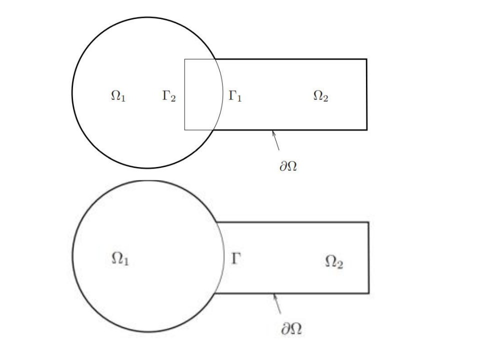
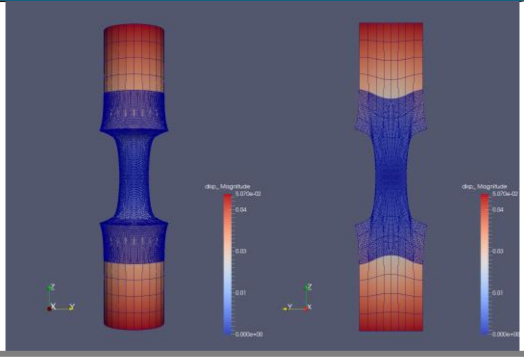
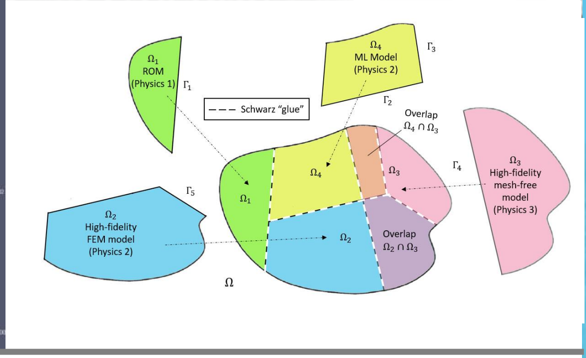
The Schwarz Alternating Method for FOM*-ROM# and ROM-ROM Coupling







* Full Order Model

\# Reduced Order Model

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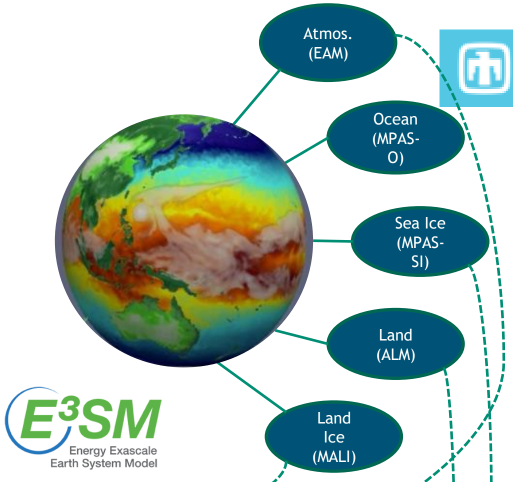
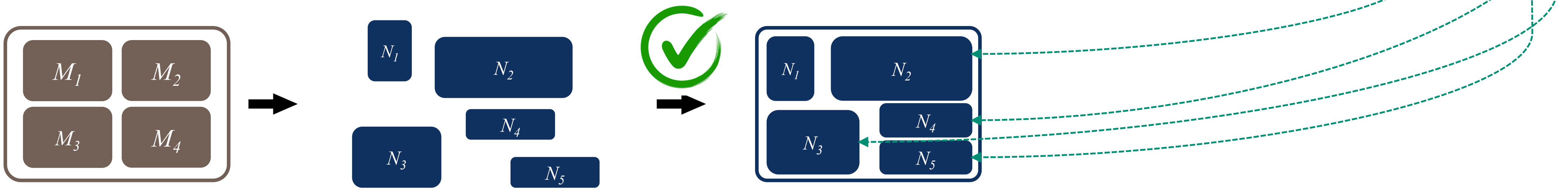
Motivation

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.





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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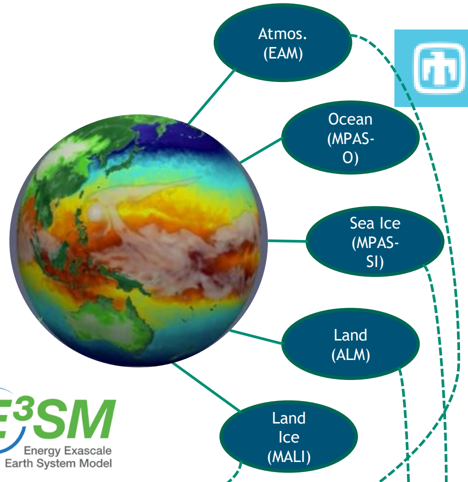

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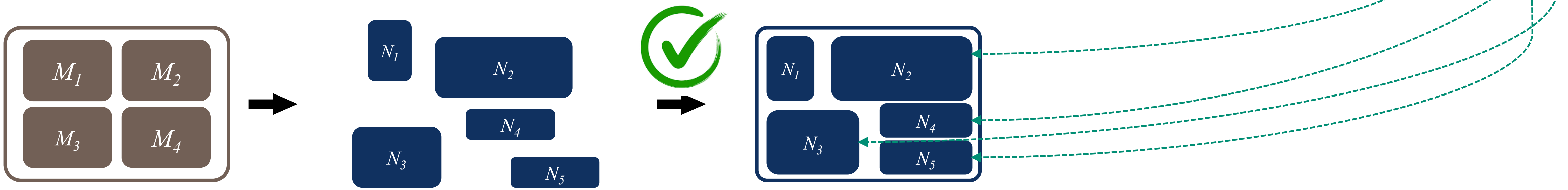
- Most existing coupling frameworks are based on **traditional discretization methods**.

E3SM Energy Exascale Earth System Model



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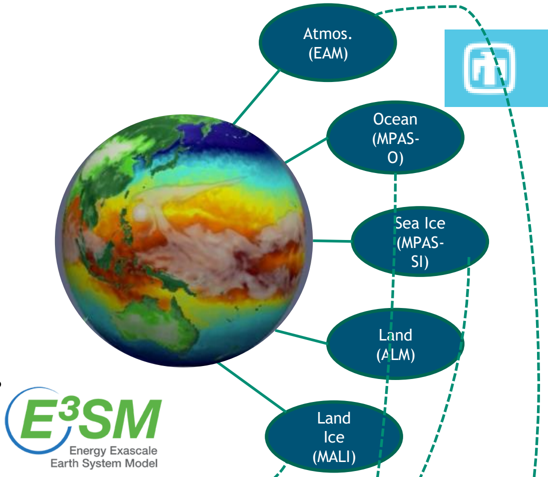

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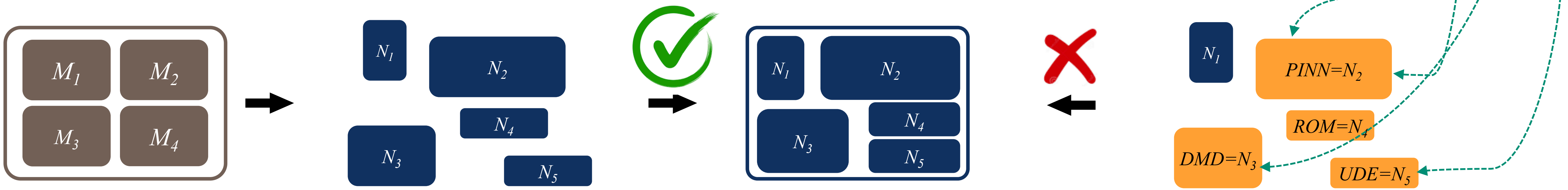

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Traditional + Data-Driven Methods
- PINNs
- Neural ODEs
- Projection-based ROMs, …

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

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

Flexible Heterogeneous Numerical Methods (fHNM) Project

Principal research objective:

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

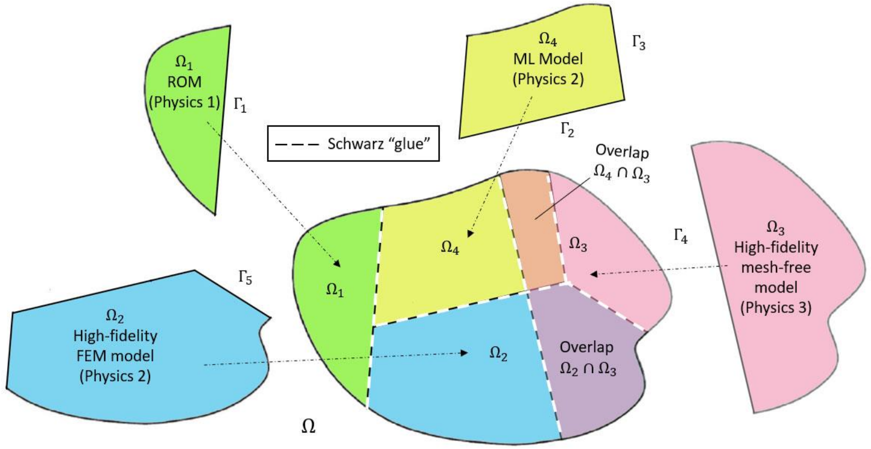
Principal research challenges: we lack mathematical and algorithmic understanding of how to

- **“Mix-and-match” standard** and **data-driven models** from three-classes
  - ➢ *Class A*: projection-based reduced order models (ROMs) ***This talk***
  - ➢ *Class B*: machine-learned models, i.e., Physics-Informed Neural Networks (PINNs)
  - ➢ *Class C*: flow map approximation models, i.e., dynamic model decomposition (DMD) models
- Ensure **well-posedness & physical consistency** of the resulting **heterogeneous models.**
- **Solve** such heterogeneous models efficiently.

Three coupling methods:

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

Talk by A. DeCastro



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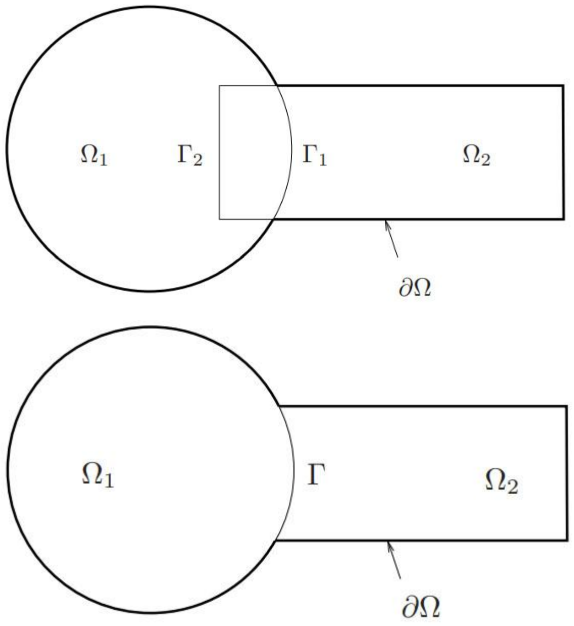
1. Overview of the Schwarz Alternating Method for Concurrent Coupling

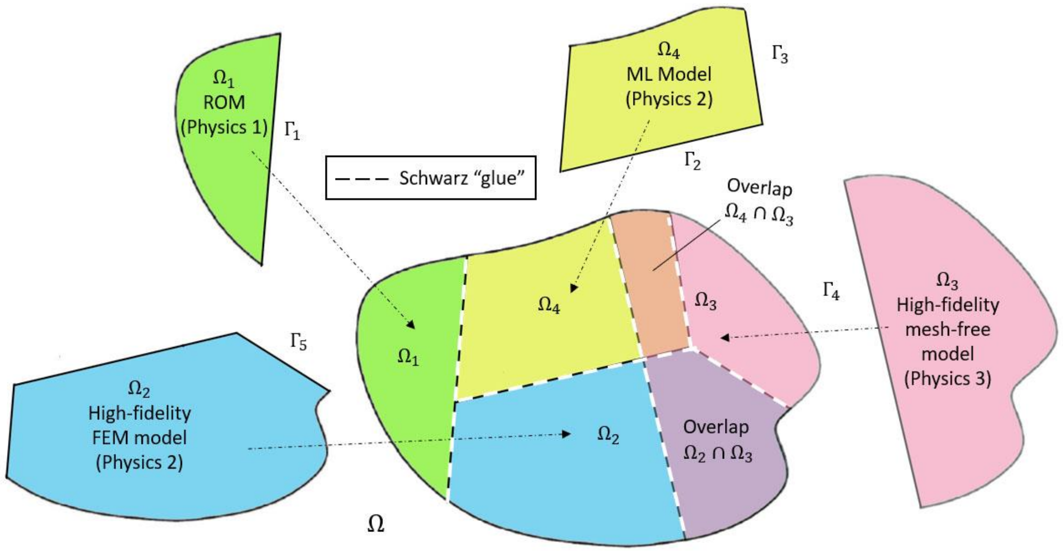
2. Overview of Projection-Based Model Order Reduction

3. Extension of Schwarz Alternating Method to FOM-ROM and ROM-ROM coupling

4. Numerical Results

5. Summary and Future Work





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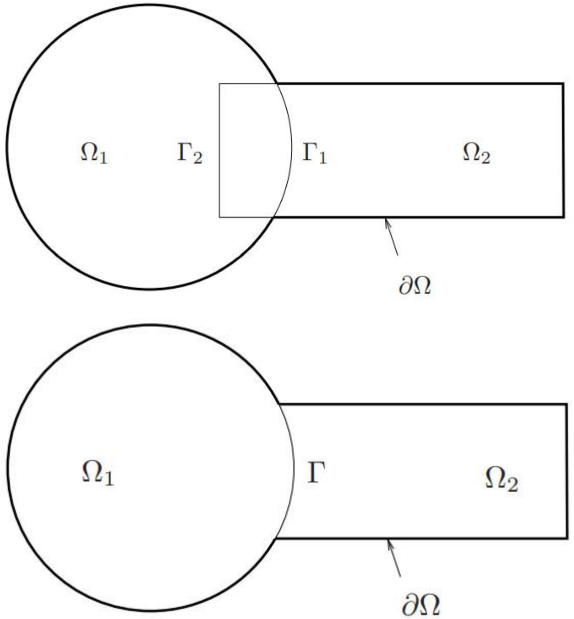
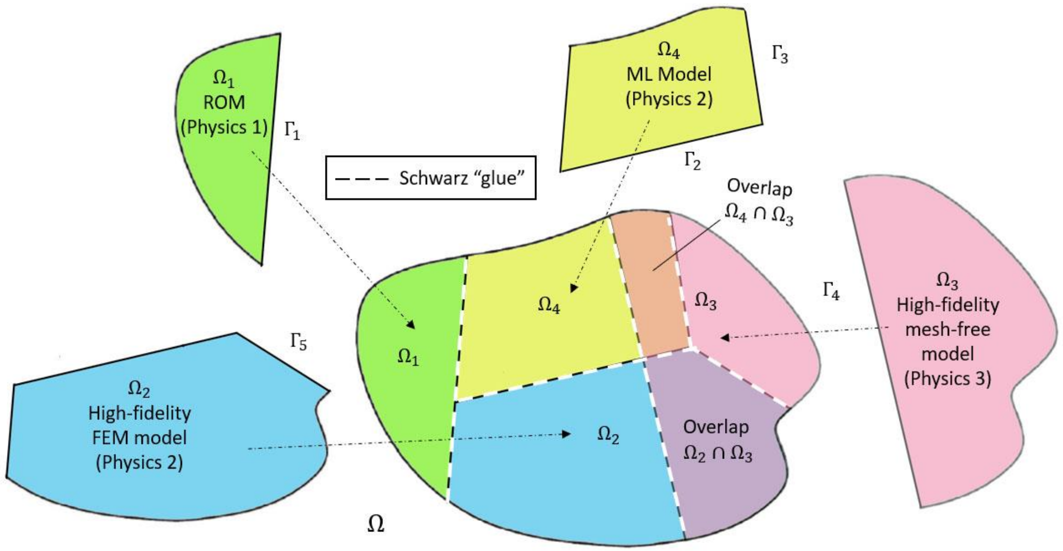
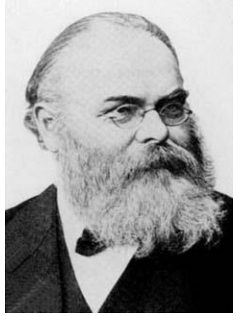




Schwarz Alternating Method for Domain Decomposition



H. Schwarz (1843–1921)

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

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

Basic Schwarz Algorithm

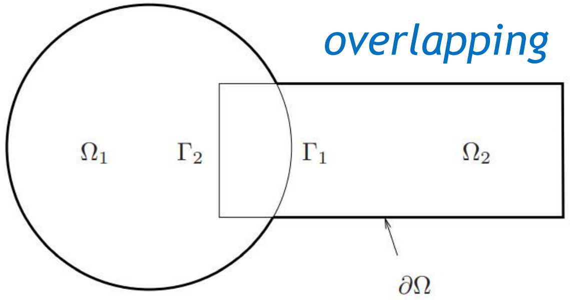
Initialize:

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

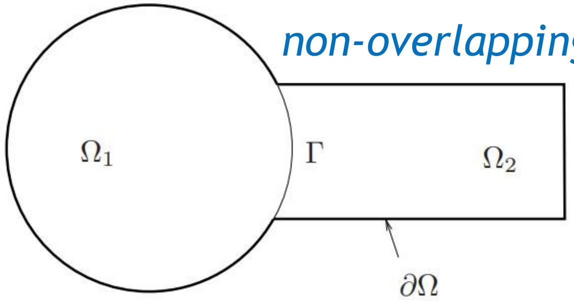
Iterate until convergence:

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

overlapping



non-overlapping



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

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

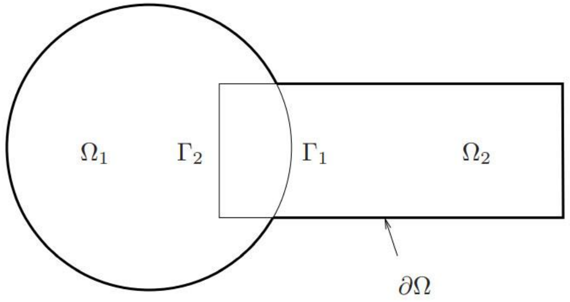
Spatial Coupling via Alternating Schwarz

Model PDE: $\begin{cases} \mathcal{L}u = f, & \text{in } \Omega, \\ u = g, & \text{on } \partial\Omega \end{cases}$

Overlapping Domain Decomposition

$$\begin{cases} \mathcal{L}u_1^{n+1} = f, & \text{in } \Omega_1, \\ u_1^{n+1} = g, & \text{on } \partial\Omega_1 \backslash \Gamma_1, \\ u_1^{n+1} = u_2^n, & \text{on } \Gamma_1, \end{cases}$$

$$\begin{cases} \mathcal{L}u_2^{n+1} = f, & \text{in } \Omega_2, \\ u_2^{n+1} = g, & \text{on } \partial\Omega_2 \backslash \Gamma_2, \\ u_2^{n+1} = u_1^{n+1}, & \text{on } \Gamma_2. \end{cases}$$



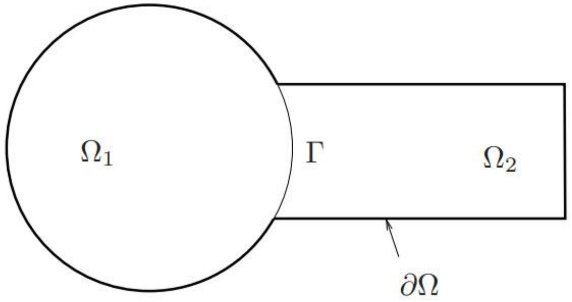
- Dirichlet-Dirichlet transmission BCs [Schwarz, 1870; Lions, 1988]

Non-overlapping Domain Decomposition

$$\begin{cases} \mathcal{L}u_1^{n+1} = f, & \text{in } \Omega_1, \\ u_1^{n+1} = g, & \text{on } \partial\Omega_1 \backslash \Gamma, \\ u_1^{n+1} = \lambda_{n+1}, & \text{on } \Gamma, \end{cases}$$

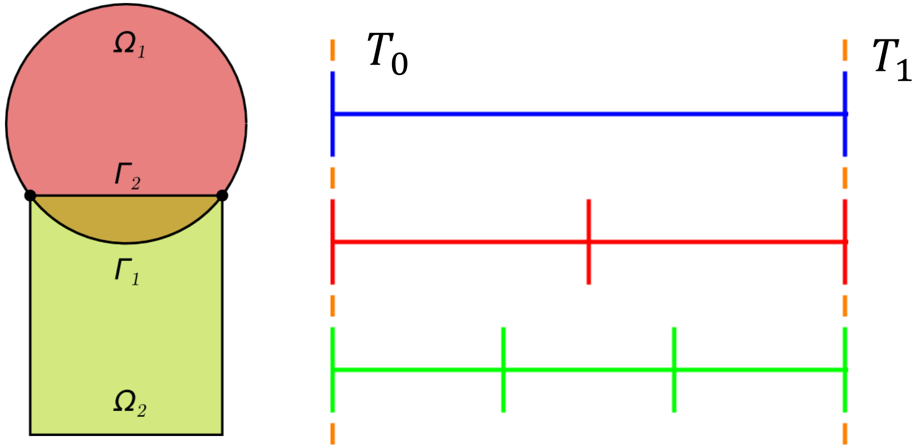
$$\begin{cases} \mathcal{L}u_2^{n+1} = f, & \text{in } \Omega_2, \\ u_2^{n+1} = g, & \text{on } \partial\Omega_2 \backslash \Gamma, \\ \frac{\partial u_2^{n+1}}{\partial \mathbf{n}_2} = \frac{\partial u_1^{n+1}}{\partial \mathbf{n}_2}, & \text{on } \Gamma, \end{cases}$$

$$\lambda_{n+1} = \theta u_2^n + (1-\theta)\lambda_n, \quad \text{on } \Gamma, \quad \text{for } n \geq 1.$$



- 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

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

Model PDE: $\begin{cases} \dot{u} = f - \mathcal{L}u, & \text{in } \Omega, \\ u(x,t) = g(t), & \text{on } \partial\Omega, \\ u(x,0) = u_0, & \text{in } \Omega \end{cases}$

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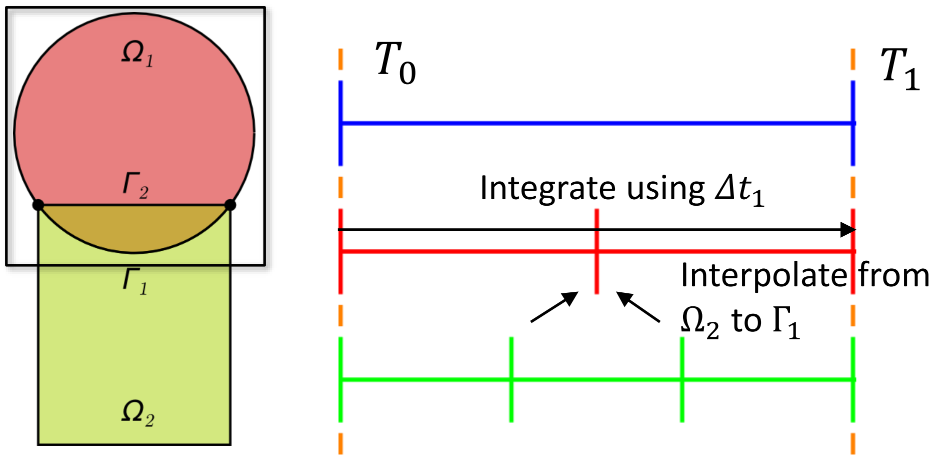

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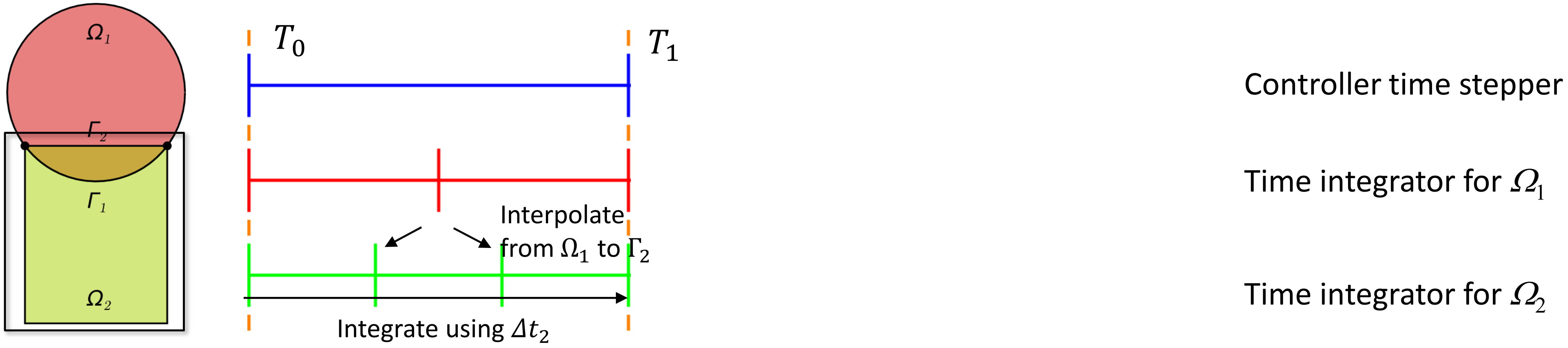

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<u>Step 2</u>: Advance Ω_2 solution from time T_i to time T_{i+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ_2 at times $T_i + n\Delta t_2$.

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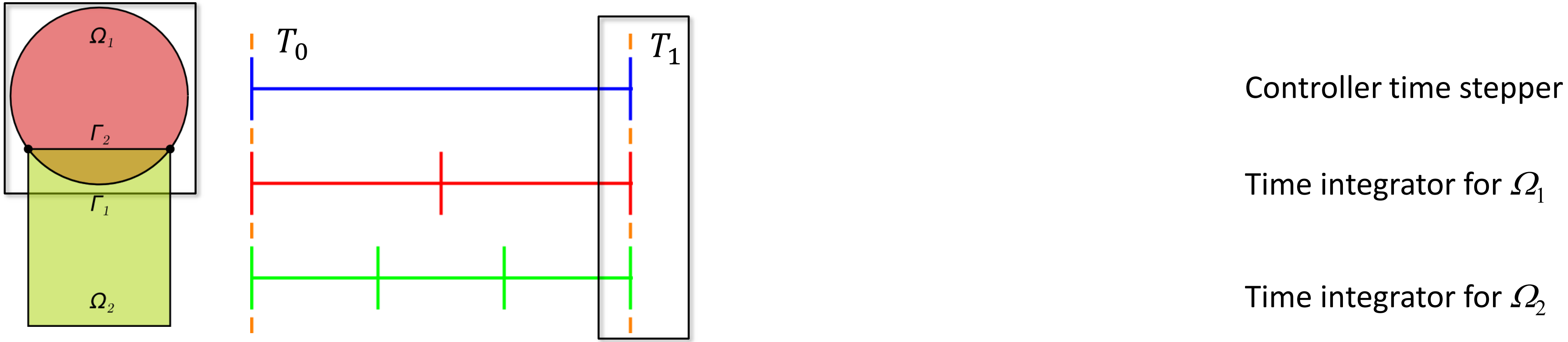

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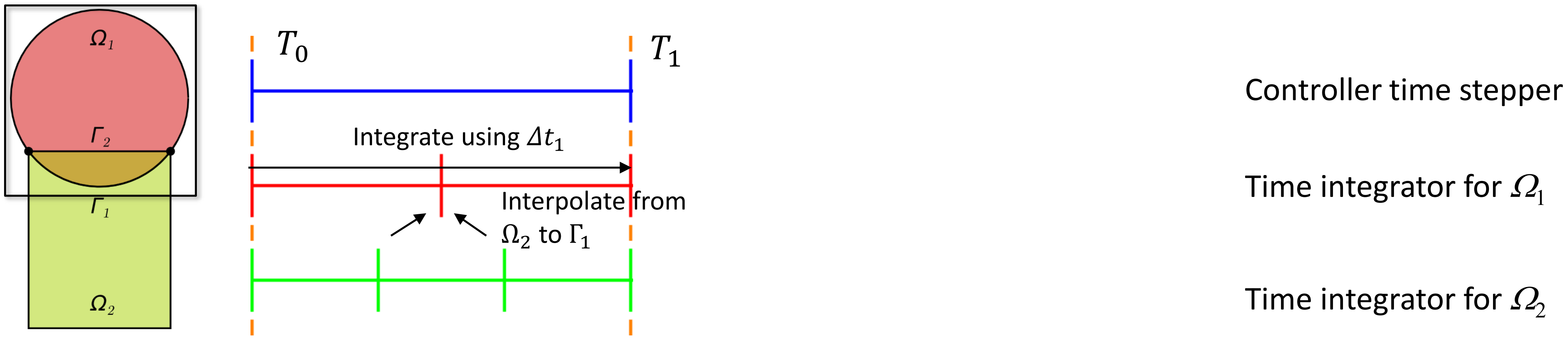

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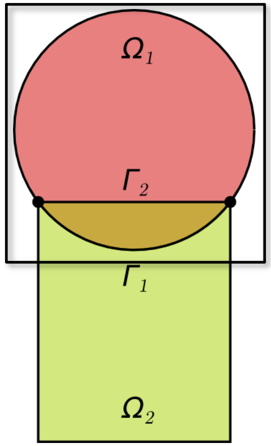

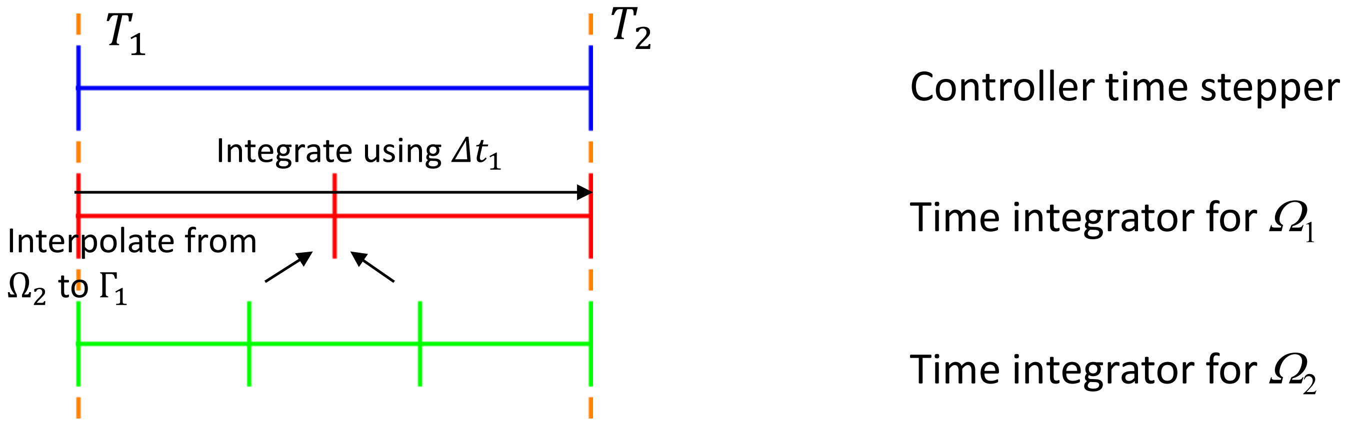

Can use ***different integrators*** with ***different time steps*** within each domain!

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

Model PDE:

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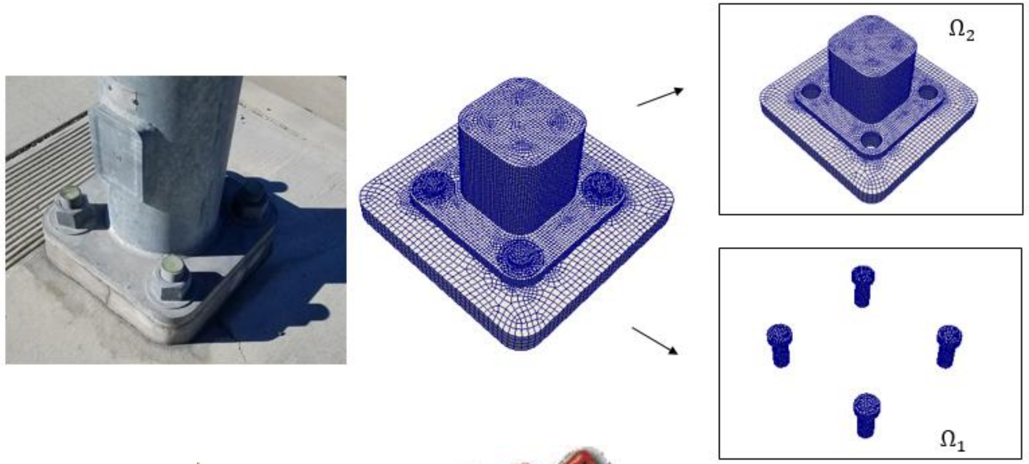
Schwarz for Multi-scale FOM-FOM Coupling in Solid Mechanics[1]

Model Solid Mechanics PDEs:

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

- Coupling is ***concurrent*** (two-way).
- ***Ease of implementation*** into existing massively-parallel HPC codes.
- ***Scalable***, ***fast***, ***robust*** (we target ***real*** engineering problems, e.g., analyses involving failure of bolted components!).
- Coupling does not introduce ***nonphysical artifacts***.
- ***Theoretical*** convergence properties/guarantees.



- ***“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.

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2. **Overview of Projection-Based Model Order Reduction**

3. Extension of Schwarz Alternating Method to FOM-ROM and ROM-ROM coupling

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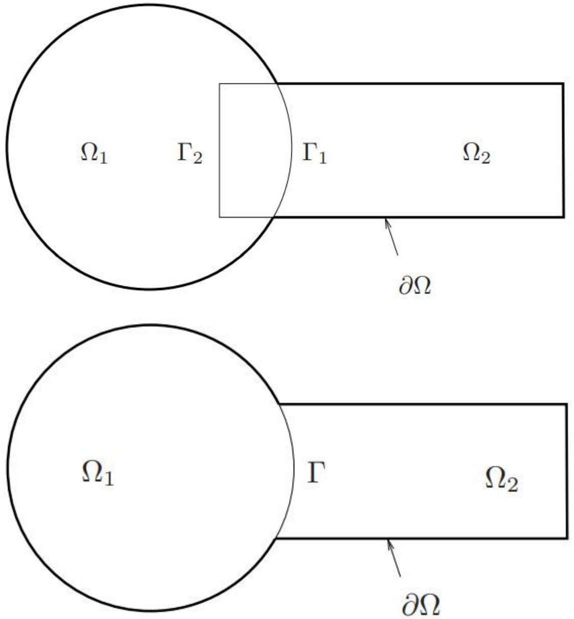
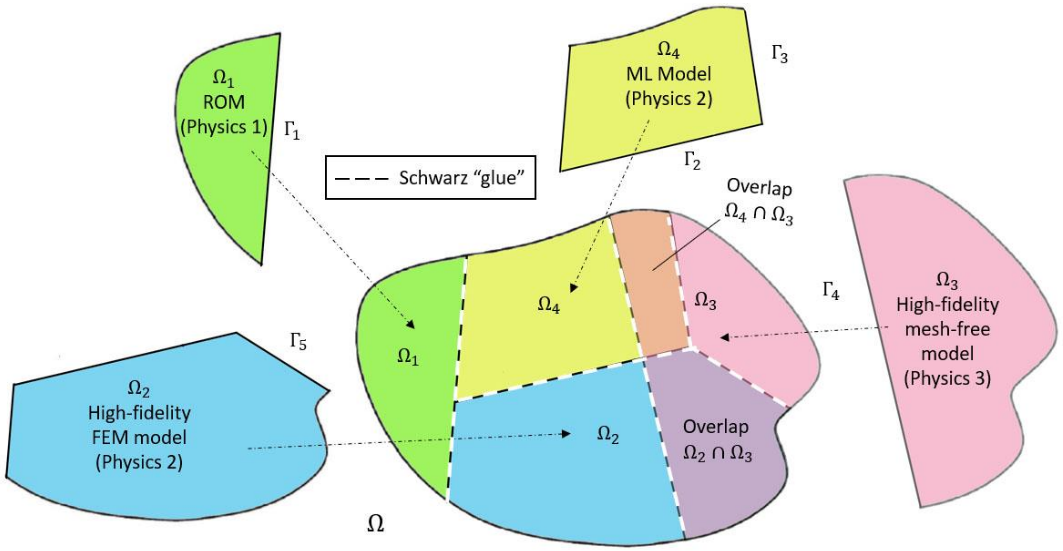
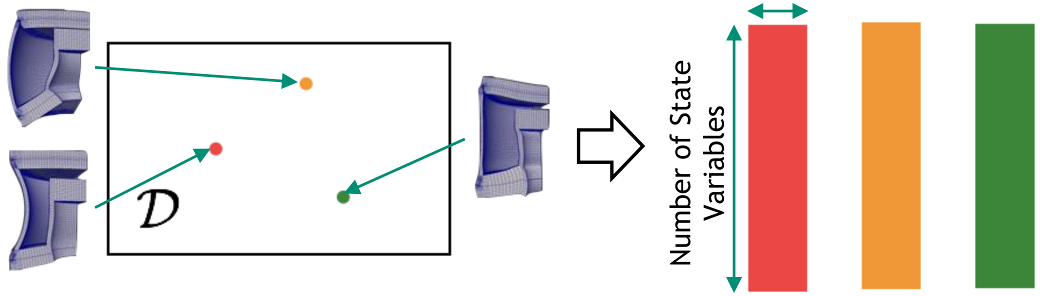




Projection-Based Model Order Reduction via the POD/Galerkin Method

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

1. Acquisition

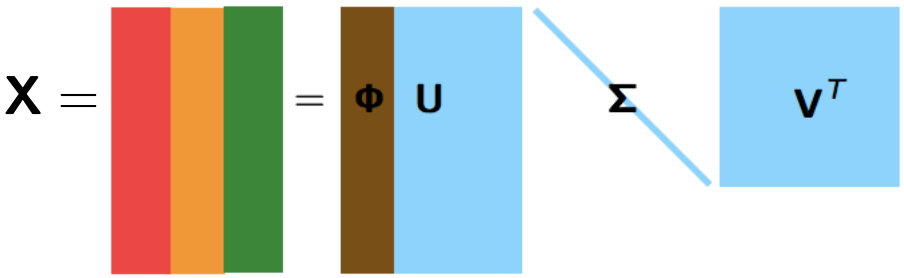


Solve ODE at different design points

Save solution data

2. Learning

Proper Orthogonal Decomposition (POD):



3. Projection-Based Reduction

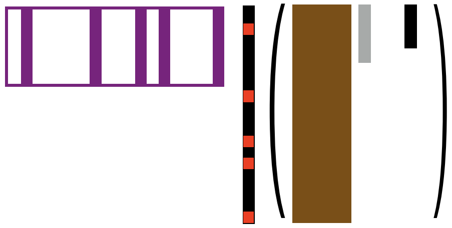
Reduce the number of unknowns

Perform Galerkin projection

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

Hyper-reduce nonlinear terms

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



Hyper-reduction/sample mesh

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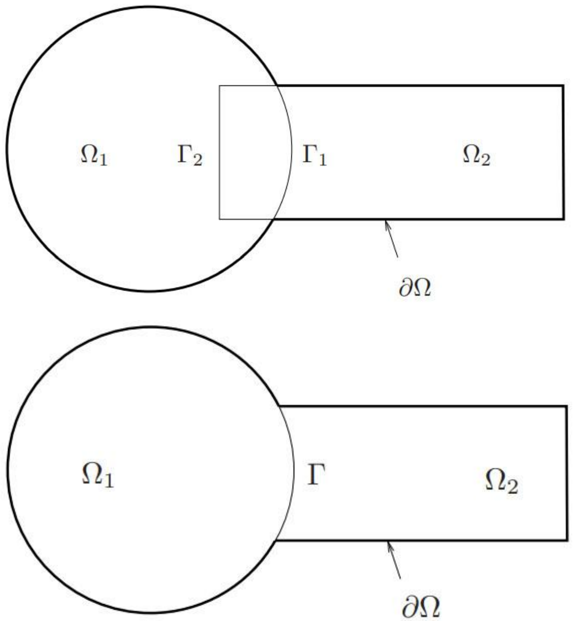

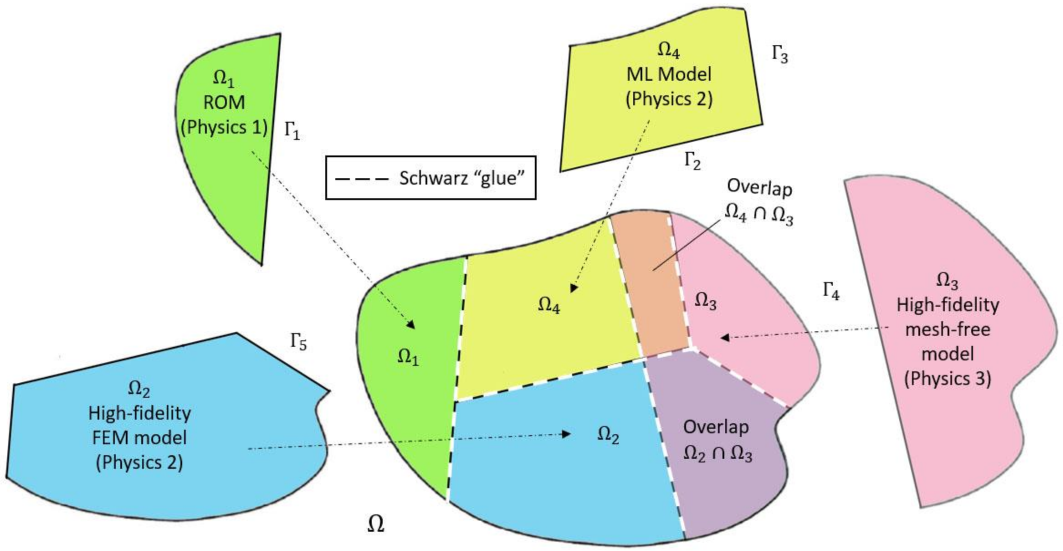

Schwarz Extensions to FOM-ROM and ROM-ROM Couplings

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

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

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

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

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 (future work) [Bergmann *et al*. 2018]

Snapshot collection and reduced basis construction

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

For nonlinear solid mechanics, special hyper-reduction methods need to preserve Hamiltonian structure, e.g., Energy-Conserving Sampling and Weighting Method (ECSW) [Farhat et al. 2015]

- Results here are for linear problem, so hyper-reduction is not required

Outline For Remainder of Presentation

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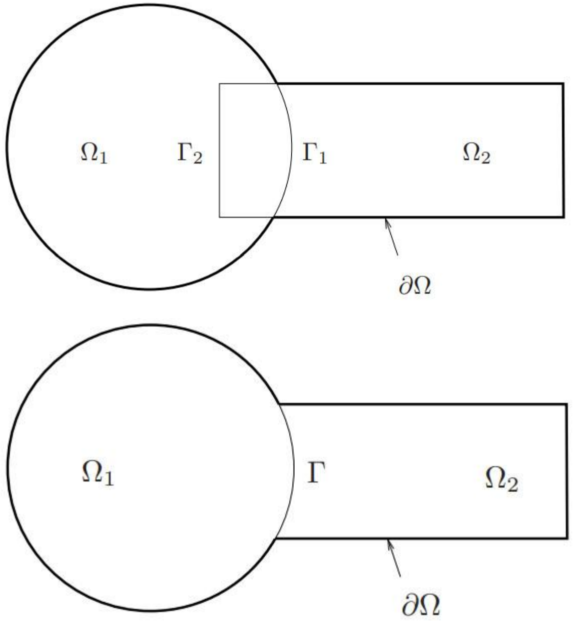
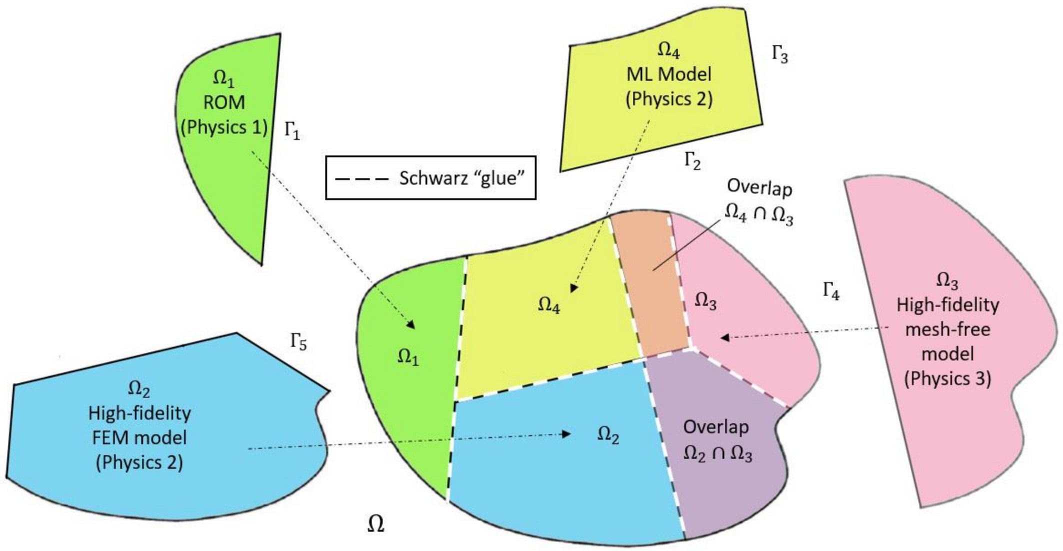
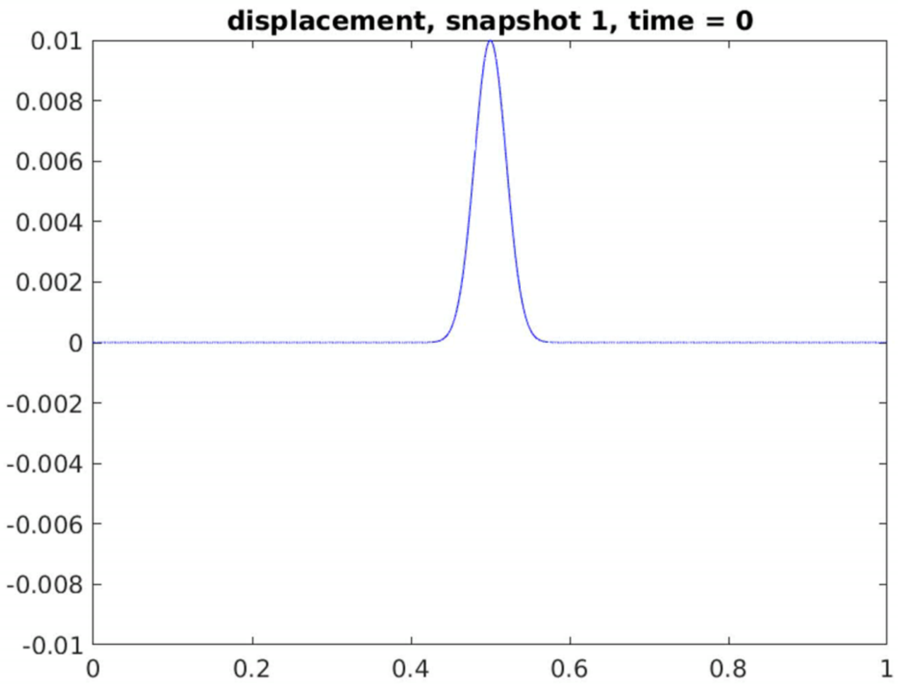
5. Summary and Future Work





Numerical Example: Linear Elastic Wave Propagation Problem

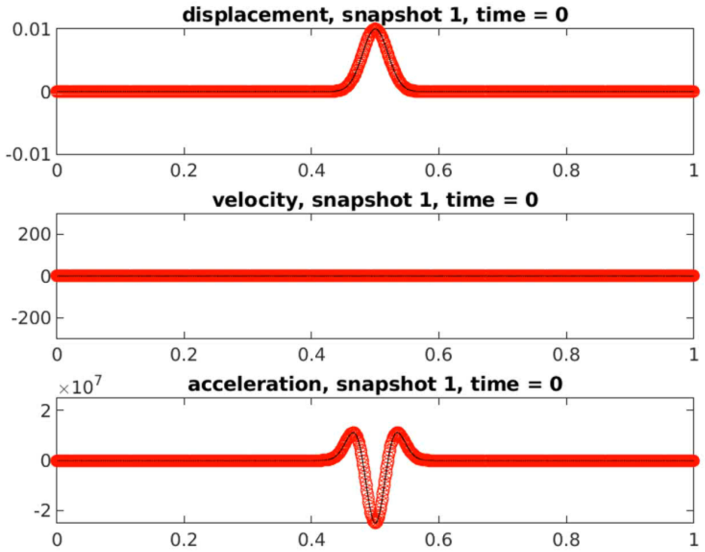
- Linear elastic ***clamped beam*** with Gaussian initial condition.
- Simple problem with analytical exact solution but very ***stringent test*** for discretization/coupling methods.
- ***Couplings tested:*** FOM-FOM, FOM-ROM, ROM-ROM, implicit-explicit, implicit-implicit, explicit-explicit.
- ROMs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

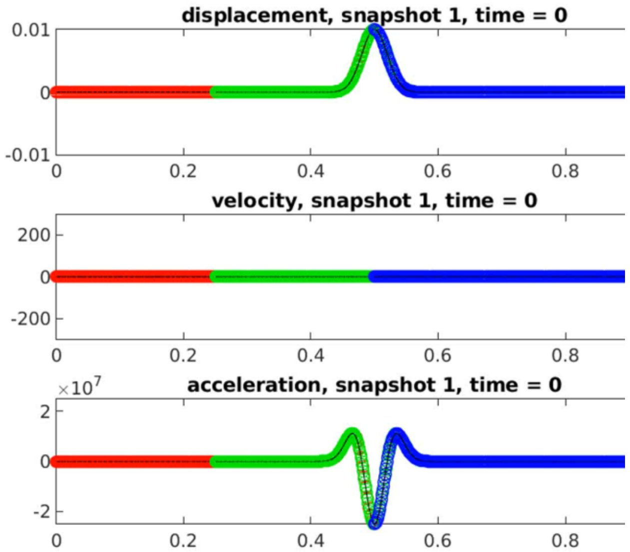


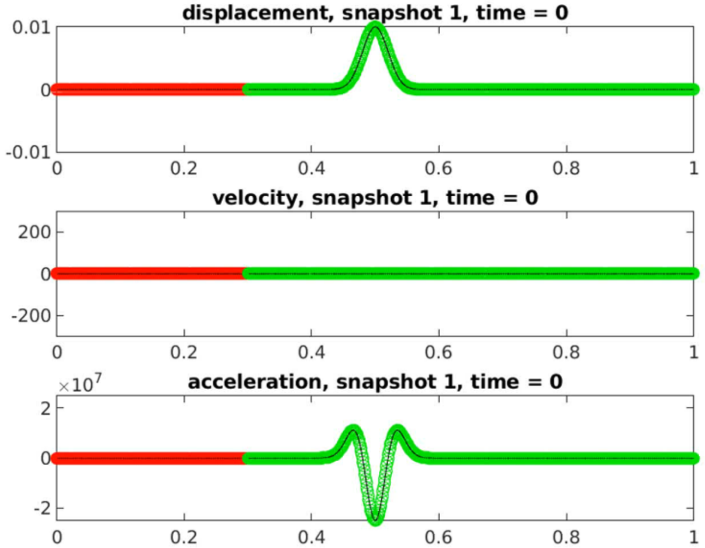
Above: 3D rendering of clamped beam with Gaussian initial condition. *Right:* Initial condition (blue) and final solution (red). Wave profile is negative of initial profile at time T = 1.0e-3.

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

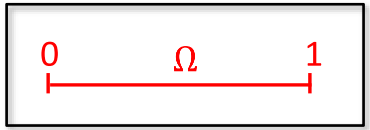
Coupling delivers accurate solution if each subdomain model is reasonably accurate, can couple different discretizations with different Δx, Δt and basis sizes.



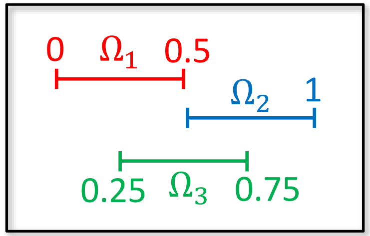




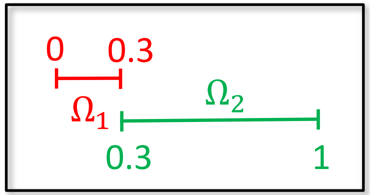
Single Domain FOM



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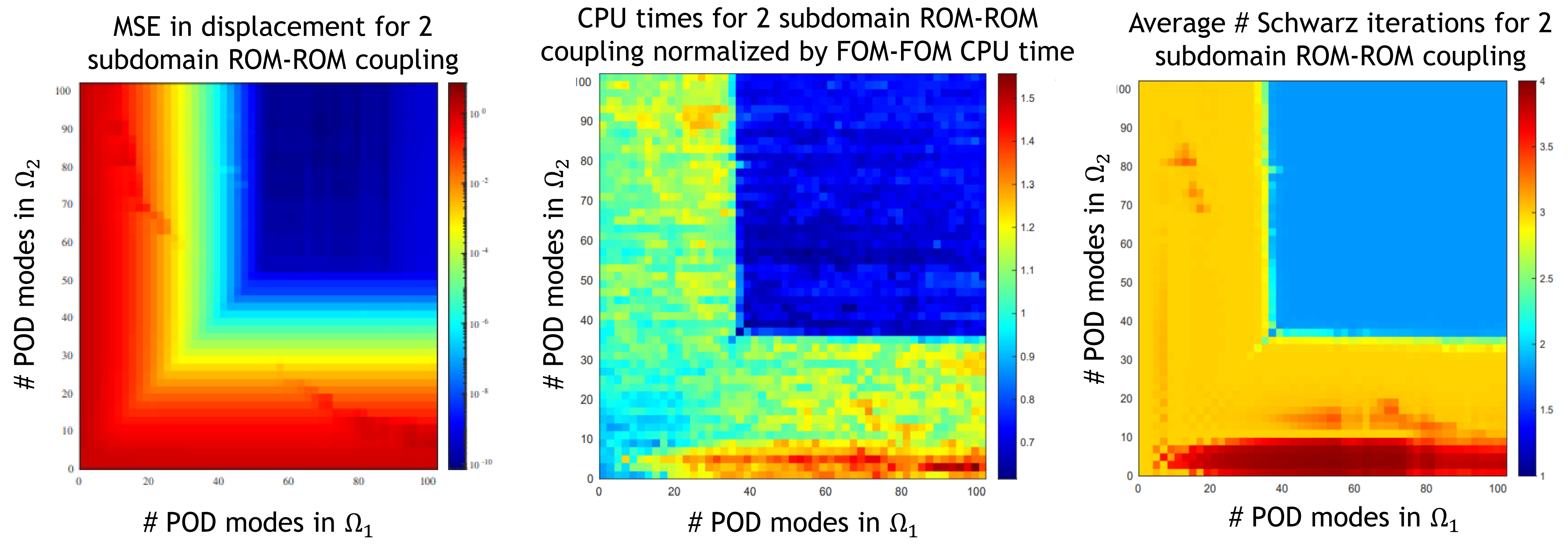
[4]Implicit FOM, Δt =2.25e-7, Δx =1e-6
[5]Explicit 50 mode POD ROM, Δt =2.25e-7, Δx =1e-6

[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.



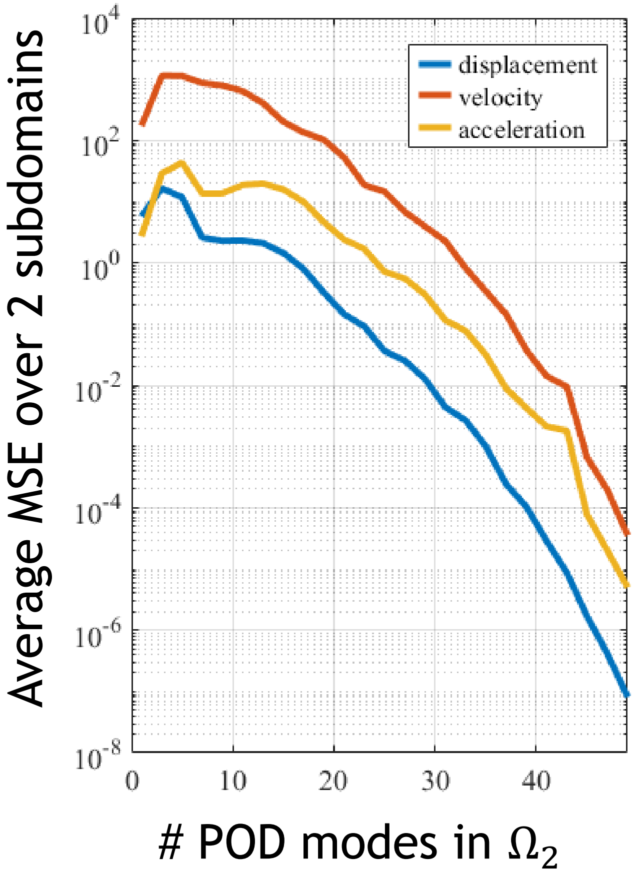
- **Smaller ROMs** are **not** the **fastest**: less accurate & require more Schwarz iterations to converge.
- All couplings converge in $\leq$ **4 Schwarz iterations** on average (FOM-FOM coupling requires average of 2.4 Schwarz iterations).

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

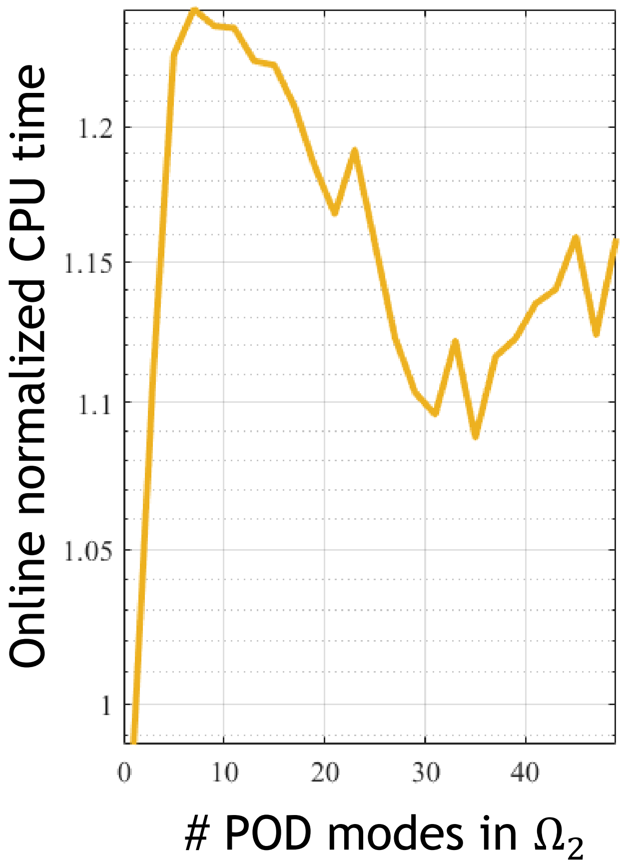
Linear Elastic Wave Propagation Problem: FOM-ROM Couplings

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.

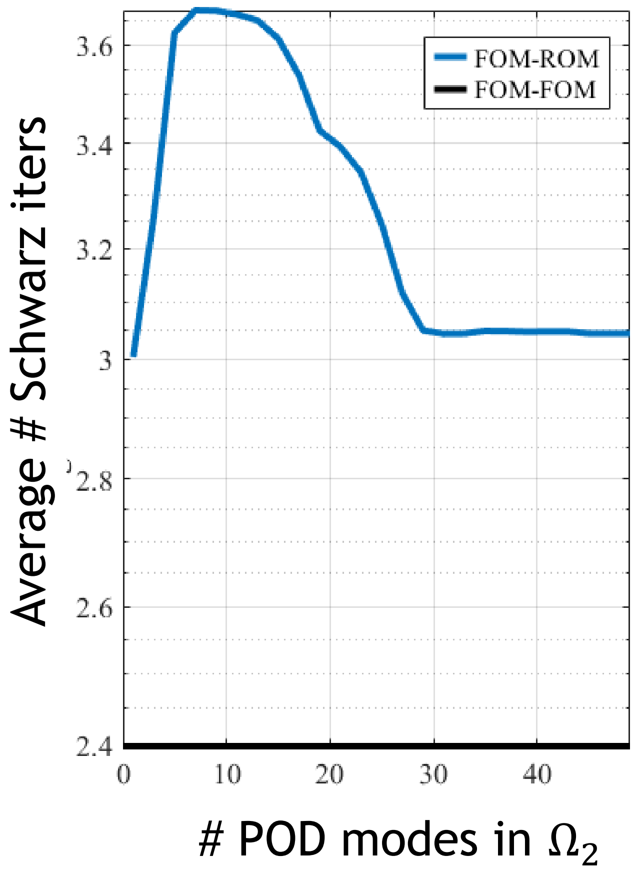
MSE for 2 subdomain FOM-ROM coupling



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



Average # Schwarz iterations for 2 subdomain couplings

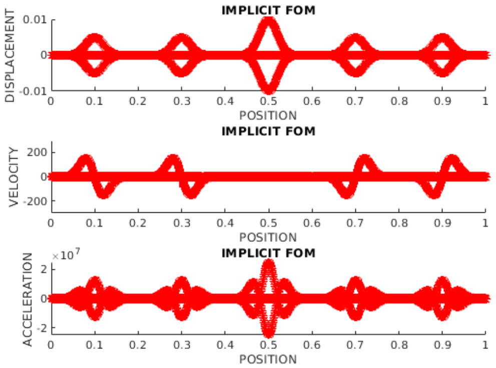


WIP: *understanding & improving FOM-ROM coupling performance.*

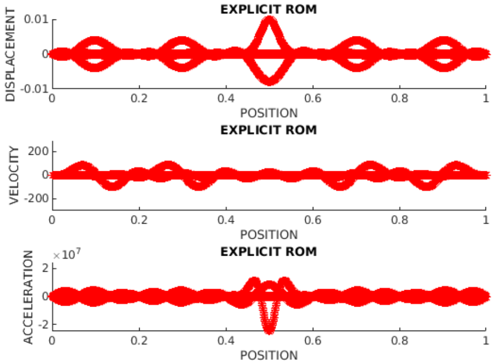
Overlapping implicit-implicit coupling with $\Omega_1 = [0, 0.75]$, $\Omega_2 = [0.25, 1]$

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

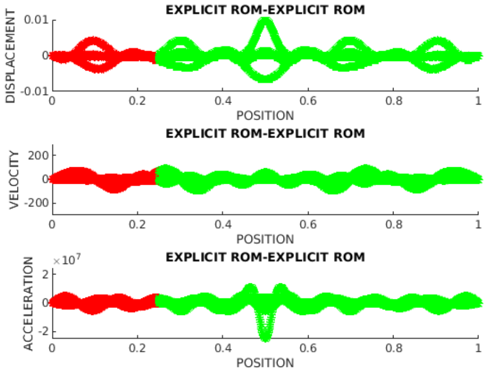
Inaccurate model + accurate model ≠ accurate model.



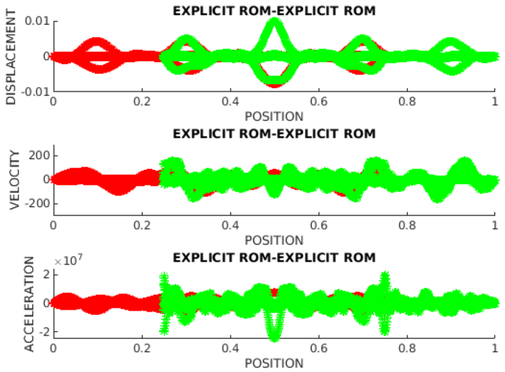
Single Domain, FOM (truth)



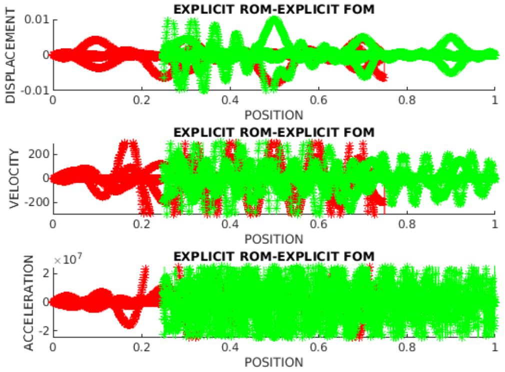
Single Domain, 10 mode POD



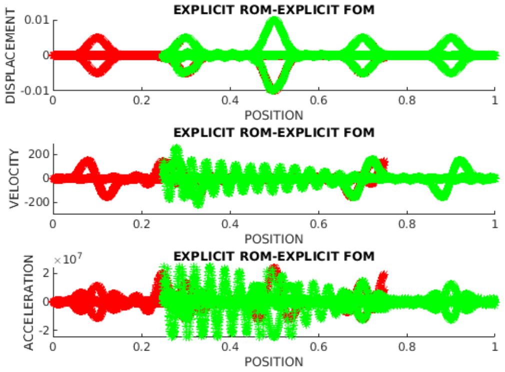
10 mode POD – 10 mode POD



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

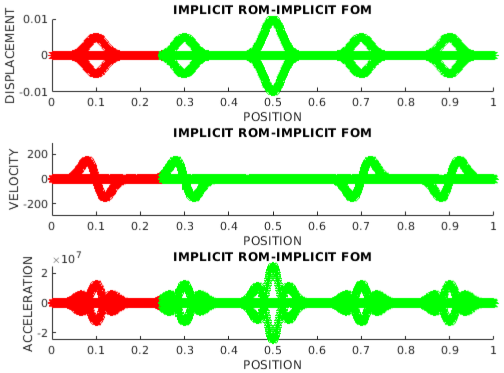
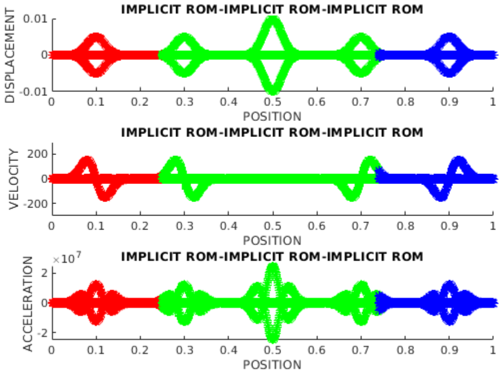


Figure above: $\Omega_1 = [0, 0.3]$, $\Omega_2 = [0.25, 1]$, 20 mode POD - FOM

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



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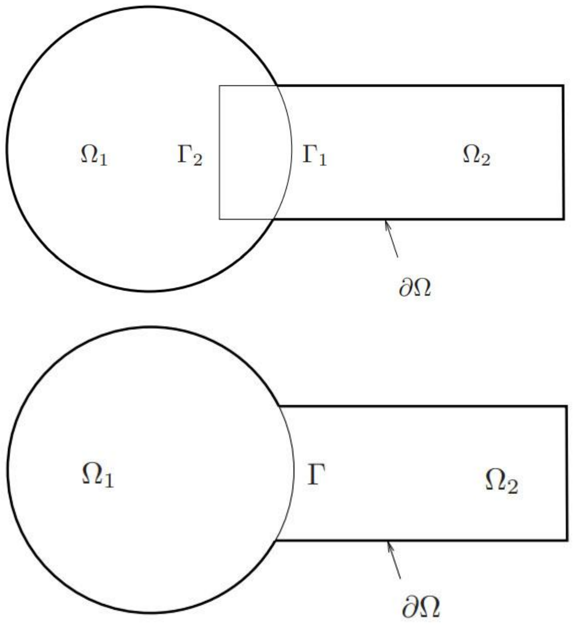

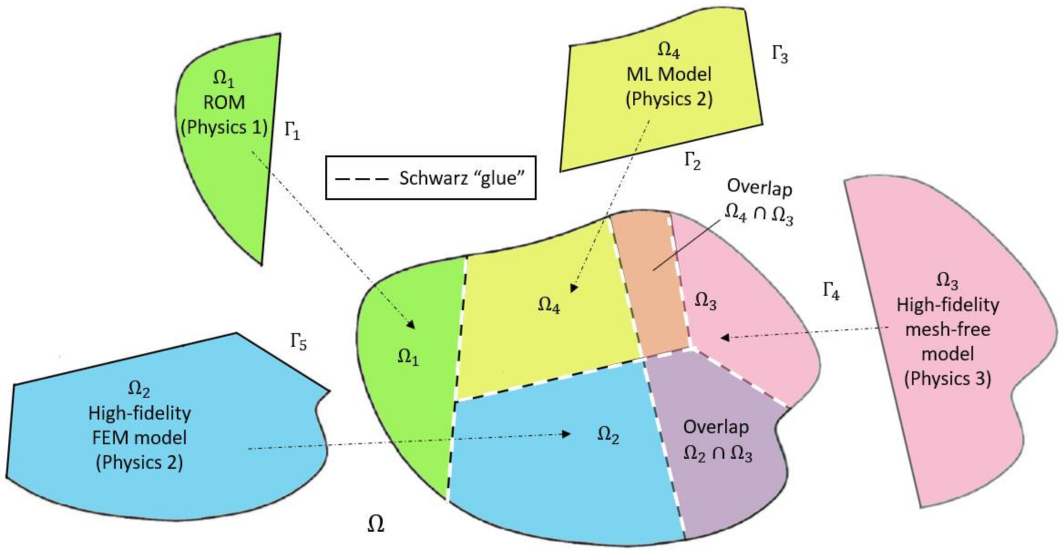

Summary & Future Work

Summary:

- Initial prototyping suggests that the Schwarz alternating method can be **effective coupling** method that enables coupling of **conventional** and **data-driven models** (projection-based ROMs).
- The coupling methodology enables the use of **different mesh resolutions, reduced basis sizes,** and **different time integrators** with **different time steps** in different subdomains.
- Preliminary results suggest that the **choice of domain decomposition** (DD) is critical to accuracy of the coupled model.

Ongoing/future work:

- Implementation/prototyping of coupling method on **non-linear problems** with ECSW-based hyper-reduction.
- Implementation/prototyping of coupling method in **multi-D**.
- **Optimizing** FOM-ROM and ROM-ROM coupling code/algorithm.
- Development of **error indicators** to guide DD in an error-controlling way, e.g., [Bergmann *et al*. 2018].
- **Analysis** of proposed coupling approach for FOM-ROM and ROM-ROM coupling.
- Development of **snapshot collection approaches** that do not require full system simulation [Hoang *et al*. 2021]
- Extension of the coupling framework to include **Physics-Informed Neural Networks (PINNs).**
- Extension of coupling method to **multi-material** and **multi-physics problems**.

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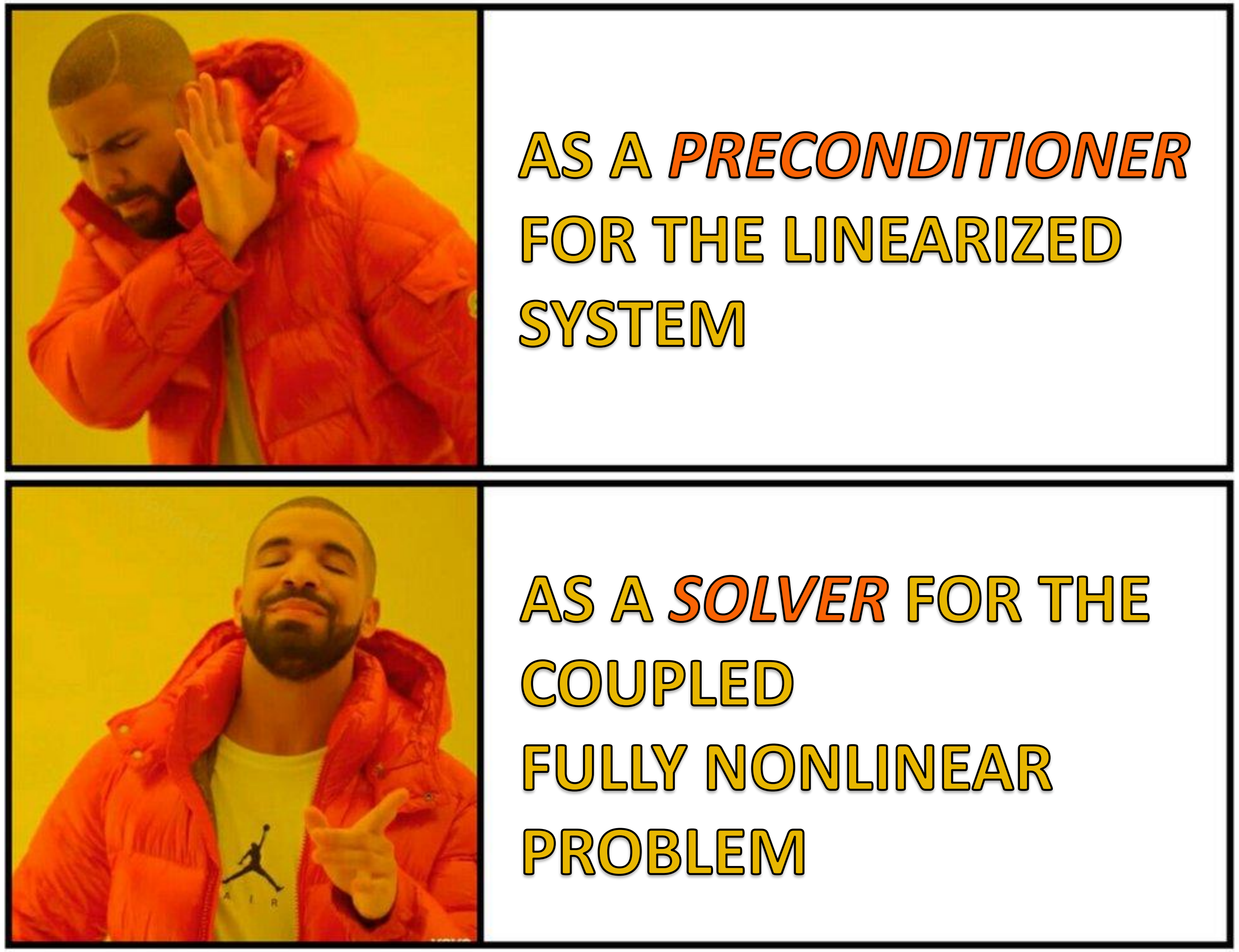
- C. Hoang, Y. Choi, K. Carlberg. Domain-decomposition least-squares Petrov-Galerkin (DD-LSPG) nonlinear model reduction. Comput. Meth. Appl. Mech. Engng. 364: 113997, 2021.

Thank you for your attention!

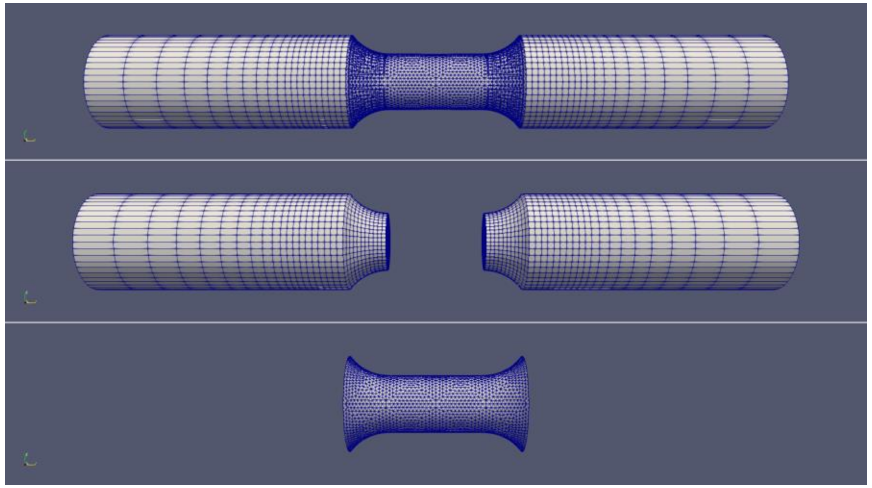
Start of Backup Slides

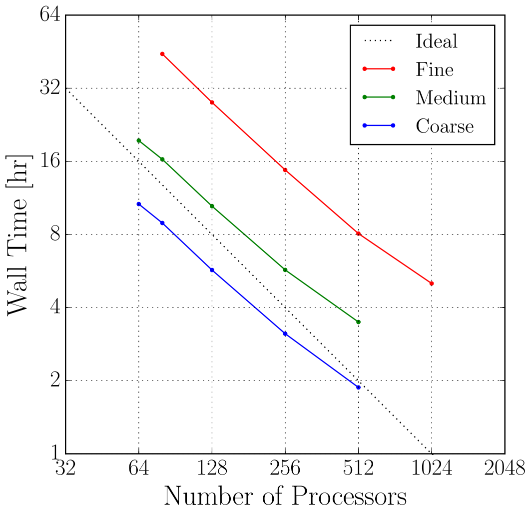
How We Use the Schwarz Alternating Method



Schwarz for Multi-scale FOM-FOM Coupling in Solid Mechanics and Contact Dynamics

The **overlapping Schwarz alternating method** has been developed/implemented for **concurrent multi-scale quasistatic**[1] **& dynamic**[2] **modeling** in Sandia's *Albany/LCM* and *Sierra/SM* codes.

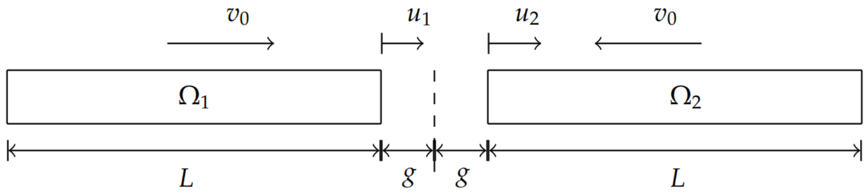


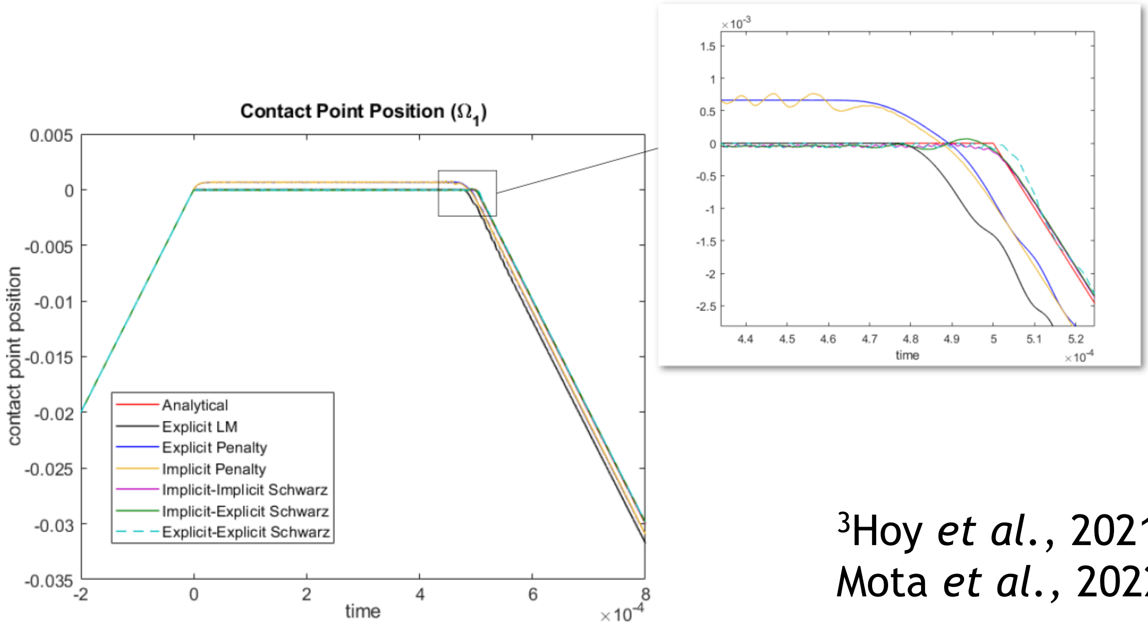


	CPU times	# Schwarz iters
Single Ω	3h 34m	–
Schwarz	2h 42m	3.22

[1]Mota *et al.*, 2017. [2]Mota *et al.*, 2022.

We are currently developing **a novel contact method**[3] based on **non-overlapping Schwarz.**





[3]Hoy *et al.*, 2021; Mota *et al.*, 2022.

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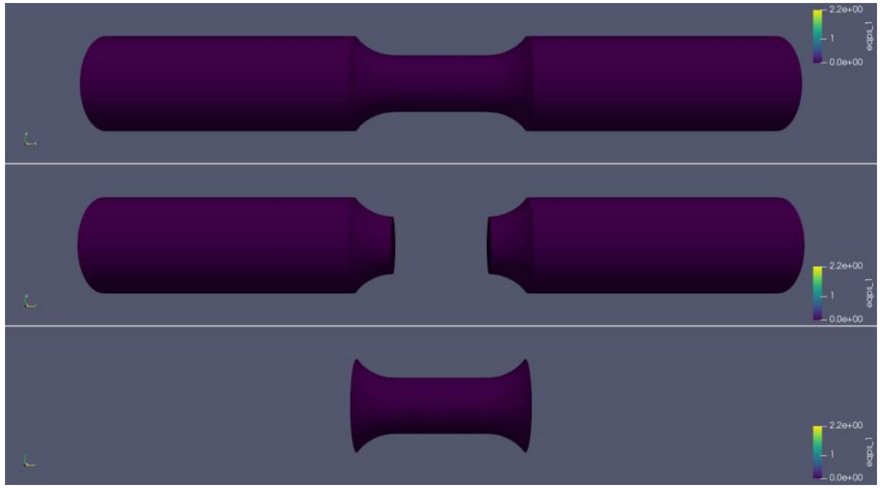

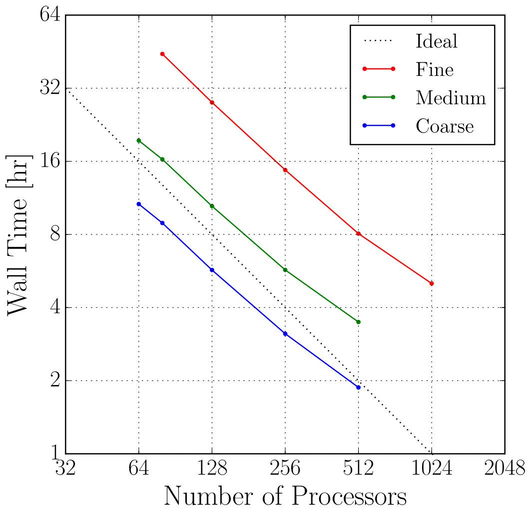

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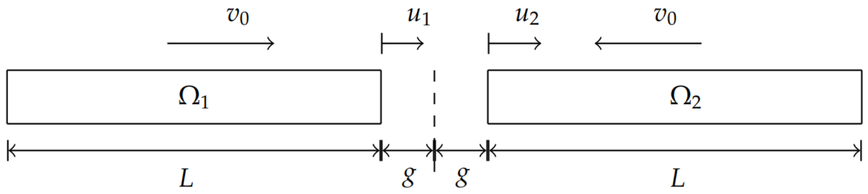
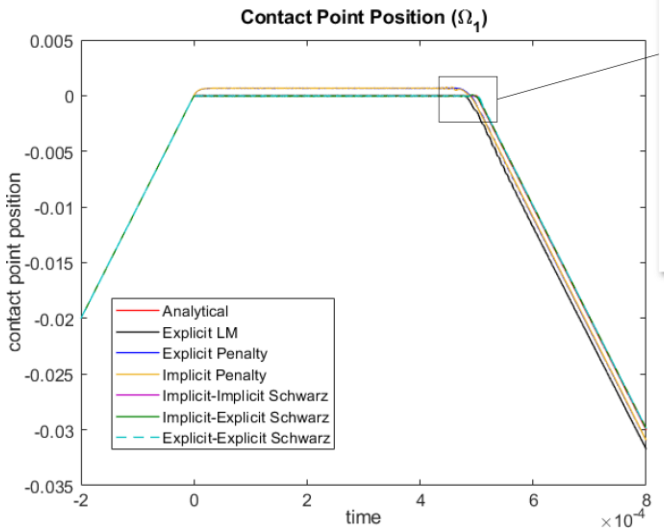
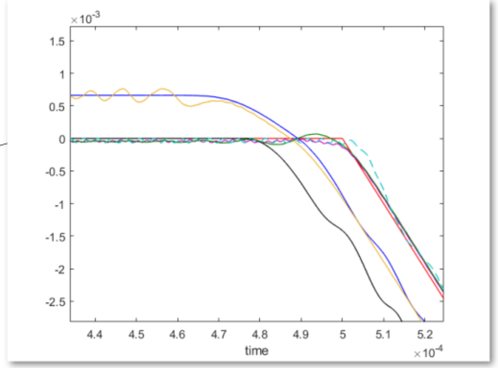


Talk by A. Mota





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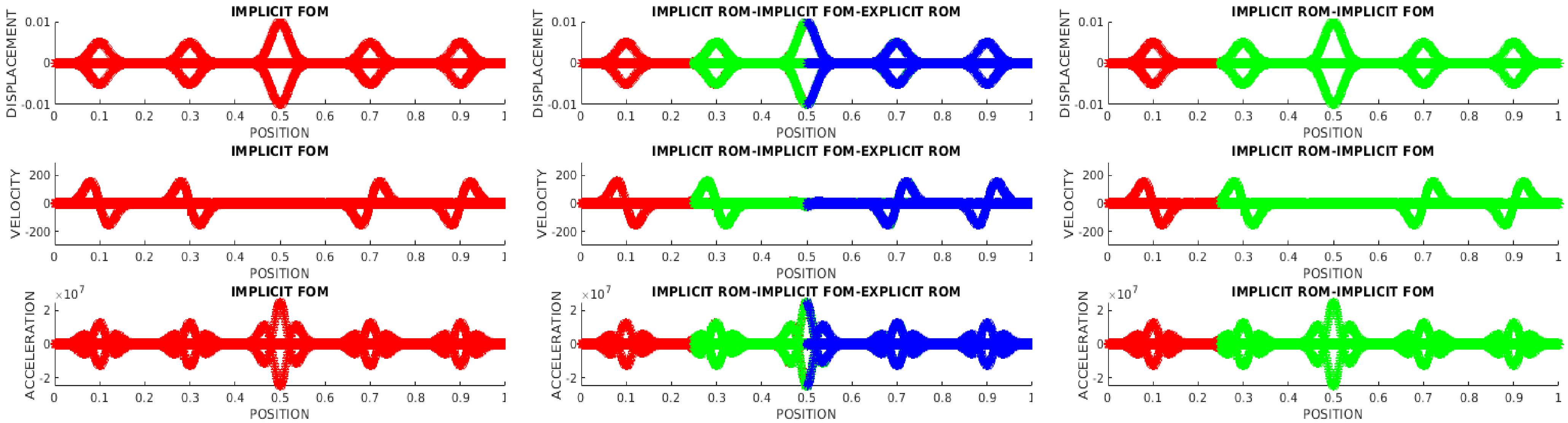
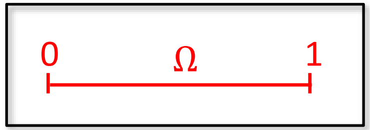
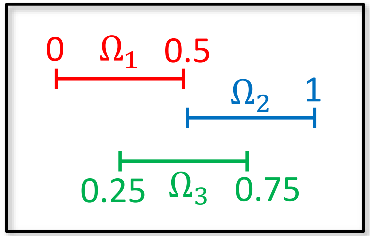


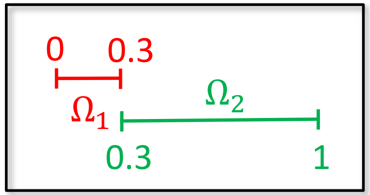
Single Domain FOM



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



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



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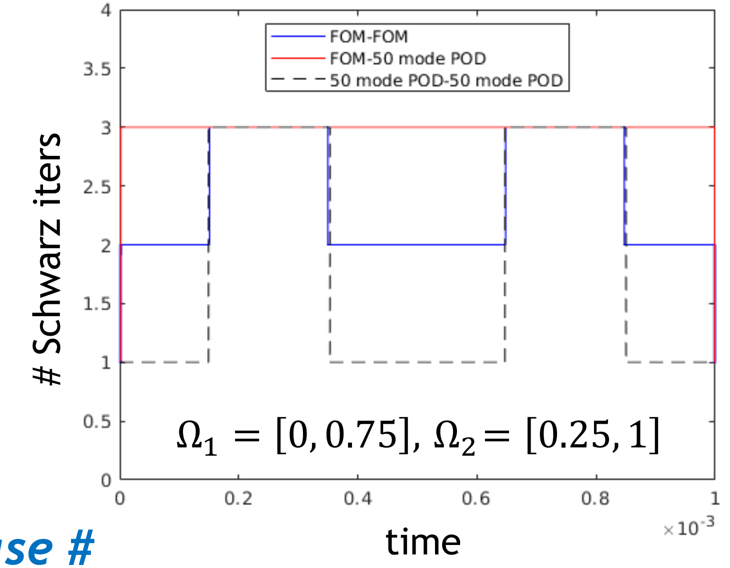
[4]Explicit 50 mode POD ROM, Δt =2.25e-7, Δx =1e-6

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

	Online CPU time	Total # Schwarz iters
Overlapping FOM[1]-FOM[2]-FOM[3]	68.7s	2972
Overlapping ROM[4]-FOM[2]-ROM[5]	81.6s	4000
Non-overlapping FOM[6]-FOM[7]	38.0s	10,516
Non-overlapping FOM[6]-ROM[8]	49.8s	13,366



CPU-Time FOM-FOM: 7.48e1
CPU-Time FOM-ROM: 1.16e2
CPU-Time ROM-ROM: 7.16e1

FOM-ROM and ROM-ROM couplings often (but not always) increase # Schwarz iterations relative to FOM-FOM coupling.

- Key to improving efficiency is reducing # Schwarz iterations.

ROMs with fewer modes do not always give rise to smaller CPU times.

- Less accurate models $\Longrightarrow$ more Schwarz iterations needed for convergence.

Using smaller time steps can decrease # Schwarz iterations.

[1]Implicit FOM, Δt =1e-6, Δx =1.25e-3
[2]Implicit FOM, Δt =1e-6, Δx =8.33e-4
[3]Explicit FOM, Δt =1e-7, Δx =1e-3
[4]Implicit 30 mode POD ROM, Δt =1e-6, Δx =1.25e-3
[5]Explicit 50 mode POD ROM, Δt =1e-7, Δx =1e-3
[6]Implicit FOM, Δt =2.25e-7, Δx =1e-6
[7]Explicit FOM, Δt =2.25e-7, Δx =1e-6
[8]Explicit 50 mode POD ROM, Δt =2.25e-7, Δx =1e-6

WIP: ***optimizing*** FOM-ROM and ROM-ROM coupling implementation and devising ways to ***reduce # Schwarz iterations*** (e.g., through relaxation parameter θ)