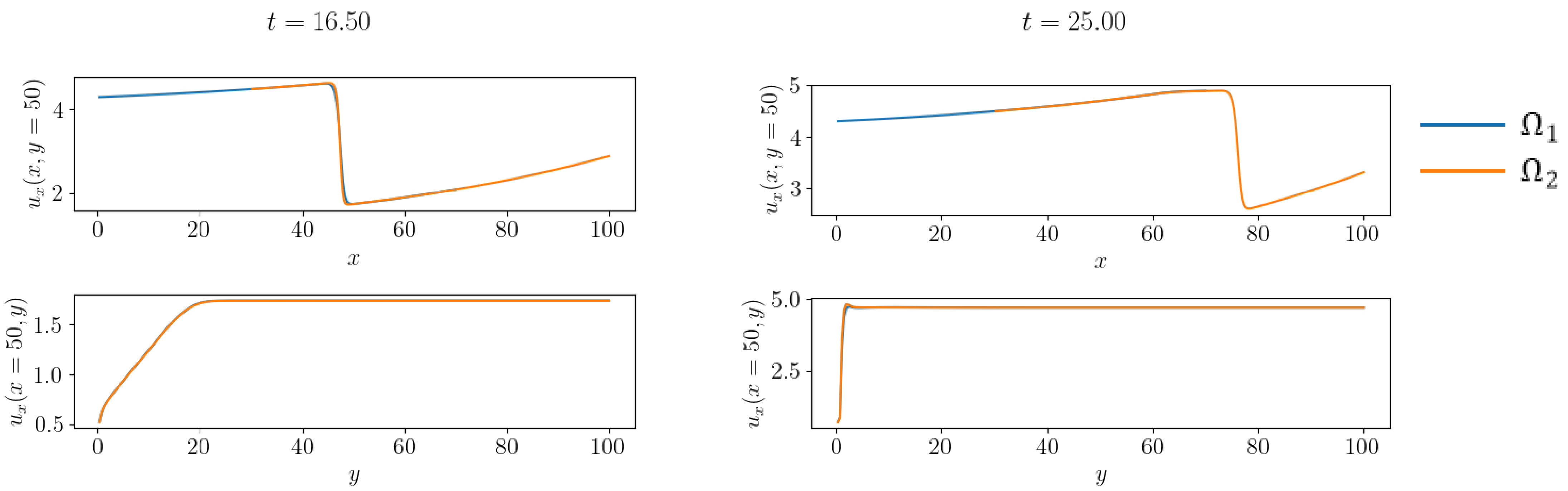
Numerical Example: 2D Inviscid Burgers Problem

- ***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, 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.

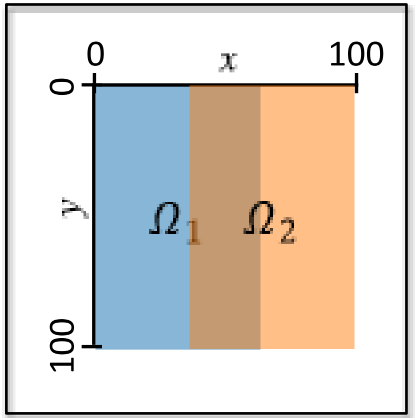
FOM-FOM Coupling: Differing Resolution



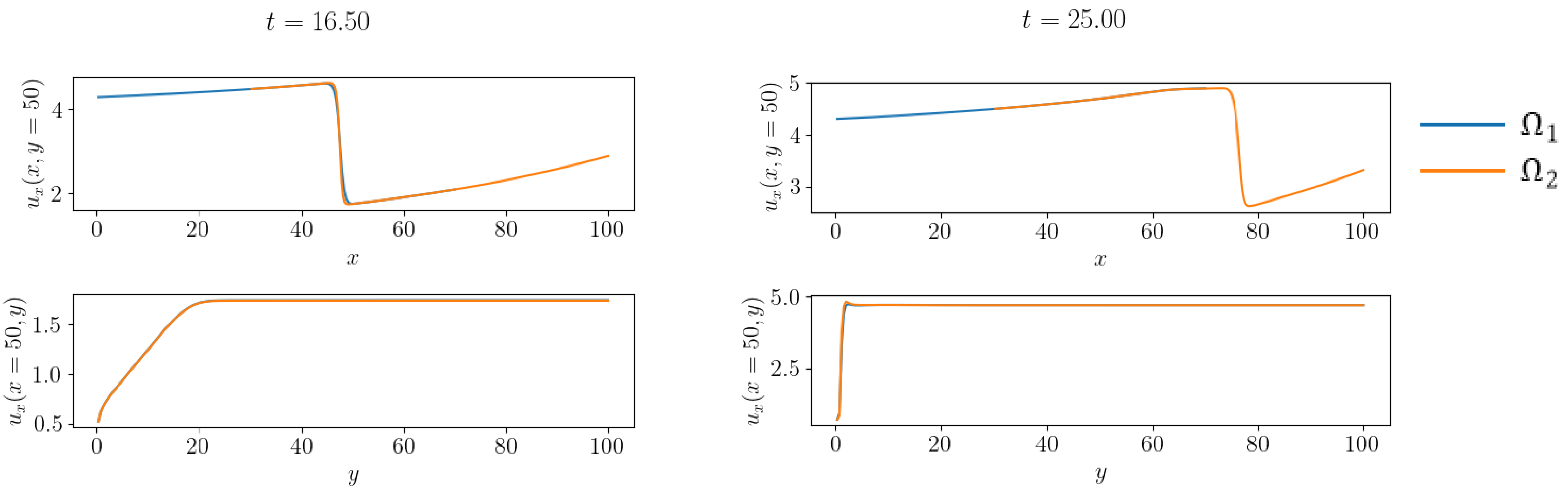
Figures above: Two-subdomain explicit-explicit overlapping coupling in x-axis [0, 70] U [30, 100] where $\mu = [4.3, 0.021]$, $\Delta t = 0.005$, $\Delta x_1 = 0.4, \Delta x_2 = 0.3$

- 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!

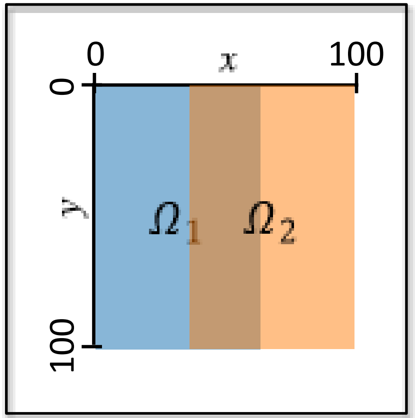


FOM-FOM Coupling: Differing Solvers

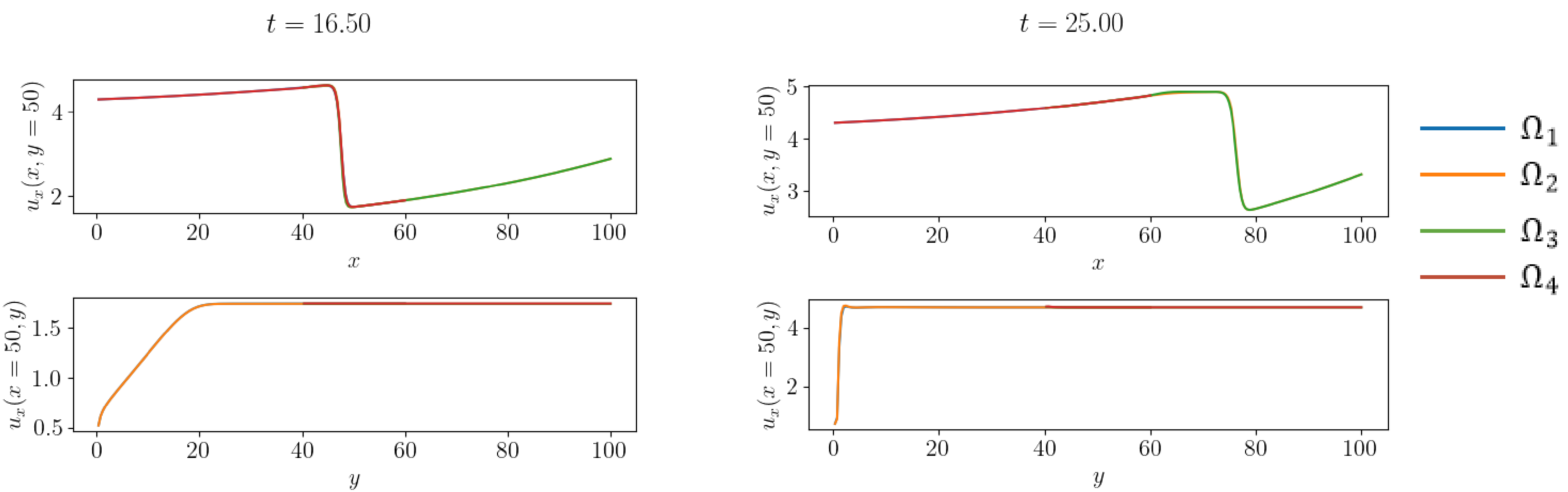


Figures above: Two-subdomain implicit-explicit overlapping coupling in x-axis [0, 70] U [30, 100], $\mu = [4.3, 0.021]$, $\Delta t_1 = 0.05$, $\Delta t_2 = 0.005$, $\Delta x_1 = 0.4, \Delta x_2 = 0.3$

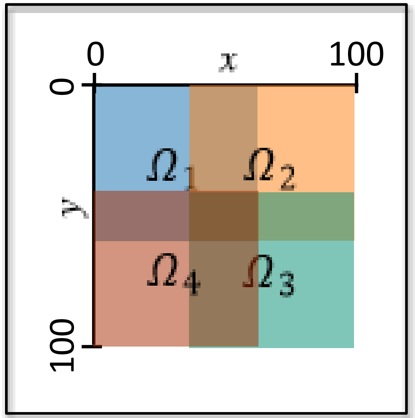
- Introducing a different time stepper in Ω_1 has not introduced artifacts and produces visually identical solution
- Choosing $\Omega_1 \rightarrow \Omega_2$ still only requires 2 Schwarz iterations per global time step



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

Single Domain ROM

- 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 $n = 95$
- 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).

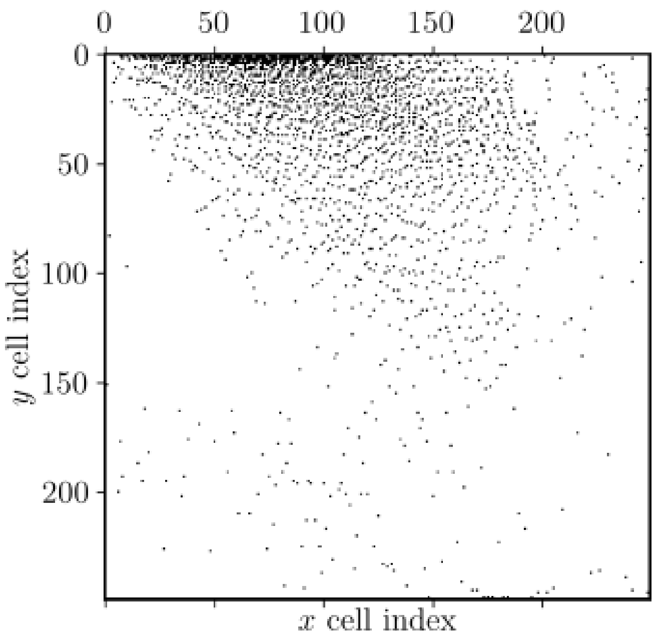


Figure above: Reduced mesh of single domain HROM

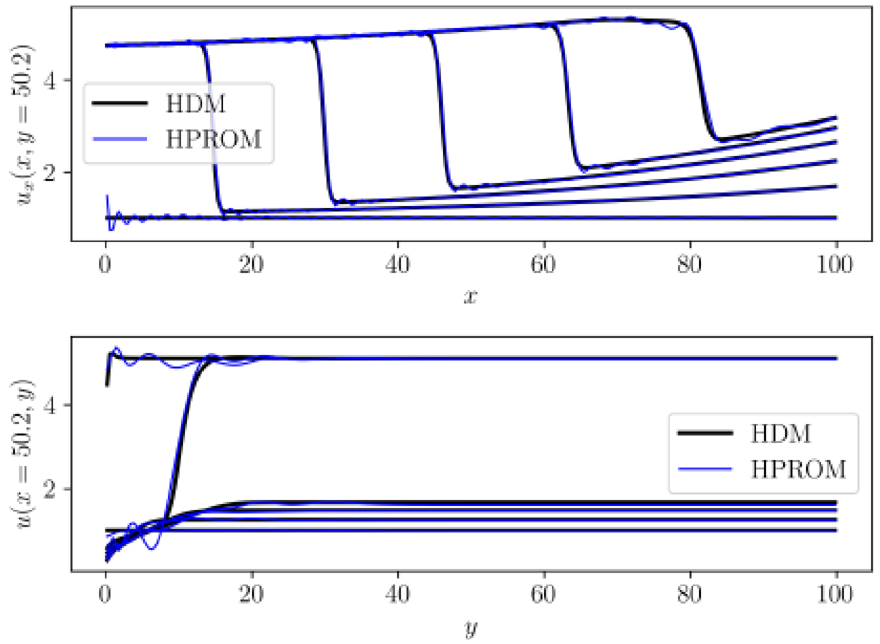
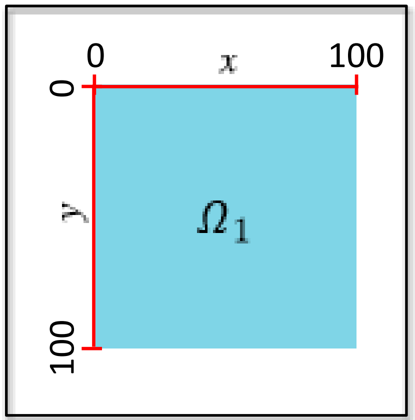


Figure above: HROM and FOM results at various time steps



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Sandia National Laboratories

LDRD
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[18] 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.

This talk

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Start of Backup Slides

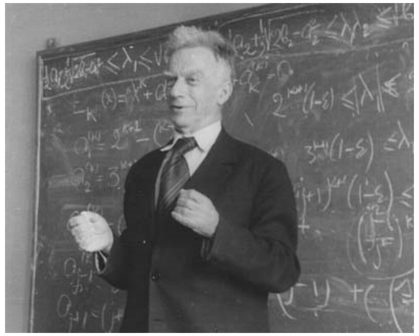
Theoretical Foundation

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

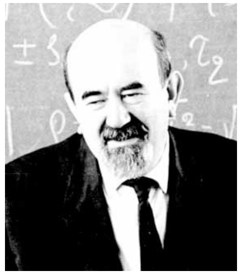
- S.L. Sobolev (1936): posed Schwarz method for ***linear elasticity*** in variational form and ***proved method's convergence*** by proposing a convergent sequence of energy functionals.
- S.G. Mikhlin (1951): ***proved convergence*** of Schwarz method for general linear elliptic PDEs.
- P.-L. Lions (1988): studied convergence of Schwarz for ***nonlinear monotone elliptic problems*** using max principle.
- A. Mota, I. Tezaur, C. Alleman (2017): proved ***convergence*** of the alternating Schwarz method for ***finite deformation quasi-static nonlinear PDEs*** (with energy functional $\boldsymbol{\Phi}[\boldsymbol{\varphi}]$) with a ***geometric convergence rate.***

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

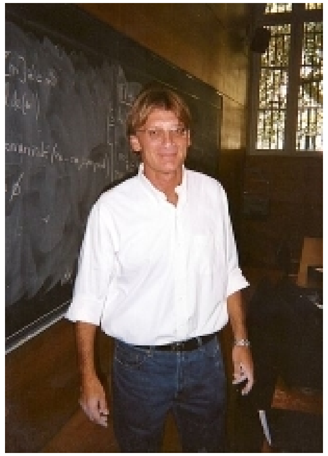
$$\nabla \cdot \boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



S.L. Sobolev (1908 – 1989)



S.G. Mikhlin (1908 – 1990)

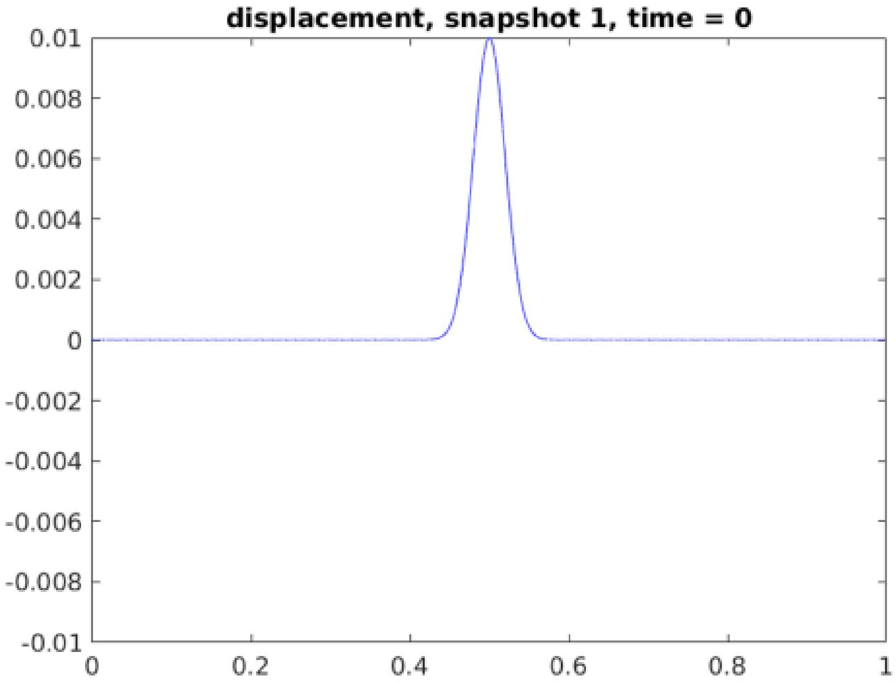


P.- L. Lions (1956-)

A. Mota, I. Tezaur, C. Alleman

Numerical Example: Linear Elastic Wave Propagation Problem

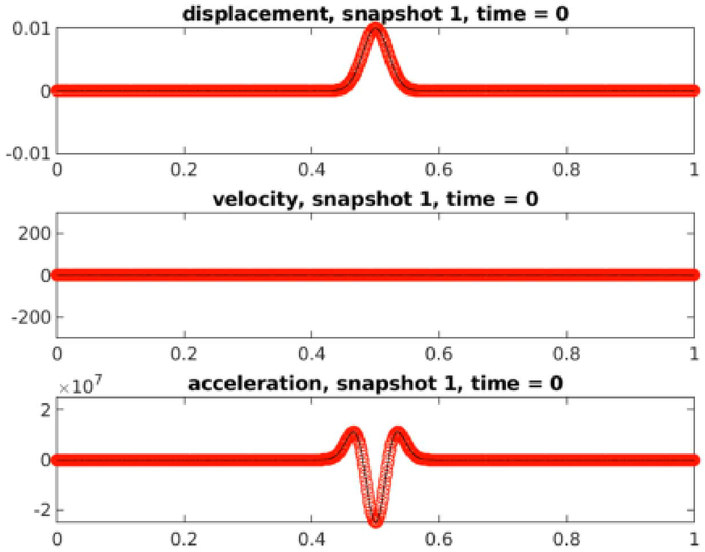
- Linear elastic ***clamped beam*** with Gaussian initial condition.
- Simple problem with analytical exact solution but very ***stringent test*** for discretization/coupling methods.
- ***Couplings tested:*** FOM-FOM, FOM-ROM, ROM-ROM, implicit-explicit, implicit-implicit, explicit-explicit.
- ROMs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



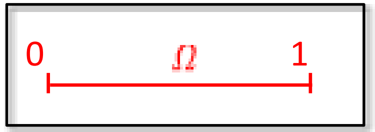
Above: 3D rendering of clamped beam with Gaussian initial condition. *Right*: Initial condition (blue) and final solution (red). Wave profile is negative of initial profile at time T = 1.0e-3.

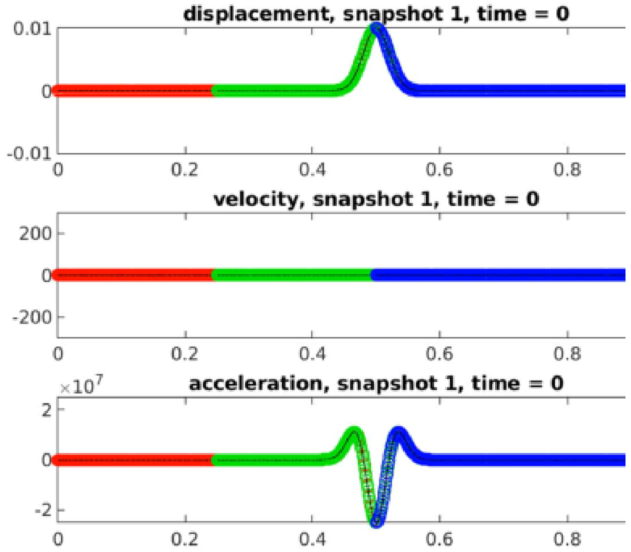
Linear Elastic Wave Propagation Problem: FOM-ROM and ROM-ROM Couplings

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

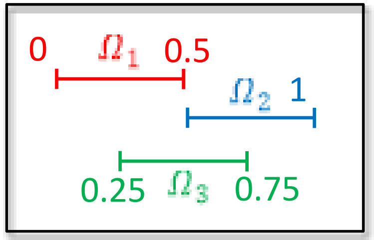


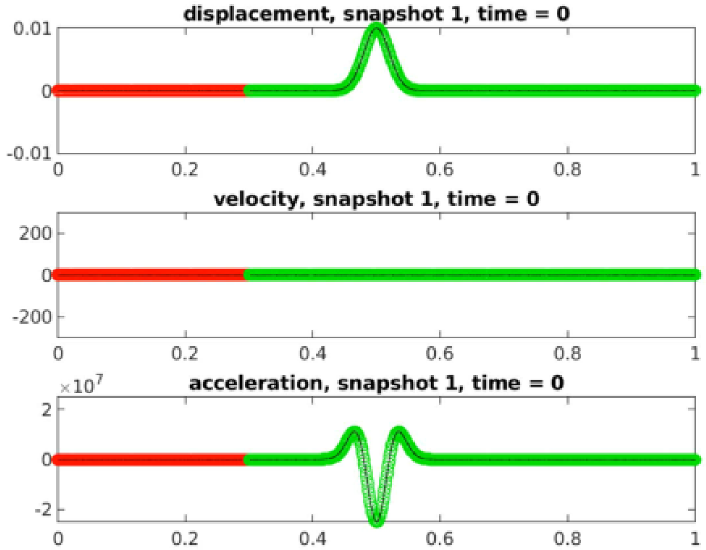
Single Domain FOM



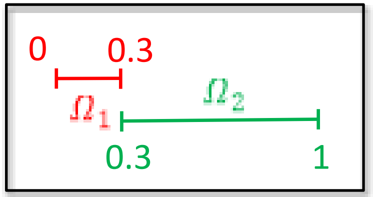


3 overlapping subdomain ROM[1]-FOM[2]-ROM[3]





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

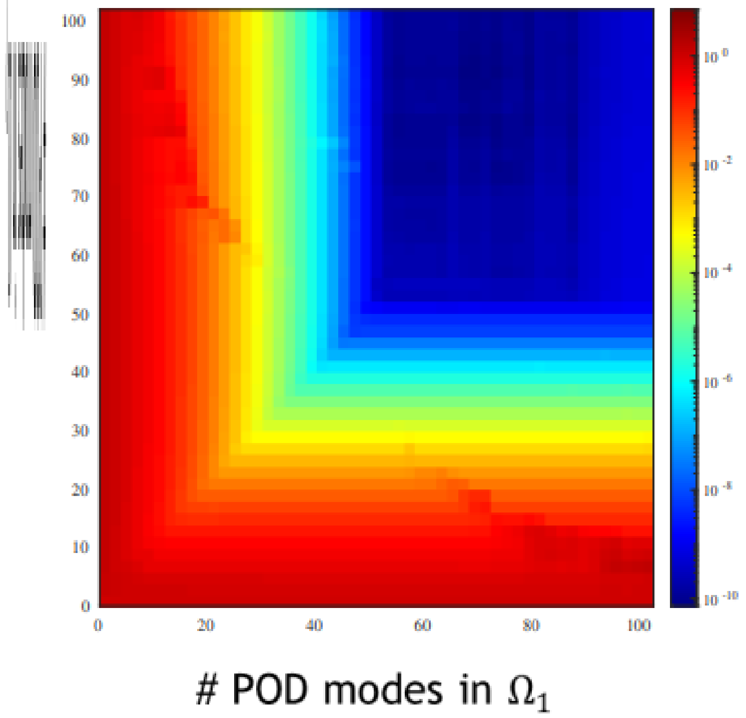
[1]Implicit 40 mode POD ROM, Δt =1e-6, Δx =1.25e-3
[2]Implicit FOM, Δt =1e-6, Δx =8.33e-4
[3]Explicit 50 mode POD ROM, Δt =1e-7, Δx =1e-3
[4]Implicit FOM, Δt =2.25e-7, Δx =1e-6
[5]Explicit 50 mode POD ROM, Δt =2.25e-7, Δx =1e-6

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

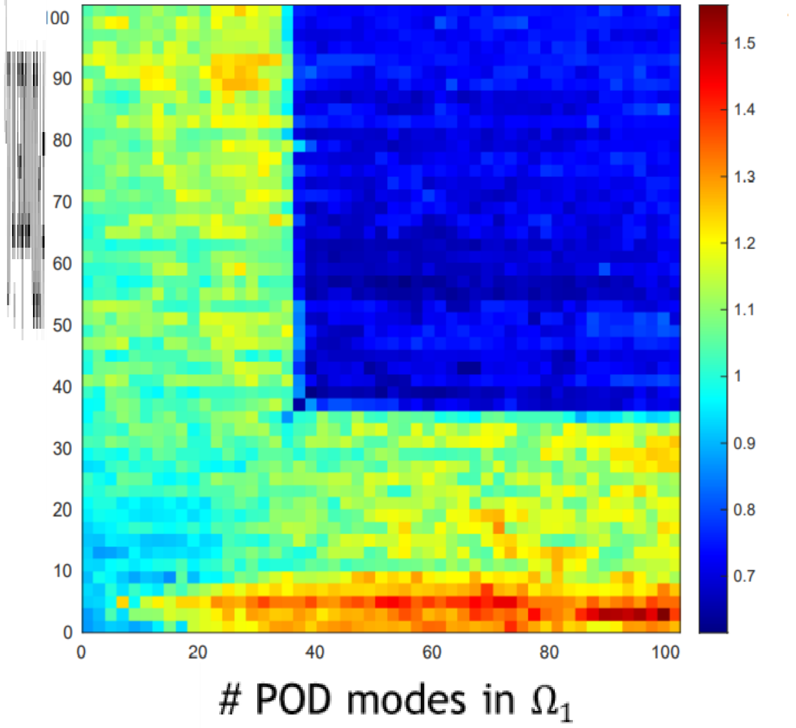
Linear Elastic Wave Propagation Problem: ROM-ROM Couplings

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

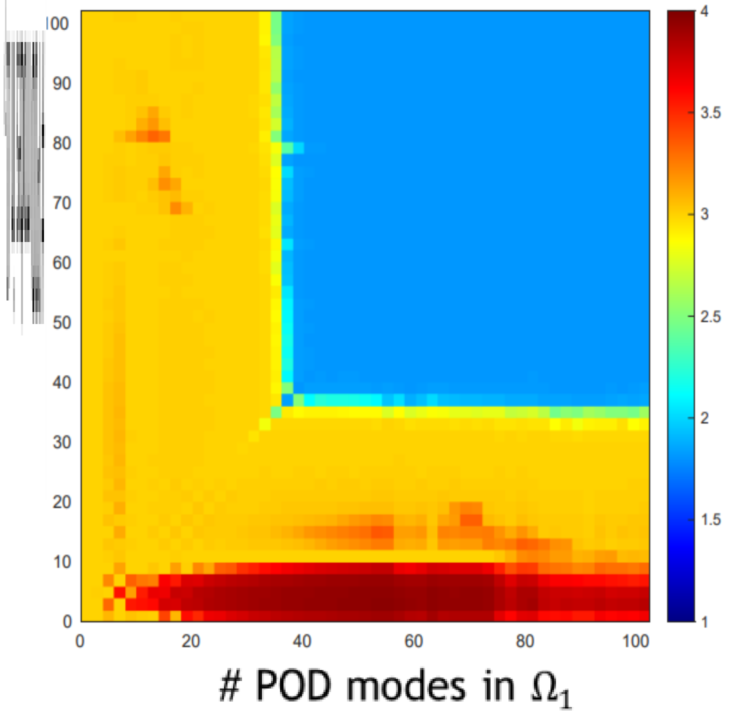
MSE in displacement for 2 subdomain ROM-ROM coupling



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



Average # Schwarz iterations for 2 subdomain ROM-ROM coupling



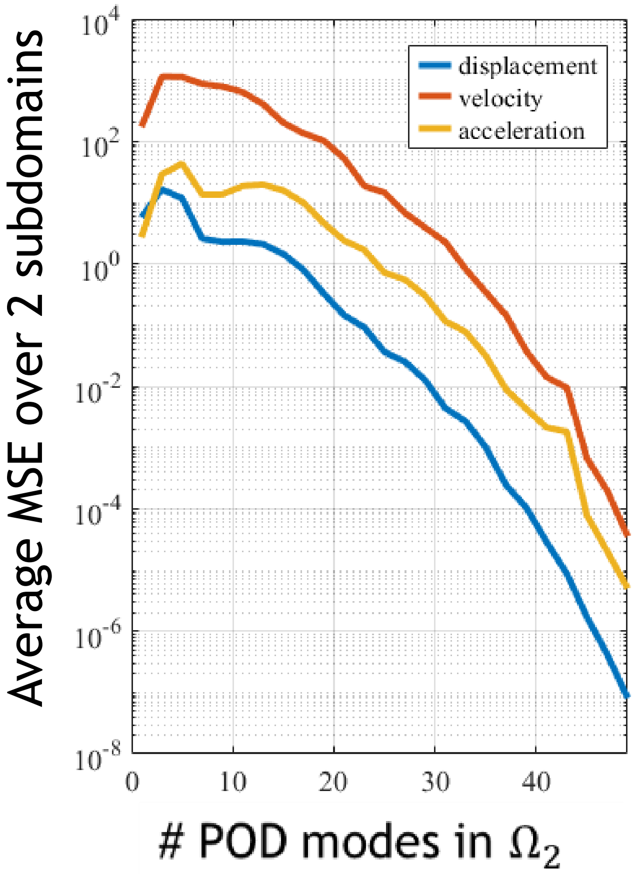
- **Smaller ROMs** are **not** the **fastest**: less accurate & require more Schwarz iterations to converge.
- All couplings converge in $\leq$ **4 Schwarz iterations** on average (FOM-FOM coupling requires average of 2.4 Schwarz iterations).

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

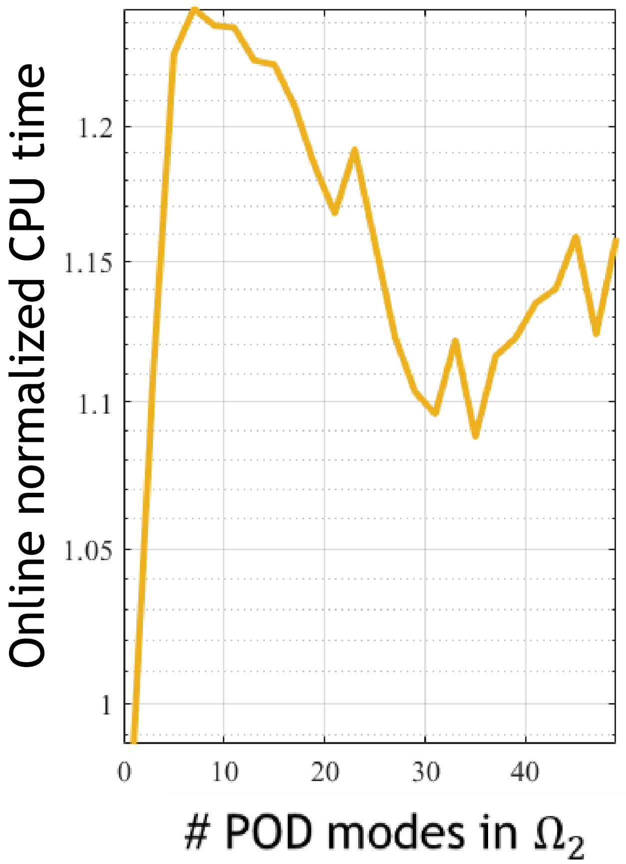
Linear Elastic Wave Propagation Problem: FOM-ROM Couplings

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.

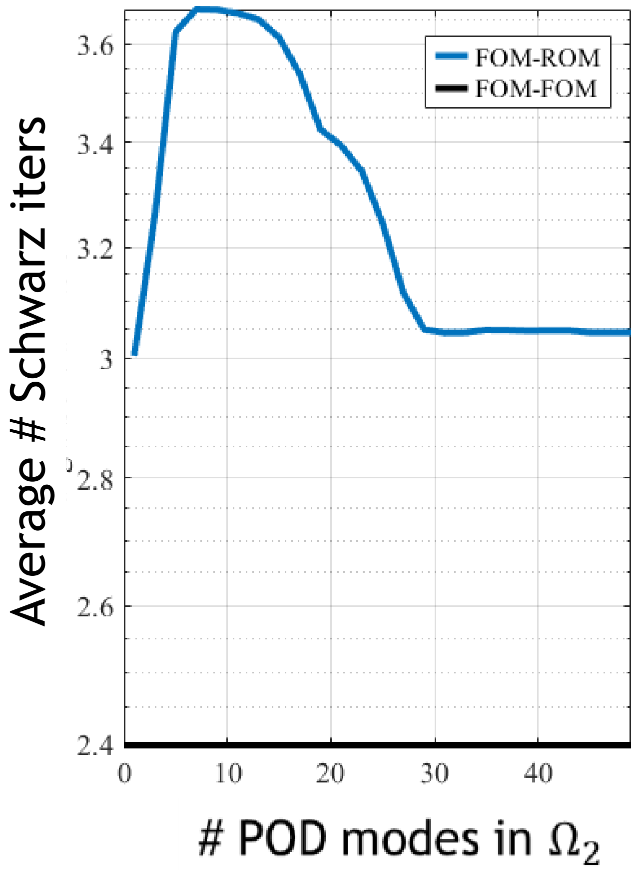
MSE for 2 subdomain FOM-ROM coupling



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



Average # Schwarz iterations for 2 subdomain couplings

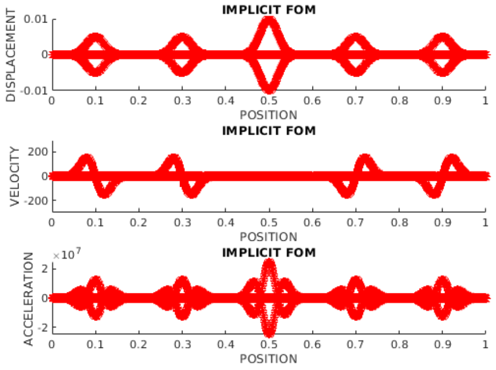


WIP: *understanding & improving FOM-ROM coupling performance.*

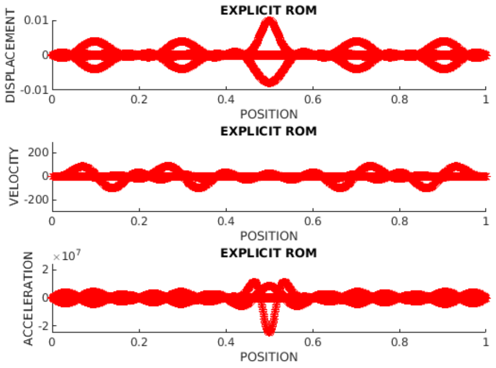
Overlapping implicit-implicit coupling with $\Omega_1 = [0, 0.75]$, $\Omega_2 = [0.25, 1]$

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

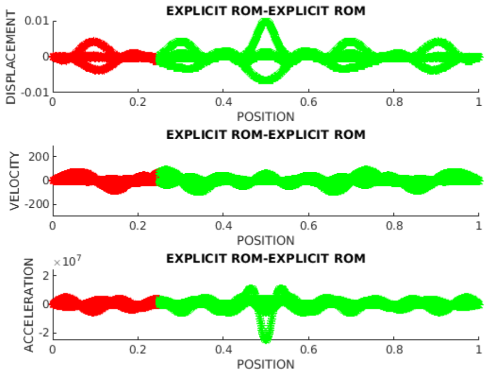
Inaccurate model + accurate model ≠ accurate model.



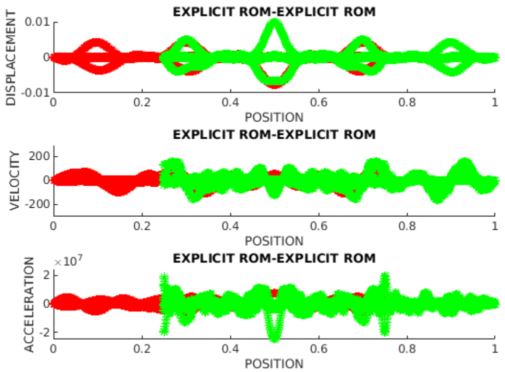
Single Domain, FOM (truth)



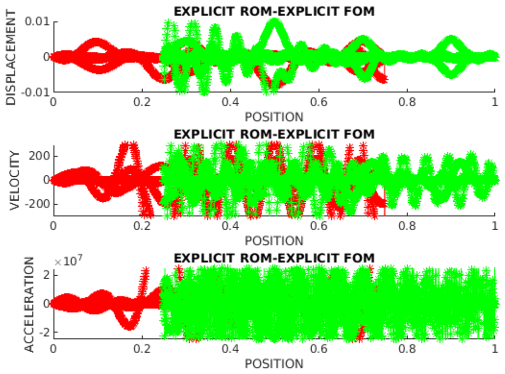
Single Domain, 10 mode POD



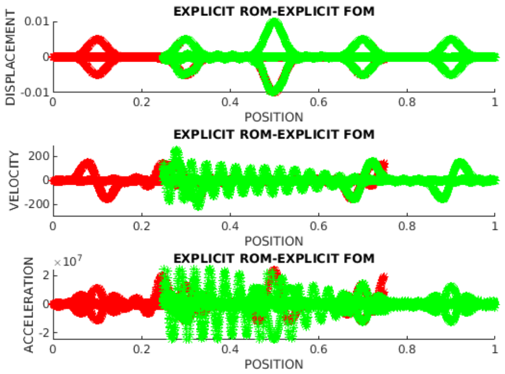
10 mode POD – 10 mode POD



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

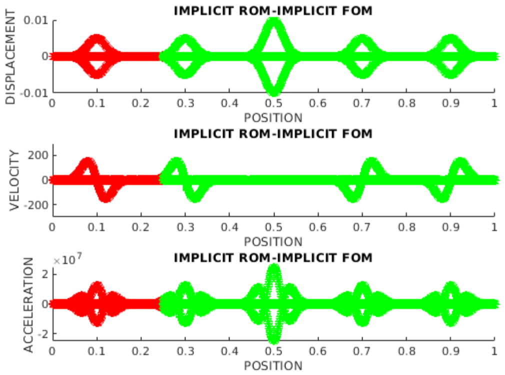
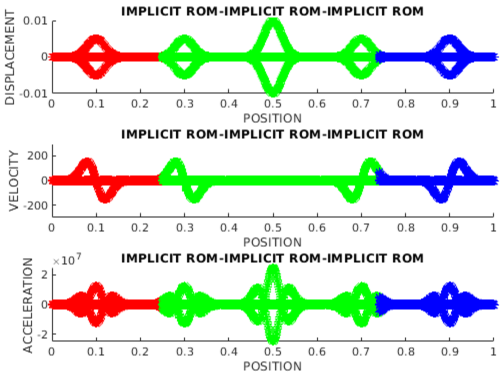


Figure above: $\Omega_1 = [0, 0.3]$, $\Omega_2 = [0.25, 1]$, 20 mode POD - FOM

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



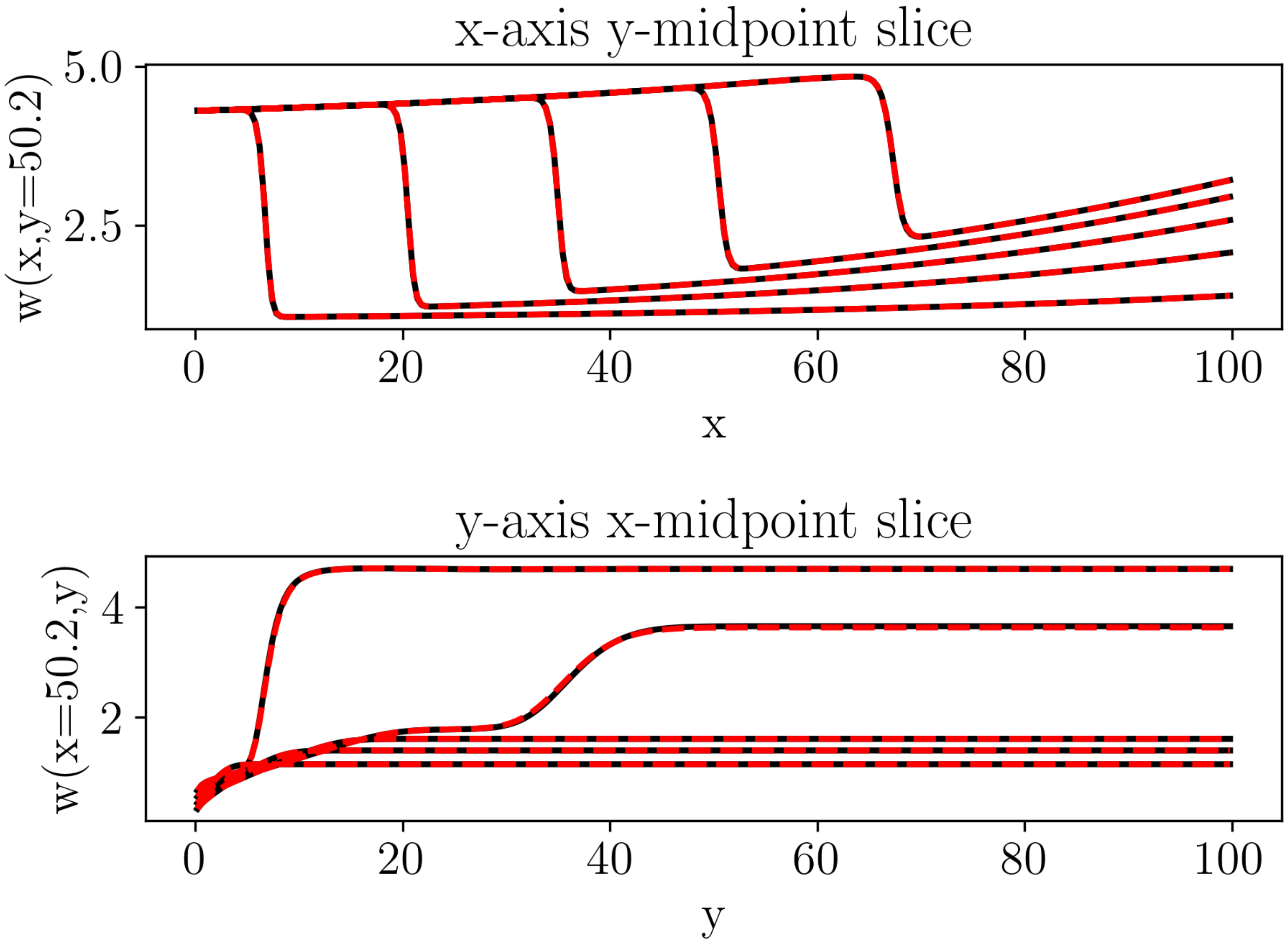
Roadmap

- Demonstrate FOM-FOM coupling with varying time-steps, domain resolutions, and time-stepping schemes
  - Try out splitting domain into four sections
- Develop FOM-ROM, ROM-ROM, HROM-HROM coupling
- Time permitting
  - Adaptive time-stepping based on local CFL number in given domain
  - OR adaptively switch to implicit time stepping after shock has left domain
  - Nonlinear approximation manifolds

2D Burgers: Verifying Implicit Implementation

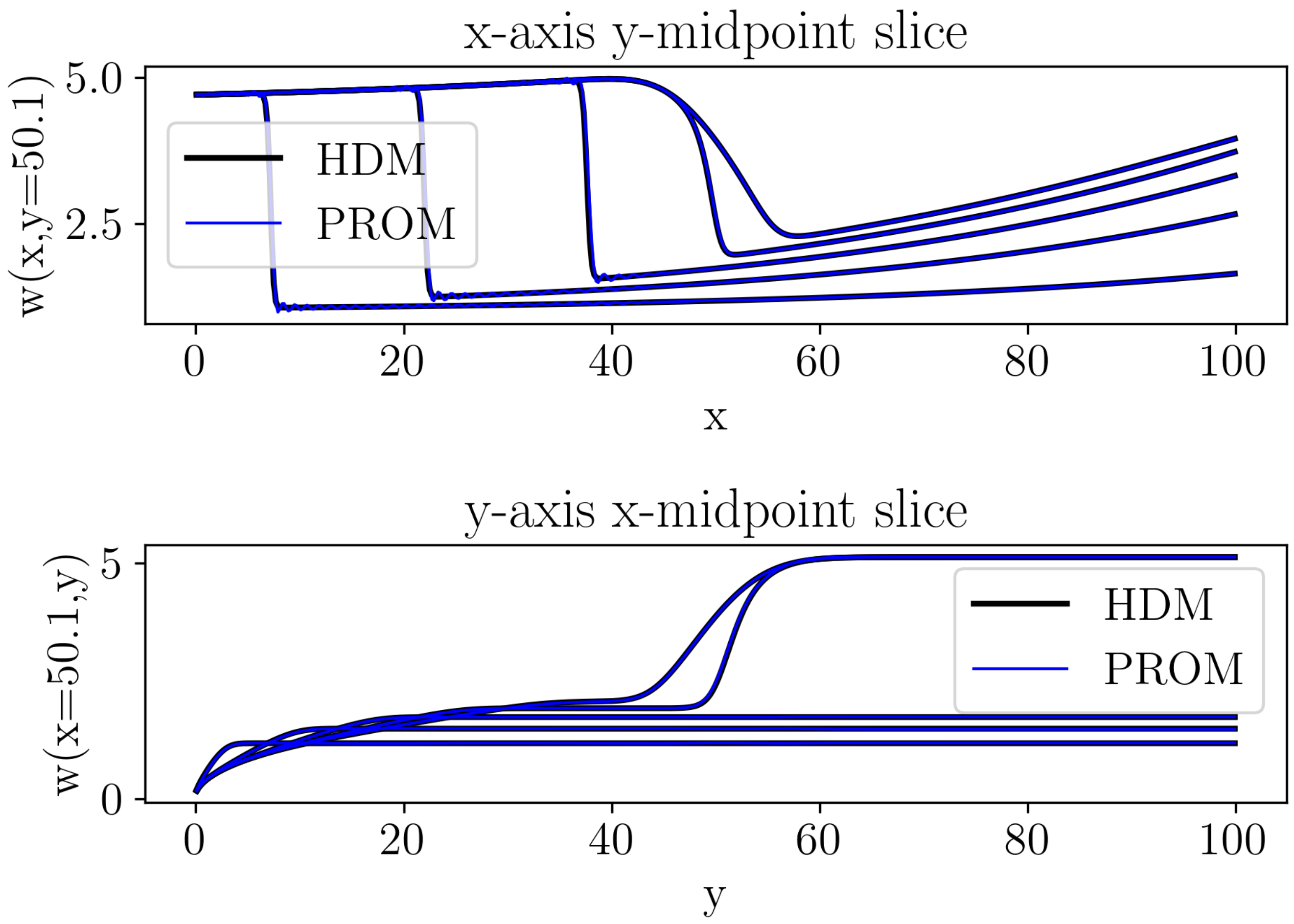
- The plot to the right shows the solution of the u component at various times along **mid-axis slices of the 2D domain**

- FOM and ROM solutions are the **same**



2D Burgers: LSPG PROM

- **Predictive case** where **μ** = [4.7, 0.026]
- Train bases using **9 total runs** of the FOM with all combinations of μ_1 = [(4.25),(4.875),(5.5)] with μ_2 = [(0.015),(0.0225),(0.03)]
- Using 113 POD modes
- Relative error of 0.61%
- 321 s wall clock time

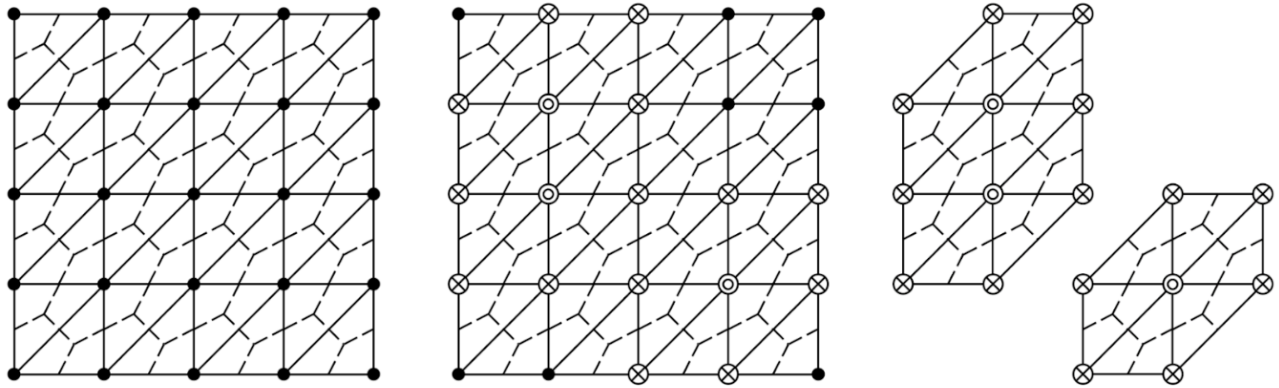


Energy-Conserving Sampling and Weighting (ECSW)

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

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

- We can then form the **system**

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

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

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

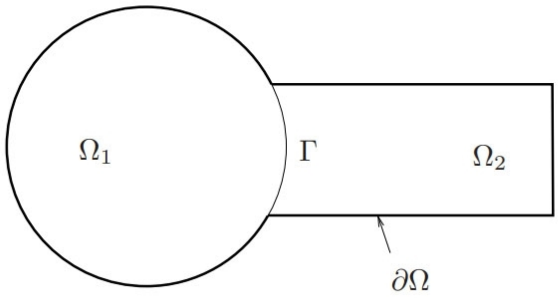
- Solve the above optimization problem using a **non-negative least squares solver** with an **early termination condition** to **promote sparsity** of the vector $\boldsymbol{\xi}$

Numerical Example: 1D Dynamic Wave Propagation Problem

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

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

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



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

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

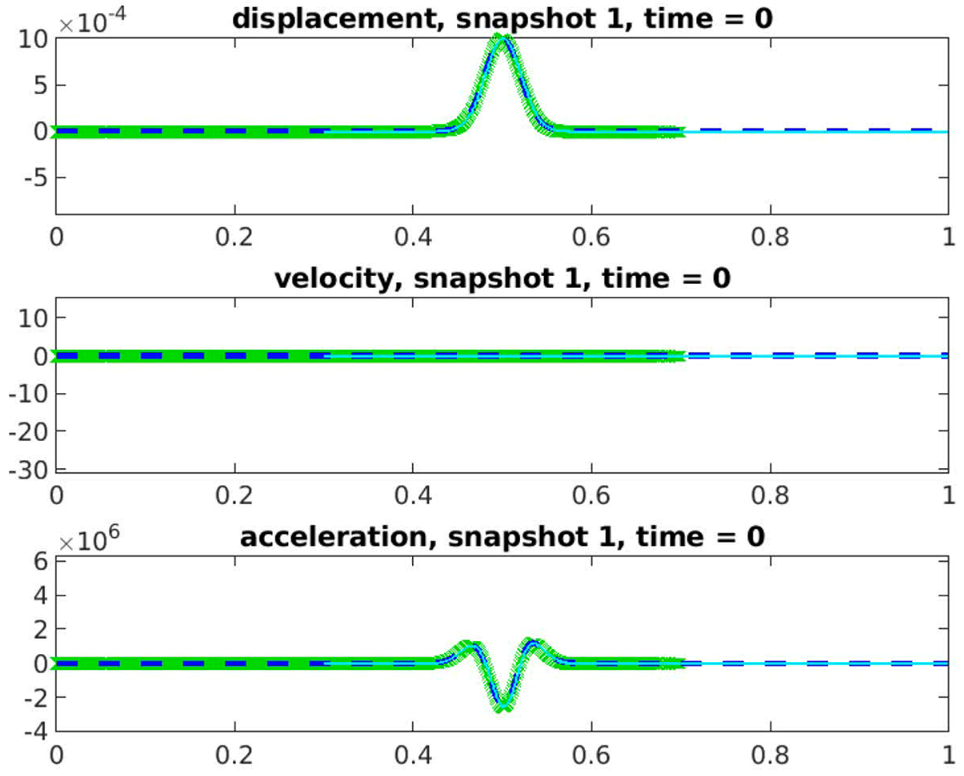
  - A **parameter sweep study** revealed $\theta = 0$ gave best performance (min # Schwarz iterations)

- 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)**:

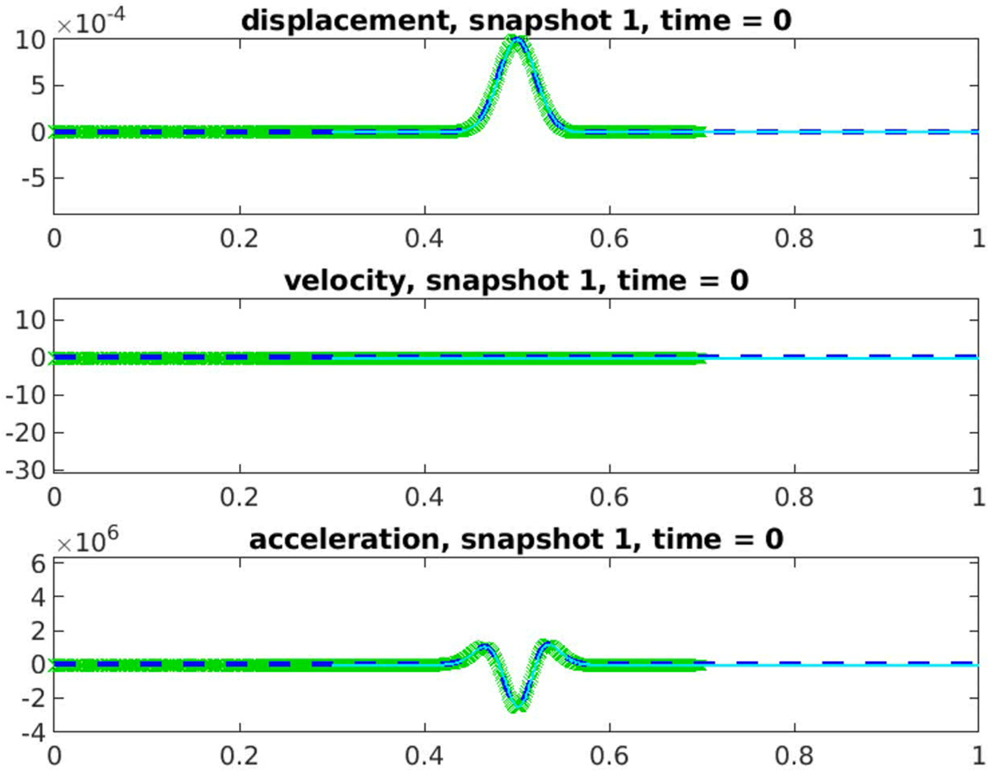
$$\varepsilon_{MSE}(\tilde{\boldsymbol{u}}_i) := \frac{\sqrt{\sum_{n=1}^{S} ||\tilde{\boldsymbol{u}}_i^n - \boldsymbol{u}_i^n||_2^2}}{\sqrt{\sum_{n=1}^{S} ||\boldsymbol{u}_i^n||_2^2}}$$

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.

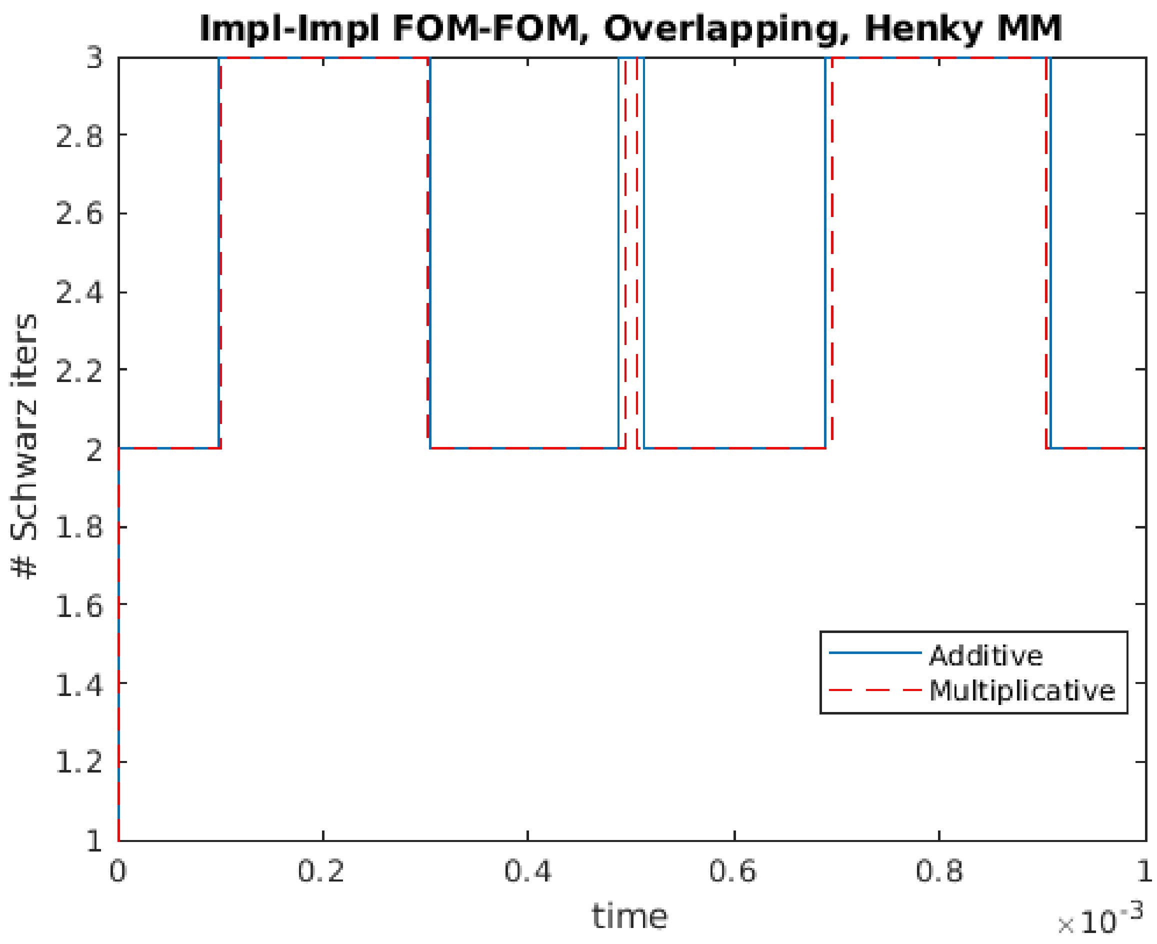


Multiplicative Schwarz



Additive Schwarz

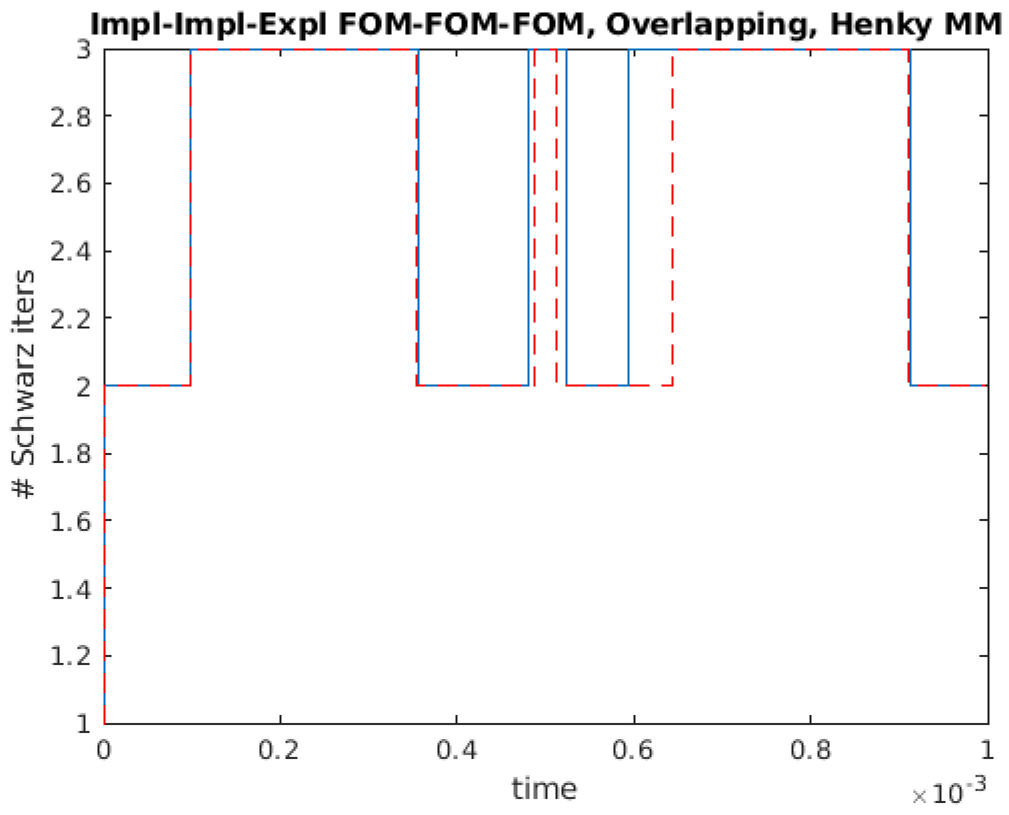
Overlapping Coupling, Nonlinear Henky MM, 2 Subdomains



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

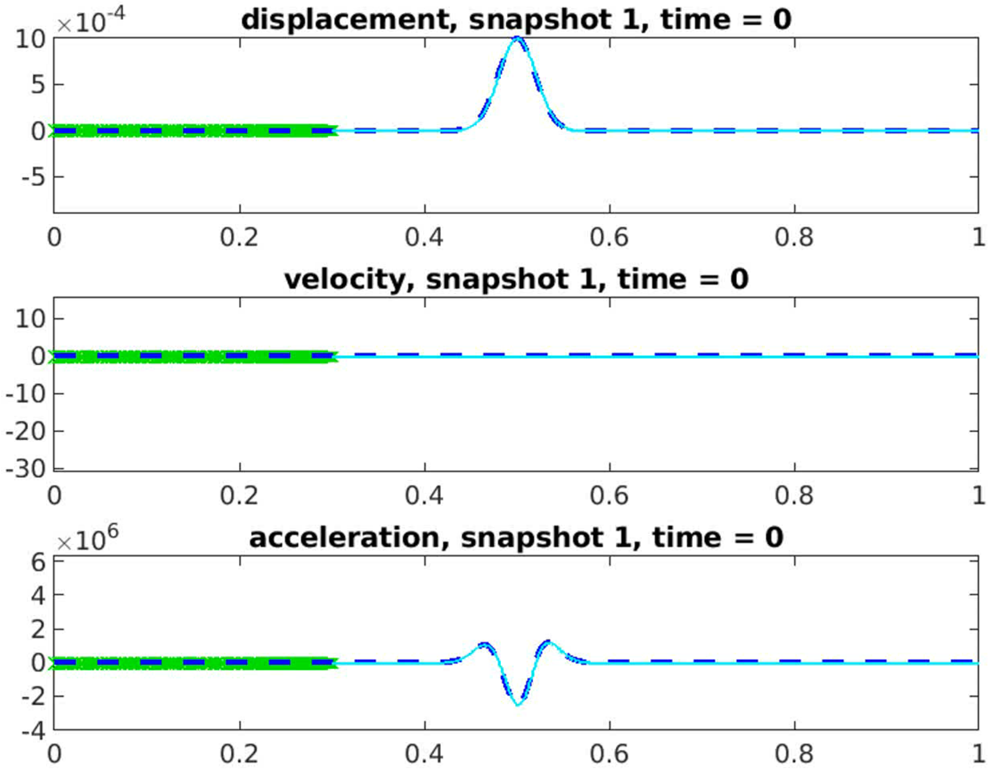


- $\Omega = [0, 0.3] \cup [0.25, 0.75] \cup [0.7, 1]$, implicit-implicit-explicit FOM-FOM-FOM coupling, dt = 1e-7, dx = 0.001.
- Solutions agree effectively to machine precision in mean square (MS) sense.
- Additive Schwarz has slightly more Schwarz iterations but is slightly faster than multiplicative.

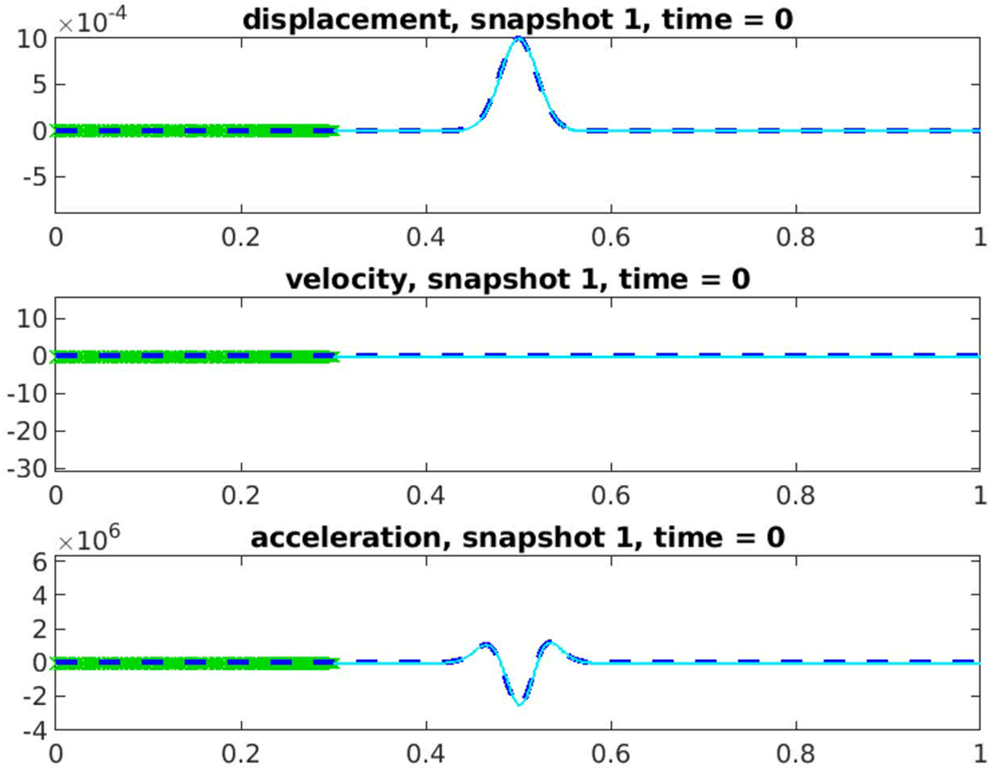
	Additive	Multiplicative
Total # Schwarz iters	26231	25459
CPU time	1.89e3s	2.05e3s
MS difference in disp	5.3052e-13/9.3724e-13/6.1911e-13	
MS difference in velo	7.2166e-12/2.2937e-11/2.4975e-11	
MS difference in acce	2.8962e-10/1.1042e-09/1.6994e-09	

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.

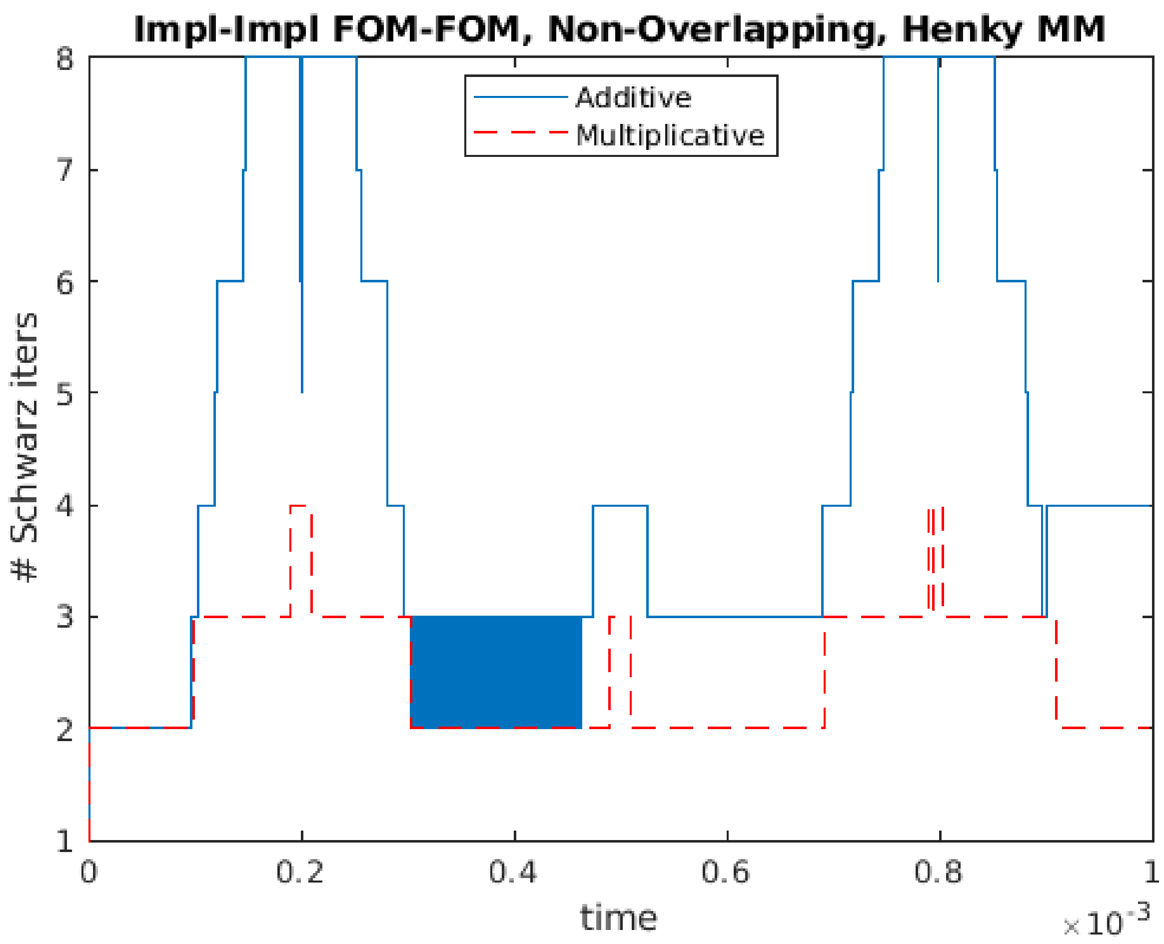


Multiplicative Schwarz



Additive Schwarz

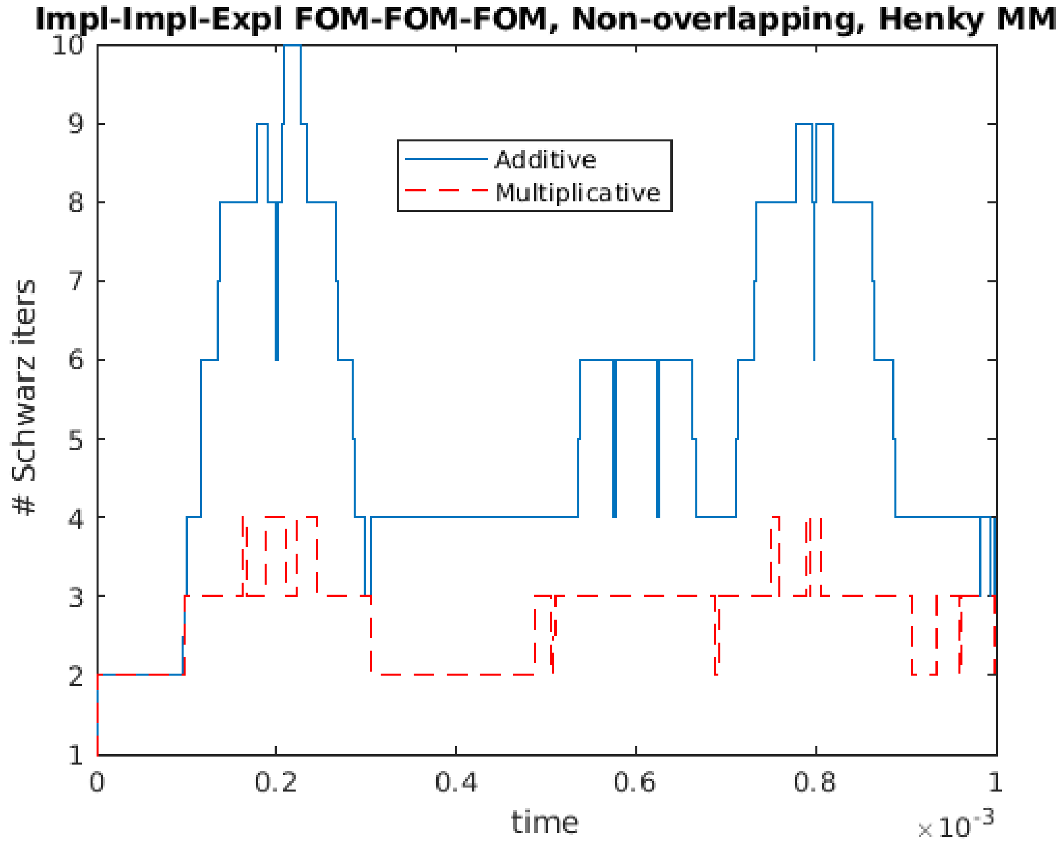
Non-overlapping Coupling, Nonlinear Henky MM, 2 Subdomains



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