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M2dt: Multifaceted Mathematics for Predictive Digital Twins

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

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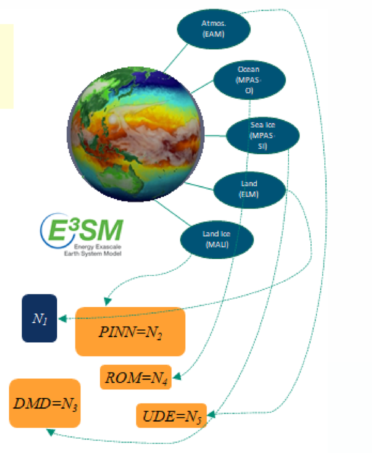
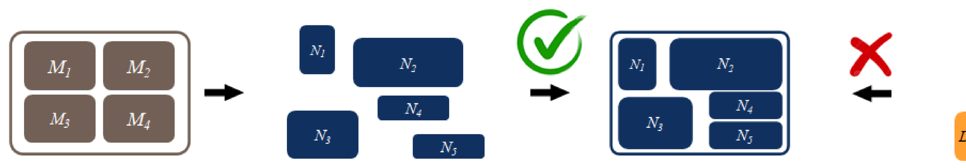
Motivation and Role in M2dt

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

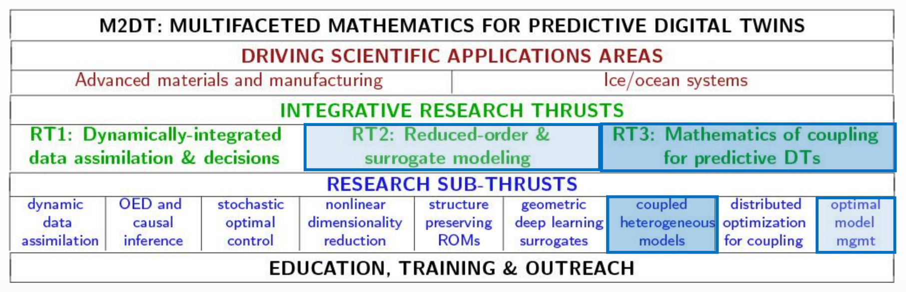
- Frameworks rely on **established mathematical theories** to couple physics components.
- Most existing coupling frameworks are based on **traditional discretization methods**, i.e., full order models (FOMs)





Unfortunately, existing algorithmic and software infrastructures are **ill-equipped** to handle plug-and-play integration of **data-driven models** (e.g., projection-based reduced order models or ROMs)!

Objective (under RT3.1 of M2dt): discover **mathematical principles** guiding assembly of **standard** and **data-driven** models in **stable, accurate** and **physically consistent** ways.



Coupling via Generalized Mortar Methods

Approach

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

$$\begin{aligned} \dot{c}_i - \nabla\cdot F_i(c_i) &= f_i, \quad \text{in } \Omega_i \times [0,T],\ i=1,2 \\ c_i &= g_i, \quad \text{on } \Gamma_i \times [0,T],\ i=1,2 \\ c_i(\boldsymbol{x},0) &= c_{i,0}(x), \quad \text{in } \Omega_i,\ i=1,2 \end{aligned} \qquad (1)$$

Compatibility conditions: on interface $\Gamma \times [0,T]$ (Figure 1)

- *Continuity of states:* $c_1(x,t) - c_2(x,t) = 0$
- *Continuity of flux:* $F_1(x,t)\cdot \boldsymbol{n}_\Gamma = F_2(x,t)\cdot \boldsymbol{n}_\Gamma$
  - ⇒ *Imposed weakly using Lagrange multiplier (LM)* λ

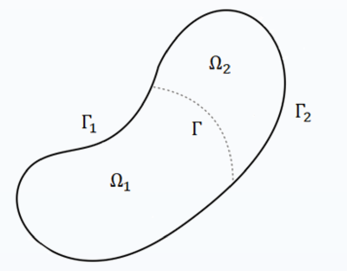


Figure 1. Non-overlapping DD of $\Omega = \Omega_1 \cup \Omega_2$.

Semi-discrete monolithic coupled formulation: obtained by discretizing weak monolithic formulation using FEM in space. *Note the alternative form of the constraint!*

$$\begin{pmatrix} M_1 & 0 & G_1^T \\ 0 & M_2 & -G_2^T \\ G_1 & -G_2 & 0 \end{pmatrix} \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \\ \lambda \end{pmatrix} = \begin{pmatrix} f_1 - K_1 c_1 \\ f_2 - K_2 c_2 \\ 0 \end{pmatrix} \qquad (2)$$

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

Decoupling via Schur complement: equation (2) equivalent to

$$\begin{pmatrix} M_1 & 0 \\ 0 & M_2 \end{pmatrix} \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \end{pmatrix} = \begin{pmatrix} f_1 - K_1 c_1 - G_1^T \lambda \\ f_2 - K_2 c_2 + G_2^T \lambda \end{pmatrix} \qquad (3)$$

where $(G_1 M_1^{-1} G_1^T + G_2 M_2^{-1} G_2^T)\lambda = G_1 M_1^{-1}(f_1 - K_1 c_1) - G_2 M_2^{-1}(f_2 - K_2 c_2)$ (4)

After solving **Schur complement problem** (4), the subdomain problems in (3) **decouple**.

Key Ingredients for Stable POD/Galerkin ROM-ROM and FOM-ROM Coupling

- Calculate **"split" reduced bases** $\boldsymbol{\Phi}_{i,\Gamma}$ and $\boldsymbol{\Phi}_{i,0}$, for interface and interior degrees of freedom (DOFs) via the Proper Orthogonal Decomposition (POD).
- Reduce LM space to size $N_{R,\Gamma} < N_{R,i\Gamma} +$ $N_{R,2\Gamma}$, 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 $N_{R,\Gamma} = N_{R,i\Gamma}$.

ROM-ROM coupling with **reduced LM space** guaranteed to have **non-singular dual Schur complement** if underlying FOM-FOM coupling satisfies conditions in [1].

Key Features of GMM-Based Coupling

- Based on a **non-overlapping** DD (ideal for transmission/multi-physics problems)
- Effective for coupling **conventional models (FOM)** and **reduced order models (ROM)**
- **Monolithic** formulation (more intrusive to implement but more efficient)
- Can couple **different mesh resolutions** and **discretization types**
- Allows the use of **different time-integrators** with **different time-steps** [3,4]
  - **Explicit time-integrators** enable **concurrent** subdomain solves
- Possesses **theoretical** convergence properties/guarantees [1,2]

Numerical Results

- **High Peclet** advection-diffusion **transmission problem** (1) on $\Omega = (0,1)\times(0,1)$ with cone, cylinder and smooth hump initial condition, Dirichlet BCs, **rotating advection field**, run for 1 full rotation (Figure 4)
- **FOM discretization**: finite elements in space ($h = \frac{1}{64}$), Crank-Nicholson in time with ($\Delta t = 6.734 \times 10^{-3}$)
- **ROM discretization**: POD/Galerkin method
  - ROMs evaluated in **predictive regime**, with prediction across κ_i
  - **Snapshots** collected by running **monolithic FOM** at testing parameters
- **Coupling specifications:**
  - **Two subdomain** non-overlapping DD with Ω split at $x = \frac{1}{2}$
  - **Dirichlet BCs** on system boundaries imposed **strongly** in ROMs [5]
  - **Training parameters**: $\kappa_1 = \kappa_2 = 10^{-5}$
  - **Testing parameters**: $\kappa_1 = 10^{-5}, \kappa_2 = 10^{-4}$
  - **Full LM space** has dimension 63
  - **Reduced LM space** has dimension $N_{R,i\Gamma} = \min\left\{\frac{1}{4} N_{R,i0}, 63\right\}$

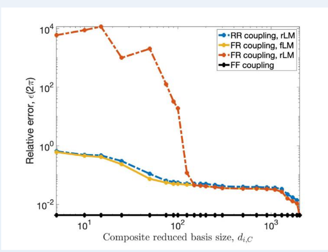


Figure 2: relative errors as a function of the reduced basis size.

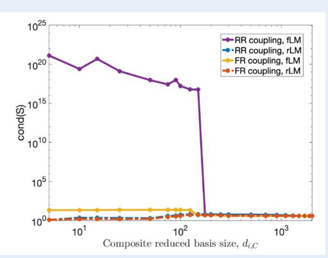


Figure 3: condition #s of (4) as a function of the reduced basis size.

Main takeaway: provably-stable ROM-ROM GMM method delivers **artifact-free solution, maintains Schur complement condition #** of O(1) regardless of basis size, and **converges** with basis refinement!

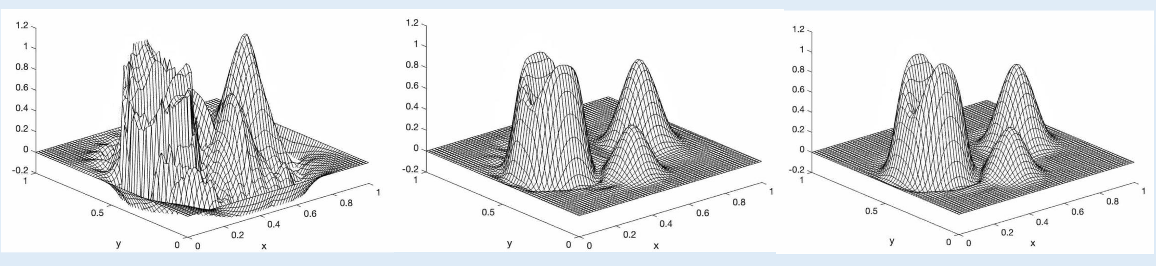


Figure 4: coupled solutions to the targeted transmission problem at the final time. Naïve ROM-ROM coupling (left), provably-stable ROM-ROM coupling (middle) and FOM-FOM coupling (left).

Alternating Schwarz-Based Coupling

Approach

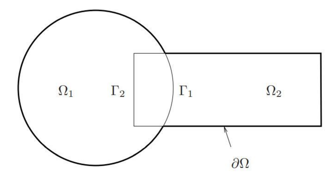
Basic Schwarz Algorithm for Spatial Coupling

Initialize:

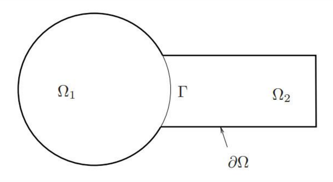
- Solve PDE by any method on Ω_1 with initial guess for transmission BCs on Γ_1 (or Γ).

Iterate until convergence:

- Solve PDE by any method on Ω_2 with transmission BCs on Γ_2 (or Γ) based on values just obtained for Ω_1.
- Solve PDE by any method on Ω_1 with transmission BCs on Γ_1 (or Γ) based on values just obtained for Ω_2.



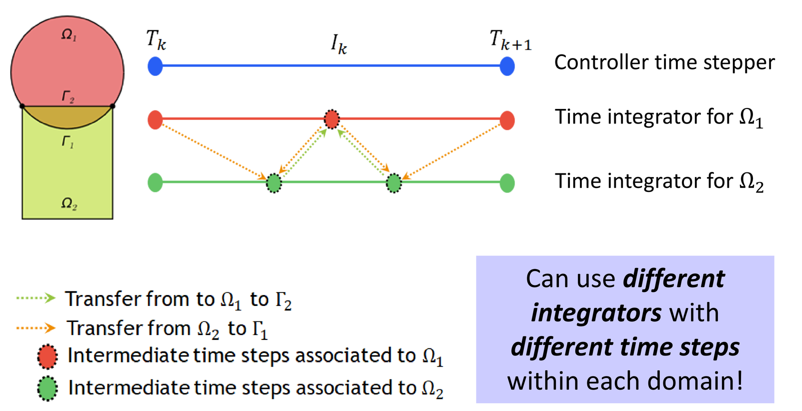
Overlapping Schwarz: convergent with all-Dirichlet transmission boundary conditions (BCs) if $\Omega_1 \cap \Omega_2 \neq \emptyset$.



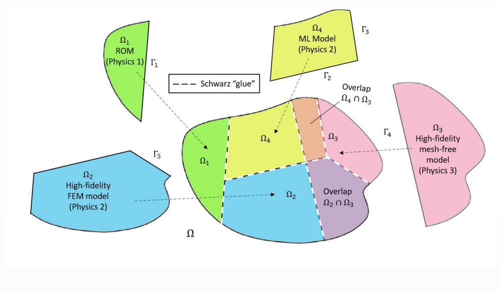
Non-overlapping Schwarz: convergent with Robin-Robin or alternating Neumann-Dirichlet transmission BCs.

Novel Idea: using Schwarz alternating method as a **discretization/coupling method** for solving multi-scale or multi-physics PDEs [6-8].

Schwarz Algorithm for Dynamics



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



Vision: create a ***"plug-and-play" framework*** for arbitrary ***mixing*** and ***matching*** of ***conventional*** and ***data-driven models*** following a domain decomposition (DD).

Key Features of Alternating Schwarz-Based Coupling

- Can handle both **overlapping** or **non-overlapping** DDs
- Can couple **arbitrary combinations** of ROMs and FOMs
- **Iterative** formulation (less intrusive to implement but may require more CPU time)
- Can couple **different mesh resolutions** and **element types**
- Allows the use of **different time-integrators** with **different time-steps** in different subdomains
- **No interface bases** are required in ROM-ROM and ROM-FOM couplings
- Requires **sequential subdomain solves** in multiplicative Schwarz variant
  - **Concurrent** subdomain solves possible with **additive Schwarz** variant
- Possesses **theoretical** convergence properties/guarantees [6-7].

Numerical Results

Model problem: Riemann problem for the **2D unsteady Euler equations**

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$$\frac{\partial}{\partial t}\begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix} + \frac{\partial}{\partial x}\begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ (E+p)u \end{pmatrix} + \frac{\partial}{\partial y}\begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ (E+p)v \end{pmatrix} = \mathbf{0}, \qquad p = (\gamma - 1)\left(\rho E - \frac{1}{2}\rho(u^2 + v^2)\right)$$

- Homogeneous Neumann BCs on system boundaries of $\Omega \times [0,\mathrm{T}] = (0,1)\times(0,1)\times[0,0.8]$.
- **FOM discretization**: 100×100 Cartesian grid, 1st order finite volume scheme, BDF1 time integration, $\Delta t = 0.005$.
- **ROM discretization**: POD/Least-Squares Petrov-Galerkin (LSPG) projection [9] with no hyper-reduction
  - Solution has **strong gradients/shocks** ⇒ poor linear representation
  - ROMs evaluated in the **predictive regime**
  - **Snapshots** collected by running **monolithic FOM** at testing parameters
- **Coupling specifications:**
  - **Four subdomain** overlapping DD: $\Omega = \bigcup_{i=1}^{4} \Omega_i$ (Figure 5)
  - **Dirichlet BCs** on Schwarz boundaries enforced **weakly**
  - **Fixed parameters**: $\rho_1 = 1.5, u_1 = v_1 = 0, p_3 = 0.029$
  - **Varied parameters:** p_1, initial condition from compatibility relations [10]
    - $p_{1,\mathrm{train}} \in [1.0, 1.25, 1.5, 1.75, 2.0]$
    - $p_{1,\mathrm{test}} \in [1.125, 1.375, 1.625, 1.875]$

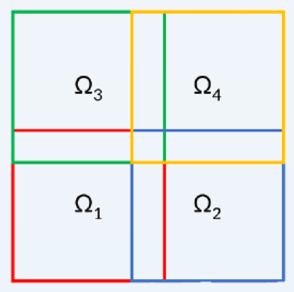


Figure 5: four subdomain overlapping DD.

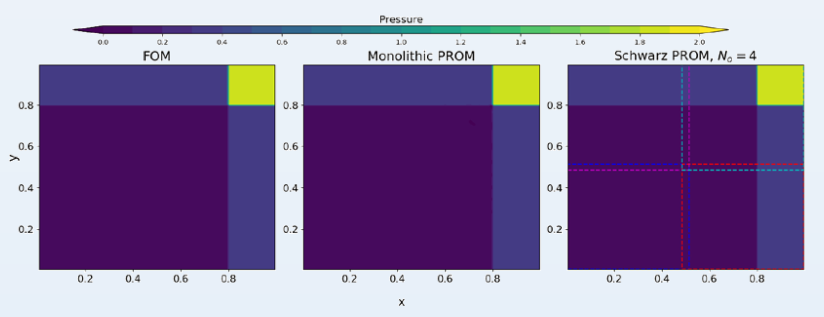


Figure 6: monolithic FOM (left), monolithic ROM (middle) and four subdomain coupled ROM (right) solutions at initial time. ROM solutions have $K = 50$ modes.

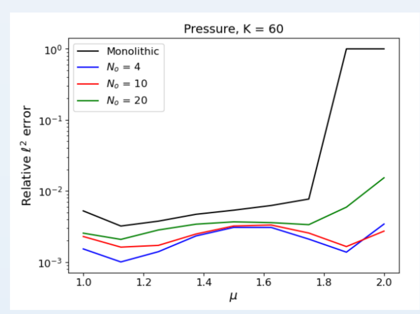


Figure 8: relative l^2 error in ROM solutions w/ and w/o DD as a function of the basis size K.

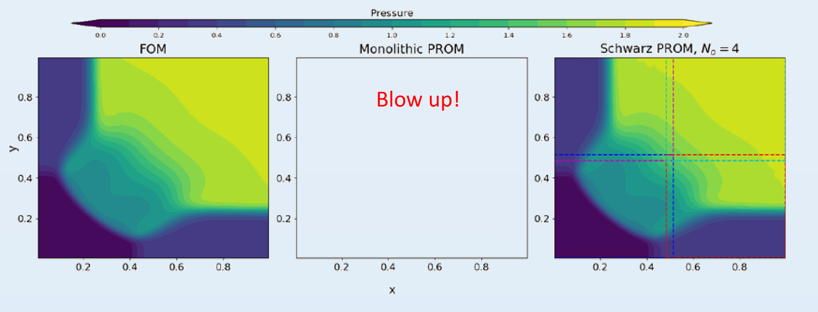


Figure 7: monolithic FOM (left), monolithic ROM (middle) and four subdomain coupled ROM (right) solutions at final time. ROM solutions have $K = 50$ modes.

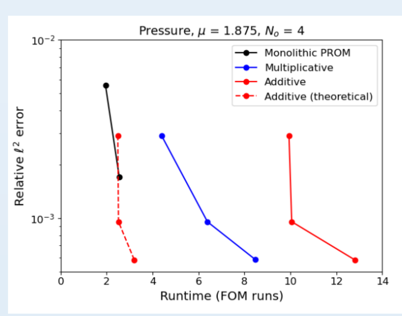


Figure 9: Pareto plots for various ROMs and alternating Schwarz-based couplings.

Main takeaways: DD and Schwarz coupling of ROMs **stabilizes** the solution! Coupled ROM has **comparable CPU time** to monolithic ROM with **additive Schwarz**. **Hyper-reduction** is needed to achieve true cost savings (WIP).

Suite of test cases (e.g., shallow water equations, compressible flow equations, etc.) available via **Pressio demo-apps** [11] open-source implementation*!

* The Pressio demo-apps library is available on github: https://github.com/Pressio/pressio-demoapps.

Ongoing and Future Work

Other Coupling Approaches

Model problem: time-dependent **advection-diffusion** problem (1)
Compatibility conditions: **continuity** of **states** and **flux** from (2)

Optimization-Based Coupling (OBC)

Key Idea: introduce **control** as the shared Neumann BC on the interface Γ (Figure 1) satisfying the continuity of flux, and form a **loss function that**, when minimized, will enforce the **continuity of states**.

- In each time-step, find $(u_1^n, u_2^n, g^n) \in X_1^n \times X_2^n \times L^2(\Gamma)$ that **minimizes**

$$J_\delta(u_1^n, u_2^n, g^n) := \frac{1}{2}||u_1^n - u_2^n||_\Gamma^2 + \frac{1}{2}\delta||g^n||_\Gamma^2 \qquad (6)$$

subject to

$$\frac{1}{\Delta t}\left(u_i^n - u_i^{n-1}, v\right) + (\sigma_i(u_i^n), \nabla v) = (f_i^n, v) + (-1)^i (g^n, v)_\Gamma, \forall v \in V_i,\ i = 1,2 \qquad (7)$$

The **control** g^n is common to both subdomains, **implicitly** enforcing **continuity of flux**

- We **relax** the constrained optimization problem with a Lagrange multiplier μ_i

$$\mathcal{L}(u_1^n, u_2^n, g^n, \mu_1, \mu_2) := J_\delta(u_1^n, u_2^n, g^n) + \sum_{i=1}^{2}\left[\frac{1}{\Delta t}\left(u_i^n - u_i^{n-1}, \mu_i\right) + (\sigma_i(u_i^n), \nabla\mu_i) = (f_i^n, \mu_i) + (-1)^i (g^n, \mu_i)_\Gamma\right]$$

and solve the optimality conditions with gradient descent and a reduced space algorithm

- This approach was developed in [12] in the setting of **coupled linear elliptic PDEs**, extended in [13] to **coupled nonlinear parabolic PDEs**, and later to **fluid-structure interaction** in [14]
- Here we further extend this approach to **ROM-ROM** and **ROM-FOM coupling**
- **Accurate results** for **ROM-ROM coupling** when using **FEM adjoints** (Figure 10)
- **Linear patch tests pass** to the tolerance of the penalty parameter δ
- Ongoing work investigating **alternative snapshot matrices** onto which the adjoint equations are projected to enable using **fewer modes**

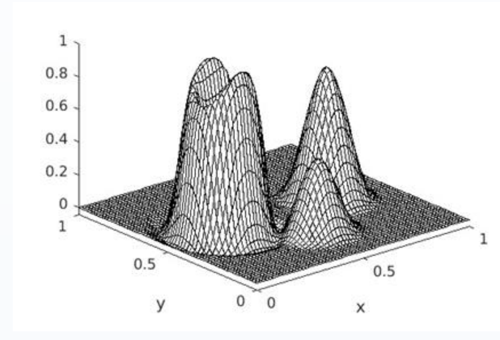


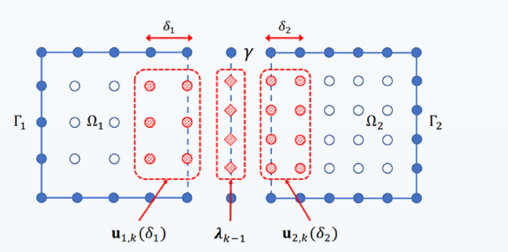
Figure 10. ROM-ROM coupling at final timestep.

Flux Surrogates

Key Idea: use data-driven techniques to **create efficient surrogates** that **approximate** the **dynamics** of the **interface flux**. This **eliminates** the more **expensive Schur complement** solves in GMM.

We consider two different **surrogates** $\boldsymbol{\lambda} = \mathcal{F}(\boldsymbol{y})$ for the **interface flux** dynamics (to replace (4)) using similar states $\boldsymbol{y}$:

- ***DMD surrogate***: $\boldsymbol{y}_{k+1} = A\boldsymbol{y}_k$
- ***nODE surrogate***: $\frac{d\boldsymbol{y}}{dt} = f(t, \boldsymbol{y}, u; \theta)$ = feed-forward NN



- **Training data** consists of both the flux ($\boldsymbol{\lambda}_{k-1}$) and patches of the states near the interface
- DMD or nODE trained to **learn** the **mapping** from $\boldsymbol{y}_{k-1} := \left(\boldsymbol{\lambda}_{k-1}, \boldsymbol{u}_{1,k}(\delta_1), \boldsymbol{u}_{2,k}(\delta_2)\right)^T$ to $\boldsymbol{y}_k$
- Preliminary results indicate that the **new DMD approach** is **more accurate** than lumped mass GMM approach and around **20× times cheaper** than a consistent mass GMM approach (Figure 11)

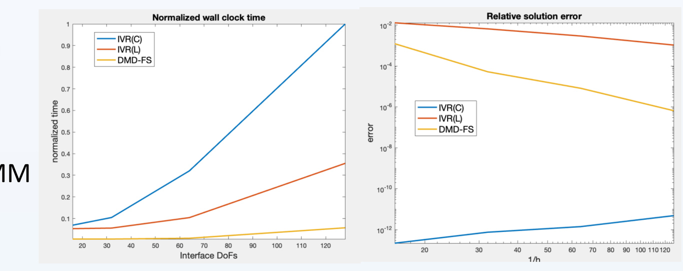
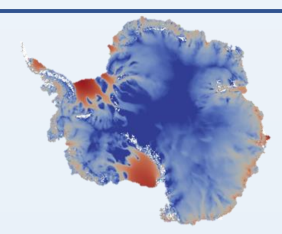


Figure 11. CPU times (left) and relative errors (right) for GMM method with consistent mass (IVR(C)), lumped mass (IVR(L)) and a DMD surrogate (DMD-FS)

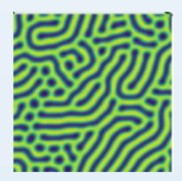
Additional Future Work

- Development of error indicator-based or reinforcement learning-based algorithm to determine **"optimal" DD** and **ROM/FOM assignment**
- Development of algorithms for **on-the-fly ROM-FOM switching** to improve predictive capabilities of the resulting hybrid model
- Incorporation of **structure preservation** into couplings
- Development/coupling of **"bottom-up" subdomain ROMs** that are **trained separately**
- **Extension** of coupling approaches to **DMD** and **non-intrusive operator inference ROMs**

Potential Impact



- New coupling methodologies enable the **rigorous integration** of **data-driven models** into **modeling & simulation toolchains** in a "plug-and-play" fashion for both multi- and mono-physics problems, including **M2dt exemplars** (land ice-ocean interaction, self-assembly of block copolymers)



- New DD-based couplings can **improve trustworthiness** and **predictive capabilities** of data-driven models by enabling **spatial localization of ROMs** (via DD) and **online integration of high-fidelity information** into these models (via FOM coupling).

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