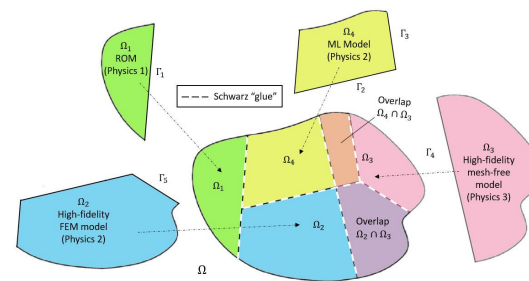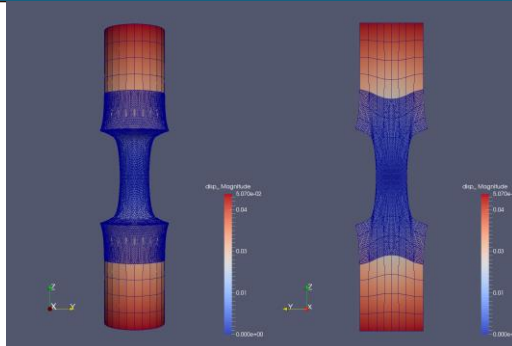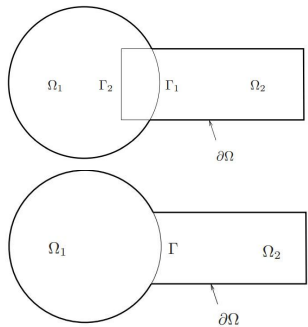# Alternating Schwarz-based coupling of conventional and data-driven models

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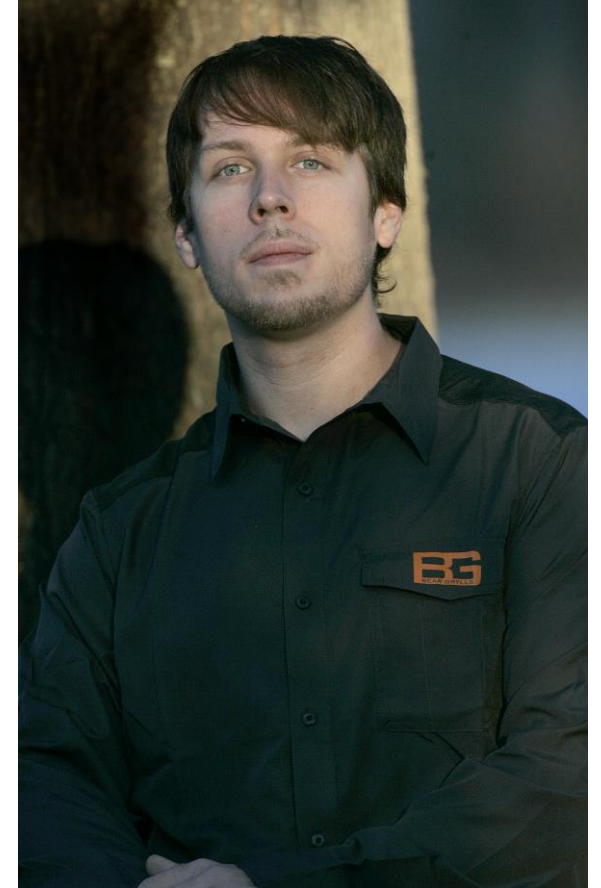Chris Wentland[1], Will Snyder[1,3]

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

COUPLED 2023
Chania, Greece, June 5-7, 2023

SAND2023-04302C

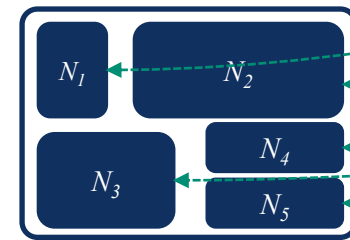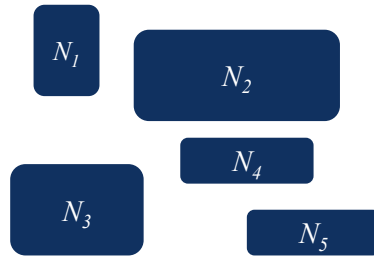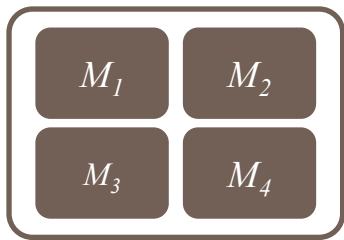# In memory of minisymposium co-organizer K. Chad Sockwell

April 30, 1991 – May 18, 2022

# 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)

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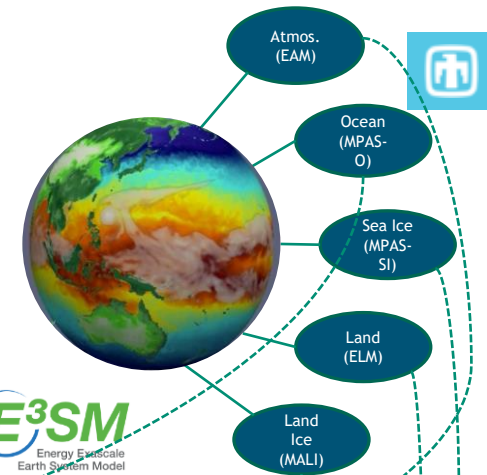- Nonlocal integral
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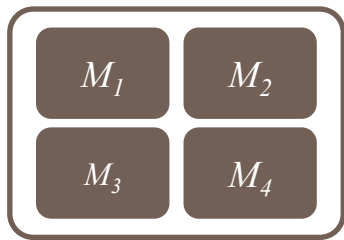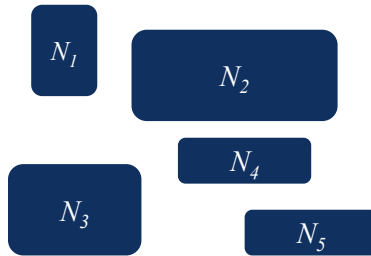- Iterative (Schwarz, optimization)

**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 Project, Models and Methods

> **fHNM (flexible Heterogeneous Numerical Methods) Project:**
> aims to **discover** the mathematical principles guiding the **assembly** of **standard** and **data-driven numerical models** in stable, accurate and physically consistent ways

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

- *Class A:* projection-based reduced order models (ROMs)
- *Class B:* machine-learned models, i.e., Physics-Informed Neural Networks (PINNs)
- *Class C:* flow map approximation models, i.e., dynamic model decomposition (DMD) models

**Coupling methods:**

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

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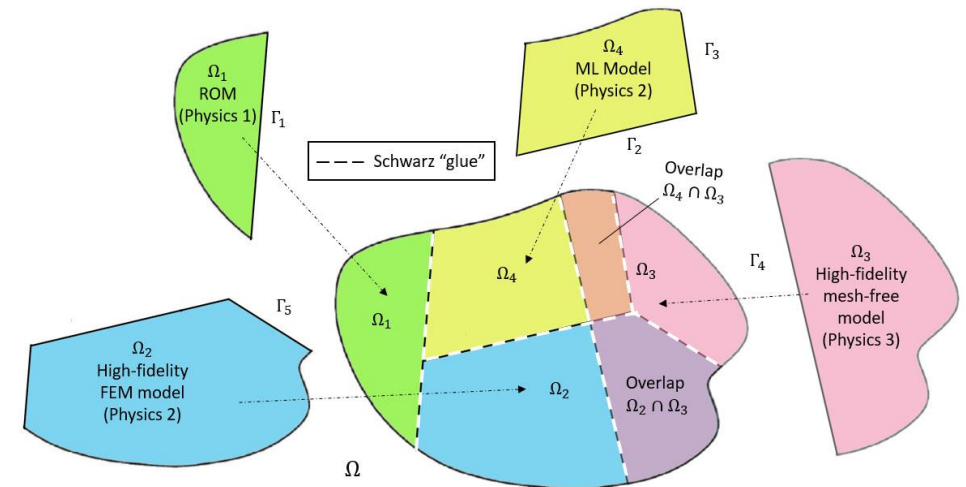
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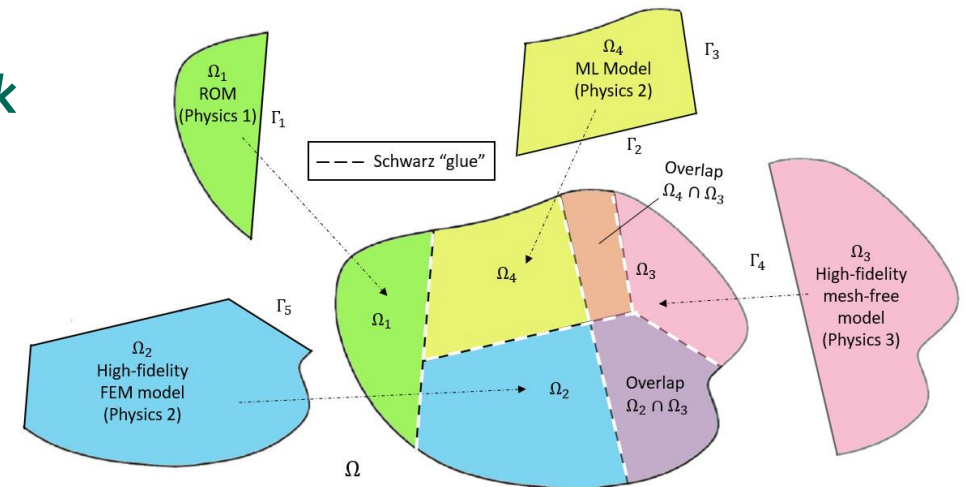- *Class A:* projection-based reduced order models (ROMs)
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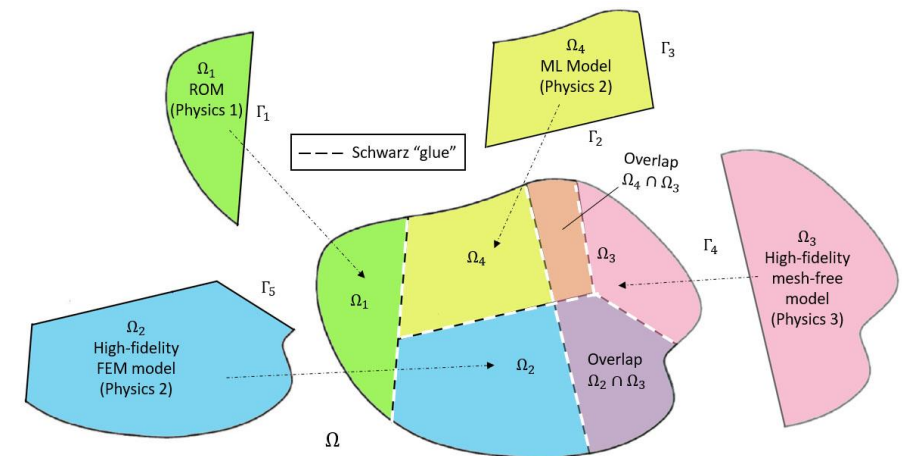- *Class C:* flow map approximation models, i.e., dynamic model decomposition (DMD) models

*This talk*

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# 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

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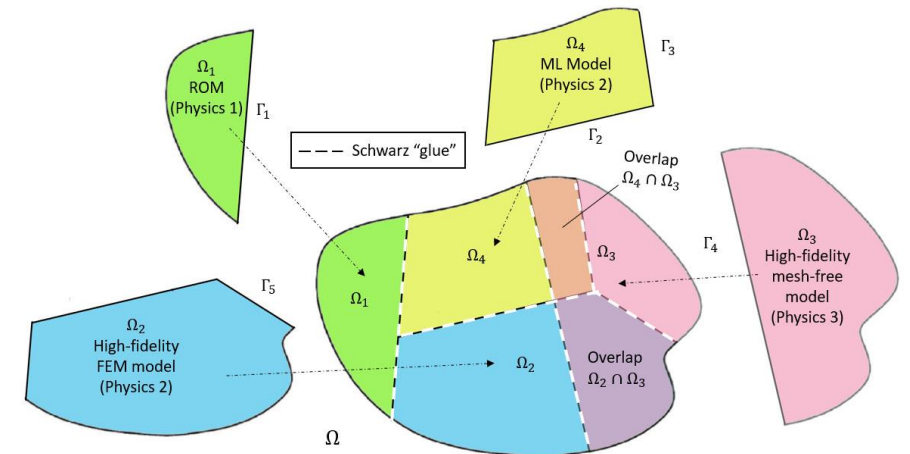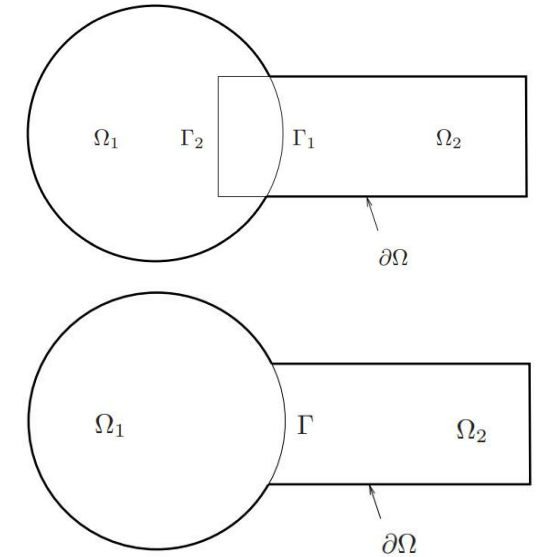
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# Schwarz Alternating Method for Domain Decomposition

- 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.
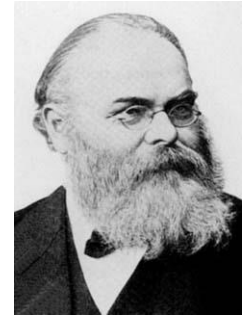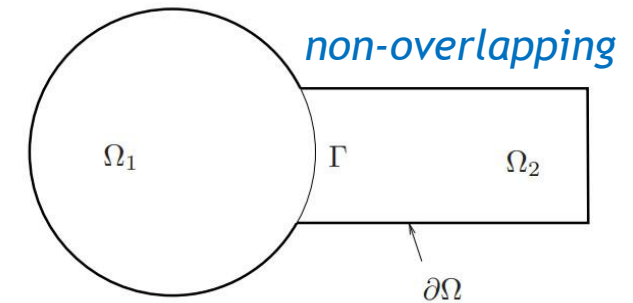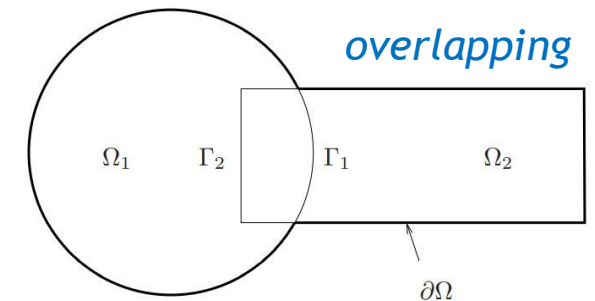
H. Schwarz (1843–1921)

### Basic Schwarz Algorithm

*Initialize:*

- Solve PDE by any method on $\Omega_1$ w/ initial guess for transmission BCs on $\Gamma_1$.

*Iterate until convergence:*

- Solve PDE by any method on $\Omega_2$ w/ transmission BCs on $\Gamma_2$ based on values just obtained for $\Omega_1$.
- Solve PDE by any method on $\Omega_1$ w/ transmission BCs on $\Gamma_1$ based on values just obtained for $\Omega_2$.

*overlapping*

$\Omega_1$ $\quad \Gamma_2$ $\quad \Gamma_1$ $\quad \Omega_2$

$\partial\Omega$

*non-overlapping*

$\Omega_1$ $\quad \Gamma$ $\quad \Omega_2$

$\partial\Omega$

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

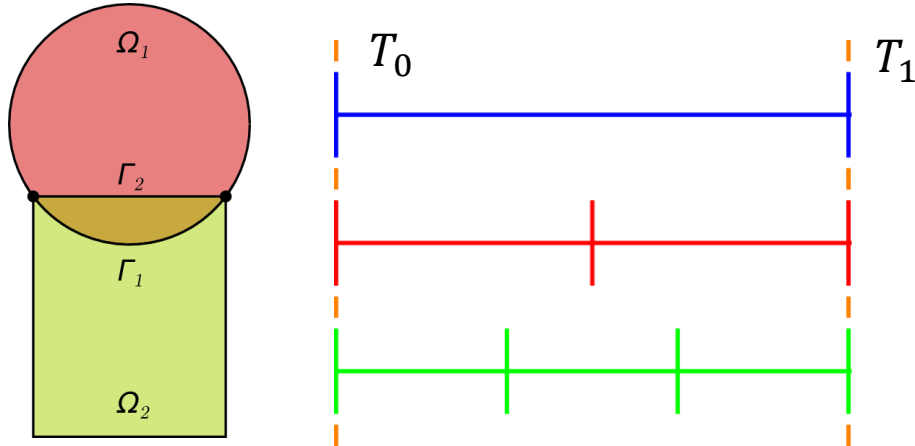**Non-overlapping Schwarz:** convergent with Robin-Robin[2] or alternating Neumann-Dirichlet[3] transmission BCs.

[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



$\Omega_1$

$\Gamma_2$

$\Gamma_1$

$\Omega_2$

$T_0$          $T_1$

Controller time stepper

Time integrator for $\Omega_1$

Time integrator for $\Omega_2$

**<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}
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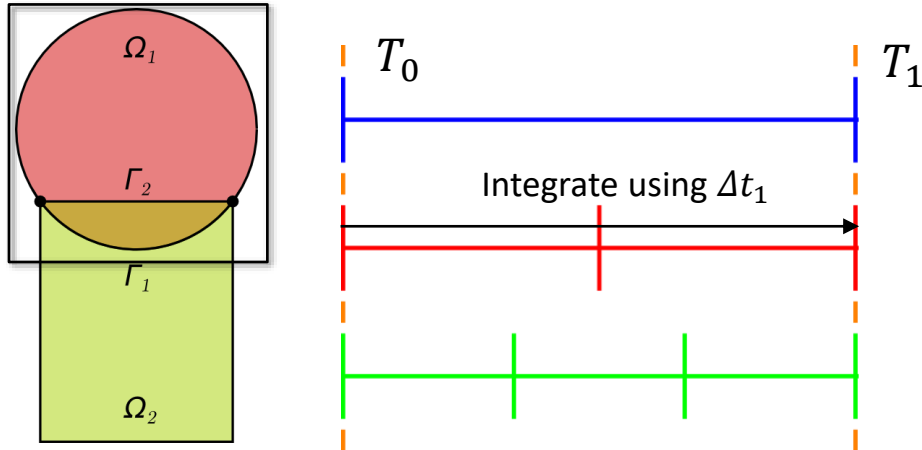
# Time-Advancement Within the Schwarz Framework



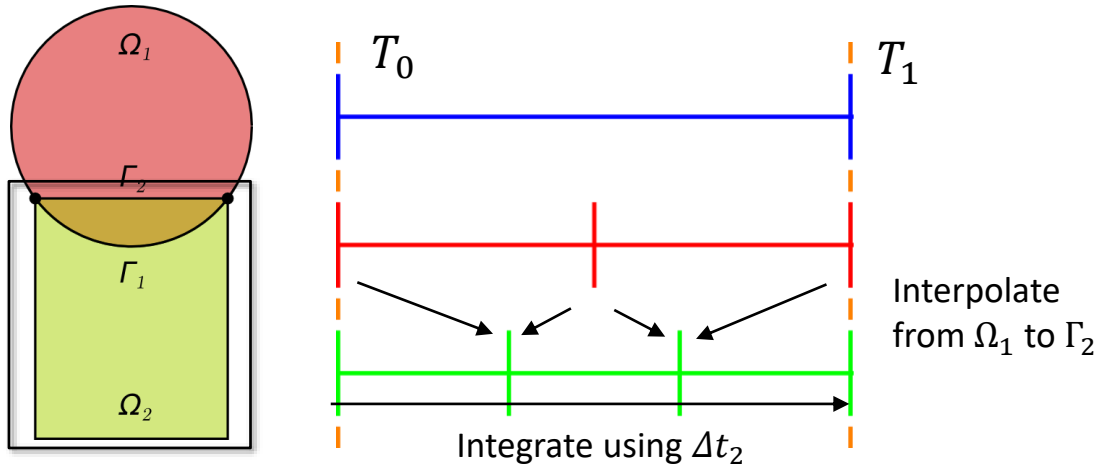Controller time stepper

Time integrator for $\Omega_1$

Time integrator for $\Omega_2$

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

**Step 1:** Advance $\Omega_1$ solution from time $T_i$ to time $T_{i+1}$ using time-stepper in $\Omega_1$ with time-step $\Delta t_1$, using solution in $\Omega_2$ interpolated to $\Gamma_1$ 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



Controller time stepper

Time integrator for $\Omega_1$

Interpolate from $\Omega_1$ to $\Gamma_2$

Time integrator for $\Omega_2$

Integrate using $\Delta t_2$

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

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# Time-Advancement Within the Schwarz Framework



Controller time stepper

Time integrator for $\Omega_1$

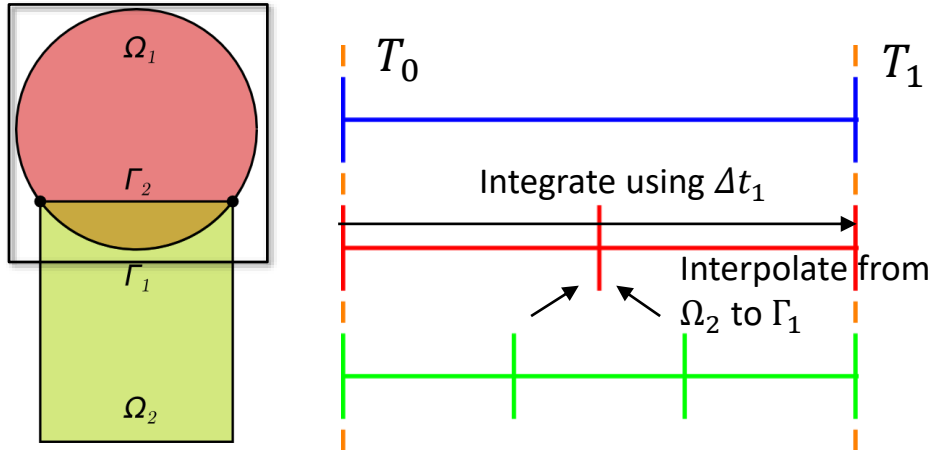Time integrator for $\Omega_2$

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

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Time integrator for $\Omega_1$

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# Time-Advancement Within the Schwarz Framework



Controller time stepper

Time integrator for $\Omega_1$

Time integrator for $\Omega_2$

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

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# Time-Advancement Within the Schwarz Framework



Controller time stepper

Time integrator for $\Omega_1$

Time integrator for $\Omega_2$

Integrate using $\Delta t_1$

Interpolate from $\Omega_2$ to $\Gamma_1$

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

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

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

**Model Solid Mechanics PDEs:**

| | |
|---|---|
| Quasistatic: | $\text{Div } \boldsymbol{P} + \rho_0 \boldsymbol{B} = \boldsymbol{0} \quad \text{in} \quad \Omega$ |
| Dynamic: | $\text{Div } \boldsymbol{P} + \rho_0 \boldsymbol{B} = \rho_0 \ddot{\varphi} \quad \text{in} \quad \Omega \times I$ |

- Coupling is **concurrent** (two-way).

- **Ease of implementation** into existing massively-parallel HPC codes.

- **Scalable**, **fast**, **robust** (we target **real** engineering problems, e.g., analyses involving failure of bolted components!).

- Coupling does not introduce **nonphysical artifacts**.

- **Theoretical** convergence properties/guarantees[1].



- **"Plug-and-play"** framework:

  ➢ Ability to couple regions with **different non-conformal meshes**, **different element types** and **different levels of refinement** to simplify task of **meshing complex geometries**.

  ➢ Ability to use **different solvers/time-integrators** in different regions.
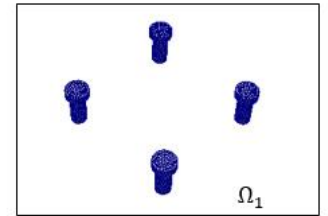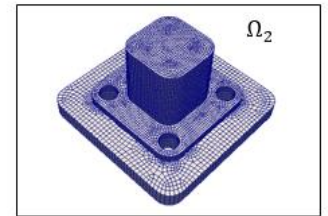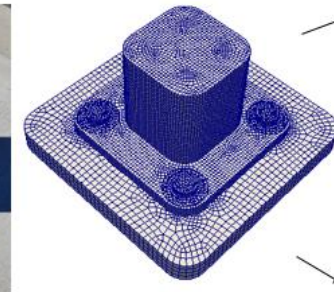
[1] Mota *et al*. 2017; Mota *et al*. 2022.   [2] https://github.com/sandialabs/LCM.

| # Outline

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

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

- ## Numerical Examples

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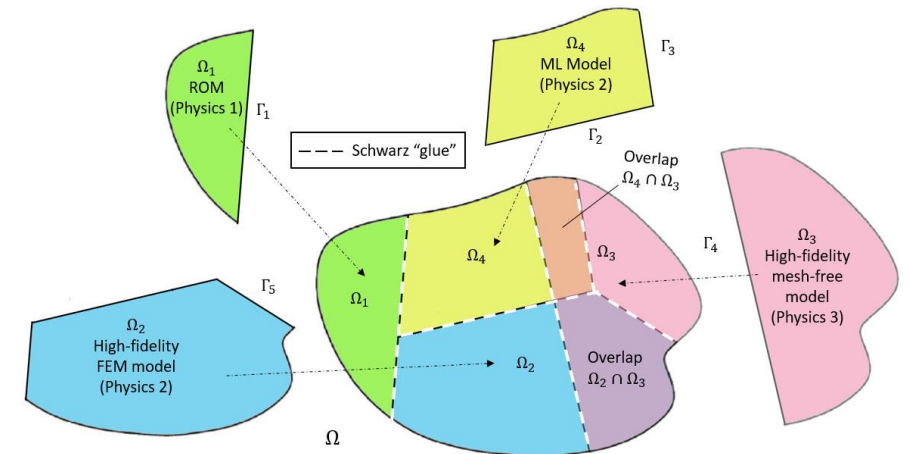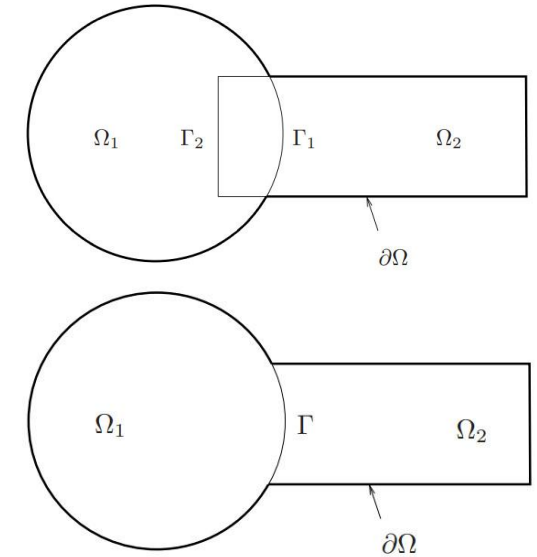
# Projection-Based Model Order Reduction via the POD/Galerkin Method

Full Order Model (FOM): $M\dfrac{d^2u}{dt^2} + f_{\text{int}}(u) = f_{\text{ext}}$

## 1. Acquisition
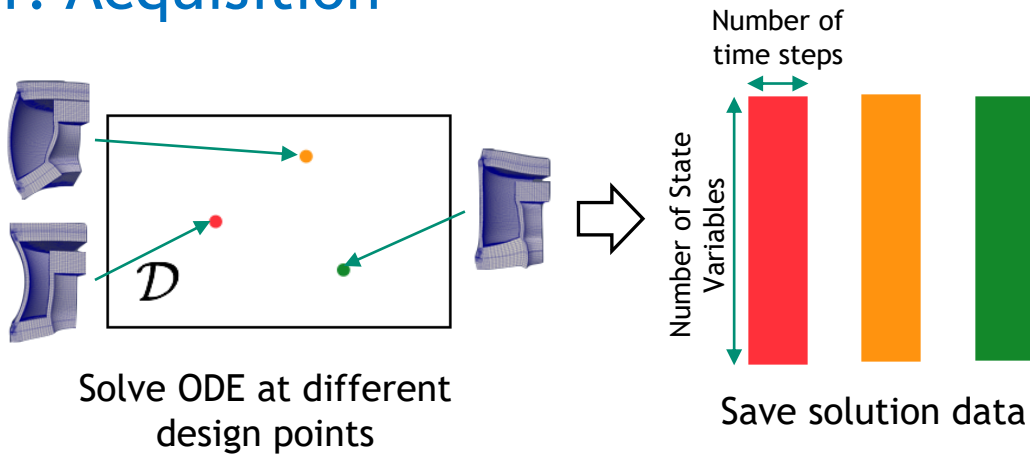


Number of time steps

Number of State Variables

Solve ODE at different design points

Save solution data

## 2. Learning

Proper Orthogonal Decomposition (POD):

$$\mathbf{X} = \quad = \quad \Phi \ \mathbf{U} \quad \Sigma \quad \mathbf{V}^T$$



ROM = projection-based Reduced Order Model

## 3. Projection-Based Reduction

Reduce the number of unknowns

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

Perform Galerkin projection

$$\Phi^T M \Phi \dfrac{d^2\hat{u}}{dt^2} + \Phi^T f_{\text{int}}(\Phi\hat{u}) = \Phi^T f_{\text{ext}}$$

Hyper-reduce nonlinear terms

$$f_{\text{int}}(\Phi\hat{u}) \approx \quad A \quad f_{\text{int}}(\Phi\hat{u})$$

Hyper-reduction/sample mesh

HROM = Hyper-reduced ROM

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

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

\* Least-Squares Petrov-Galerkin

## 1. Acquisition
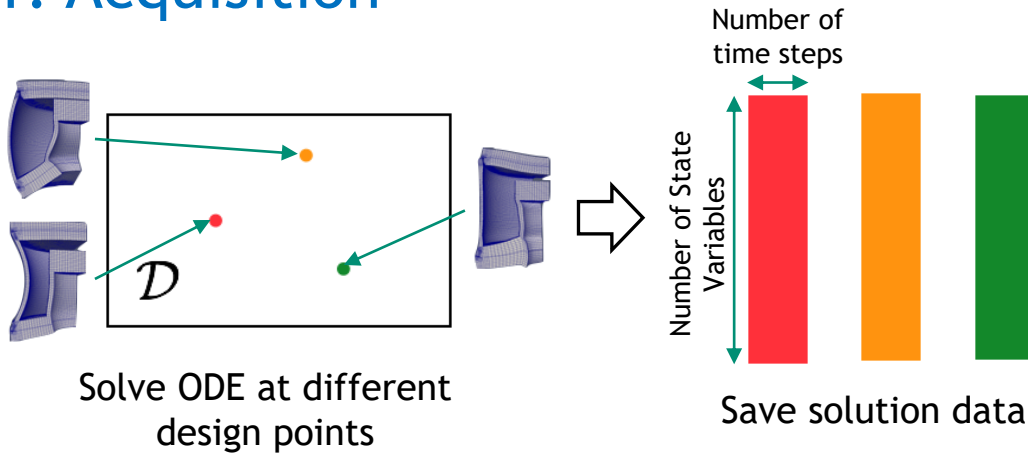
Number of time steps

Number of State Variables

$\mathcal{D}$

Solve ODE at different design points

Save solution data

## 2. Learning

Proper Orthogonal Decomposition (POD):

$$\mathbf{X} = \quad = \boldsymbol{\Phi}\ \mathbf{U} \qquad \boldsymbol{\Sigma} \qquad \mathbf{V}^T$$

ROM = projection-based Reduced Order Model

## 3. Projection-Based Reduction

Choose ODE temporal discretization

$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{f}(\boldsymbol{u}; t, \boldsymbol{\mu})$$

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

Reduce the number of unknowns

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

Minimize residual

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

$$\left\| \quad \left( \quad ; \quad \right) \right\|_2$$

Hyper-reduction/sample mesh

HROM = Hyper-reduced ROM

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

## *Enforcement of Dirichlet boundary conditions (DBCs) in ROM at indices $i_{\text{Dir}}$*

- 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 $\overline{\boldsymbol{u}}, \overline{\boldsymbol{v}}, \overline{\boldsymbol{a}}$: $\overline{\boldsymbol{u}}(\boldsymbol{i}_{\text{Dir}}) \leftarrow \boldsymbol{\chi}_u, \overline{\boldsymbol{v}}(\boldsymbol{i}_{\text{Dir}}) \leftarrow \boldsymbol{\chi}_v, \overline{\boldsymbol{a}}(\boldsymbol{i}_{\text{Dir}}) \leftarrow \boldsymbol{\chi}_a$

## *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*

- 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 $\Omega = \cup_i \ \Omega_i$
- Future work: generate snapshots/bases separately in each $\Omega_i$ [Hoang *et al.* 2021, Smetana *et al.* 2022]

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- Summary & Future Work

*Full-Order Model.  #Reduced Order Model.
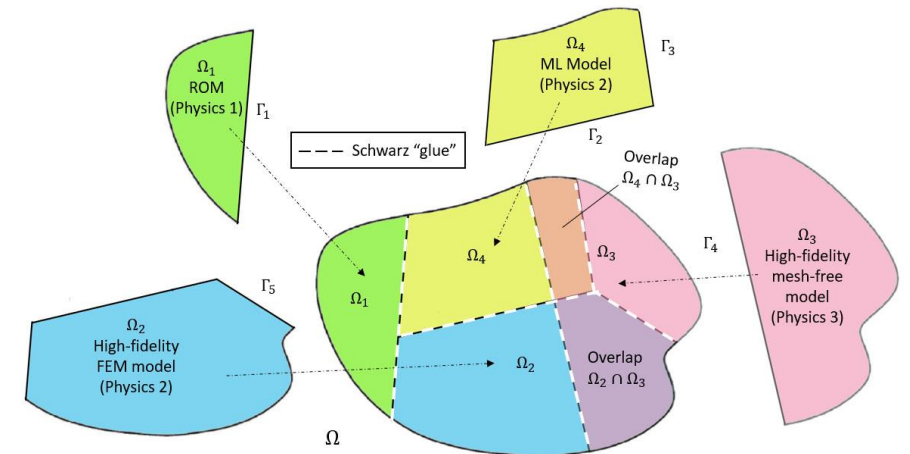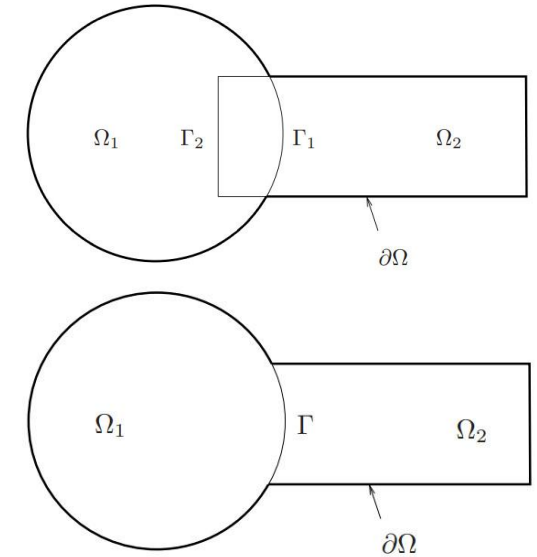
# Numerical Example: 1D Dynamic Wave Propagation Problem

- **1D beam** geometry $\Omega = (0,1)$, clamped at both ends, with prescribed initial condition discretized using FEM + Newmark-$\beta$

- 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**
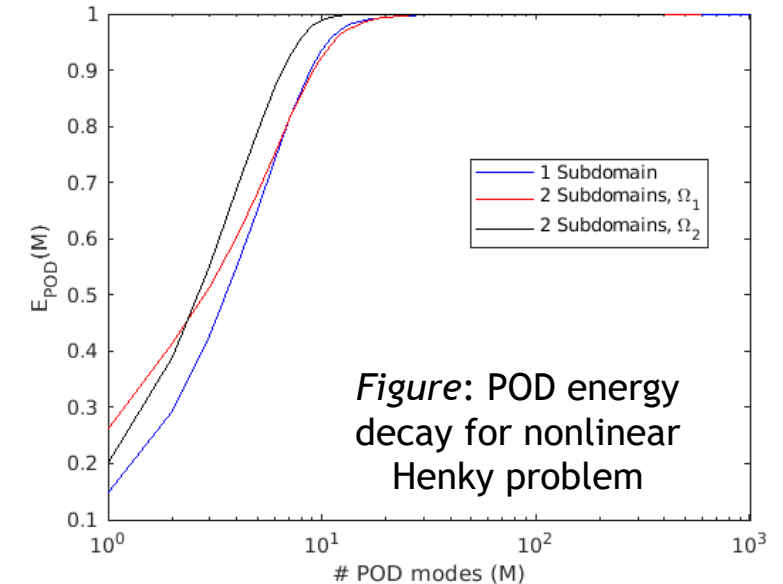
# Numerical Example: 1D Dynamic Wave Propagation Problem

- **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 $\Omega_1$ = [0, 0.6] and $\Omega_2$ = [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 $\Omega_1$, 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**
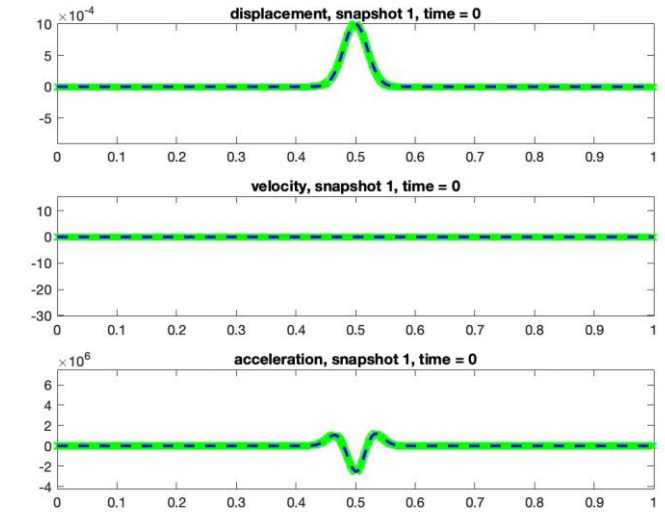


*Figure above*: Symmetric Gaussian IC problem solution
*Figure below*: Rounded Square IC problem solution
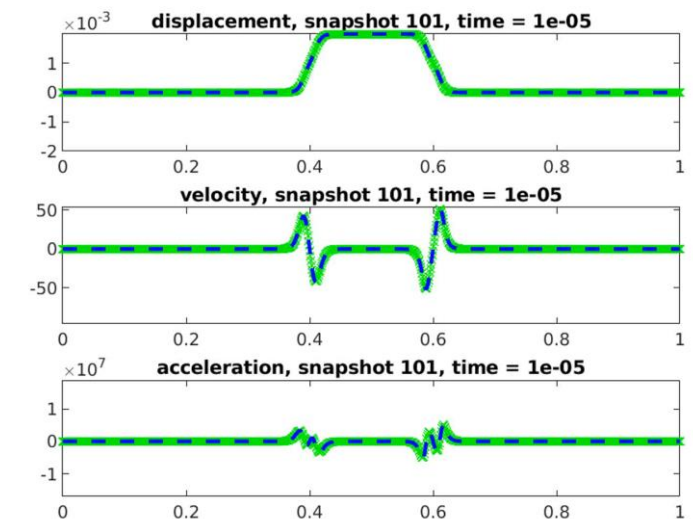
# Numerical Example: Reproductive Problem Results
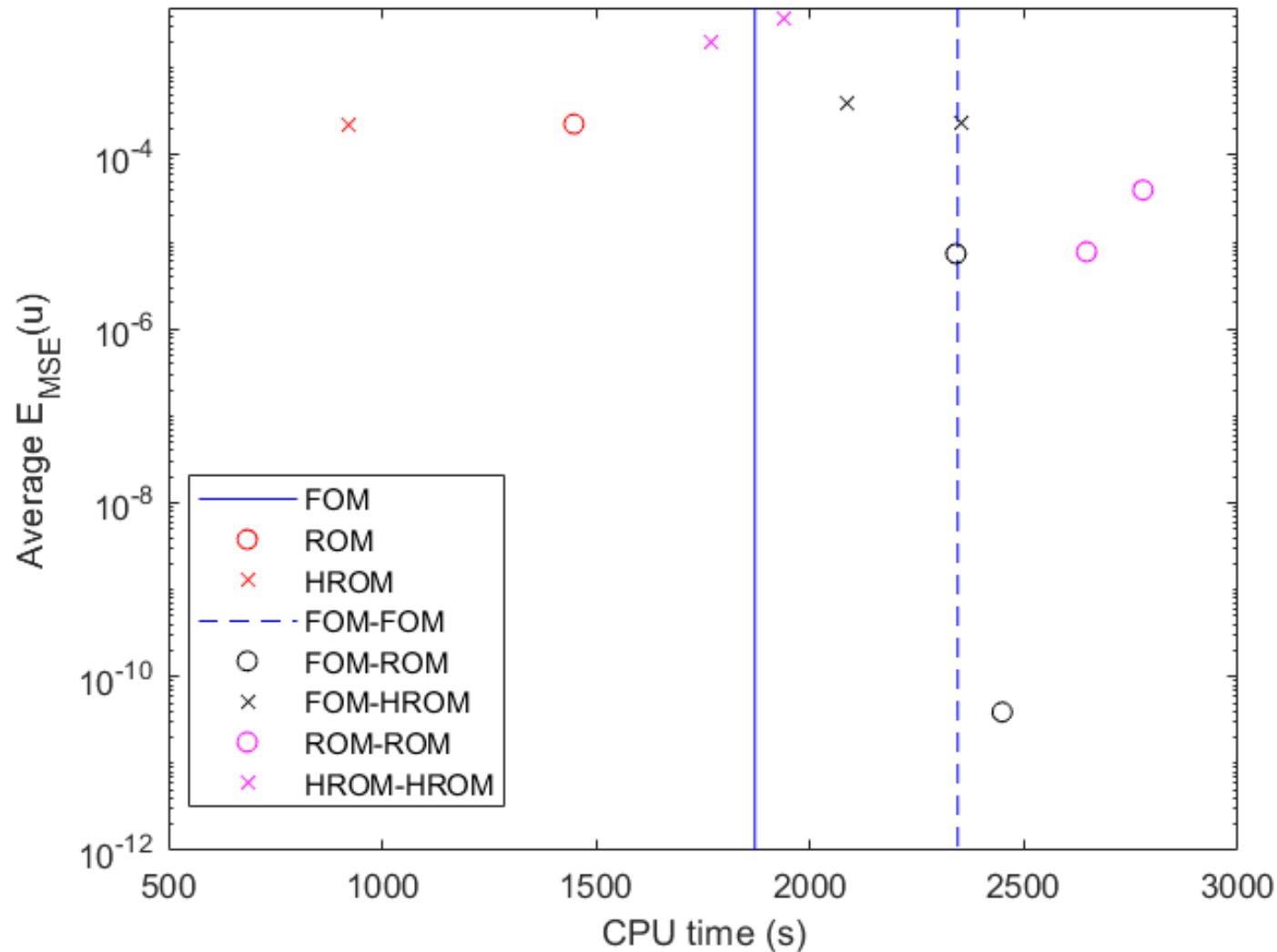


- **Single-domain** ROM and HROM are most **efficient**

- 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
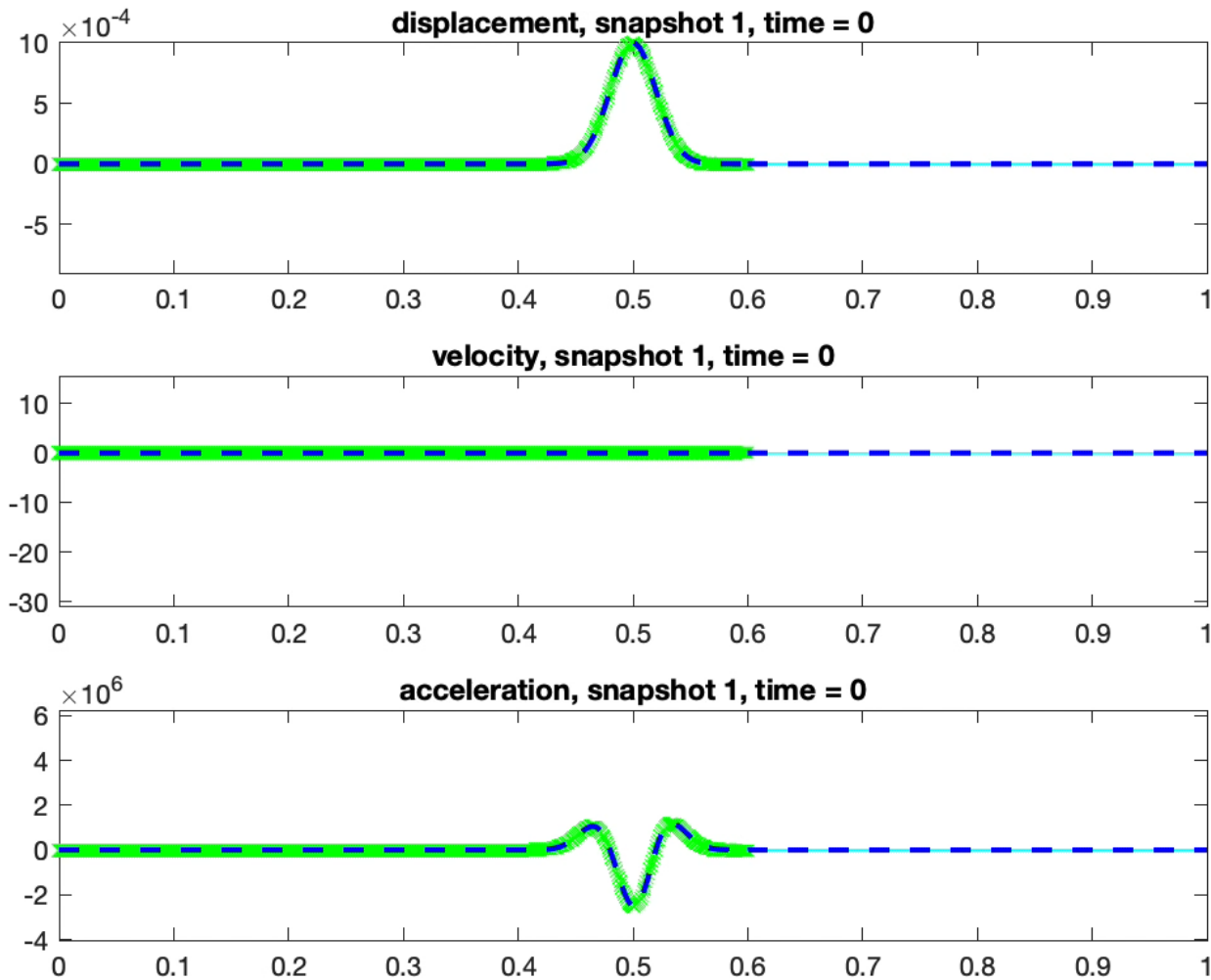


*Figure left*: FOM (green) – HROM (cyan) coupling compared with single-domain FOM solution (blue).  HROM has 200 modes.

*Figure below*: ECSW algorithm samples 253/400 elements
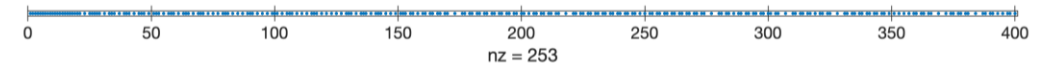
# Numerical Example: Predictive Problem Results

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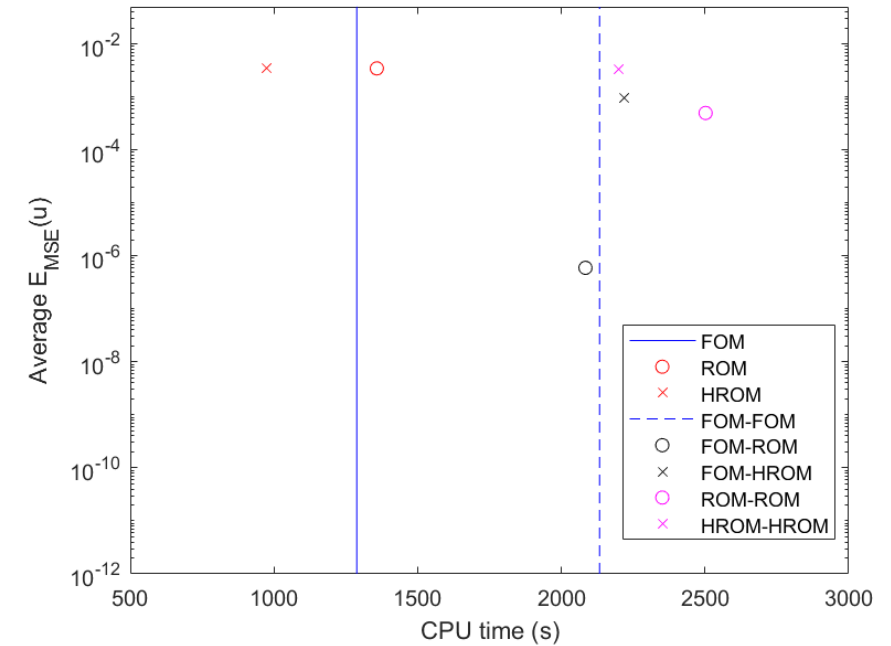


- Results indicate that **predictive accuracy/robustness** can be **improved** by **coupling** ROM or HROM to FOM
  - ➤ FOM-ROM coupling is **remarkably accurate,** achieving displacement error $O(1 \times 10^{-8})$
  - ➤ FOM-HROM and ROM-ROM couplings are **more accurate** than single-domain ROMs
 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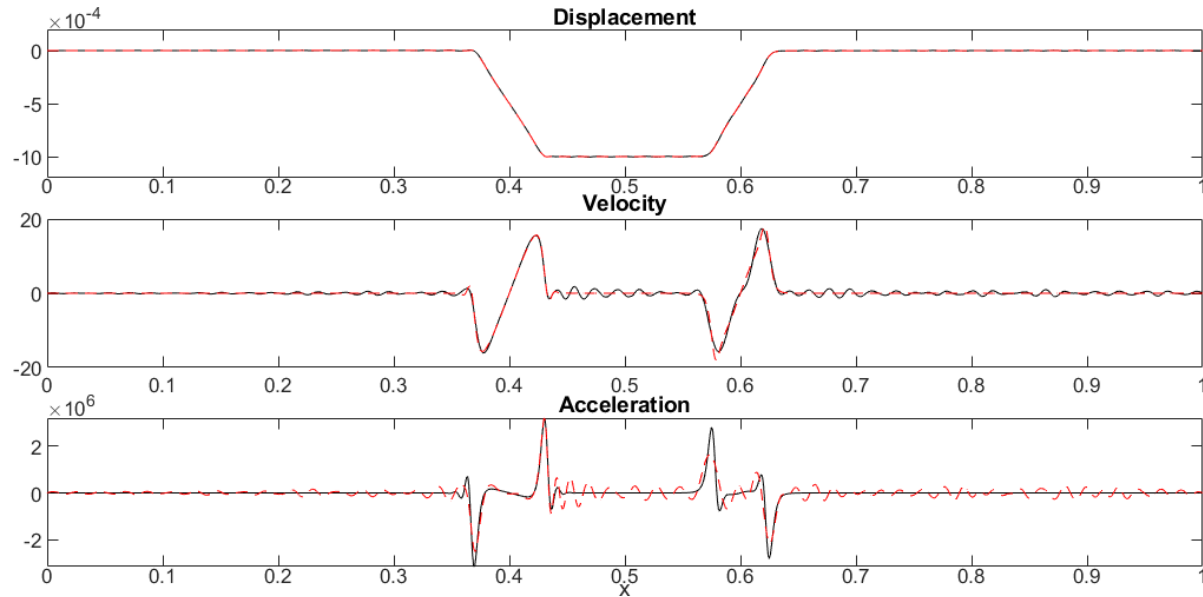


Predictive single-domain ROM ($M_1$= 300)
solution at final time
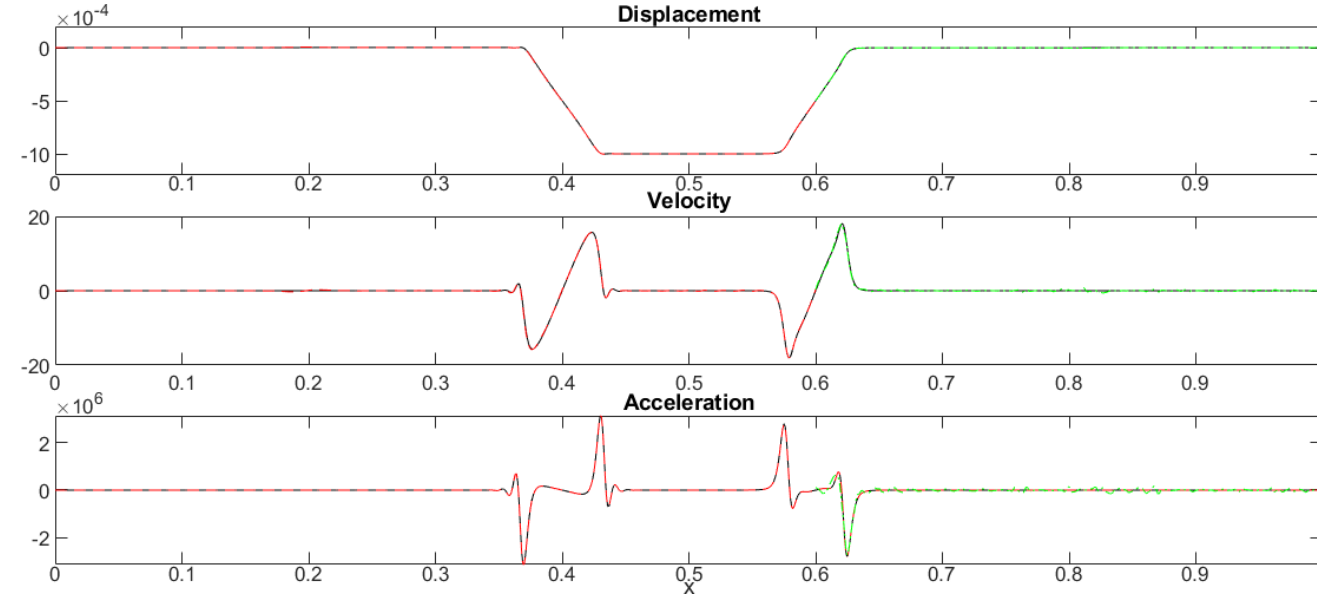
Predictive FOM-HROM ($M_2$= 200)
solution at final time

| — Single-domain FOM solution | — Solution in $\Omega_1$ | — Solution in $\Omega_2$ |
| --- | --- | --- |

- 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
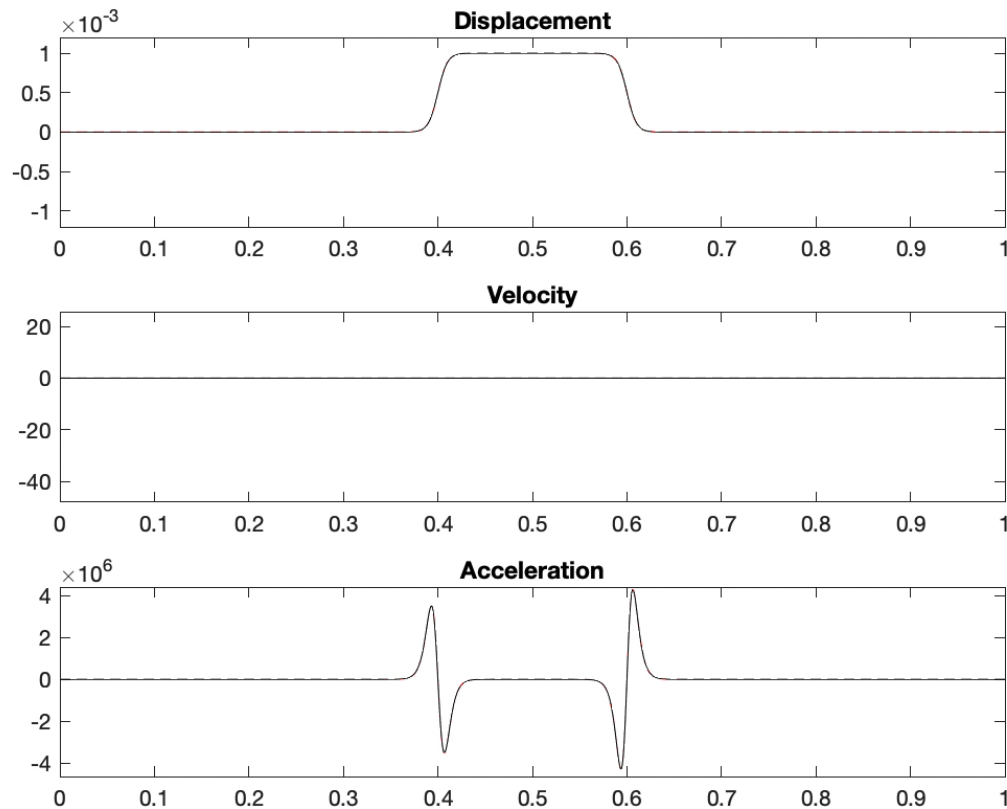


Predictive single-domain ROM ($M_1 = 300$)
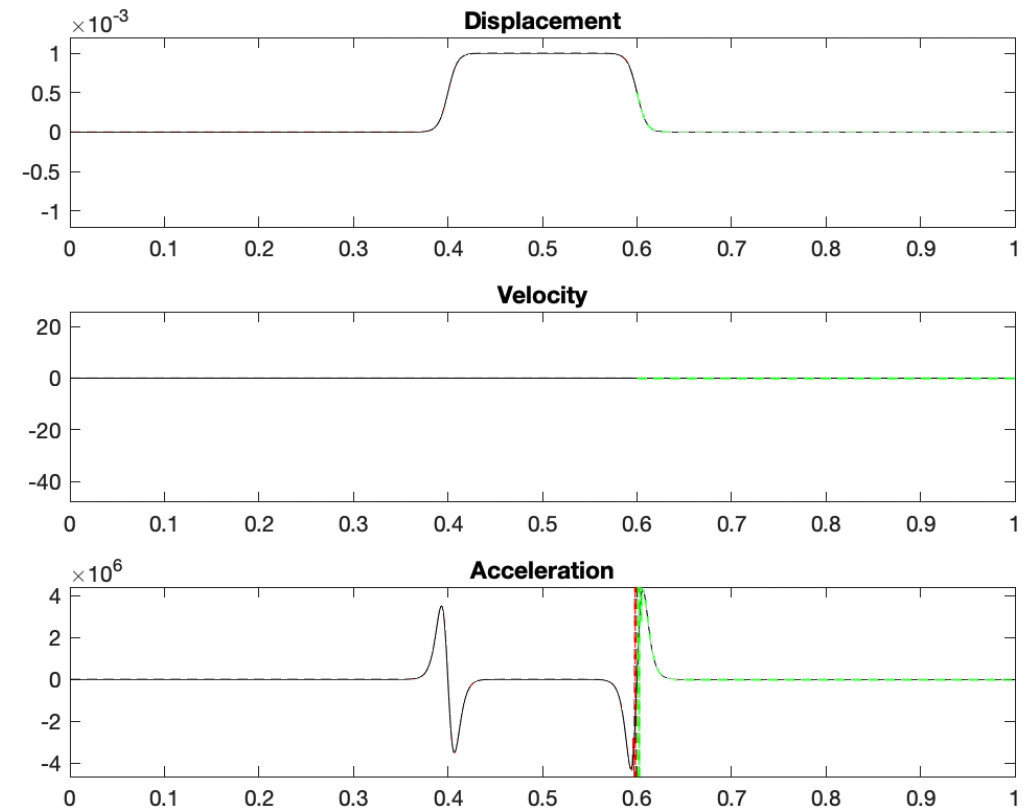
Predictive FOM-HROM ($M_2 = 200$)

— Single-domain FOM solution — Solution in $\Omega_1$ — Solution in $\Omega_2$

# 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.
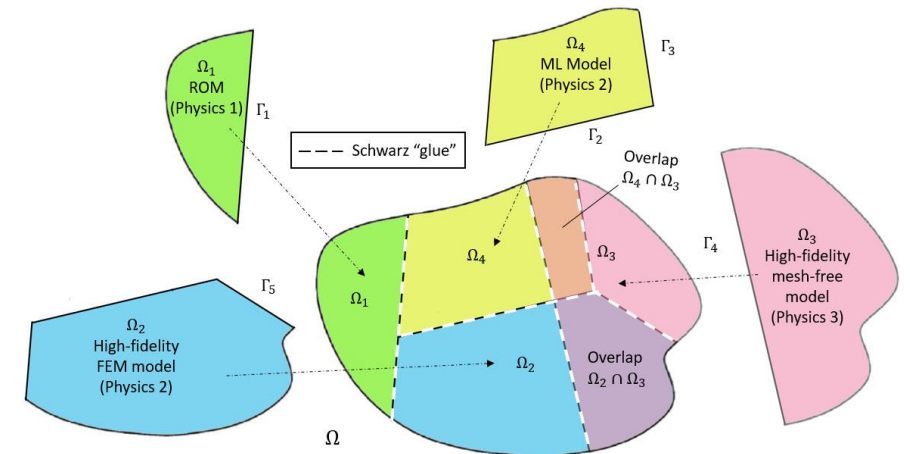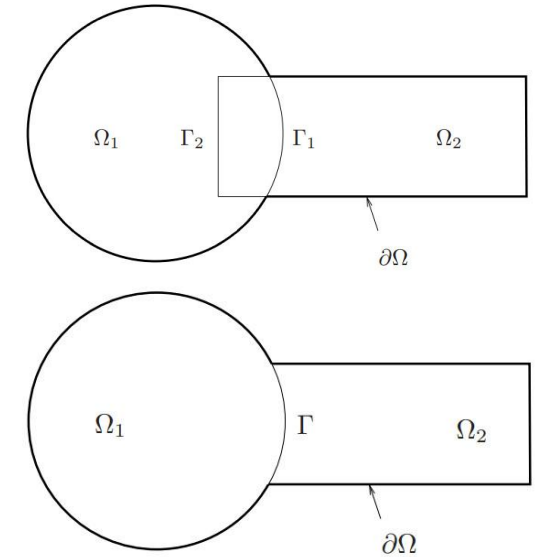
# Numerical Example: 2D Inviscid Burgers Problem

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

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

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

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

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

## 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 $T_f = 25.0$
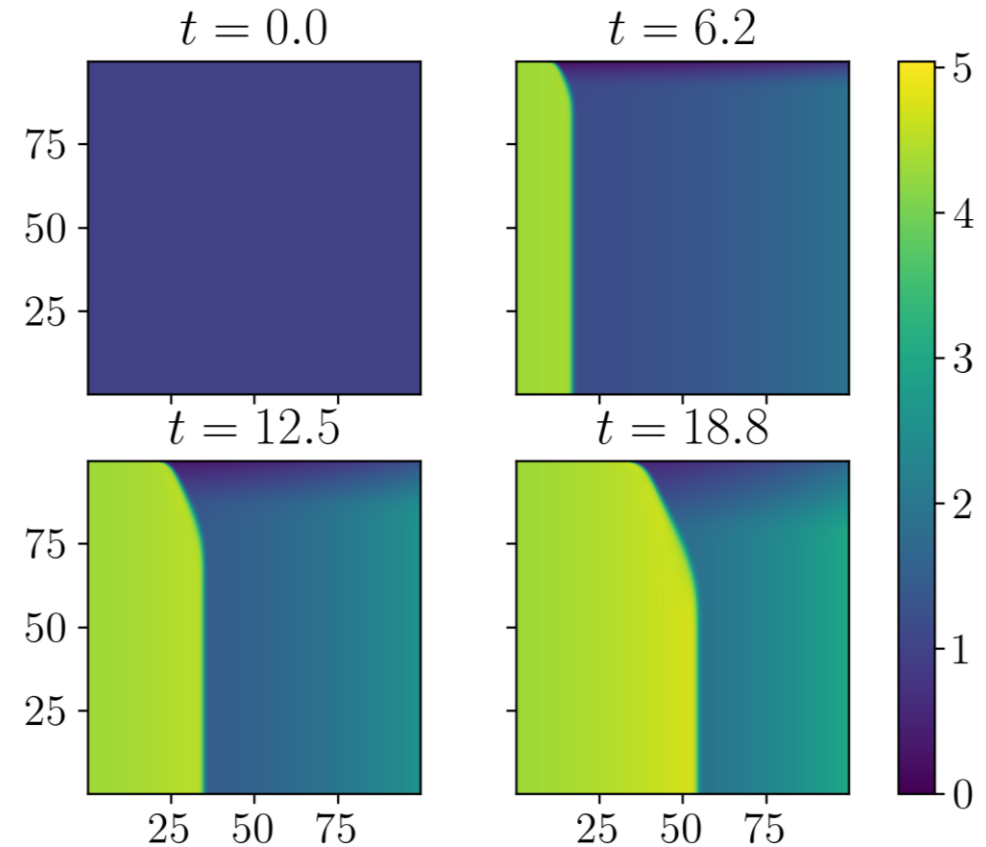


*Figure above:* solution of $u$ component at various times
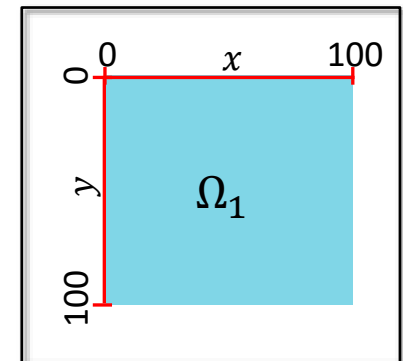
# Numerical Example: 2D Inviscid Burgers Problem

- **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, and is particularly difficult for conventional projection-based ROMs



- Two **parameters** considered:
  - ➢ Dirichlet BC parameterization $\mu_1$
  - ➢ Source term parameterization $\mu_2$

- 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.
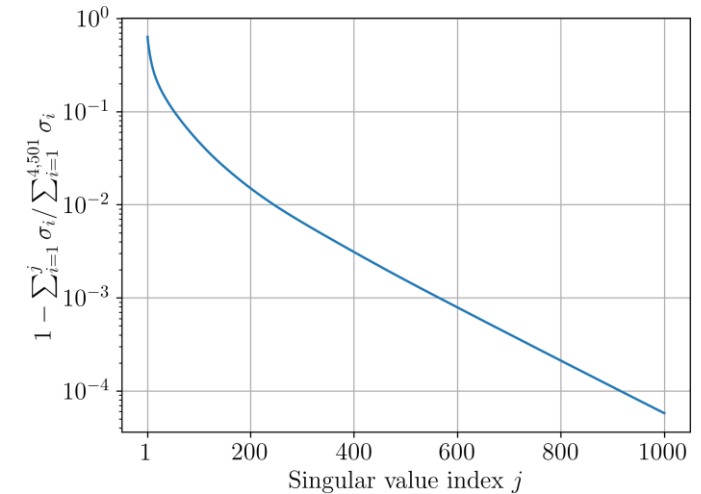
  *This talk*

# 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 $\Rightarrow$ **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).
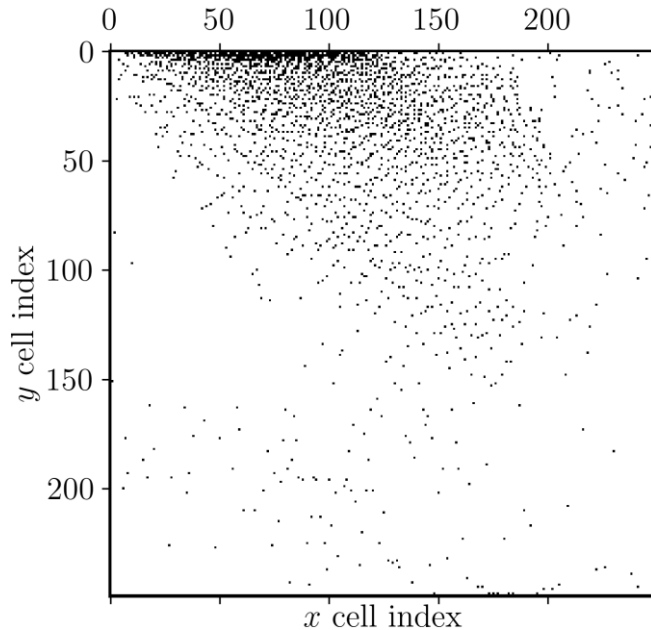


*Figure above: Reduced mesh of single domain HROM*
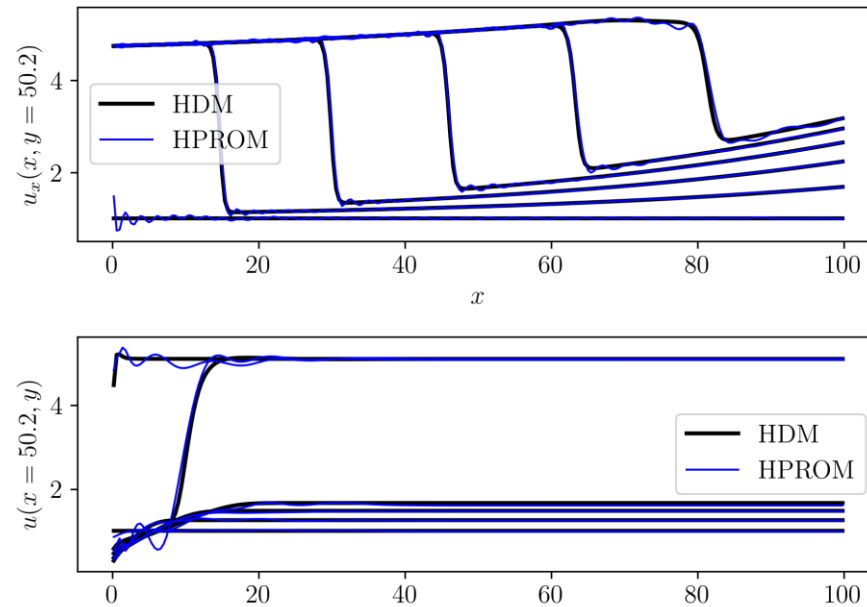


*Figure above: HROM and FOM results at various time steps*

| % 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

### 95% Singular Value (SV) Energy Retention

### 99% Singular Value (SV) Energy Retention

- $\Omega_1$
- $\Omega_2$
- $\Omega_3$
- $\Omega_4$
- —— 1 SD
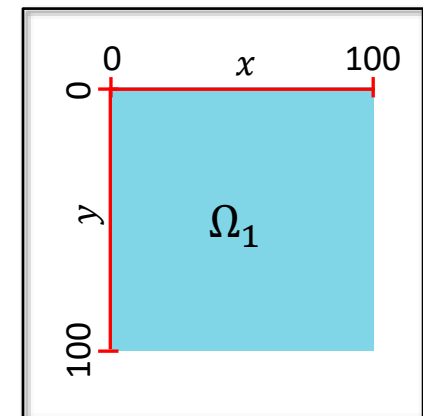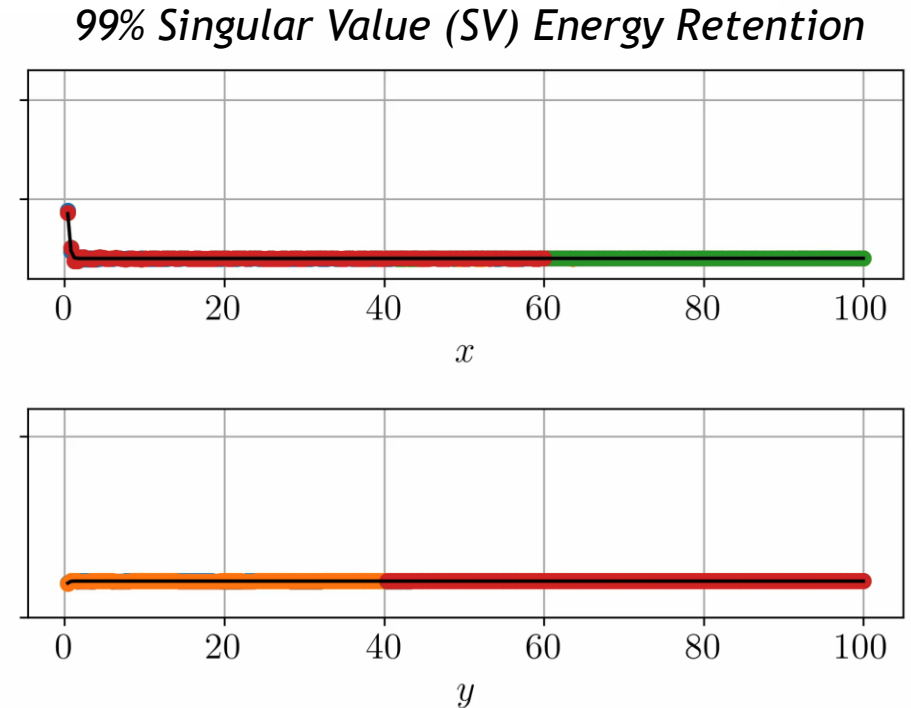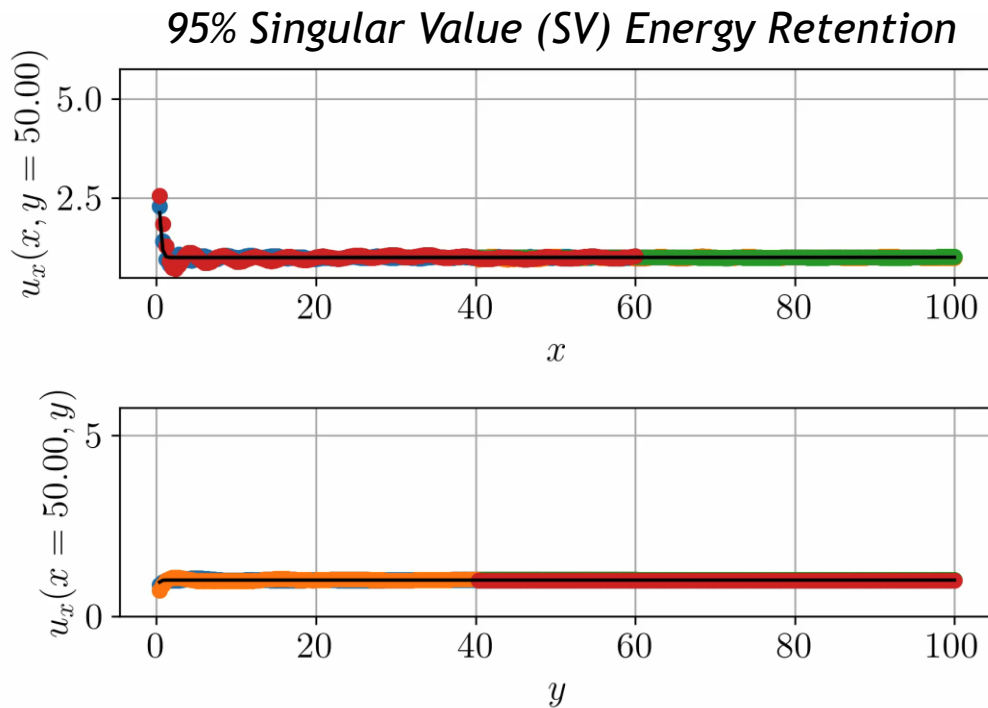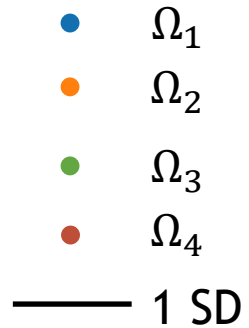


- Method converges in **only 3 Schwarz iterations** per controller time-step
- **Errors** $O$(1%) or less
- **1.47× speedup** over all-FOM coupling for 95% SV energy retention case

| Subdomains | 95% SV Energy | | | 99% SV Energy | | |
|---|---|---|---|---|---|---|
| | $M$ | MSE (%) | CPU time (s) | $M$ | MSE (%) | CPU time (s) |
| $\Omega_1$ | 57 | 1.1 | 85 | 146 | 0.18 | 295 |
| $\Omega_2$ | 44 | 1.2 | 56 | 120 | 0.18 | 216 |
| $\Omega_3$ | 24 | 1.4 | 43 | 60 | 0.16 | 89 |
| $\Omega_4$ | 32 | 1.9 | 61 | 66 | 0.25 | 100 |
| **Total** | | | **245** | | | 700 |
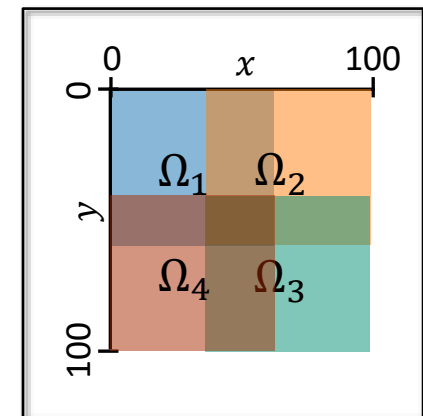
# FOM-HROM-HROM-HROM Coupling



| Subdomains | 99% SV Energy | | |
|---|---|---|---|
| | $M$ | MSE (%) | CPU time (s) |
| $\Omega_1$ | – | 0.0 | 95 |
| $\Omega_2$ | 120 | 0.26 | 26 |
| $\Omega_3$ | 60 | 0.43 | 17 |
| $\Omega_4$ | 66 | 0.34 | 21 |
| Total | | | 159 |
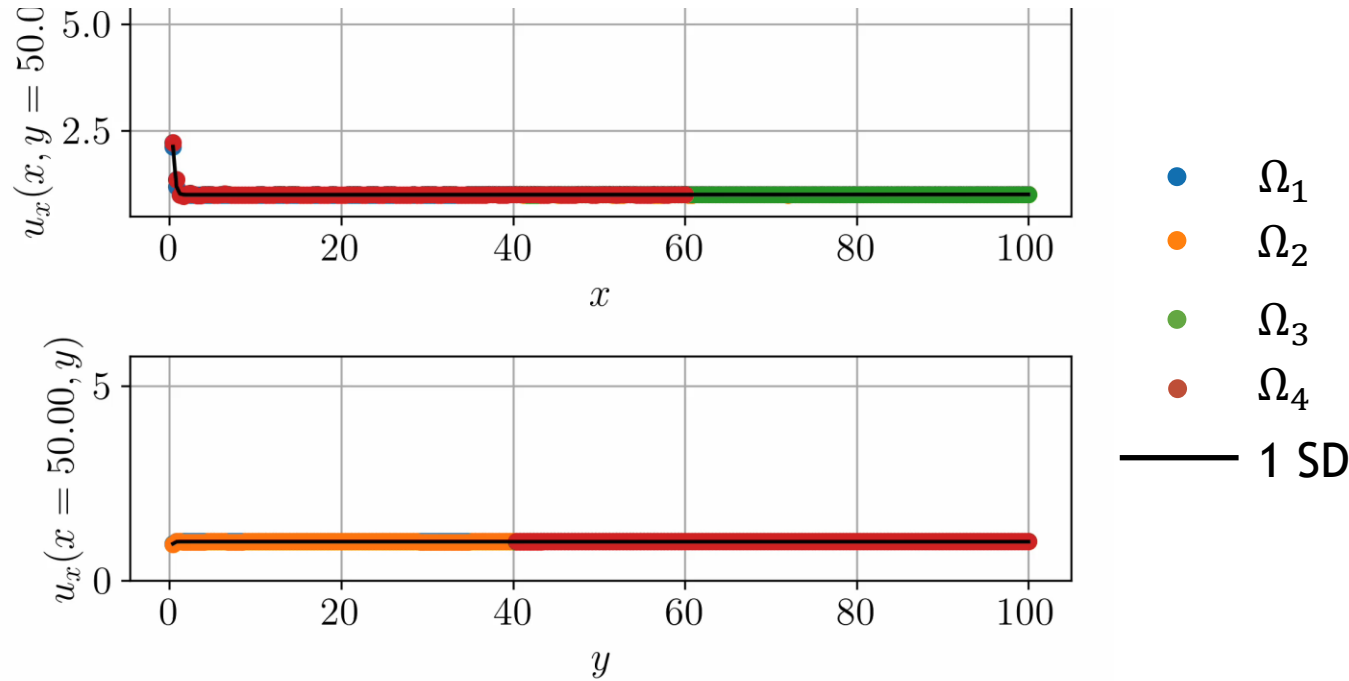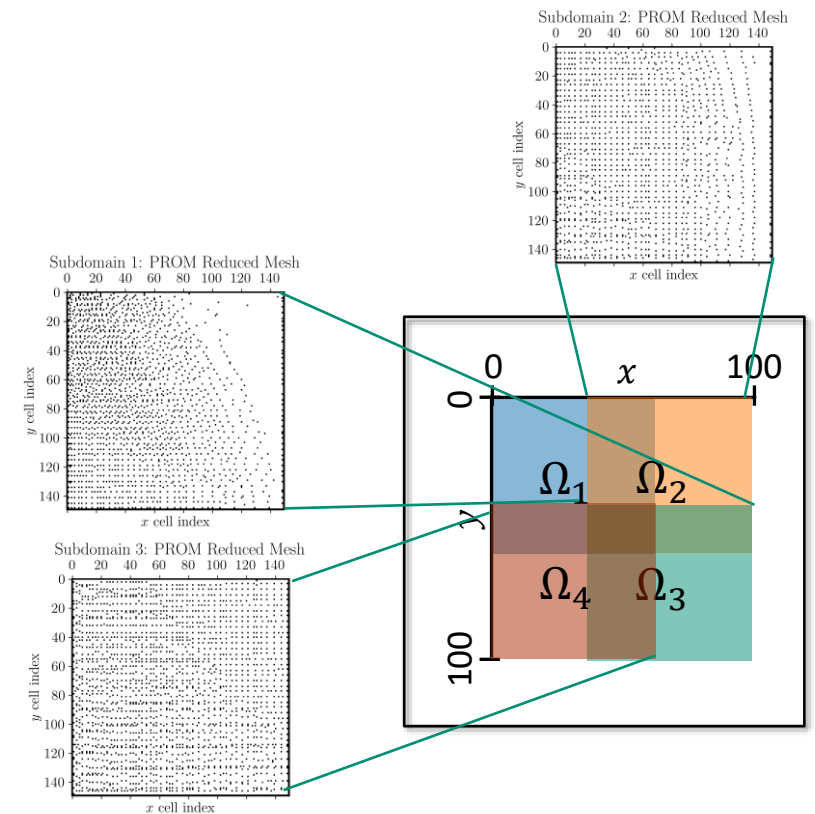


- **FOM** in $\Omega_1$ as this is **"hardest" subdomain** for ROM
- **HROMs** in $\Omega_2$, $\Omega_3$, $\Omega_4$ capture **99% snapshot energy**
- Method converges in **3 Schwarz iterations** per controller time-step
- Errors $O(0.1\%)$ with 0 error in $\Omega_1$
- **2.26× speedup** achieved over 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
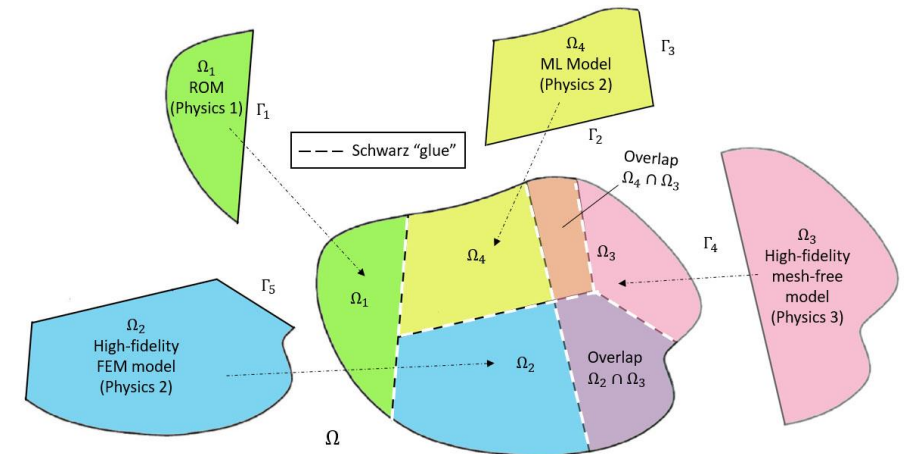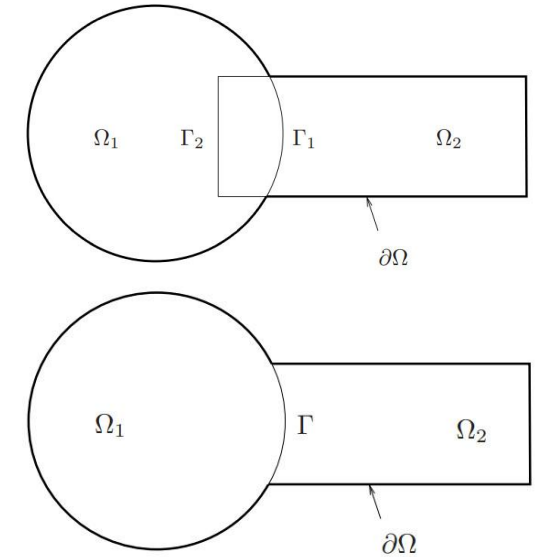
## Summary:

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

## Ongoing & future work:

- Extension to **other applications** and **HPC codes**
- Improving method **efficiency** (e.g., **additive Schwarz**)
- Coupling **nonlinear approximation manifold methods**
- Dynamic **adaptation of domain** partitioning & "on-the-fly" **ROM-FOM switching**
- **Learning** of "optimal" **transmission conditions** to ensure **structure preservation**
- Extension of Schwarz to coupling of **Physics Informed Neural Networks (PINNs)**
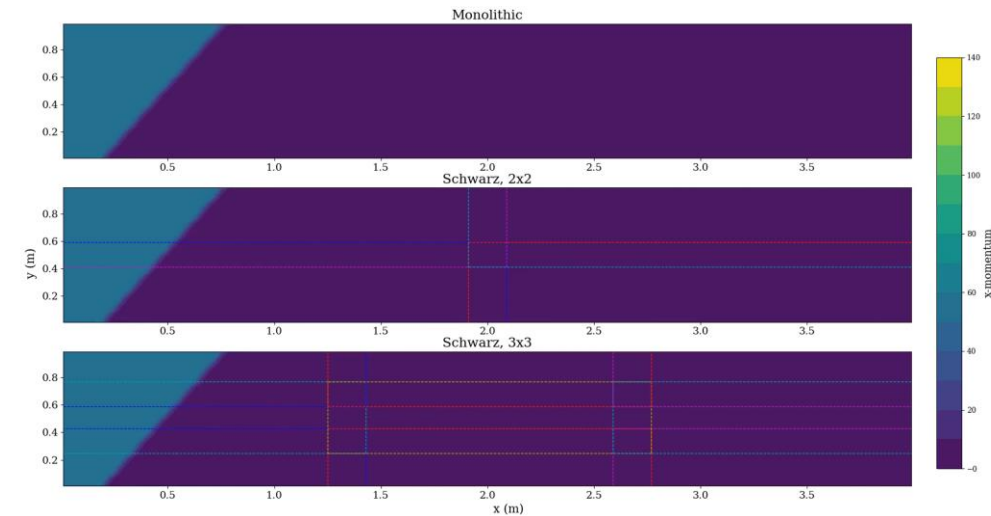
*Movie above*: FOM-FOM coupling via Schwarz for 2D Euler problem using pressio-demoapps*

\* https://https://pressio.github.io
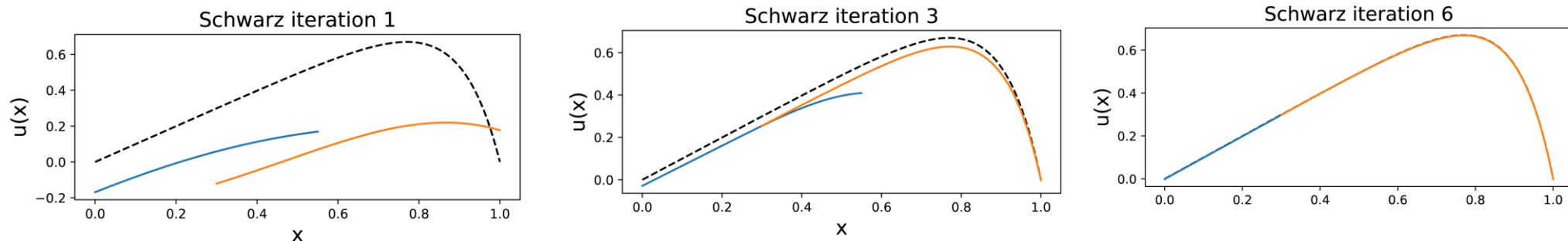
*Figure above*: overlapping alternating Schwarz PINN-PINN coupling for advection-diffusion problem.

# Team & Acknowledgments
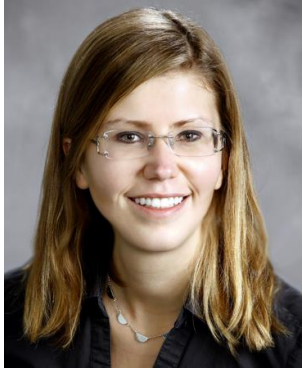

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RESEARCH & DEVELOPMENT


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## *Thank you!  Questions?*

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# 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 Partioned Heterogeneous Time-Integration Methods. *Methods Numer. Meth. PDEs*, 2023 (in press). *Talk by P. Kuberry (IS03-II)*

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

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*URL:* www.sandia.gov/~ikalash

# Start of Backup Slides

# Spatial Coupling via Alternating Schwarz

## Overlapping Domain Decomposition

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

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

$\Omega_1 \quad \Gamma_2 \quad \Gamma_1 \quad \Omega_2$

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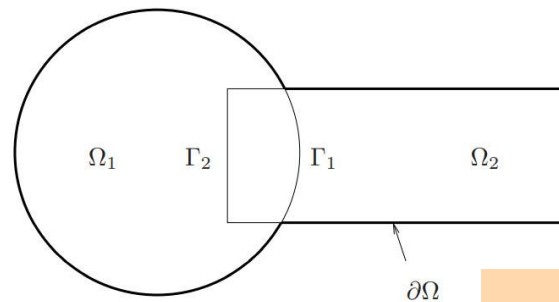
$$\text{Model PDE:} \begin{cases} N(\boldsymbol{u}) = \boldsymbol{f}, \text{ in } \Omega \\ \boldsymbol{u} = \boldsymbol{g}, \quad \text{ on } \partial\Omega \end{cases}$$

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

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

## Non-overlapping Domain Decomposition

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

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

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

$\Omega_1 \quad \Gamma \quad \Omega_2$

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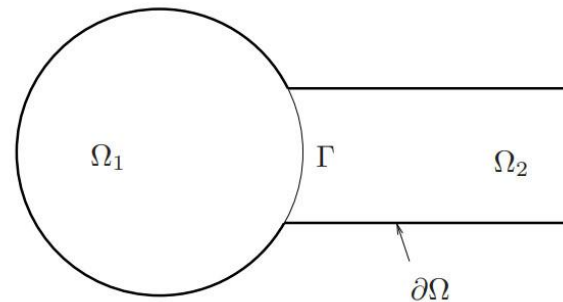
- Relevant for multi-material and multi-physics coupling
- Alternating Dirichlet-Neumann transmission BCs [Zanolli *et al.* 1987]
- Robin-Robin transmission BCs also lead to convergence [Lions 1990]
- $\theta \in [0,1]$: relaxation parameter (can help convergence)

Numerical Example: 1D Dynamic Wave Propagation Problem

- **Basis sizes** $M_1$ and $M_2$ vary from 60 to 300
  - ➢ Larger ROM used in $\Omega_1$, 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
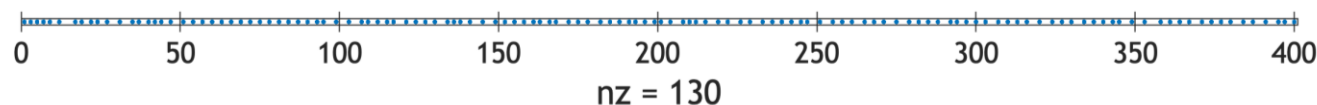


| Figure left: sample sample mesh for 1D wave propagation problem |

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

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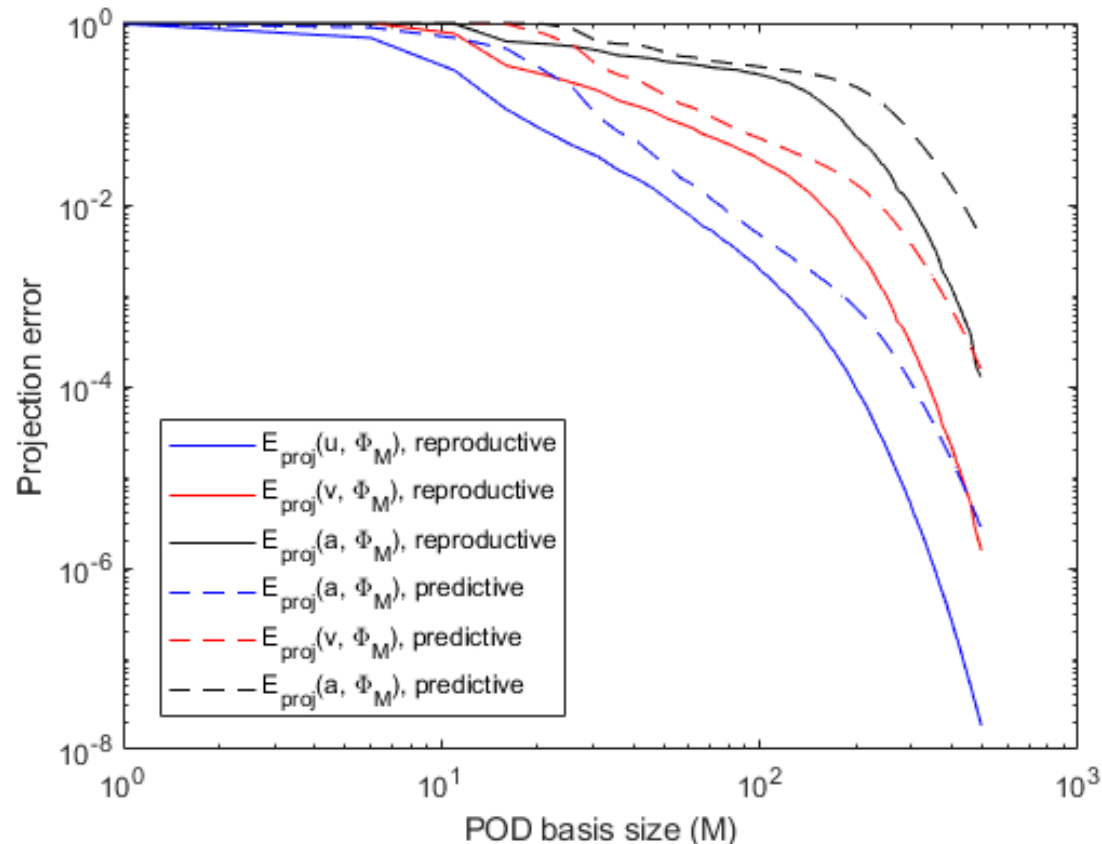


- Projection error suggests **predictive ROM** can achieve **accuracy** and **convergence** with **basis refinement**

- **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 (1908 – 1989)

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

- **S.G. Mikhlin (1951):** *proved convergence* of Schwarz method for general linear elliptic PDEs.

- **P.-L. Lions (1988):** studied convergence of Schwarz for  *nonlinear monotone elliptic problems* using max principle*.*

- **A. Mota, I. Tezaur, C. Alleman (2017):** proved *convergence* of the alternating Schwarz method for *finite deformation quasi-static nonlinear PDEs* (with energy functional $\boldsymbol{\Phi}[\boldsymbol{\varphi}]$) with a *geometric convergence rate.*
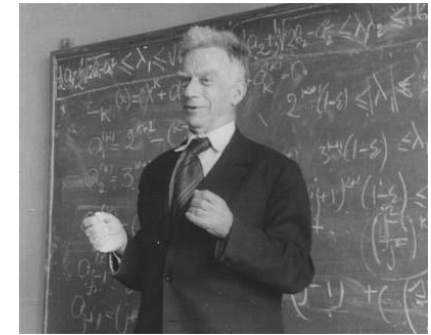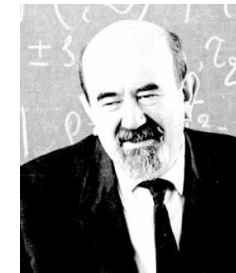


S.G. Mikhlin
(1908 – 1990)



P.- L. Lions (1956-)

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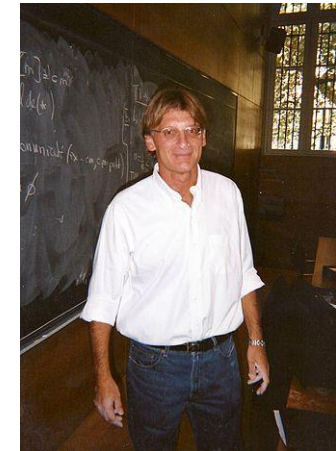


A. Mota, I. Tezaur, C. Alleman

# 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 $\varphi$ is the minimizer of $\Phi[\varphi]$ over $\mathcal{S}$.*

(b) *The sequence $\{\tilde{\varphi}^{(n)}\}$ defined in (39) converges to the minimizer $\varphi$ 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 $\Delta t$.

- **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** $\Delta t$

  ➤ Numerical experiments reveal that $\Delta t$ requirements for **stability/accuracy** typically lead to automatic satisfaction of this bound.

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



y-displacement      EQPS



Single Ω      Schwarz



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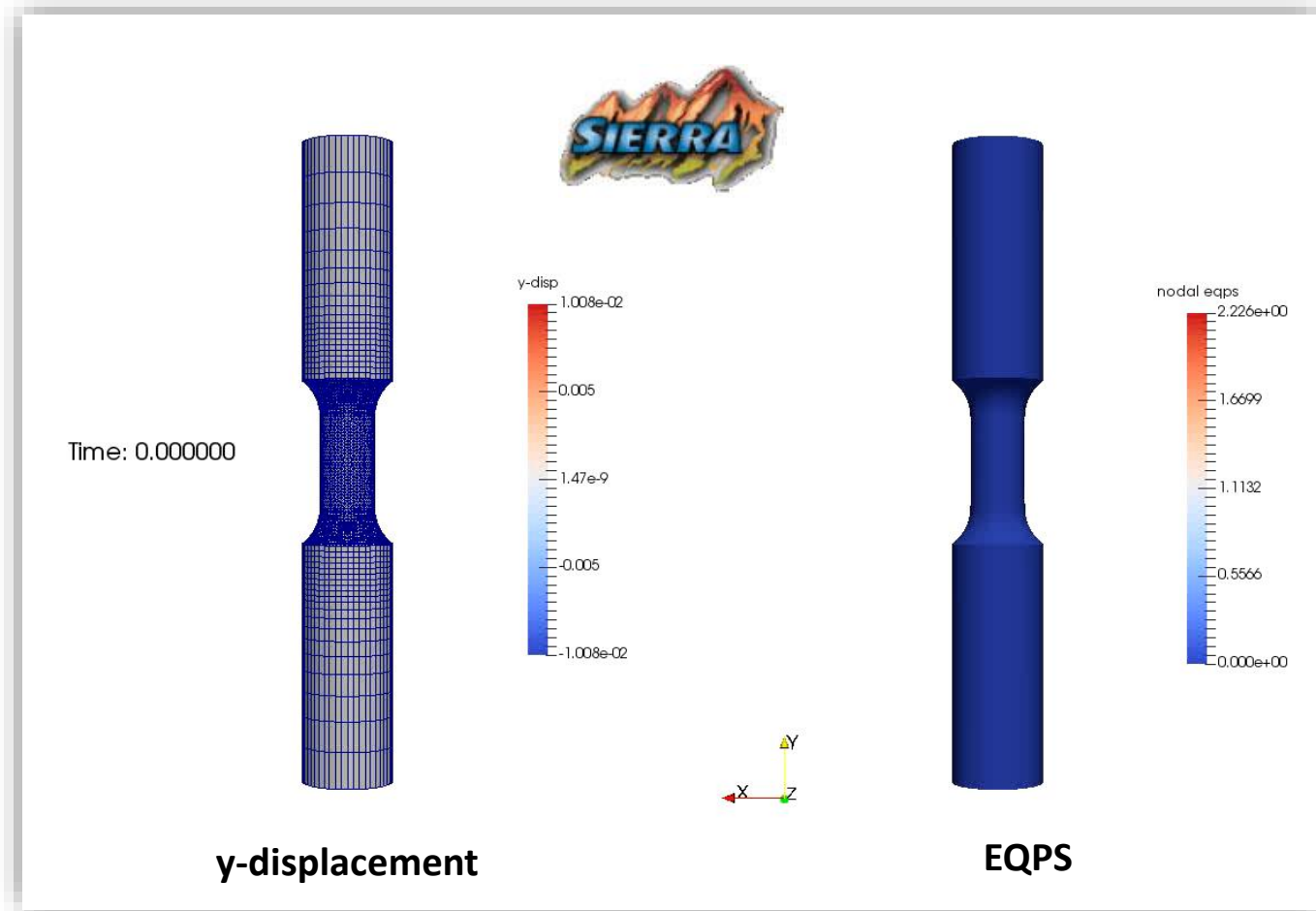
*Figure above:* tension specimen simulation coupling composite TET10 elements with HEX elements in Sierra/SM.

*Figures right:* bolted joint simulation coupling composite TET10 elements with HEX elements in Sierra/SM.
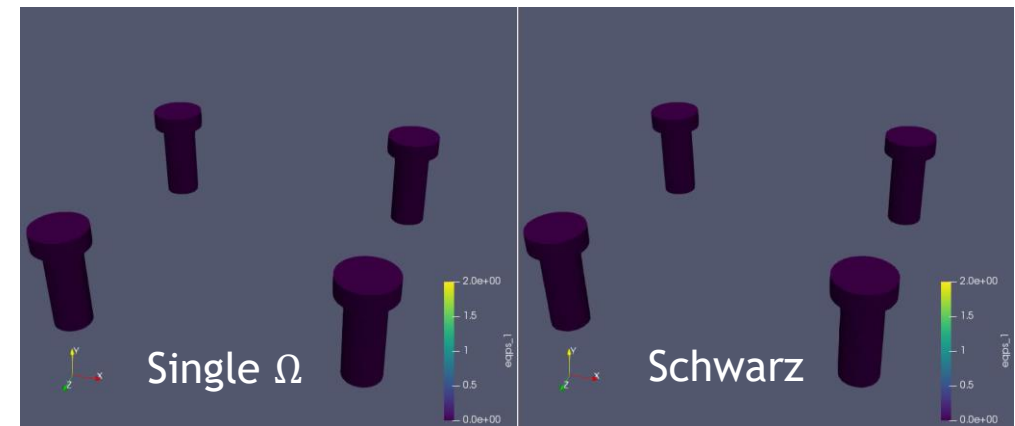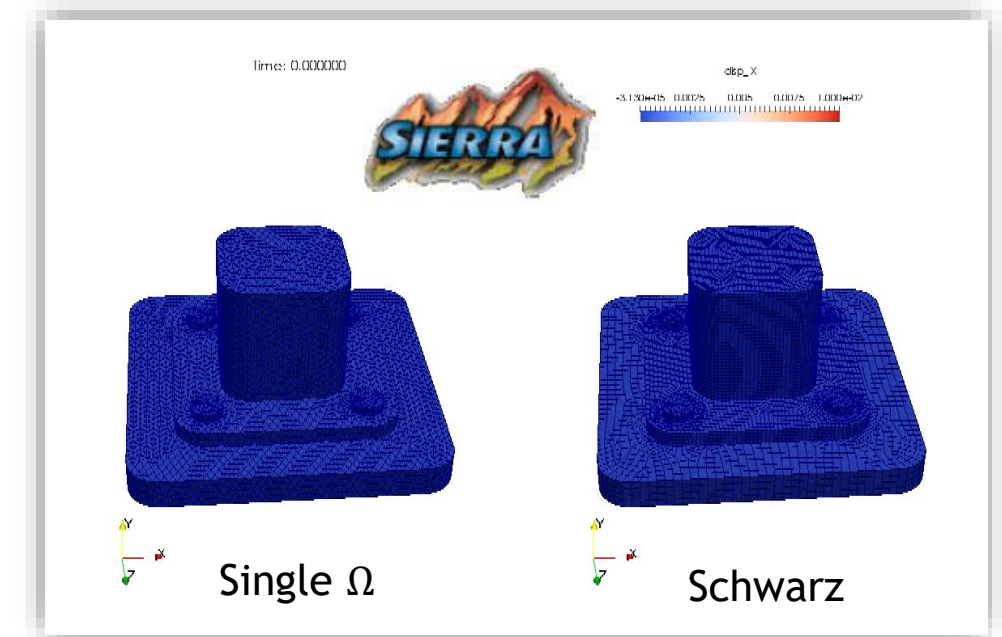
[1] Mota *et al.* 2017; Mota *et al.* 2022.

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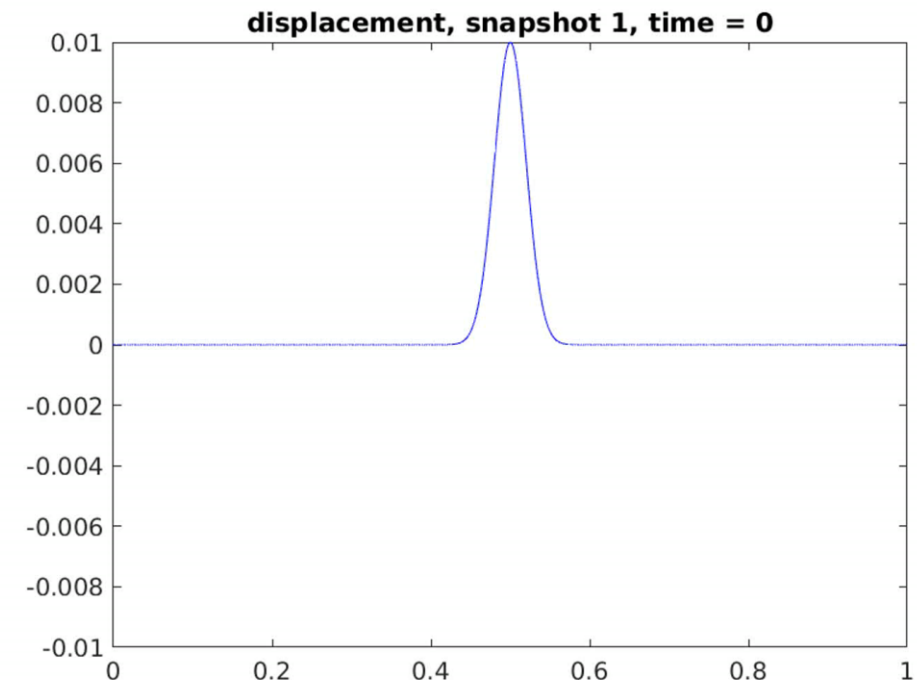
# Linear Elastic Wave Propagation Problem: FOM-ROM and ROM-ROM Couplings

*Coupling delivers accurate solution if each subdomain model is reasonably accurate, can couple different discretizations with different $\Delta x$, $\Delta t$ and basis sizes.*
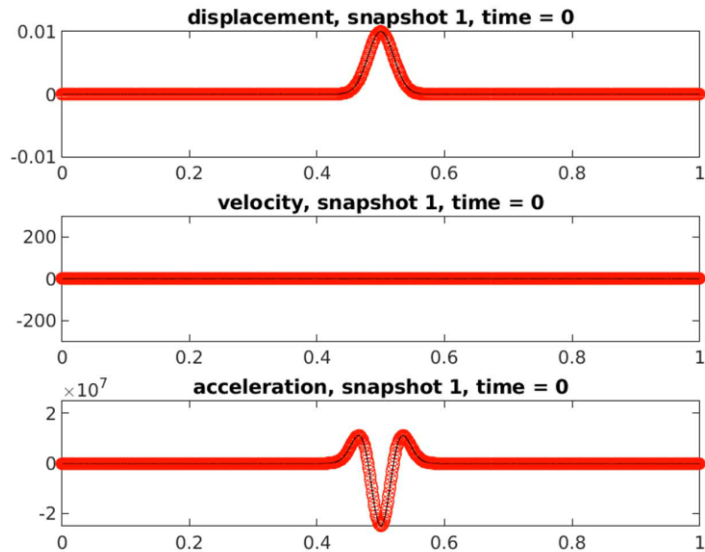


Single Domain FOM
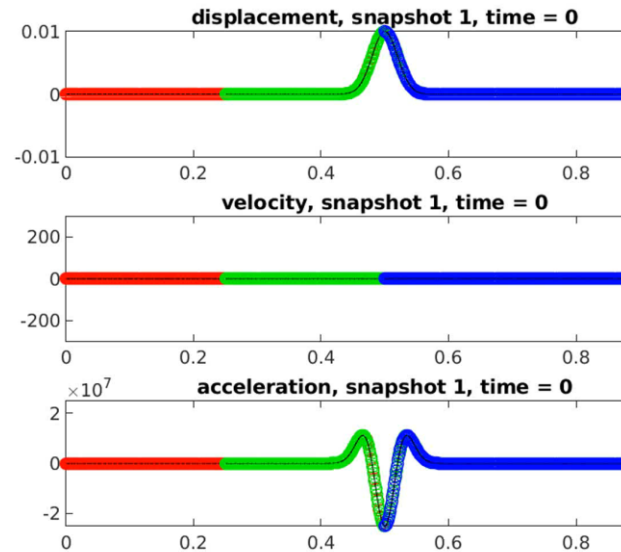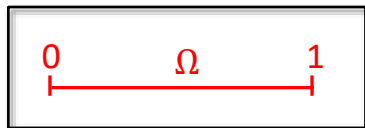
3 overlapping subdomain
$ROM^1$-$FOM^2$-$ROM^3$
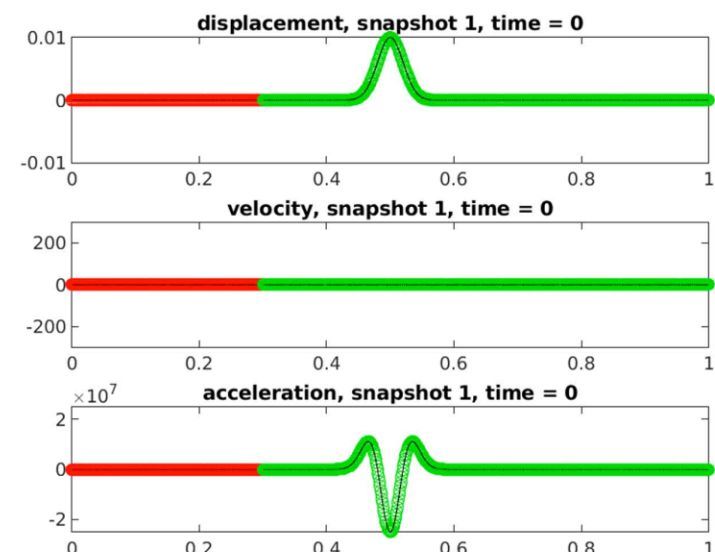
2 non-overlapping subdomain
$FOM^4$-$ROM^5$ ($\theta = 1$)
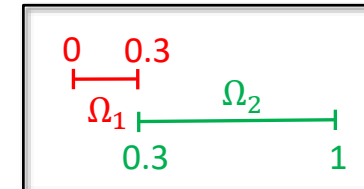
[1]Implicit 40 mode POD ROM, $\Delta t$=1e-6, $\Delta x$=1.25e-3
[2]Implicit FOM, $\Delta t$ =1e-6, $\Delta x$ =8.33e-4
[3]Explicit 50 mode POD ROM, $\Delta t$ =1e-7, $\Delta x$ =1e-3

[5]Implicit FOM, $\Delta t$ =2.25e-7, $\Delta x$ =1e-6
[4]Explicit 50 mode POD ROM, $\Delta t$ =2.25e-7, $\Delta x$ =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, $\Delta t$ =1e-6, $\Delta x$ =1.25e-3
[2]Implicit FOM, $\Delta t$ =1e-6, $\Delta x$ =8.33e-4
[3]Explicit 50 mode POD ROM, $\Delta t$ =1e-7, $\Delta x$ =1e-3
[4]Implicit FOM, $\Delta t$ =2.25e-7, $\Delta x$ =1e-6
[5]Explicit 50 mode POD ROM, $\Delta t$ =2.25e-7, $\Delta x$ =1e-6

[6]MSE= 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
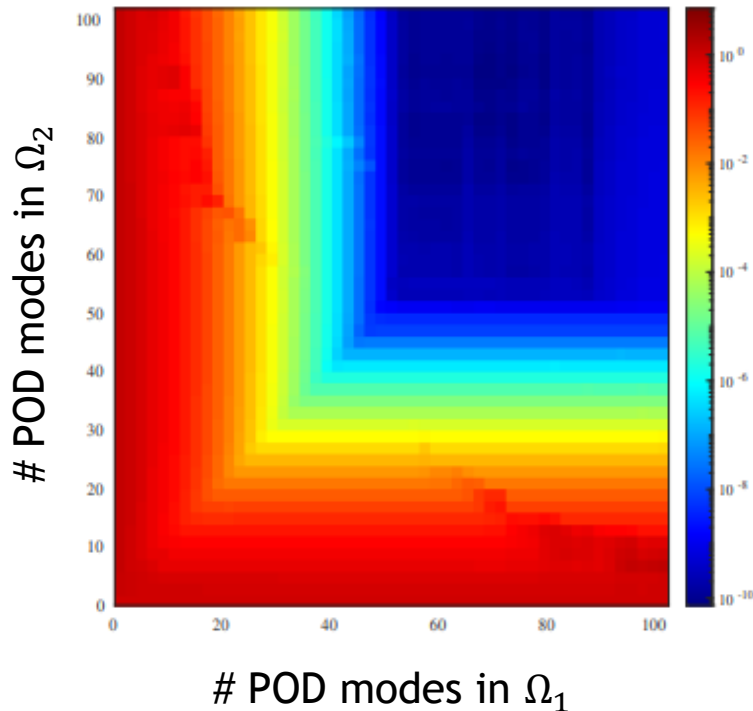
CPU times for 2 subdomain ROM-ROM coupling normalized by FOM-FOM CPU time
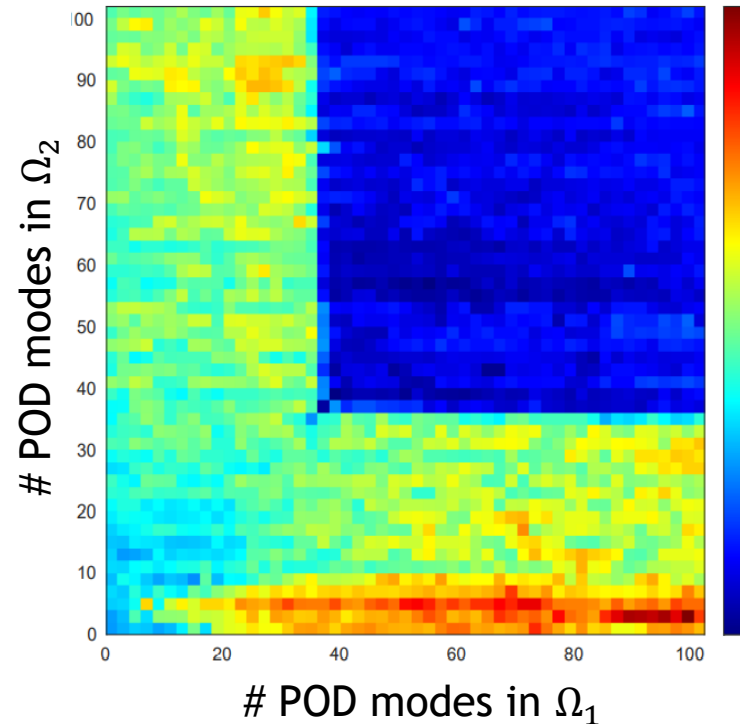
Average # Schwarz iterations for 2 subdomain ROM-ROM coupling
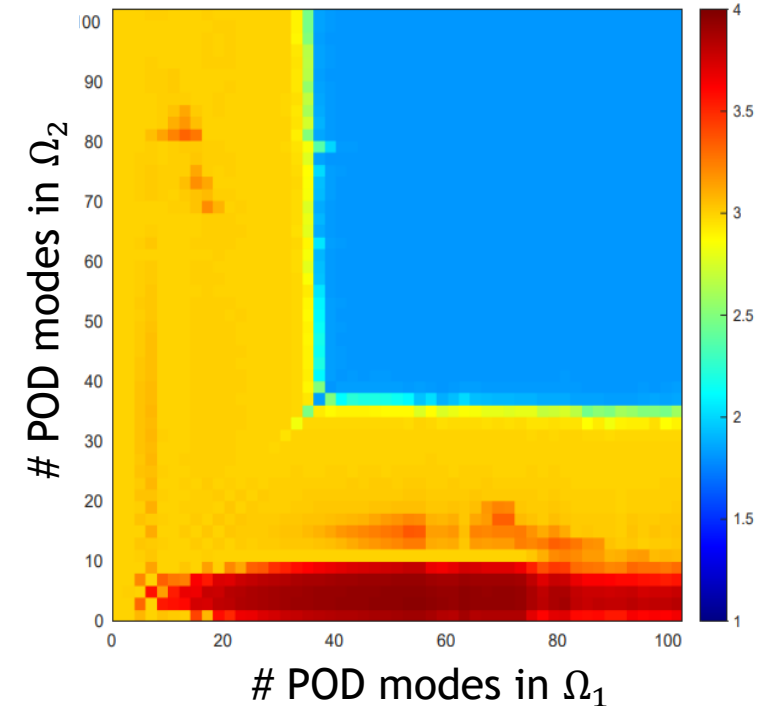
- **Smaller ROMs** are **not** the **fastest**: less accurate & require more Schwarz iterations to converge.

- 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
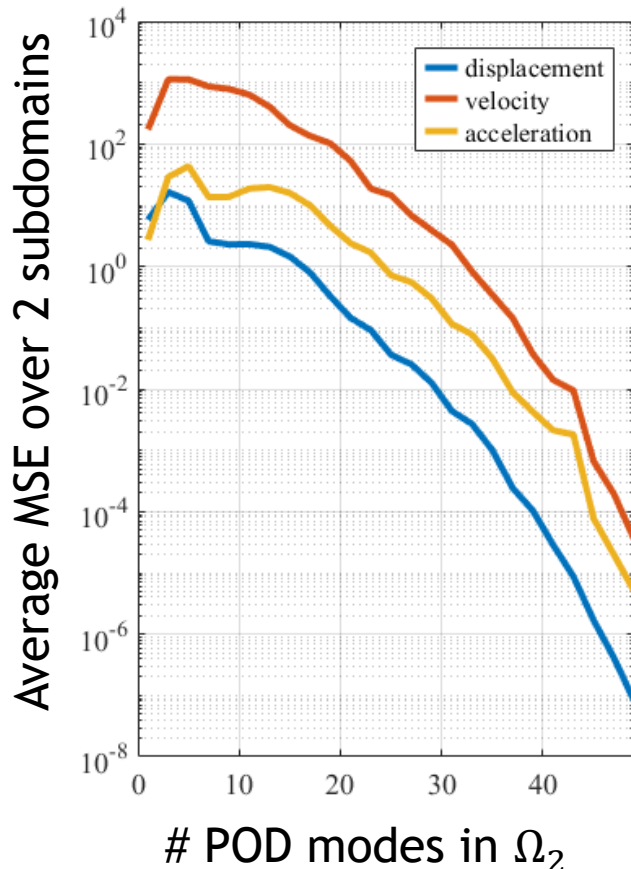
CPU times for 2 subdomain FOM-ROM coupling normalized by FOM-FOM CPU time
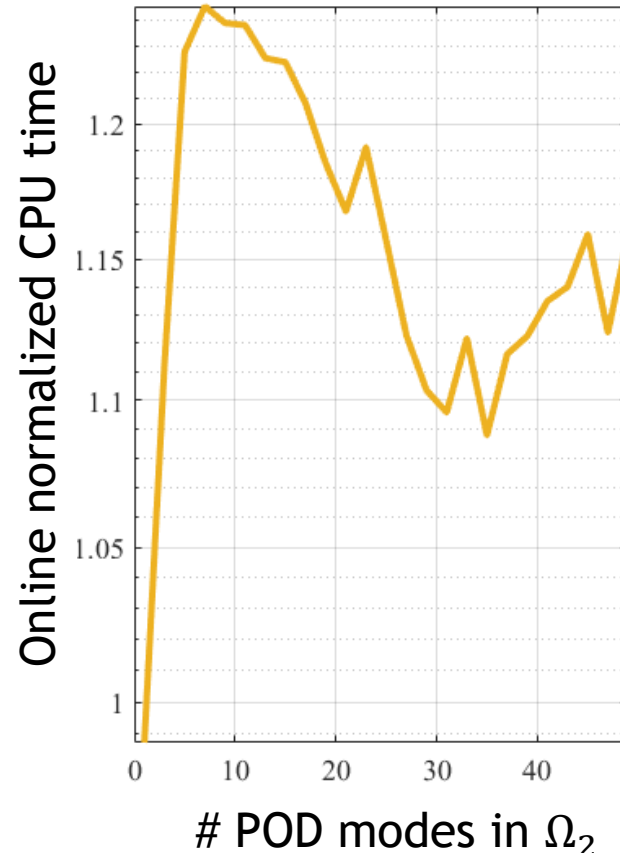
Average # Schwarz iterations for 2 subdomain couplings



Average MSE over 2 subdomains

- displacement
- velocity
- acceleration

# POD modes in $\Omega_2$

Online normalized CPU time

# POD modes in $\Omega_2$

Average # Schwarz iters

- FOM-ROM
- FOM-FOM

# POD modes in $\Omega_2$
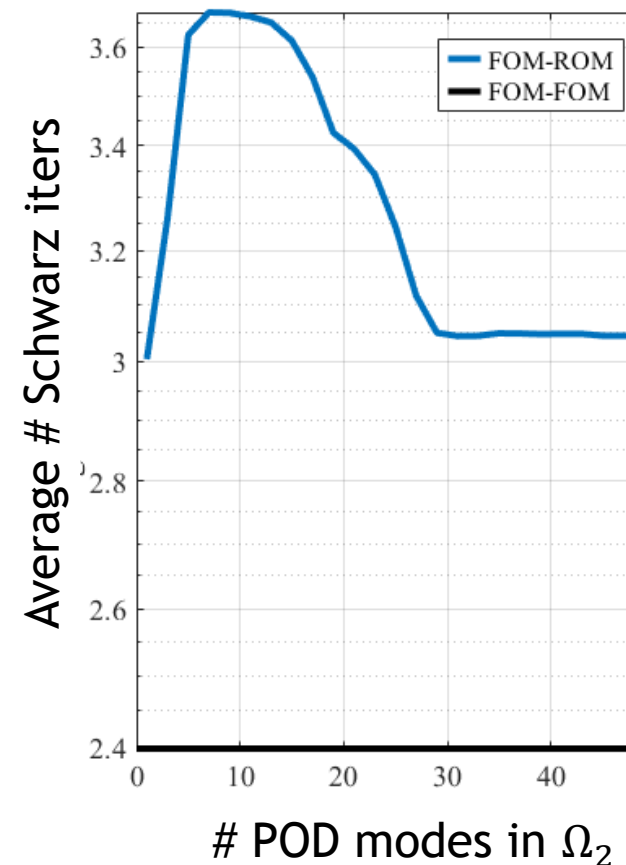
**WIP:** *understanding & improving FOM-ROM coupling performance.*

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

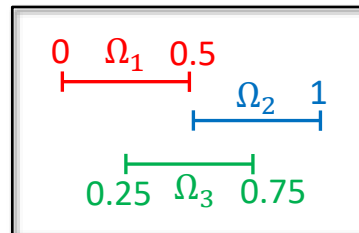# Linear Elastic Wave Propagation Problem: FOM-ROM and ROM-ROM Couplings

*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*
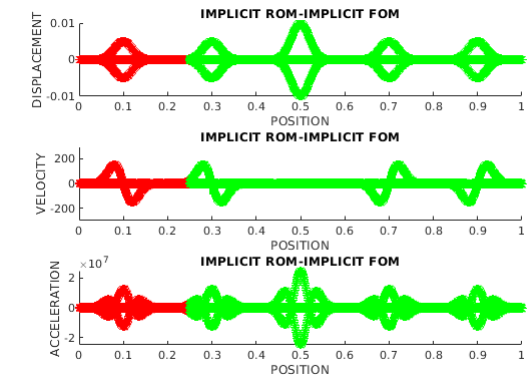


*Figure above*: $\Omega_1 = [0, 0.3]$, $\Omega_2 = [0.25, 1]$, 20 mode POD – FOM

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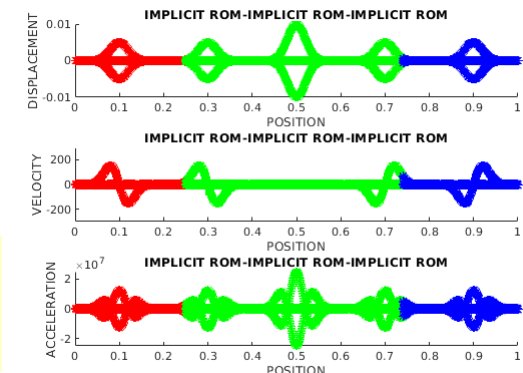
- **Project-then-approximate** paradigm (as opposed to approximate-then-project)

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

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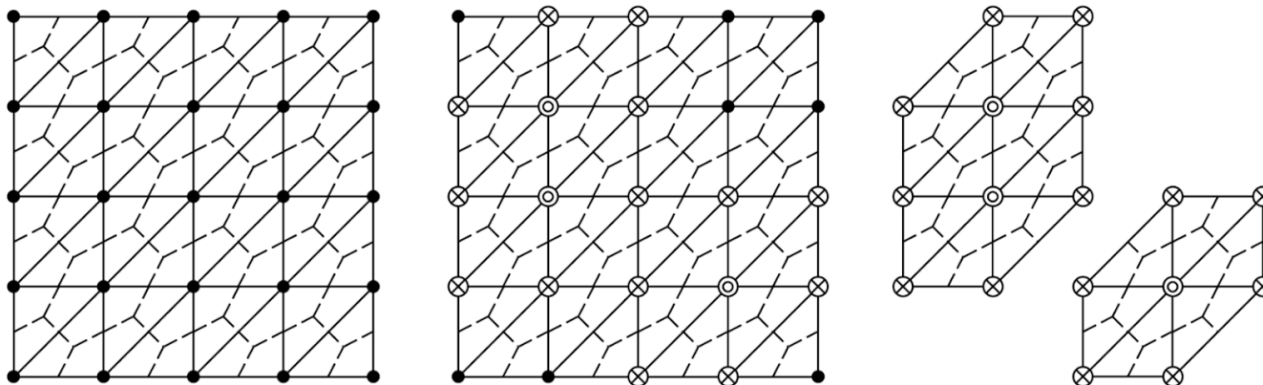


Augmented reduced mesh: ⊙ represents a selected node attached to a selected element; and ⊗ represents an added node to enable the full representation of the computational stencil at the selected node/element

# 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**

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

- We can then form the **system**

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

- Where $C\xi = d, \xi \in \mathbb{R}^{N_e}, \xi = 1$ must be the solution

- Further relax the equality to yield **non-negative least-squares problem:**

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

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

# Numerical Example: 1D Dynamic Wave Propagation Problem

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

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

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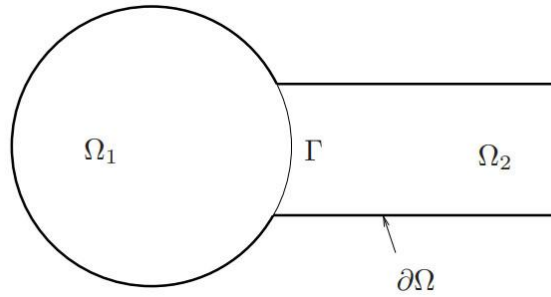
$$\boldsymbol{\lambda}_{n+1} = \theta \boldsymbol{\varphi}_2^{(n)} + (1 - \theta)\boldsymbol{\lambda}_n, \text{ on } \Gamma, \text{ for } n \geq 1$$

| $\theta$ | 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)**:

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

# Overlapping Coupling, Nonlinear Henky MM, 2 Subdomains

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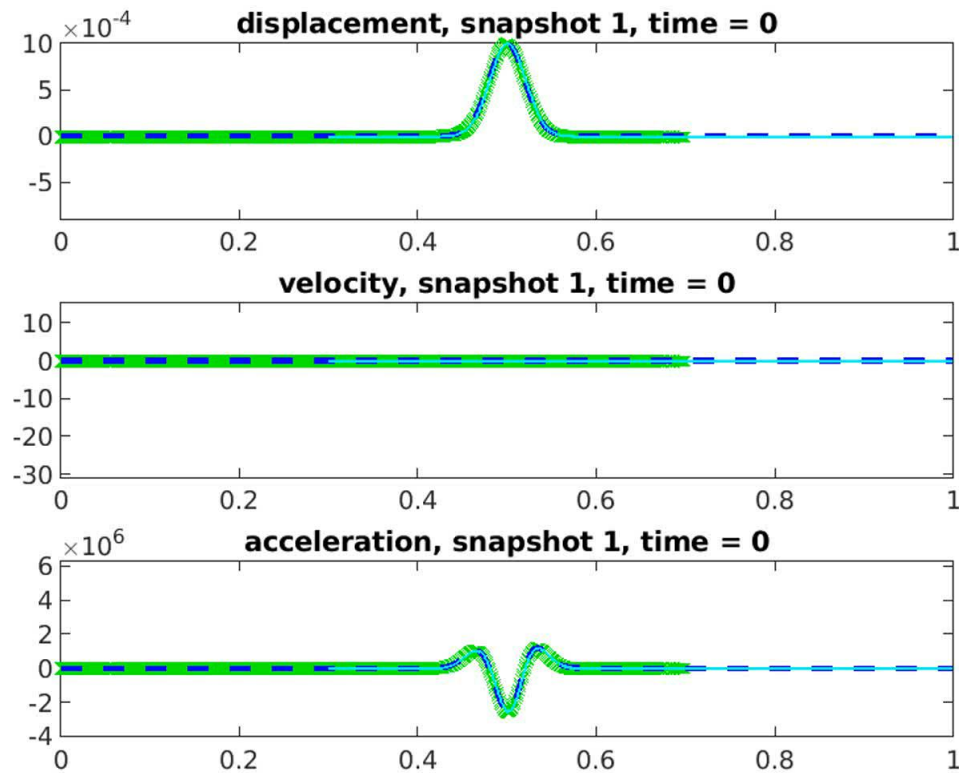


Multiplicative Schwarz
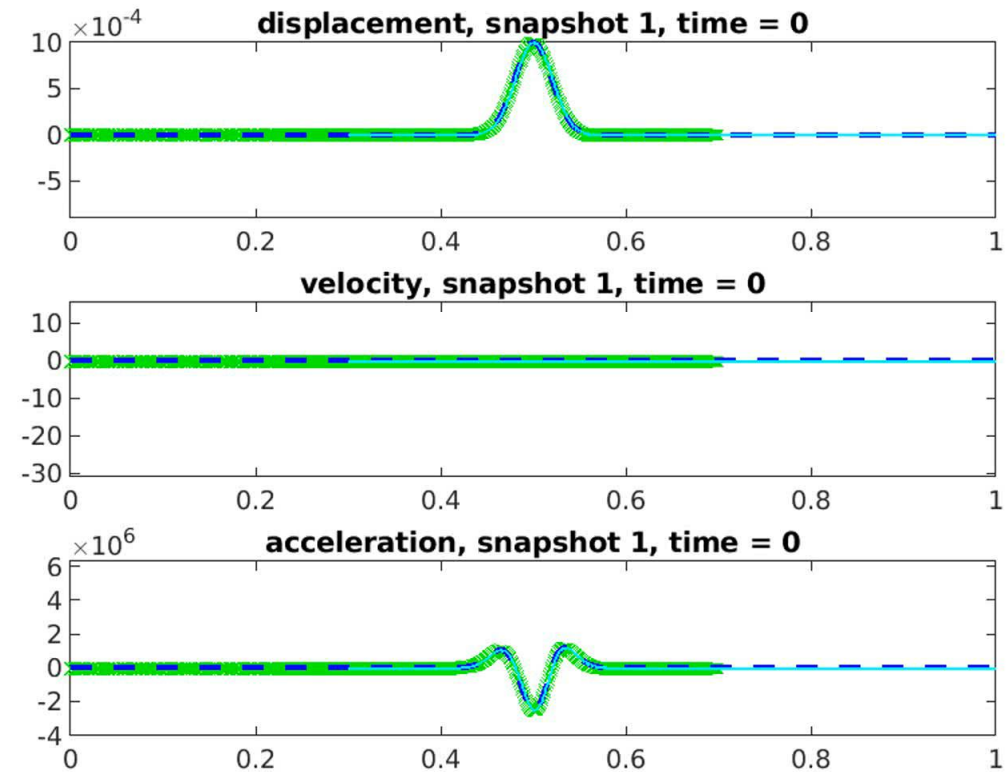
Additive Schwarz

# Overlapping Coupling, Nonlinear Henky MM, 2 Subdomains



Impl-Impl FOM-FOM, Overlapping, Henky MM

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



Impl-Impl-Expl FOM-FOM-FOM, Overlapping, Henky MM
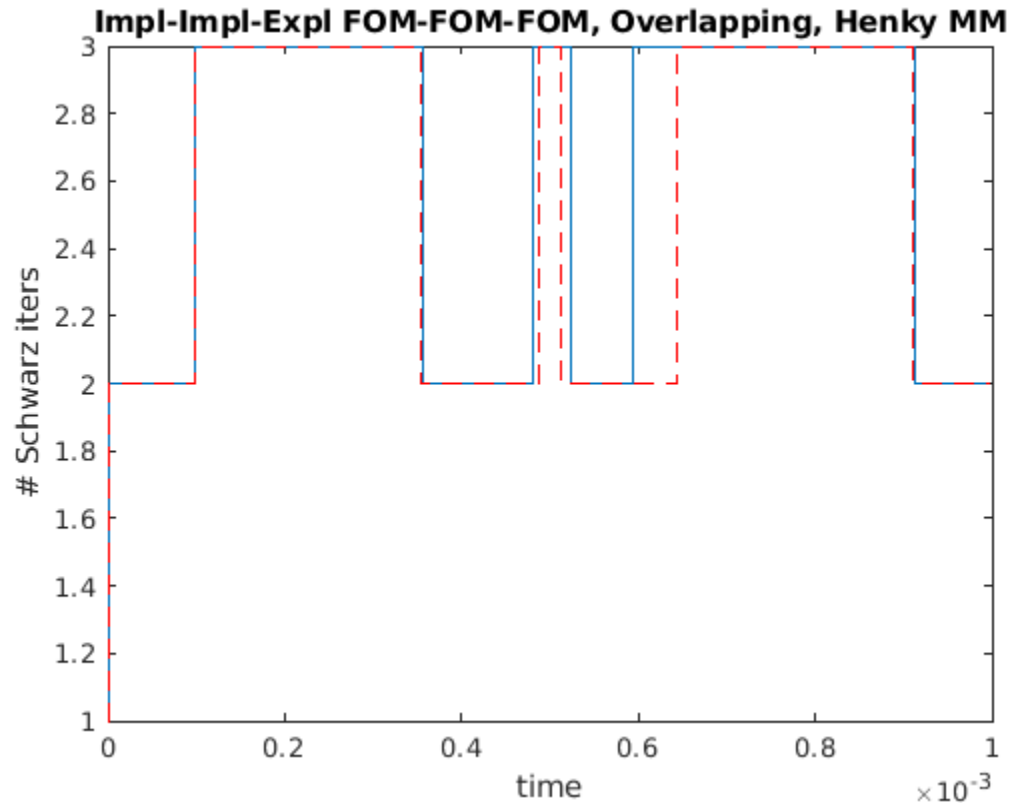
- $\Omega = [0, 0.3] \cup [0.25, 0.75] \cup [0.7, 1]$, implicit-implicit-explicit FOM-FOM-FOM coupling, dt = 1e-7, dx = 0.001.

- 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.
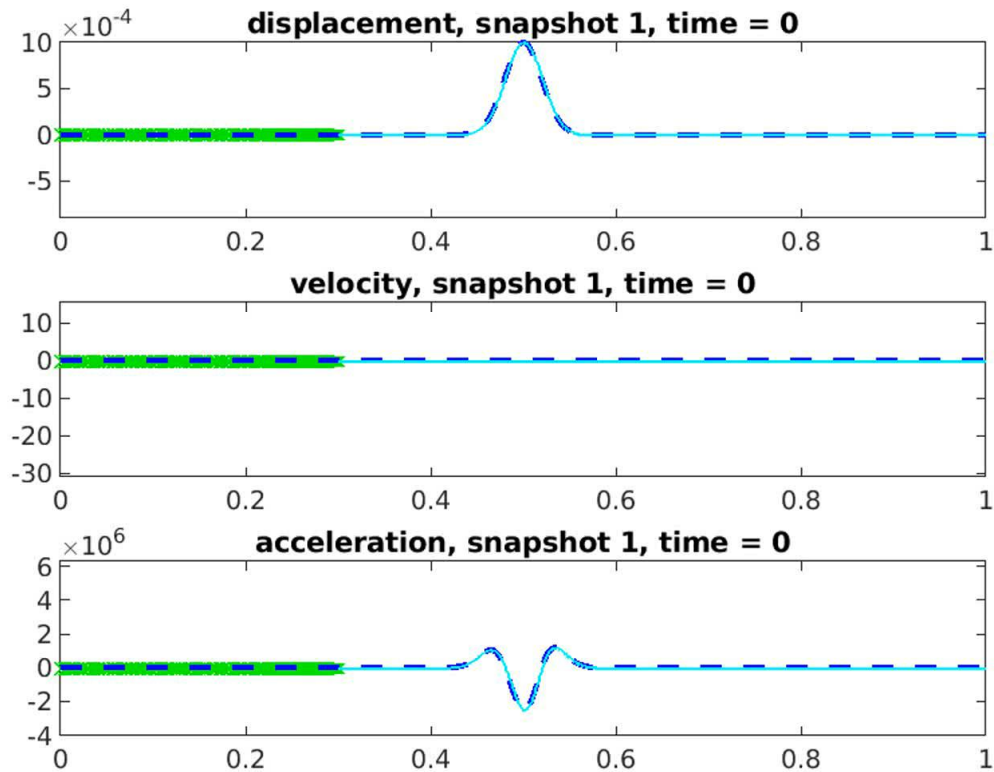


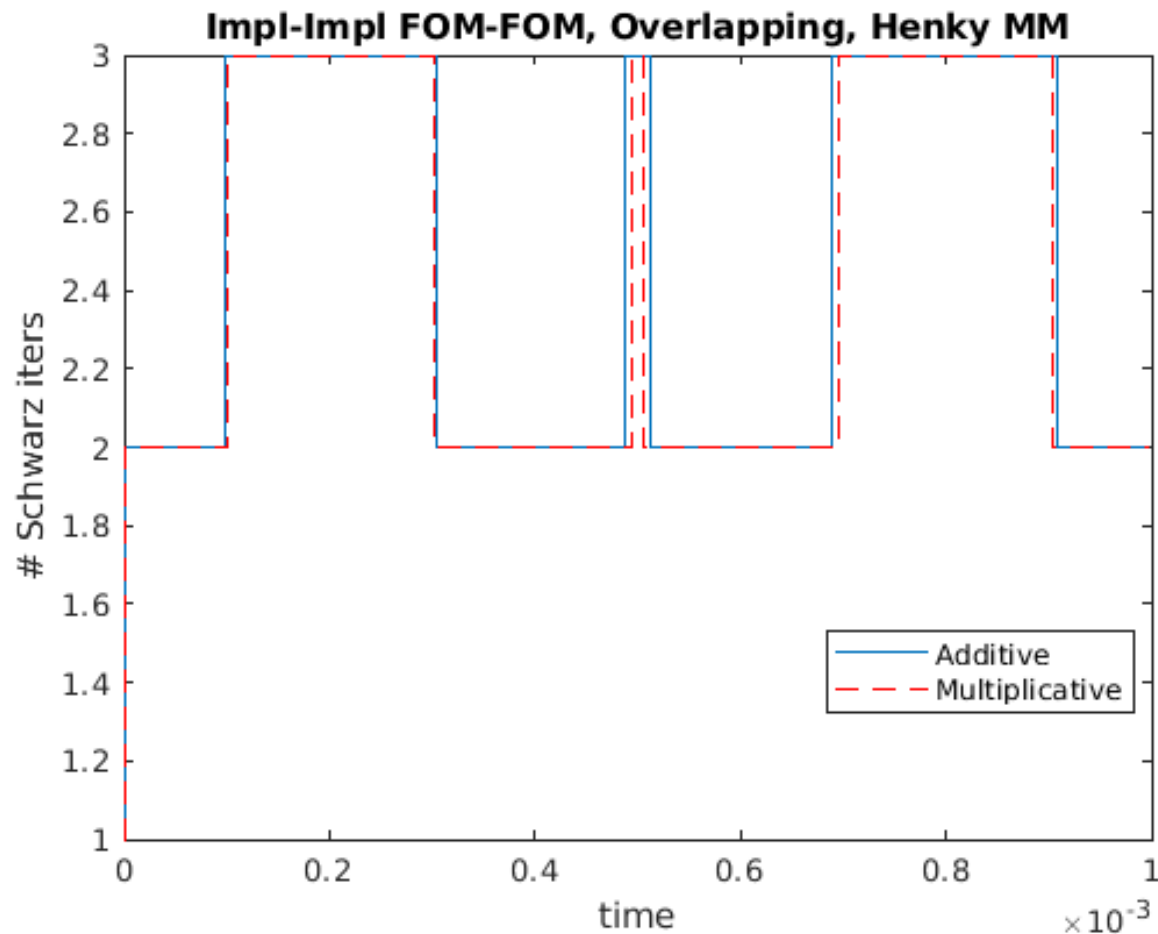Multiplicative Schwarz
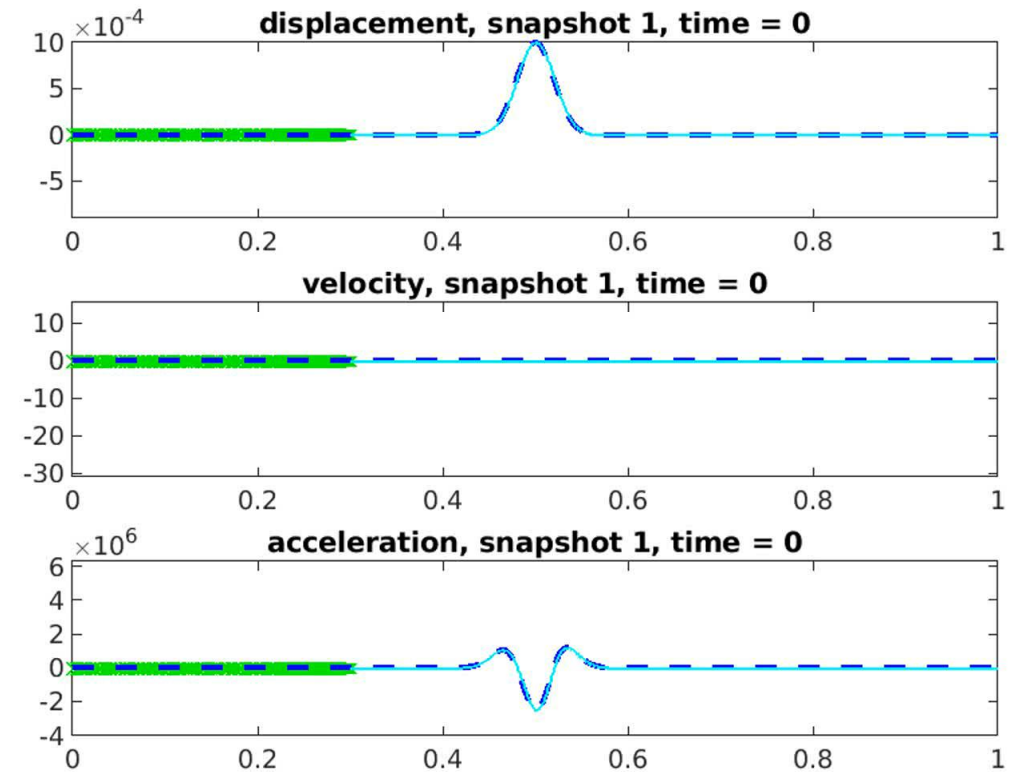
Additive Schwarz

# Non-overlapping Coupling, Nonlinear Henky MM, 2 Subdomains



**Impl-Impl FOM-FOM, Non-Overlapping, Henky MM**
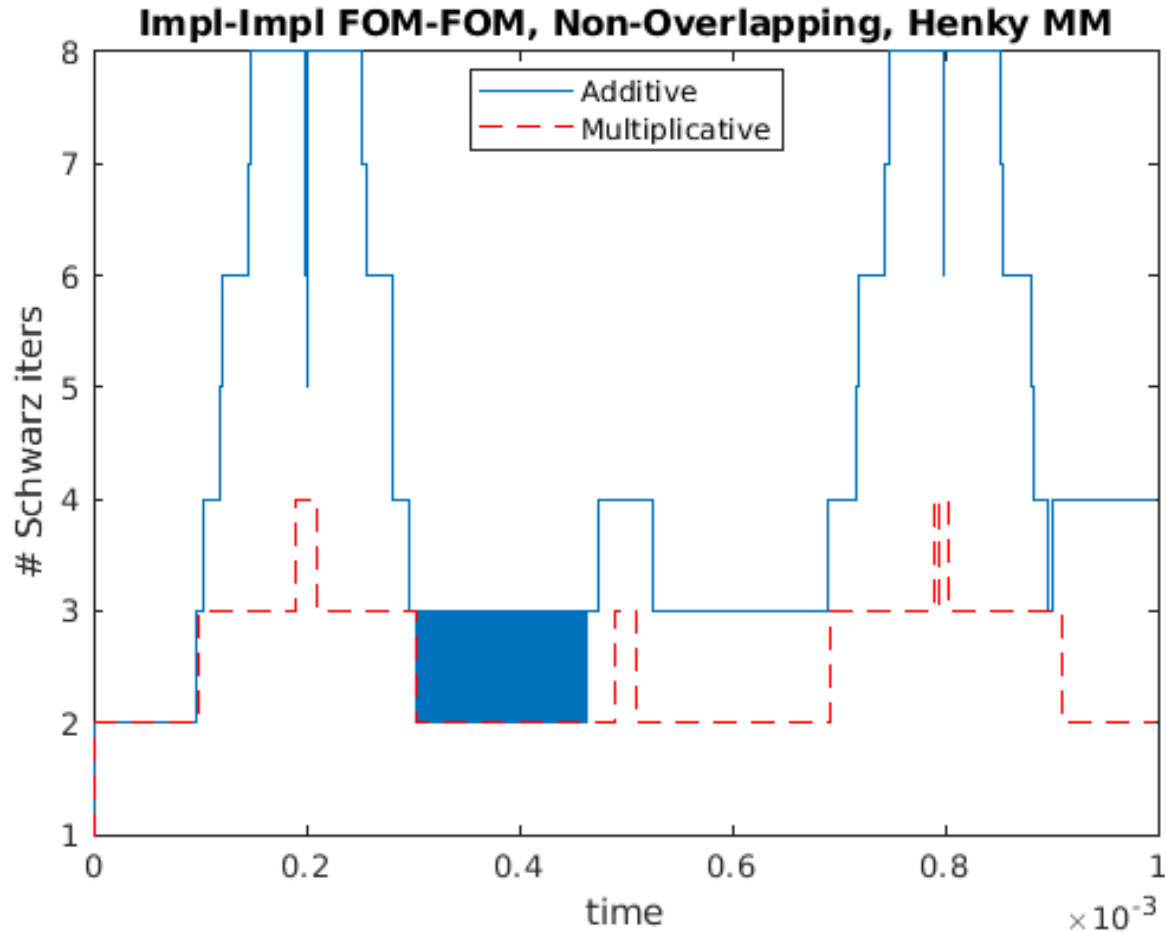
- $\Omega = [0, 0.3] \cup [0.3, 1]$, implicit-implicit FOM-FOM coupling, dt = 1e-7, dx = 1e-3.

- 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

**Impl-Impl-Expl FOM-FOM-FOM, Non-overlapping, Henky MM**
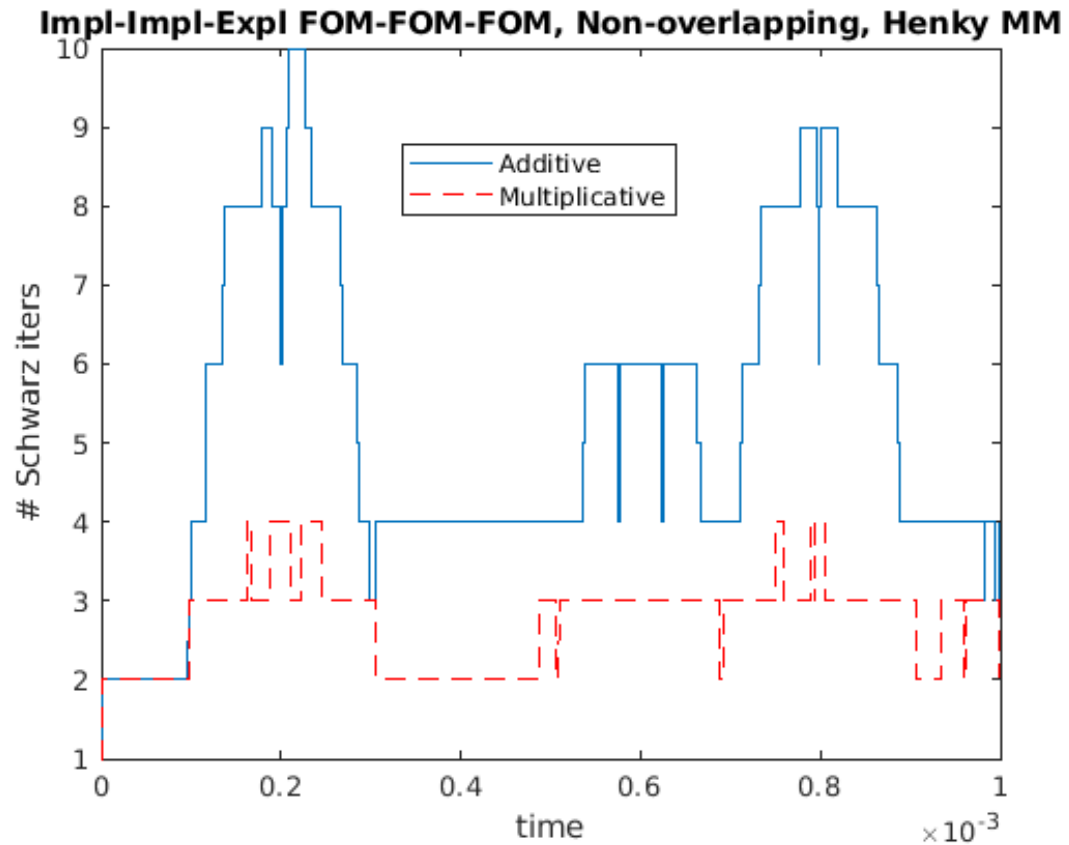


- $\Omega = [0, 0.3] \cup [0.3, 0.7] \cup [0.7, 1]$, implicit-implicit-explicit FOM-FOM-FOM coupling, dt = 1e-7, dx = 0.001.

- 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

$t = 16.50$

$t = 25.00$
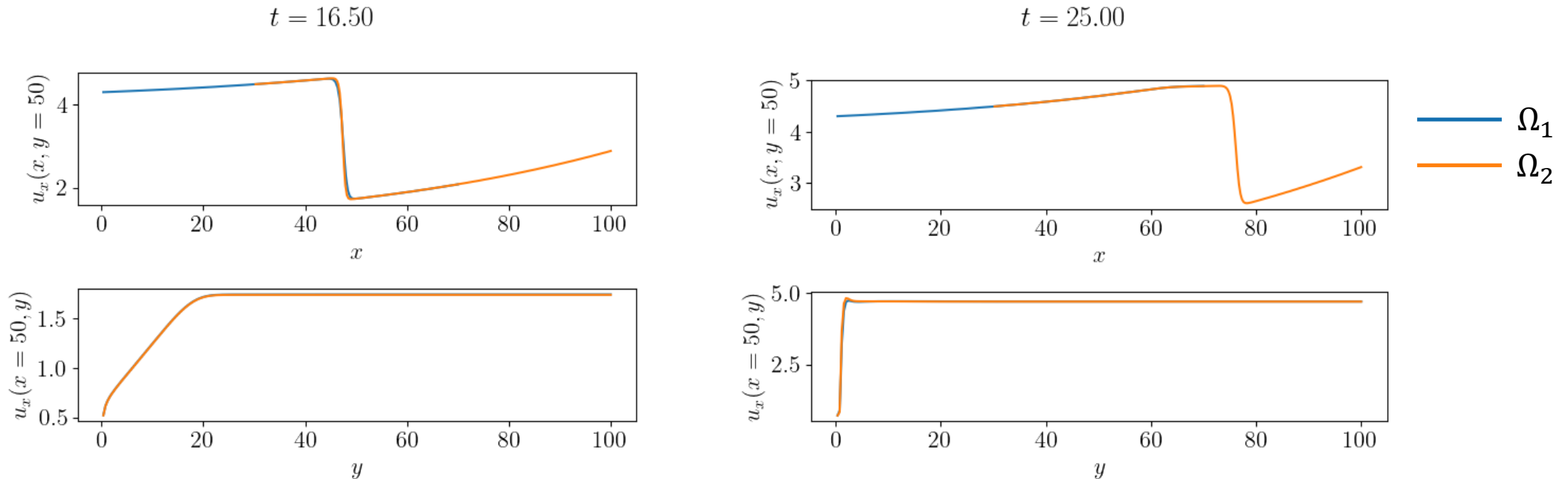


*Figures above: Two-subdomain explicit-explicit overlapping coupling in x-axis*
*[0, 70] U [30, 100] where $\mu = [4.3, 0.021]$, $\Delta t = 0.005$, $\Delta x_1 = 0.4$, $\Delta x_2 = 0.3$*

- 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!**
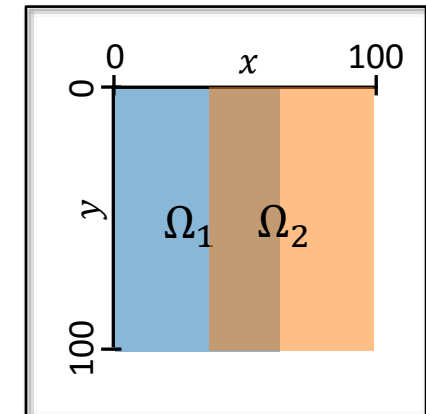
# FOM-FOM Coupling: Differing time integrators and $\Delta t$



$t = 16.50$      $t = 25.00$
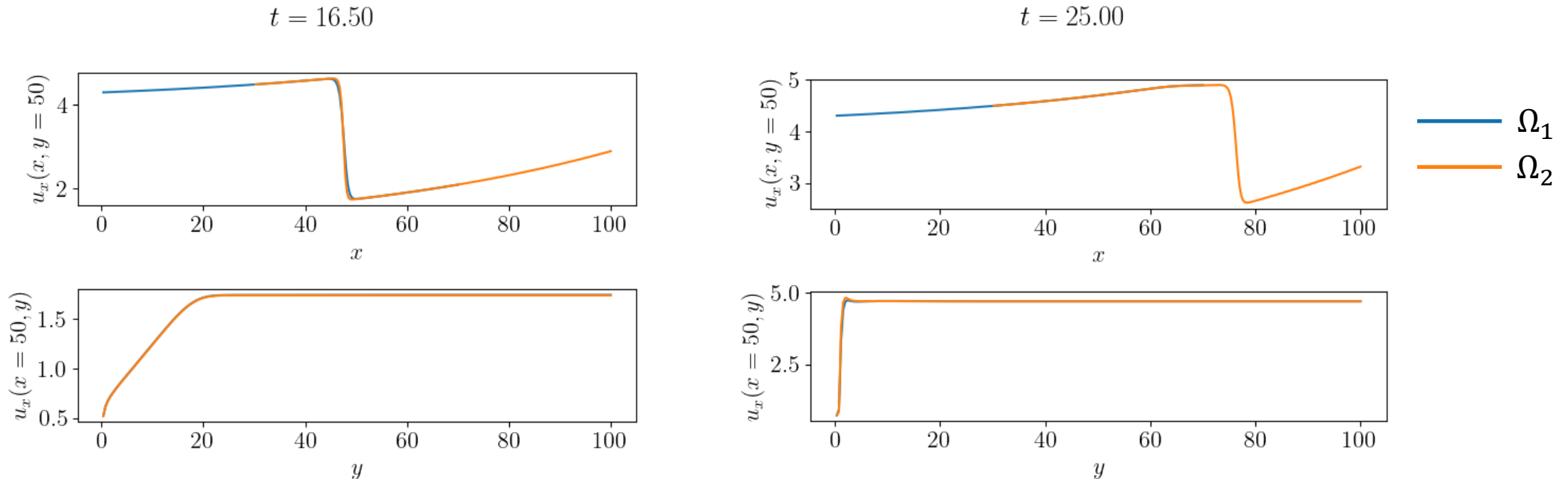
*Figures above: Two-subdomain implicit-explicit overlapping coupling in x-axis [0, 70] U [30, 100], $\mu = [4.3, 0.021]$, $\Delta t_1 = 0.05$, $\Delta t_2 = 0.005$, $\Delta x_1 = 0.4, \Delta x_2 = 0.3$*

- Introducing a different time stepper in $\Omega_1$ 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

$$t = 16.50$$

$$t = 25.00$$

$\Omega_1$
$\Omega_2$
$\Omega_3$
$\Omega_4$
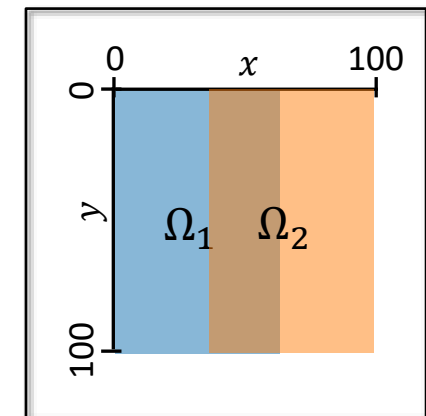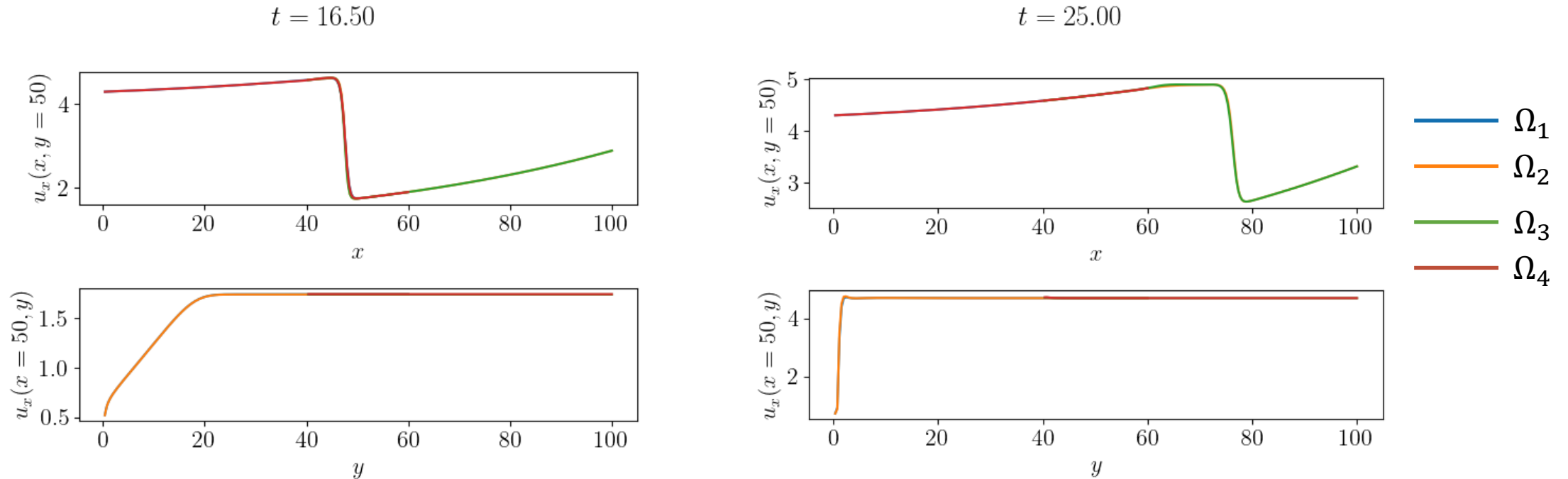
*Figures above: Four-subdomain implicit-explicit-implicit-explicit overlapping coupling in x-axis [0, 60] U [40, 100] and y-axis [0,60] U [40, 100], $\mu = [4.3, 0.021]$, $\Delta t_1 = \Delta t_3 = 0.05$, $\Delta t_2 = \Delta t_4 = 0.005$, $\Delta x_1 = \Delta x_4 = 0.4$, $\Delta x_2 = \Delta x_3 = 0.3$*

- 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
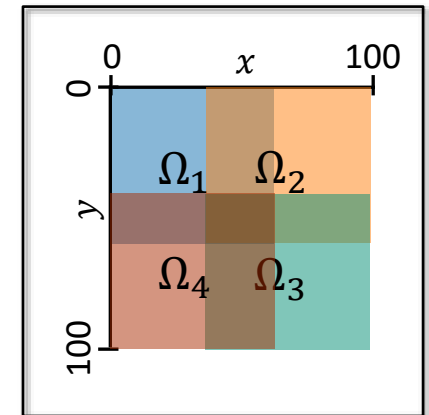
# FOM-FOM Coupling: >2 Subdomains

| Subdomain | Wall Clock Time (s) | Total (s) |
|---|---|---|
| Monolithic | 124 | 124 |
| $\Omega_1$ | 75 | |
| $\Omega_2$ | 62 | 300 |
| $\Omega_3$ | 62 | |
| $\Omega_4$ | 77 | |

$t = 0.00$



- $\Omega_1$
- $\Omega_2$
- $\Omega_3$
- $\Omega_4$
— 1 SD

*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], $\mu = [4.3, 0.021]$, $\Delta t = 0.05$, $\Delta x_1 = \Delta x_4 = 0.4$, $\Delta x_2 = \Delta x_3 = 0.3$*
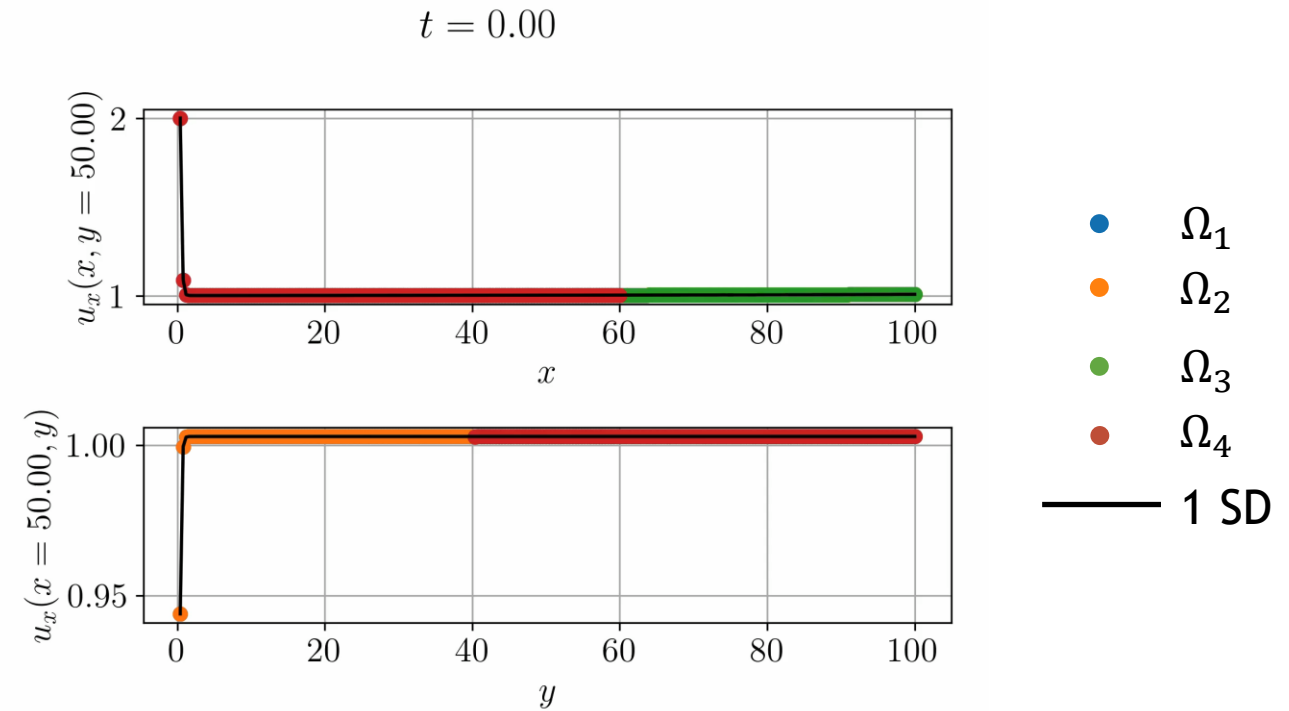
- Despite a heterogeneous mixture of different subdomains coupled in multiple dimensions with different solvers, resolutions, etc. the solution is still consistent

- Choosing $\Omega_1 \rightarrow \Omega_2 \rightarrow \Omega_3 \rightarrow \Omega_4$ requires 3 Schwarz iterations per global time step
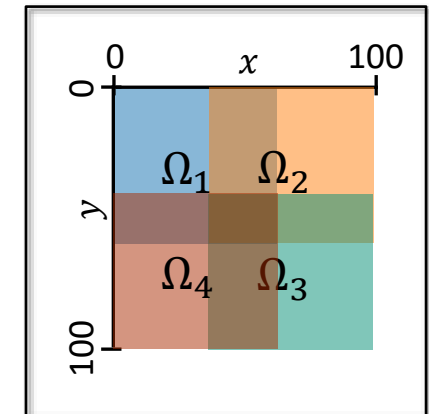
# HROM-FOM-FOM-FOM Coupling



$t = 0.00$

$\Omega_1$
$\Omega_2$
$\Omega_3$
$\Omega_4$
— 1 SD
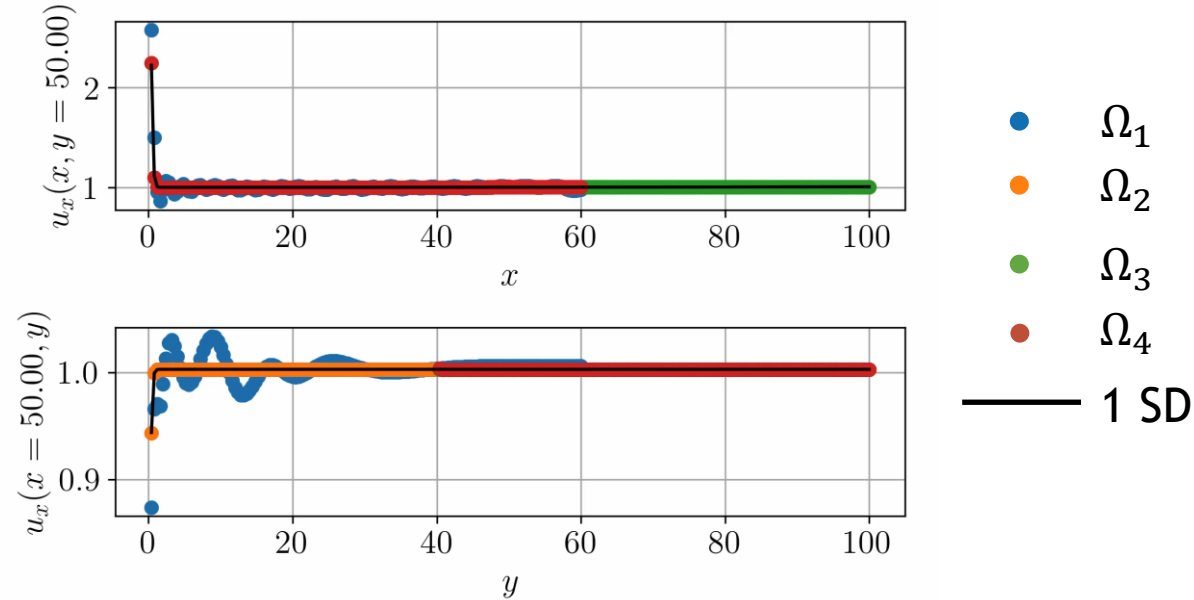
$n_e = 4{,}346$ (19% of $N_e$)

| Domain | $M$ | MSE (%) | HROM-FOM-FOM-FOM Wall Clock Time (s) | FOM-FOM-FOM-FOM Wall Clock Time (s) | Speedup |
|--------|-----|---------|--------------------------------------|-------------------------------------|---------|
| $\Omega_1$ | 76 | 1.5 | 30 | 68 | 2.3 |
| Total | — | — | 276 | 300 | 1.1 |
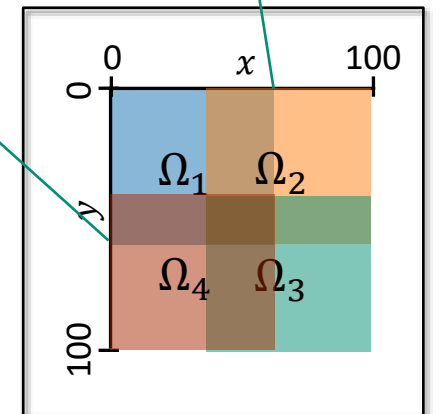
- We have **computational gain** even when choosing the "worst" subdomain for HROM
- No speedup over single-domain FOM (wall clock time = $124\,s$)
  - ➤ **Mitigation:** additive Schwarz, which admits more parallelism

# HROM-FOM-FOM-FOM Coupling



$\Omega_1$
$\Omega_2$
$\Omega_3$
$\Omega_4$
—— 1 SD
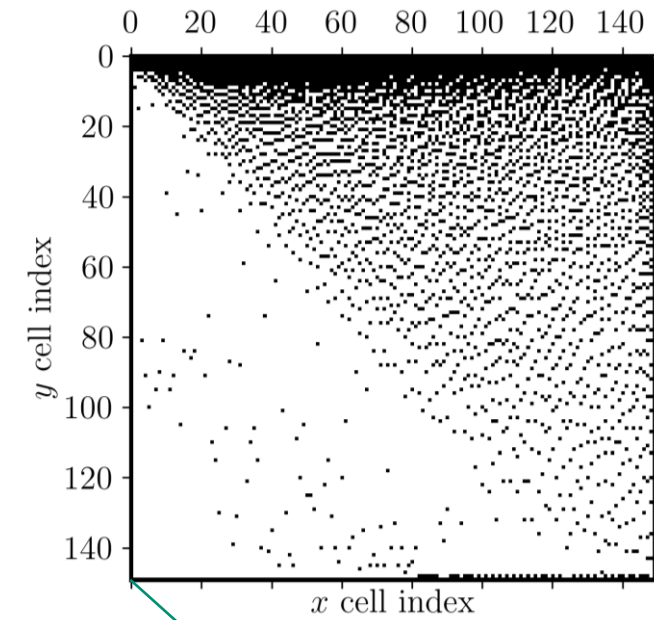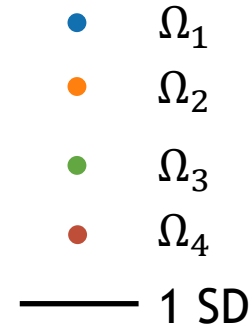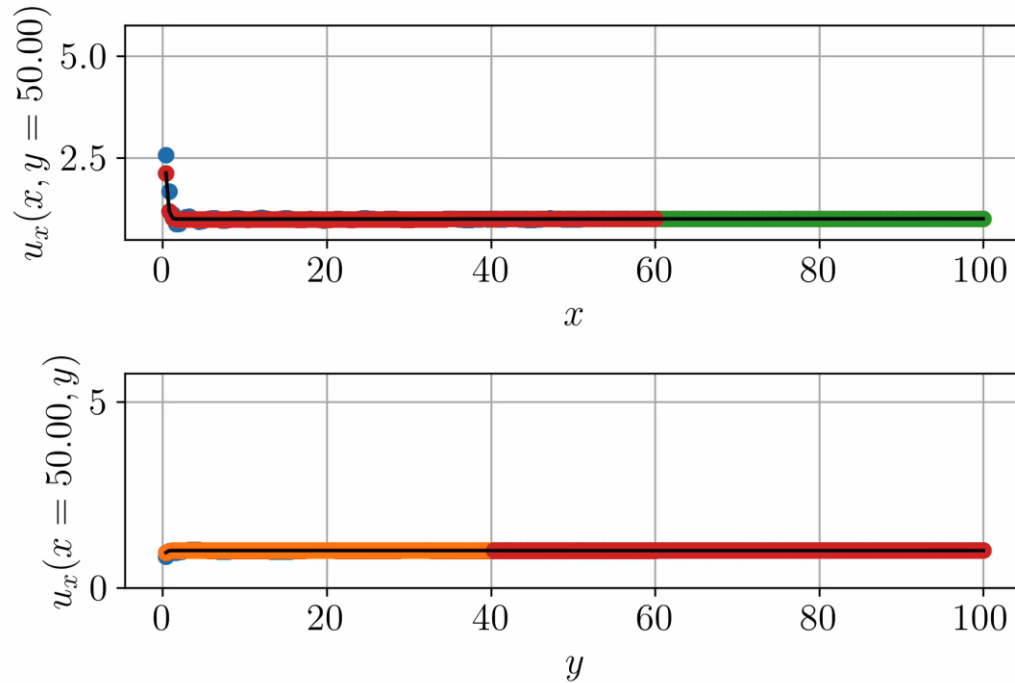
$n_e = 4{,}346$ (19% of $N_e$)
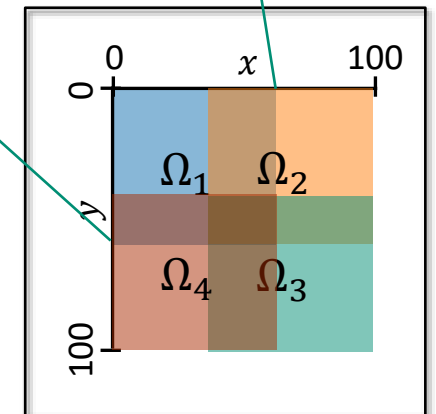
- HROM is in $\Omega_1$ and retains **95% of snapshot energy** $\Rightarrow$ 57 modes
  - ➤ HROM assignment is **"worst-case-scenario"**
- **Reduced mesh** trained only using a single parameter instance of $\boldsymbol{\mu} = [4.25, 0.0225]$
- Method converges in **3 Schwarz iterations** per controller 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