Sandia National Laboratories

Component-Based Coupling of First-Principles and Data-Driven Models

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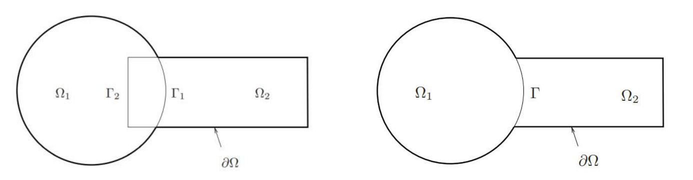
Alternating Schwarz-Based Coupling

Alternating Schwarz Method for Domain Decomposition (DD) and Coupling

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

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



Overlapping Schwarz: convergent with all-Dirichlet transmission boundary conditions (BCs) if $\Omega_1 \cap \Omega_2 \neq \emptyset$.

Non-overlapping Schwarz: convergent with Robin-Robin or alternating Neumann-Dirichlet transmission BCs.

Basic Schwarz Algorithm for Spatial Coupling

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

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

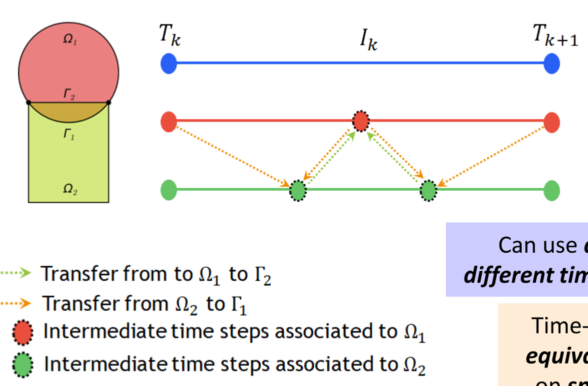
- Schwarz alternating method most commonly used as a ***preconditioner*** for Krylov iterative methods to solve linear algebraic equations.

Novel Idea: using Schwarz alternating method as a ***discretization method*** for solving multi-scale or multi-physics PDEs.

Schwarz Algorithm for Dynamics

Initialize:
- Set $k = 0$ (controller time index).

Iterate until convergence:
- ***Step 1:*** Advance Ω_1 solution from time T_k to time T_{k+1} using time-stepper in Ω_1 with time-step Δt_1, using solution in Ω_2 interpolated to Γ_1 at times $T_k + n\Delta t_1$
- ***Step 2:*** Advance Ω_2 solution from time T_k to time T_{k+1} using time-stepper in Ω_2 with time-step Δt_2, using solution in Ω_1 interpolated to Γ_2 at times $T_k + n\Delta t_2$.
- ***Step 3:*** Check for convergence at time T_{k+1}.
  If unconverged, return to Step 1.
  If converged, set $k = k + 1$ and return to Step 1.



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

Time-stepping procedure is ***equivalent*** to doing Schwarz on ***space-time domain*** [2].

Schwarz for Multi-Scale Coupling of Full Order Models (FOMs) in Solid Mechanics

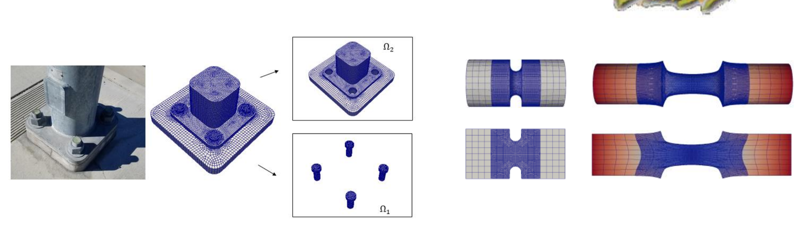
- Coupling is ***concurrent*** (two-way).
- ***Easy to implement*** into existing massively-parallel HPC codes.
- ***Scalable, fast, robust*** (we target ***real*** engineering problems, e.g., analyses involving failure of bolted components!).
- Coupling does not introduce ***nonphysical artifacts.***
- ***Theoretical*** convergence properties/guarantees [1, 2].
- ***"Plug-and-play" framework***:
  - Ability to couple regions with ***different non-conformal meshes***, ***different element types*** and ***different levels of refinement*** to simplify task of ***meshing complex geometries.***
  - Ability to use ***different solvers/time-integrators*** in different regions.

Model Solid Mechanics PDEs:

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

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

Albany-LCM* SIERRA



* https://github.com/sandialabs/LCM.

Schwarz Extensions to ROM-FOM and ROM-ROM Couplings

Enforcement of Dirichlet boundary conditions (DBCs) in ROM at indices i_{Dir}

- Method I in [3] is employed

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

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

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).

Snapshot collection and reduced basis construction

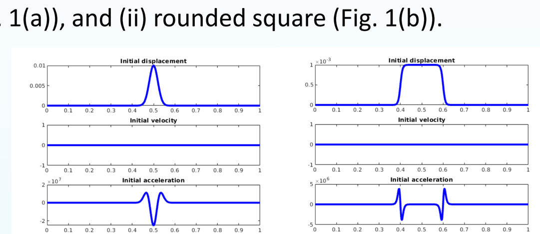
- POD results presented herein use snapshots obtained via FOM-FOM coupling on $\Omega = \bigcup_i \Omega_i$.
- Future work: generate snapshots/bases separately in each Ω_i.

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

- We employ the Energy-Conserving Sampling & Weighting Method (ECSW).
- Boundary points must be included in sample mesh for DBC enforcement.

Numerical Example: Nonlinear Hyper-Elastic Wave Propagation Problem [4]

- ***Dynamic solid mechanics*** problem with ***nonlinear hyperelastic Hencky*** constitutive model.
- ***1D beam*** geometry $\Omega = (0,1)$, clamped at both ends, with prescribed initial condition discretized using FEM + implicit Newmark-β.
- ***Two initial conditions***: (i) Gaussian (Fig. 1(a)), and (ii) rounded square (Fig. 1(b)).
  - ***Reproductive case:*** generate snapshots with initial condition (i) and predict solution with initial condition (i)
  - ***Predictive case:*** generate snapshots with initial condition (ii) and predict solution with initial condition (i)



(a) Gaussian (b) Rounded Square

Figure 1: Initial conditions considered.

- Very ***stringent test case*** for coupling and for ROMs (traveling wave, sharp gradients in solution)!
- **Non-overlapping domain decomposition (DD)** of $\Omega = \Omega_1 \cup \Omega_2$, where $\Omega_1 = [0, 0.6]$ and $\Omega_2 = [0.6, 1.0]$ and same $\Delta x = 10^{-3}$ and $\Delta t = 10^{-7}$ in both subdomain.
  - ***Transmission BCs:*** alternating Dirichlet-Neumann with no relaxation.

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

Table 1. CPU times, mean square errors ($\varepsilon_{\mathrm{MSE}}$) and total # Schwarz iterations (N_S) for different couplings for reproductive problem. Couplings outperforming the FOM-FOM model in terms of CPU-time and with reasonable errors are highlighted in green.

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	1.288×10^3	−/−	−/−	−/−	−/−	−
ROM	1.358×10^3	−/−	3.451×10^{-3}/−	6.750×10^{-2}/−	3.021×10^{-1}/−	−
HROM	9.759×10^2	614/−	3.463×10^{-3}/−	6.750×10^{-2}/−	3.021×10^{-1}/−	−
FOM-FOM	2.133×10^3	−/−	−/−	−/−	−/−	23,280
FOM-ROM	2.084×10^3	−/−	1.907×10^{-8}/ 1.170×10^{-6}	1.461×10^{-6}/ 9.882×10^{-5}	3.973×10^{-5}/ 1.757×10^{-3}	23,288
FOM-HROM	2.219×10^3	−/253	1.967×10^{-4} 1.720×10^{-3}	4.986×10^{-3} 4.185×10^{-2}	2.768×10^{-2} 2.388×10^{-1}	29,700
ROM-ROM	2.502×10^3	−/−	5.592×10^{-4}/ 4.346×10^{-4}	1.575×10^{-2}/ 1.001×10^{-2}	9.197×10^{-2}/ 5.304×10^{-2}	26,220
HROM-HROM	2.200×10^3	405/253	4.802×10^{-3} 1.960×10^{-3}	8.500×10^{-2} 4.630×10^{-2}	3.744×10^{-1} 2.580×10^{-1}	30,067

Table 2. CPU times, mean square errors ($\varepsilon_{\mathrm{MSE}}$) and total # Schwarz iterations (N_S) for different couplings for predictive problem. Couplings outperforming the FOM-FOM model in terms of CPU-time and with reasonable errors are highlighted in green.

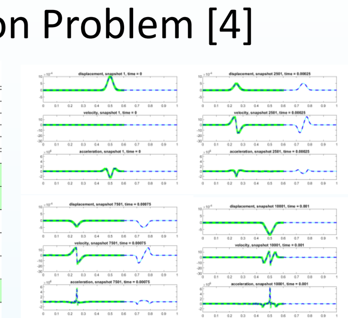


Figure 2. Plots of the HROM-HROM coupled solutions with $M_1 = 200$ (green), $M_2 = 80$ (cyan) compared to a single-domain FOM solution (blue) for reproductive problem.

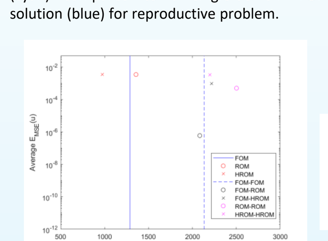
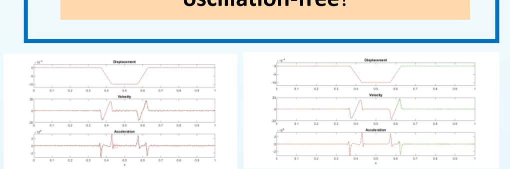


Figure 3: Pareto plot showing CPU time (s) vs average displacement MSE over all subdomains coupled for predictive problem.



(a) Single-domain ROM (M_1= 300) solution (red) compared to FOM. (b) FOM-HROM (M_2= 200) solution (red-green) compared to FOM.

Figure 4: Solutions to predictive problem at the final time $T = 10^{-3}$. FOM solution shown in black.

Key Takeaways

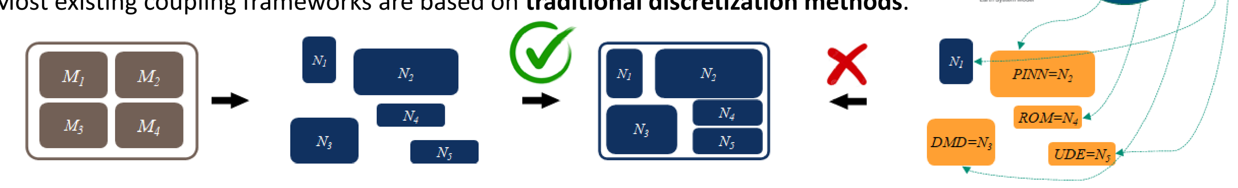
- All coupled models evaluated converge in <3 Schwarz iterations/Δt.
- **FOM-HROM & HROM-HROM** couplings **outperform FOM-FOM** coupling in CPU time by 12.5-32.6%. ***Greater speedups expected in multi-D.***
- All couplings involving ROMs/HROMs are **at least as accurate** as single-domain ROMs/HROMs.

Predictive couplings involving ROMs/HROMs are **smooth** and **oscillation-free**!

Motivation for Coupling

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

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

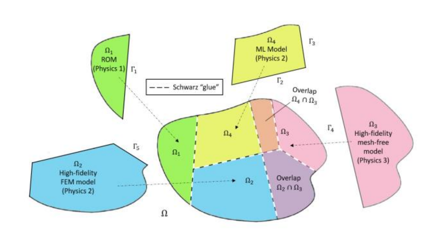


Complex System Model
- PDEs, ODEs
- Nonlocal integral
- Atomistic, ...

Traditional Methods
- Mesh-based (FE, FV, FD)
- Meshless (SPH, MLS)
- Eulerian, Lagrangian, ...

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

Traditional + Data-Driven Methods
- Physics-Informed Neural Networks (PINNs)
- Neural ODEs
- Projection-based ROMs, ...

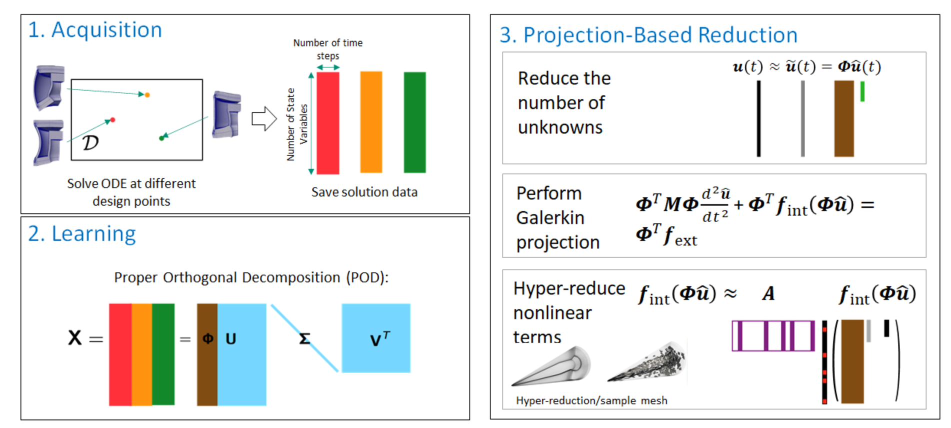


Unfortunately, existing algorithmic and software infrastructures are **ill-equipped** to handle plug-and-play integration of **data-driven models**!

Objective: discover **mathematical principles** guiding assembly of standard and data-driven models in **stable, accurate and physically consistent** ways.

Projection-Based Model Order Reduction

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



ROM = Reduced Order Model
HROM = Hyper-reduced ROM

Coupling methods are **not limited** to linear bases (e.g., POD) and Galerkin projection.

Comparison of Coupling Methods

Alternating Schwarz-Based Coupling

- 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/Dynamic Mode Decomposition (DMD)** data-driven model

Lagrange Multiplier-Based IVR Coupling

- 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** or **IMEX 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**

Current & Future Work

- Extension of Schwarz method to **multi-D** problems.
- Extension of Lagrange multiplier-based method to **predictive** and **nonlinear problems.**
- Extension of methods to **PINN-PINN coupling.**
- Development of **error indicator-based DD approaches**, to determine optimal ROM-FOM placement (including **on-the-fly ROM-FOM switching**).
- Extension of couplings to POD modes built from snapshots on **independently-simulated subdomains.**
- Application to **multi-physics problems.**

Journal articles on new methods are in preparation.

References

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Coupling via Generalized Mortar Methods

Lagrange Multiplier-Based Partitioned Coupling Formulation

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

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

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

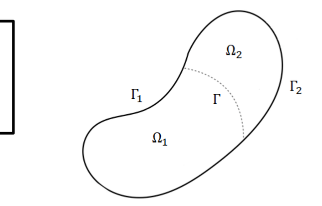

Figure 5. Non-overlapping DD of $\Omega = \Omega_1 \cup \Omega_2$

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

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

$\boldsymbol{M}_i$: mass matrices, $\boldsymbol{K}_i$: stiffness matrices, $\boldsymbol{G}_i$: constraint matrices

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

- ***Continuity of states***: $c_1(\boldsymbol{x},t) - c_2(\boldsymbol{x},t) = 0$
- ***Continuity of total flux***: $F_1(\boldsymbol{x},t) \cdot \boldsymbol{n}_\Gamma = F_2(\boldsymbol{x},t) \cdot \boldsymbol{n}_\Gamma$

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

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

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

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

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

Implicit Value Recovery (IVR) Algorithm [5]

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

* Ensures that dual Schur complement of (2) is symmetric positive definite

Lagrange Multiplier-Based Coupling of FOMs

"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 [6,7]
- Coupling is ***non-iterative*** (single pass)

Method is theoretically rigorous [5]:

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

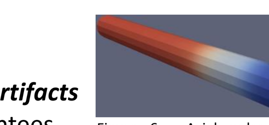

Figure 6. Axial pulse bar test simulated with variable resolution

Figure 7. Patch test (ALEGRA-Sierra coupling)

Method has been applied to several application spaces:

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

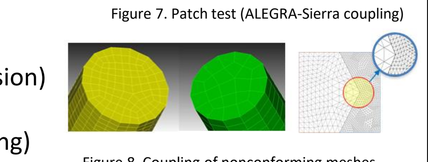

Figure 8. Coupling of nonconforming meshes

Lagrange Multiplier-Based FOM-ROM and ROM-ROM Coupling

- Collect **snapshots** using suitable monolithic FOM solve for equation (1) and **subtract Dirichlet BC data** on $\Gamma_1 \cup \Gamma_2$.
- **Partition** modified snapshots into **subdomain snapshot matrices** $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ on Ω_1 and Ω_2, respectively.
- Calculate **"split" reduced bases** $\boldsymbol{\Phi}_{i,\Gamma}$ and $\boldsymbol{\Phi}_{i,0}$, for interface and interior degrees of freedom (DOFs).
- **Approximate** the solution as a **linear combination** of the POD modes in each subdomain and on each boundary:

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

- **Reduce LM space** to size $N_{R,\Gamma} < N_{R,1\Gamma} + N_{R,2\Gamma}$, where $N_{R,i\Gamma}$ = # POD modes in $\boldsymbol{\Phi}_{i,\Gamma}$, and approximate $\boldsymbol{\lambda} \approx \boldsymbol{\Phi}_{\mathrm{LM}}\hat{\boldsymbol{\lambda}}$ where $\boldsymbol{\Phi}_{\mathrm{LM}} = \boldsymbol{\Phi}_{i,\Gamma}$ for $i = 1,2$, so that $N_{R,\Gamma} = N_{R,i\Gamma}$.
- Substitute above expansions into (2) and **project** equations onto reduced bases to obtain:

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

Extensions to **FOM-ROM coupling** is straight-forward.

Online ROM-ROM IVR Solution Algorithm: at each time step t^n

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

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

- Advance the following systems forward in time:

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

ROM-ROM coupling with **reduced LM space** guaranteed to have **non-singular dual Schur complement** if underlying FOM-FOM coupling satisfies conditions in [5].

Numerical Example: High-Peclet Advection-Diffusion Problem [8]

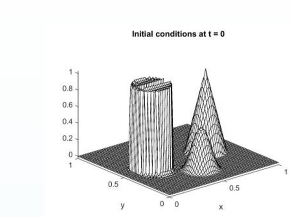

Figure 9. Initial condition.

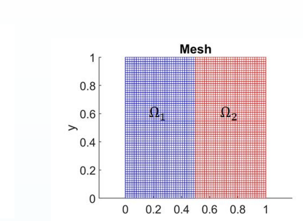

Figure 10. Mesh and DD.

- Cone, cylinder and smooth hump **initial condition** (Fig. 9).
- **Rotating advection field** $(0.5 - y, x - 0.5)$ for 1 rotation.
- Snapshots from **monolithic FEM** on Ω with 4225 DOFs ($h = \frac{1}{64}$).
- **Two subdomains** with 2145 DOFs/subdomain (Fig. 10).
- **High Peclet regime:** $\kappa_i = 10^{-5}$, for $i = 1,2$.
- **Homogeneous** Dirichlet BCs.
- **IMEX** version of **Crank-Nicholson** (treating LM explicitly), with snapshot time step $\Delta t_s = 6.734 \times 10^{-3}$.
- **~20 interior modes** are needed and only **5 interface modes** are needed to capture 99% of their respective snapshot energies.
- **Full LM space** has dimension 63.
- **Reduced LM space** has dimension:

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

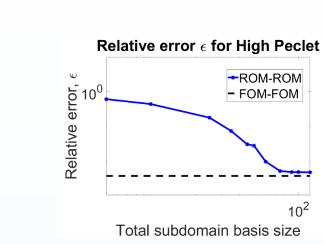

Figure 11. Relative errors w.r.t FOM at $t = 2\pi$

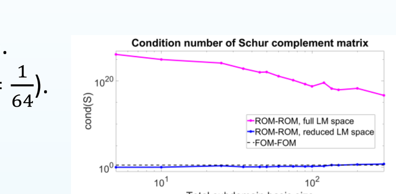

Figure 12. Condition numbers of Schur complement

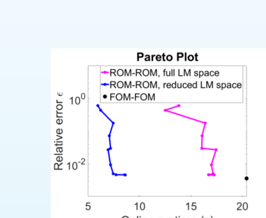

Figure 13. Pareto plot for various couplings. Relative errors are w.r.t. FOM at $t = 2\pi$

- Errors for **ROM-ROM coupling** with **full** and **reduced LM spaces** are **identical** to machine precision (Fig. 11).
- As expected, using **reduced LM space** improves **condition number** (Fig. 12).
- **Conditioning** of the Schur complement for **ROM-ROM** with reduced LM space is essentially **the same** as for the **FOM-FOM coupling** (proven to be well-conditioned in [5]) (Fig. 12).
- Each coupling is capable of attaining an **error** on **the order of the relative error for the FOM-FOM coupling** (Fig. 13).
- **Reduced LM** ROM-ROM coupling achieves **optimal errors** in **less time** (Fig. 13).
- Couplings deliver solutions which are **smooth** and **artifact-free** (Fig. 14).

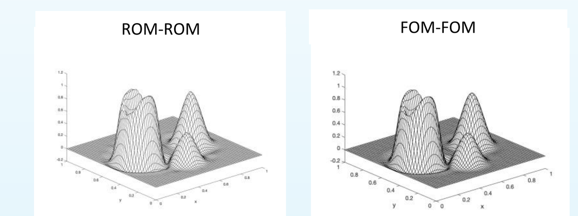

Figure 14. ROM-ROM (left) and FOM-FOM (right) solutions at final time

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