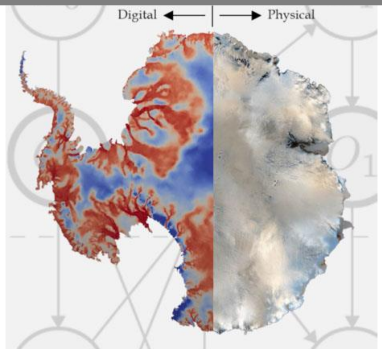
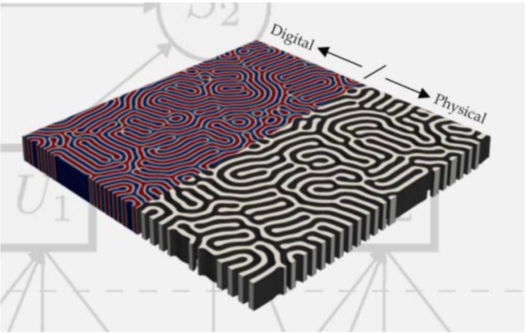
SNL progress highlights: data-driven couplings (RT3.1) and preservation of geometric structure in ROM (RT2.2)



$$\int \mathcal{M}^2 dt$$



__Speakers__: Irina Tezaur and Anthony Gruber

Sandia National Laboratories

M2dt Project All-Hands Meeting

Wednesday, October 25, 2023

SAND2023-10975PE

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Research thrust organization

$\int \mathcal{M}^2 dt$

DRIVING SCIENTIFIC APPLICATION AREA: PREDICTIVE DIGITAL TWINS

Testbed 1: Self-assembling thin films testbed	Testbed 2: Coupled ice shelf-ocean cavity testbed
Alexander & Biros	Heimbach & Urban

INTEGRATIVE RESEARCH THRUSTS

Dynamically-integrated data assimilation & decisions	Reduced-order & surrogate modeling	Mathematics of coupling for predictive DTs
Marzouk & Leyffer	Ghattas & Tezaur	Bochev & Willcox

RESEARCH SUB-THRUSTS

dynamic data assimilation	OED and causal inference	stochastic optimal control	nonlinear dimensionality reduction	structure preserving ROMs	geometric deep learning surrogates	coupled heterogeneous models	distributed optimization for coupling	optimal model mgmt
Marzouk	Uhler	Gunzburger	Ward/Willcox	Tezaur	Ghattas	Bochev	Leyffer	Biros

EDUCATION, TRAINING & OUTREACH

Leyffer & Willcox

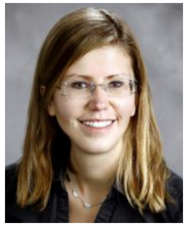
ROM = reduced order model

Part 2 of talk (RT2.2)
Anthony Gruber

Part 1 of talk (RT3.1)
Irina Tezaur

Team

Core Sandia M2dt team


Irina Tezaur


Pavel Bochev


Chris Eldred


Anthony Gruber


Eric Parish


Patrick Blonigan


Paul Kuberry

Other Sandia contributors not officially part of M2dt


Joshua Barnett


Chris Wentland

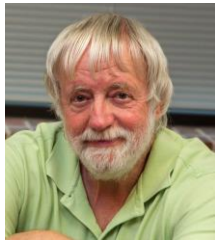

Amy de Castro


Alejandro Mota


Francesco Rizzi

Sandia National Laboratories

Collaborations within M2dt

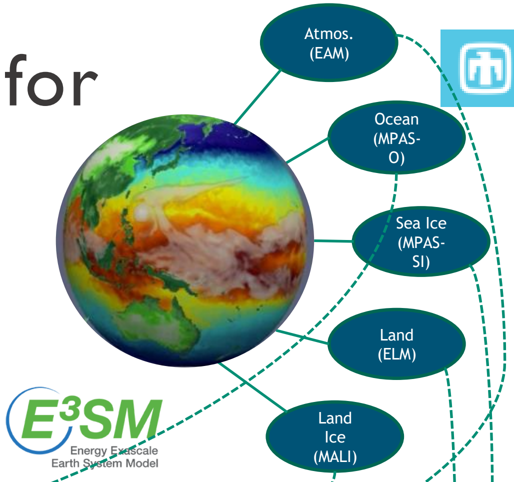

Max Gunzburger


Rudy Geelen

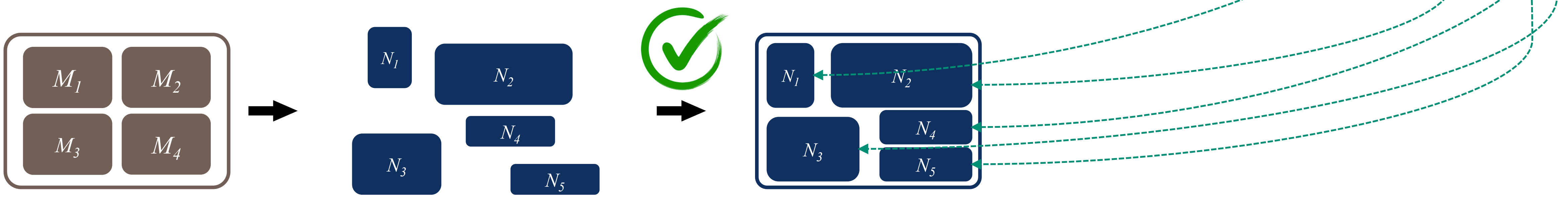

Nicole Aretz

THE UNIVERSITY OF TEXAS AT AUSTIN
PRAESIDIUM
DISCIPLINA CIVITATIS

Motivation for RT3.1: coupled heterogeneous methods for 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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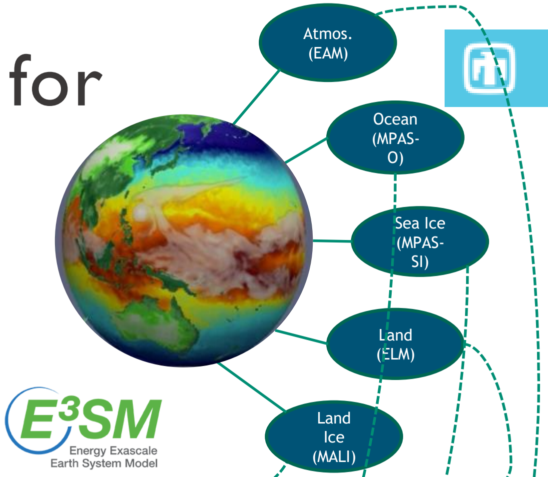

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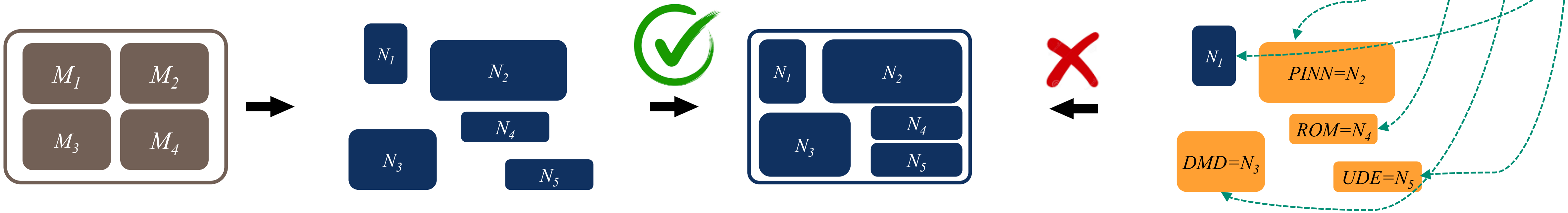

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Traditional + Data-Driven Methods

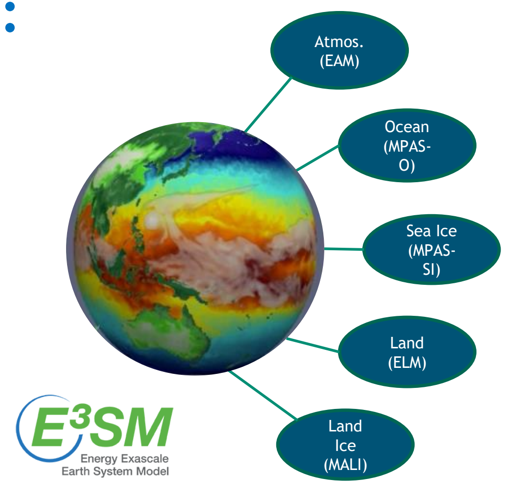
- PINNs
- Neural ODEs
- Projection-based ROMs, …

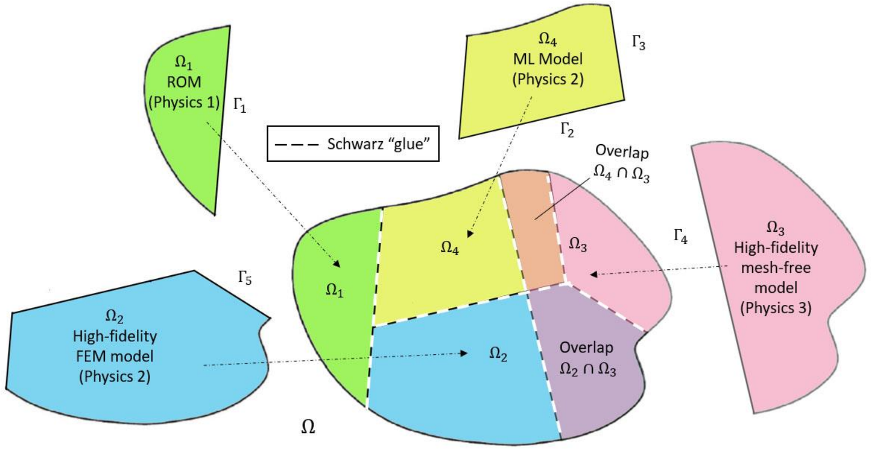
While there is currently a big push to integrate **data-driven methods** into modeling & simulation toolchains, existing algorithmic and software infrastructures are **ill-equipped** to handle **rigorous** plug-and-play integration of **non-traditional, data-driven models**!

Coupling scenarios, models and methods

Coupling scenarios:

Scenario I:
multi-component coupling with a given domain/component decomposition (for reuse of single-component codes)





Scenario II:
multi-scale coupling where decomposition can be chosen to maximize accuracy, robustness & efficiency of coupled model

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., Neural Networks (NNs)
- *Class C*: flow map approximation models, i.e., dynamic model decomposition (DMD) models

Coupling methods:

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

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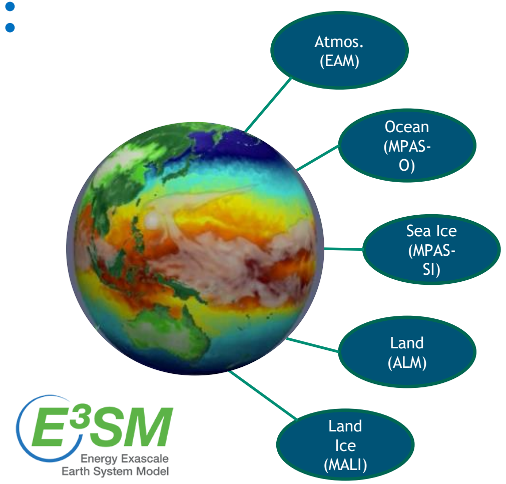

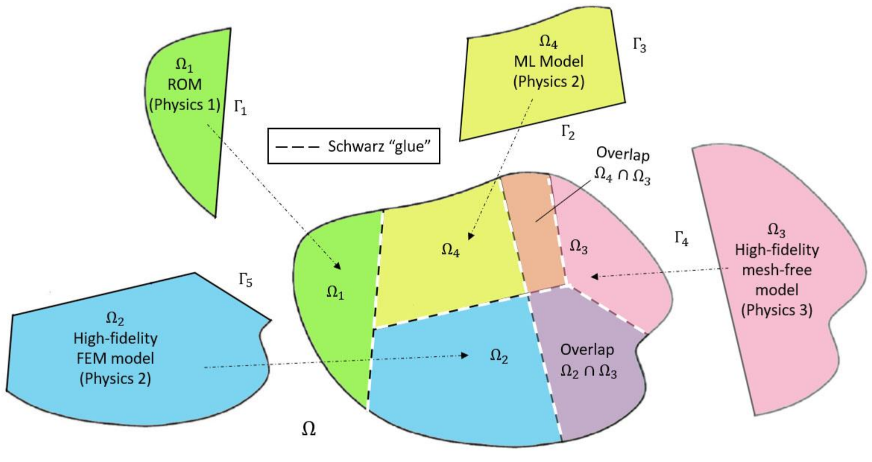

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This talk

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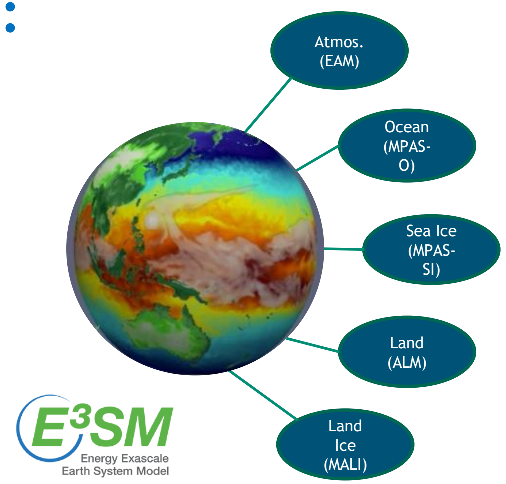

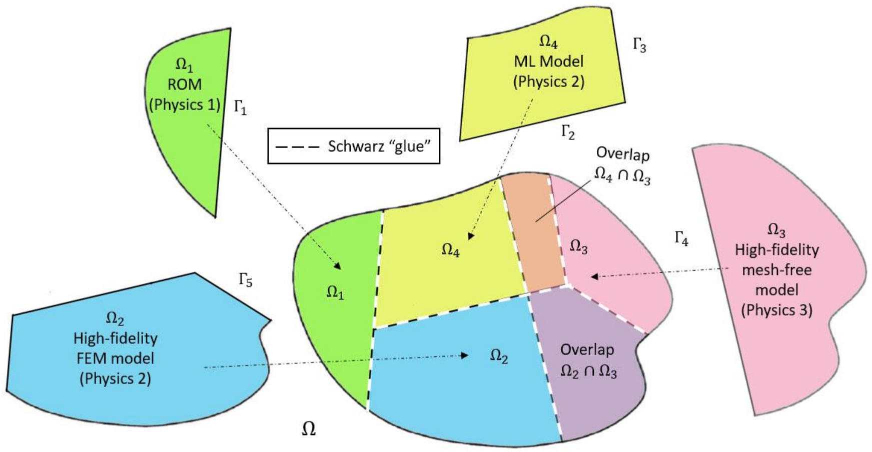

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This talk

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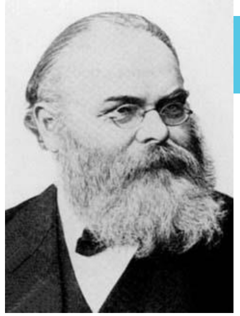
Schwarz alternating method for domain decomposition (DD)

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



H. Schwarz (1843–1921)

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

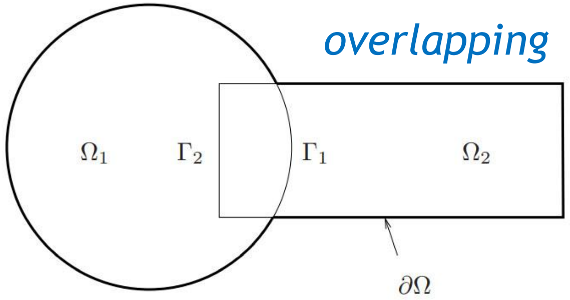
Initialize:

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

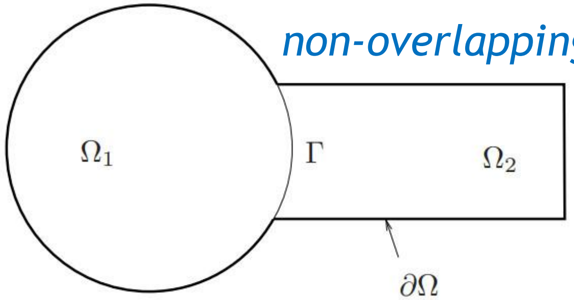
Iterate until convergence:

- 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



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

AS A *PRECONDITIONER* FOR THE LINEARIZED SYSTEM

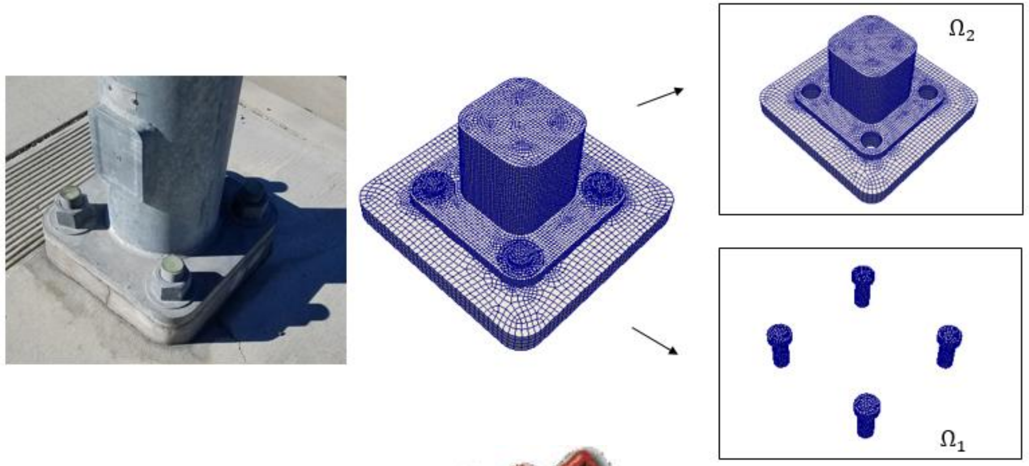
AS A *SOLVER* FOR THE COUPLED FULLY NONLINEAR PROBLEM

Schwarz for multiscale FOM-FOM coupling in solid mechanics[1]

Model Solid Mechanics PDEs:

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

- 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.



Albany-LCM[2]   SIERRA

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

Schwarz extensions to FOM-(H)ROM and (H)ROM-(H)ROM couplings

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

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

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

HROM = hyper-reduced ROM

  - 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 (for Coupling Scenario II)

- *Future work*: error indicator-based or reinforcement learning-based algorithms to determine "optimal" domain decomposition and ROM/FOM assignment, and possibly online ROM-FOM switching

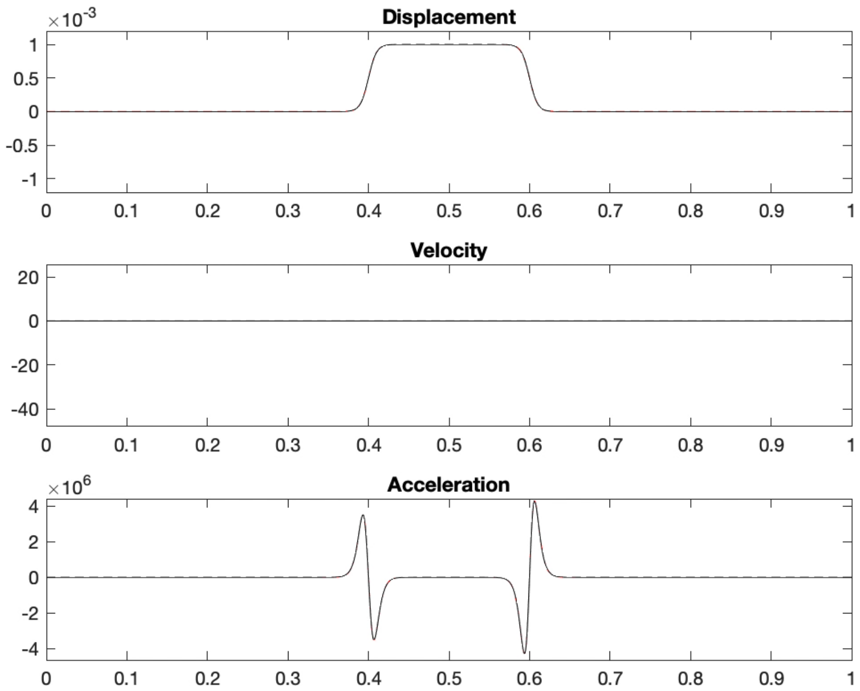
Snapshot collection and reduced basis construction (for Coupling Scenario I)

- 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 Ω_i [Hoang *et al*. 2021, Smetana *et al*. 2022]

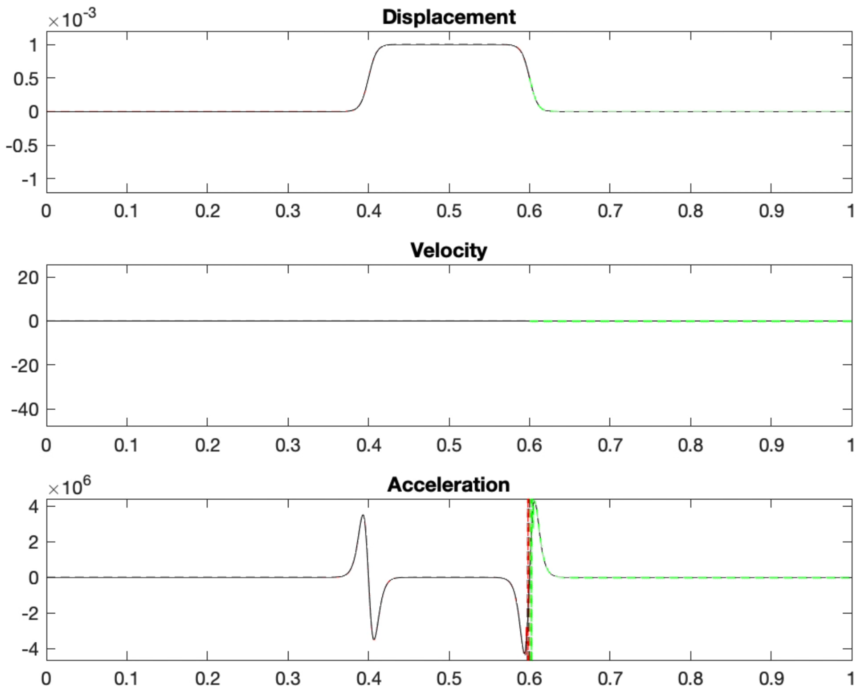
Numerical results

Model Problem 1: Dynamic wave propagation in 1D nonlinear hyper-elastic beam

- **Non-overlapping DD** of $\Omega = \Omega_1 \cup \Omega_2$, where Ω_1 = [0, 0.6] and Ω_2 = [0.6, 1.0]
- **(H)ROM-(H)ROM/FOM-(H)ROM couplings** for POD/Galerkin ROM with Energy-Conserving Sampling & Weighting (ECSW) hyper-reduction
- **Prediction** across initial condition (IC)



Predictive single-domain ROM (M_1= 300)



Predictive FOM-HROM (M_2= 200)

Predictive single-domain ROM solution exhibits **spurious oscillations** whereas coupled FOM-HROM solution is **smooth** and **oscillation-free**!

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

Numerical results

Model Problem 2: 2D inviscid Burgers equation with moving shock

$$\frac{\partial u}{\partial t} + \frac{1}{2}\left(\frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial y}\right) = 0.02\exp(\mu_2 x)$$
$$\frac{\partial v}{\partial t} + \frac{1}{2}\left(\frac{\partial vu}{\partial x} + \frac{\partial v^2}{\partial y}\right) = 0$$
$$u(x=0, y, t; \boldsymbol{\mu}) = \mu_1$$
$$u(x, y, t=0) = v(x, y, t=0) = 1$$
$$x, y \in [0, 100], t \in [0, T_f]$$

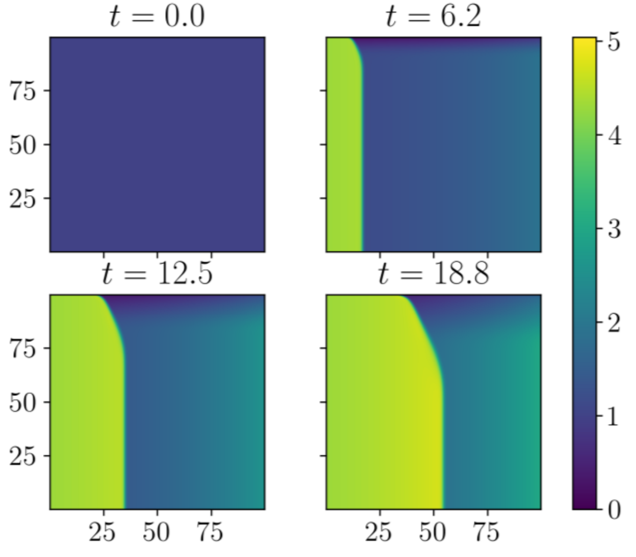


Figure 1: solution of u component at various times

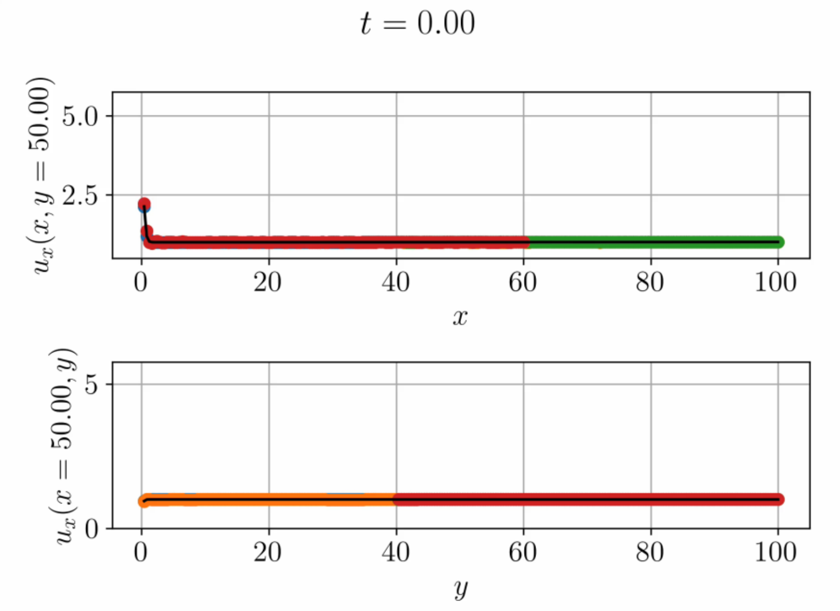


Figure 2: 1D cross-sections of solution u for FOM-HROM-HROM-HROM coupling

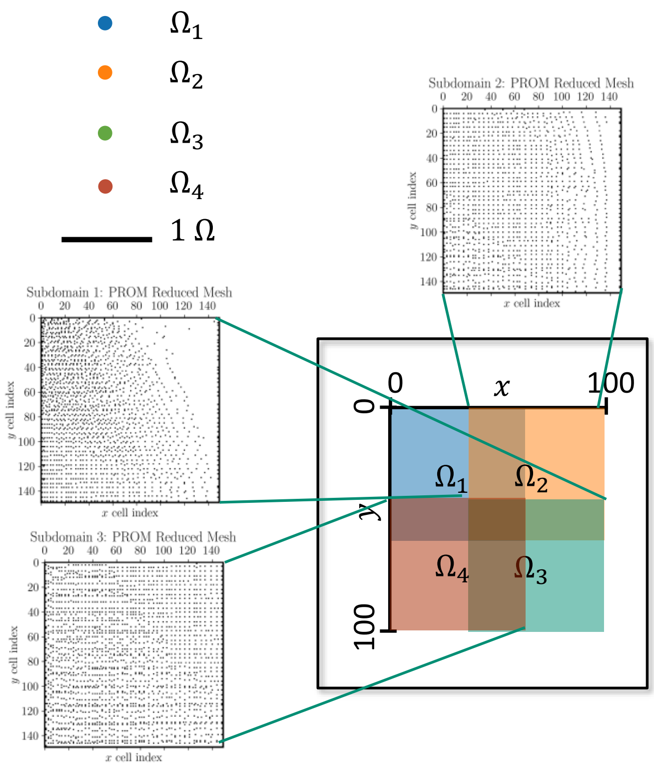


Figure 3: 4 overlapping subdomain DD

- **FOM-HROM couplings** of POD/LSPG ROMs w/ ECSW hyper-reduction, FOM in "hardest" subdomain Ω_1
- **Prediction** across parameters μ_1 and μ_2
- Schwarz converges in **3 iterations** per time-step

Further **speedups** possible via **code optimizations** and **additive Schwarz.**

Subdomains	99% SV Energy		
	M	MSE (%)	CPU time (s)
Ω_1	–	0.0	95
Ω_2	120	0.26	26
Ω_3	60	0.43	17
Ω_4	66	0.34	21
Total			159

*Errors O(0.1%), 2.26× **speedup** over all-FOM coupling*

Numerical results

Model Problem 3: Riemann problem for 2D Euler equations

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho E\end{bmatrix}+\frac{\partial}{\partial x}\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ (E+p)u\end{bmatrix}+\frac{\partial}{\partial y}\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ (E+p)v\end{bmatrix}=0$$

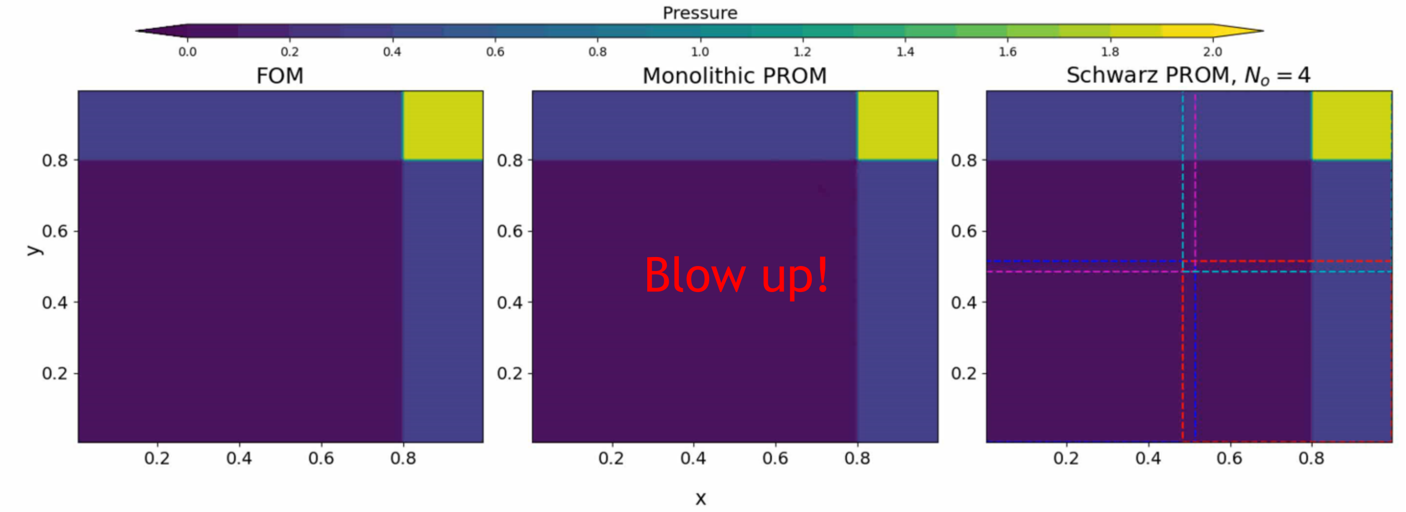
$$p=(\gamma-1)\left(\rho E-\frac{1}{2}\rho(u^2+v^2)\right)$$

- POD/LSPG **all-ROM** coupling, **no hyper-reduction**, **prediction** across initial condition
- Solution has strong gradients/shocks ⇒ POD is **poor (linear) representation**

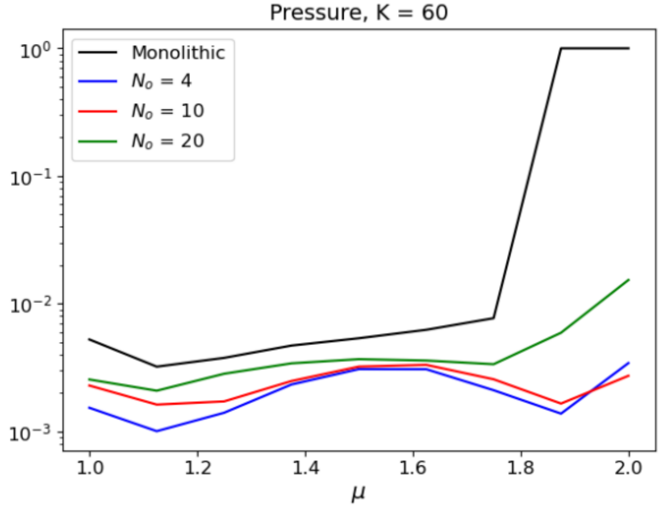
DD and Schwarz coupling of ROMs **stabilizes** the solution! Coupled ROM has **comparable CPU time** to monolithic ROM with additive Schwarz.

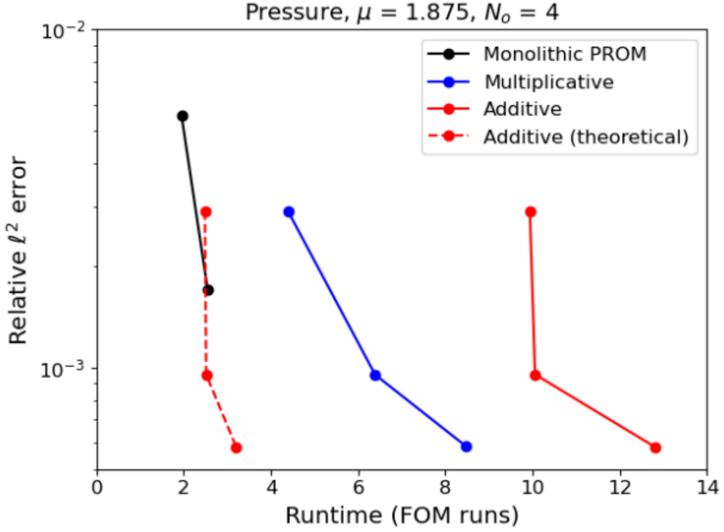
- **Hyper-reduction** is needed to achieve true **cost savings**
- Suite of test cases (e.g., shallow water equations) available via **Pressio demo-apps** open-source implementation*!

* https://github.com/Pressio/pressio-demoapps



Movie above: monolithic FOM (left), monolithic 50 mode ROM (middle) and 4 overlapping 50 mode subdomain all-ROM coupled (right) pressure solutions





Lagrange multiplier-based partitioned coupling formulation

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

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

- $i \in \{1,2\}$
- 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

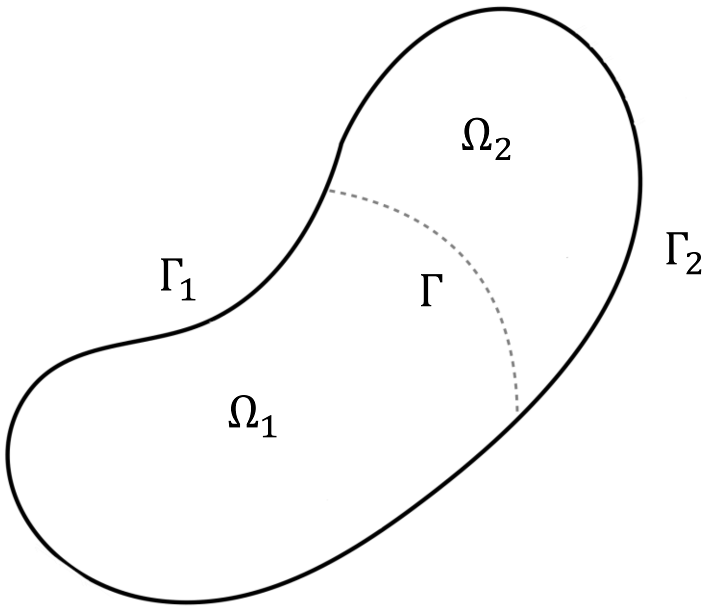


Figure 4: example non-overlapping DD of $\Omega = \Omega_1 \cup \Omega_2$

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***: $F_1(\boldsymbol{x},t) \cdot \boldsymbol{n}_\Gamma = F_1(\boldsymbol{x},t) \cdot \boldsymbol{n}_\Gamma$

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

A Lagrange multiplier-based partitioned scheme

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

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

- $\boldsymbol{M}_i$: mass matrices
- $\boldsymbol{K}_i := \boldsymbol{D}_i + \boldsymbol{A}_i$: stiffness matrices, where $\boldsymbol{D}_i$ and $\boldsymbol{A}_i$ are matrices for diffusive and advective terms, respectively
- $\boldsymbol{G}_i$: constraints matrices enforcing constraints in weak sense

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

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

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

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

Time integration schemes** and **time-steps** in Ω_1 and Ω_2 can be **different!

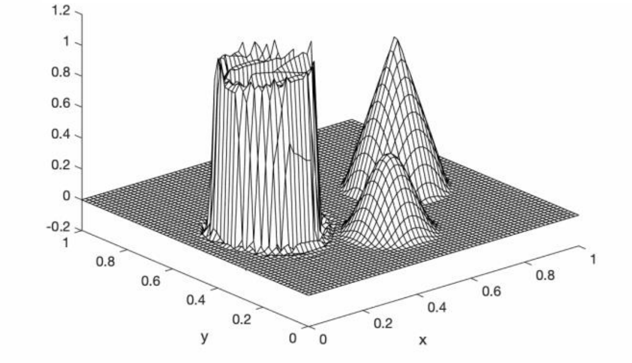
Implicit Value Recovery (IVR) Algorithm [Peterson *et al*. 2019]

- Pick explicit or IMEX time-integration scheme for Ω_1 and Ω_2
- Approximate LM space as trace of FE 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

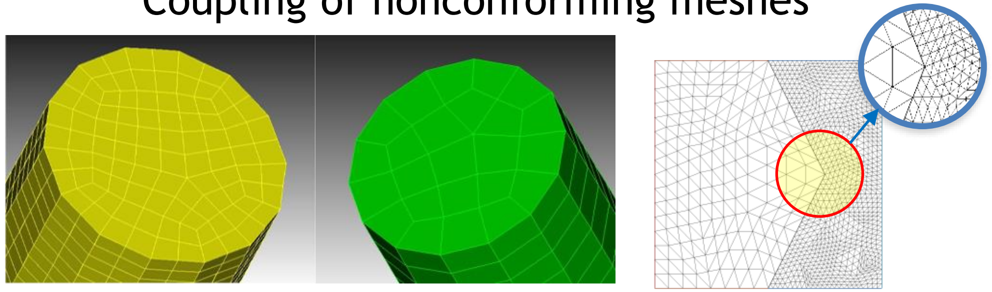
* Ensures that dual Schur complement of (2) is s.p.d.

Lagrange multiplier-based partitioned FOM-FOM coupling

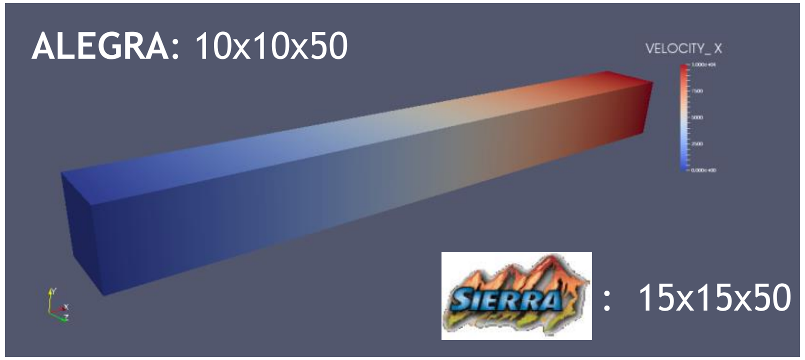
FEM-FEM coupling for high Peclet transport problem



Coupling of nonconforming meshes



Patch test (ALEGRA-Sierra/SM coupling)



"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[1,2]
- Coupling is ***non-iterative*** (single pass)

Method is theoretically rigorous[3]:

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

Method has been applied to several application spaces:

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

[1]Connors *et al*. 2022. [2]Sockwell *et al*. 2023. [3]Peterson *et al*. 2019.

ROM-ROM/ROM-FOM coupling: split bases & reduced LM spaces

- Consider two **separate expansions** for **interface** and **interior DOFs** for $i = 1{,}2$:

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

- Substituting expansions into (2) and projecting PDEs onto RBs gives:

Split basis + reduced LM space guarantees ROM-ROM/ROM-FOM coupling has **non-singular dual Schur complement***.

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

For details, see:

Computer Methods in Applied Mechanics and Engineering

Available online 25 September 2023, 116398

In Press, Corrected Proof What's this?

Explicit synchronous partitioned scheme for coupled reduced order models based on composite reduced bases ☆

Amy de Castro [a b], Pavel Bochev [b], Paul Kuberry [b], Irina Tezaur [c]

Online ROM-ROM IVR Solution Algorithm with Split Bases & Reduced LM Spaces: 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:

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

- Advance the following systems forward in time:

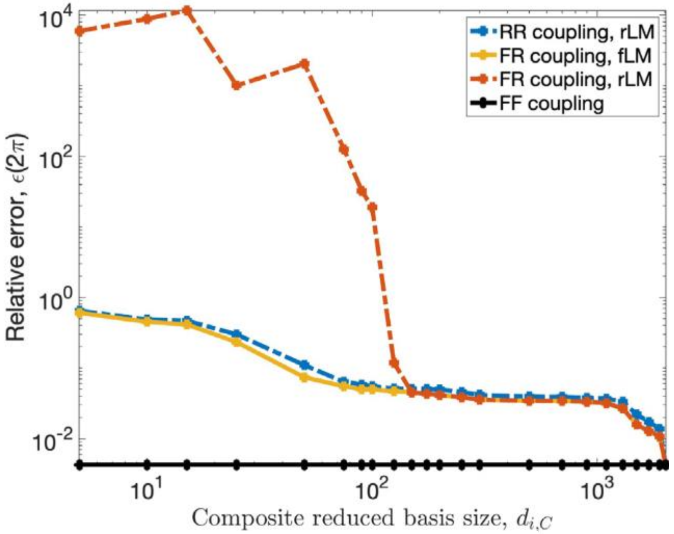
$$\begin{pmatrix} \widetilde{\boldsymbol{M}}_{i,\Gamma} & \widetilde{\boldsymbol{M}}_{i,\Gamma 0} \\ \widetilde{\boldsymbol{M}}_{i,\Gamma 0} & \widetilde{\boldsymbol{M}}_{i,\Gamma} \end{pmatrix} \begin{pmatrix} \dot{\hat{\boldsymbol{c}}}_{i,\Gamma}^n \\ \dot{\hat{\boldsymbol{c}}}_{i,0}^n \end{pmatrix}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

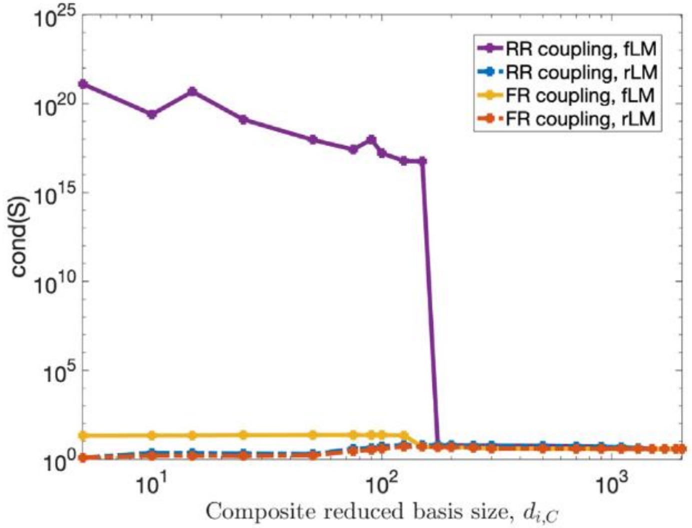
* If conditions in [Peterson *et al.*, 2019] are satisfied for underlying FOM-FOM coupling.

Numerical results

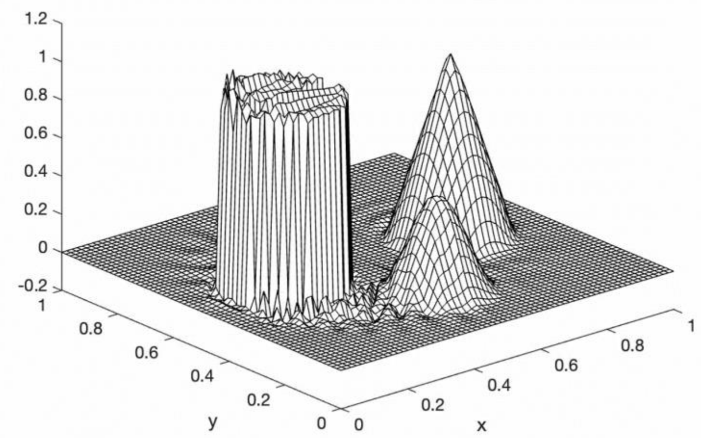
Model Problem: 2D advection-diffusion transmission problem (TP)

- Cone, cylinder & smooth hump **IC**
- **Non-overlapping** DD w/ Γ at $x = 0.5$
- **Rotating advection field** $(0.5 - y, x - 0.5)$ for one full rotation
- **High Peclet predictive problem:** $\kappa_1 = \kappa_2 = 10^{-5}$ for training, $\kappa_1 = 10^{-5}$ and $\kappa_2 = 10^{-4}$ for prediction
- Provably-stable methods **maintain condition number** of O(1) regardless of basis size and **converge** with basis refinement

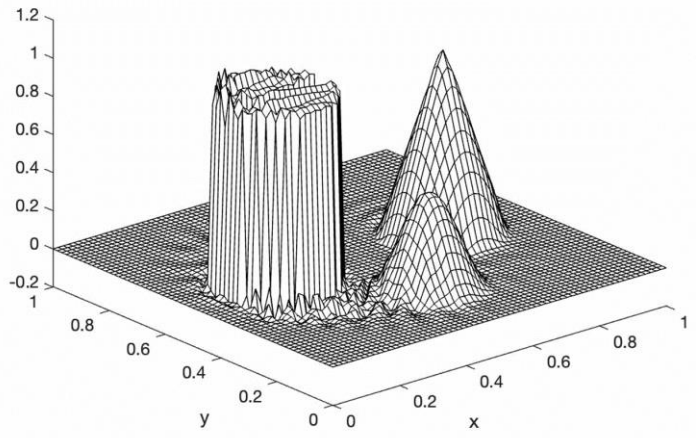




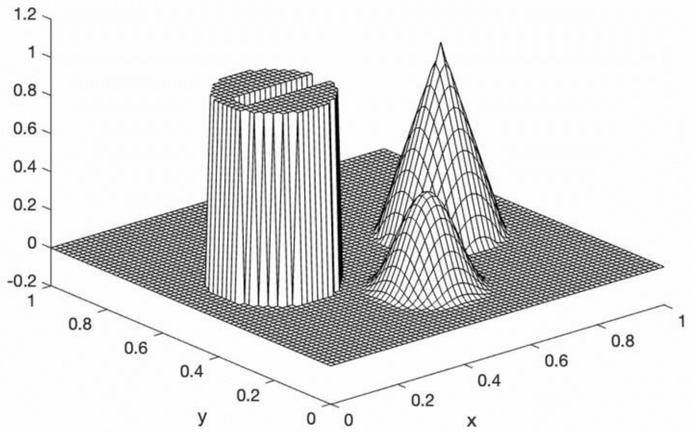
“Naïve” ROM-ROM coupling



Provably-stable ROM-ROM coupling



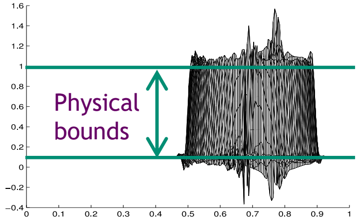
FOM-FOM

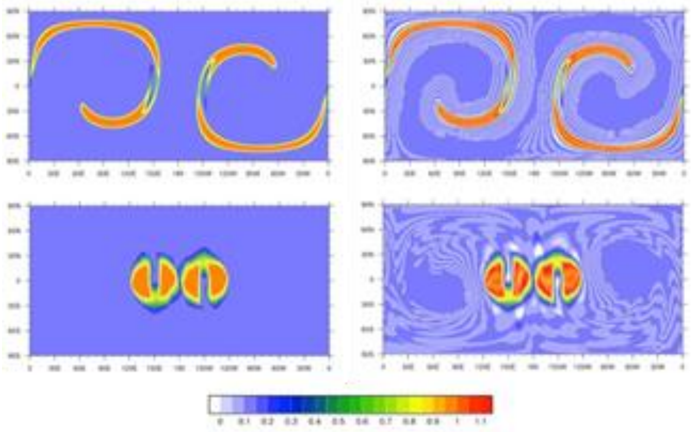


Motivation for RT2.2: structure-preserving ROM (SP-ROM)

Motivation

- To be **reliable predictive tools**, ROMs & surrogates must preserve **key properties** of underlying PDEs (e.g., Hamiltonian structure, conservation, energy/entropy-stability, physical bounds, etc.)





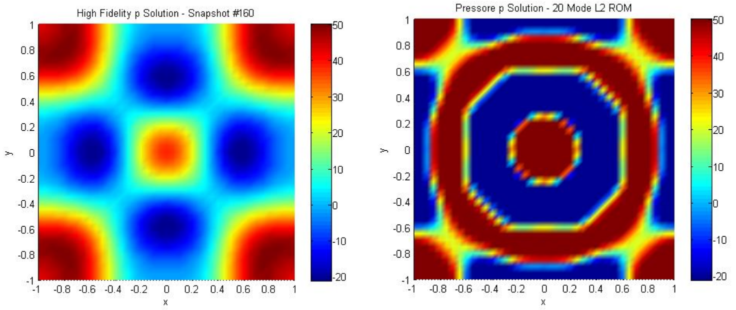
ROMs in general will ***NOT*** automatically inherit the properties of the FOMs from which they are constructed!

Above: bounds-preserving (left) vs. bounds-violating (right) tracer-transport solution [Peterson et al., 2014].

Below: energy-stable (left) vs. unstable (right) compressible flow pressure solutions [Tezaur et al., 2017].

Objective

- Develop **new property-preserving nonlinear dimensionality reduction methods** that will support **new classes of compatible ROMs** mirroring the properties of established compatible discretization methods for FOMs



SP-ROM: research themes & methods

We have identified **three research themes**, informed by many years of research in discretization and geometric methods communities. **Structure preservation** related **to one or more of these themes** is a **prerequisite** for the **stable**, **accurate** and **physically-consistent** solution of PDEs underpinning the **M2dt exemplars**.

Theme A. Geometric Property Preservation

- ***A.1.*** Symplectic structure
- ***A.2.*** Metriplectic structure
- ***A.3.*** Energy/entropy stability

Theme B. Topological property preservation

- ***B.1.*** Hodge decomposition
- ***B.2.*** de Rham complex

Theme C. Qualitative properties

- ***C.1.*** Bounds/positivity
- ***C.2.*** Monotonicity, max principle
- ***C.3.*** Total Variation Diminishing (TVD)

*Themes are crucial to **many applications**, including **solid mechanics/material design** (**Testbed 1**) & **ice/ocean flow** (**Testbed 2**).*

The above three **research themes** will be pursued using the following **methods** and their **combination**:

Method (i). Structure-preserving Operator Inference (OpInf) learning methods

Method (ii). Nonlinear manifold structure-preserving ROMs

Method (iii). Structure-preserving hyper-reduction

Method (iv). Conservation and energy-/entropy-stability

Method (v). Structure-preservation in multi-physics/multi-component ROMs

Method (vi). Optimization-based methods

SP-ROM: research themes & methods

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- ***A.3.*** Energy/entropy stability

Theme B. **Topological property preservation**

- ***B.1.*** Hodge decomposition
- ***B.2.*** de Rham complex

Theme C. **Qualitative properties**

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Deep dive in this talk

(for discussion of other themes/methods, see next talk by Pavel)

Method (i). Structure-preserving Operator Inference (OpInf) learning methods

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Hamiltonian Operator Inference (H-OpInf)

- Hamiltonian systems $\dot{\boldsymbol{x}} = \{\boldsymbol{x}, H(\boldsymbol{x})\} = \boldsymbol{L}(\mathbf{x})\nabla \mathrm{H}(\mathbf{x})$ are archetypically conservative.
  - Governed by scalar potential H and skew-symmetric matrix operator $\boldsymbol{L}$.
- $\boldsymbol{L}$ defines (potentially degenerate) Poisson bracket $\{F, G\} = \nabla F \cdot \boldsymbol{L} \nabla G$.
  - Satisfies Jacobi identity: $\{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\} = 0.$
- Guarantees that flow is perpendicular to ∇H and energy is conserved.

$$\dot{H}(\boldsymbol{x}) = \dot{\boldsymbol{x}} \cdot \nabla H = \boldsymbol{L} \nabla H \cdot \nabla H = -\boldsymbol{L} \nabla H \cdot \nabla H = 0.$$

Examples: Incompressible Euler, Maxwell, shallow water, Monge-Ampere, sine-Gordon, nonlinear Schrodinger, …

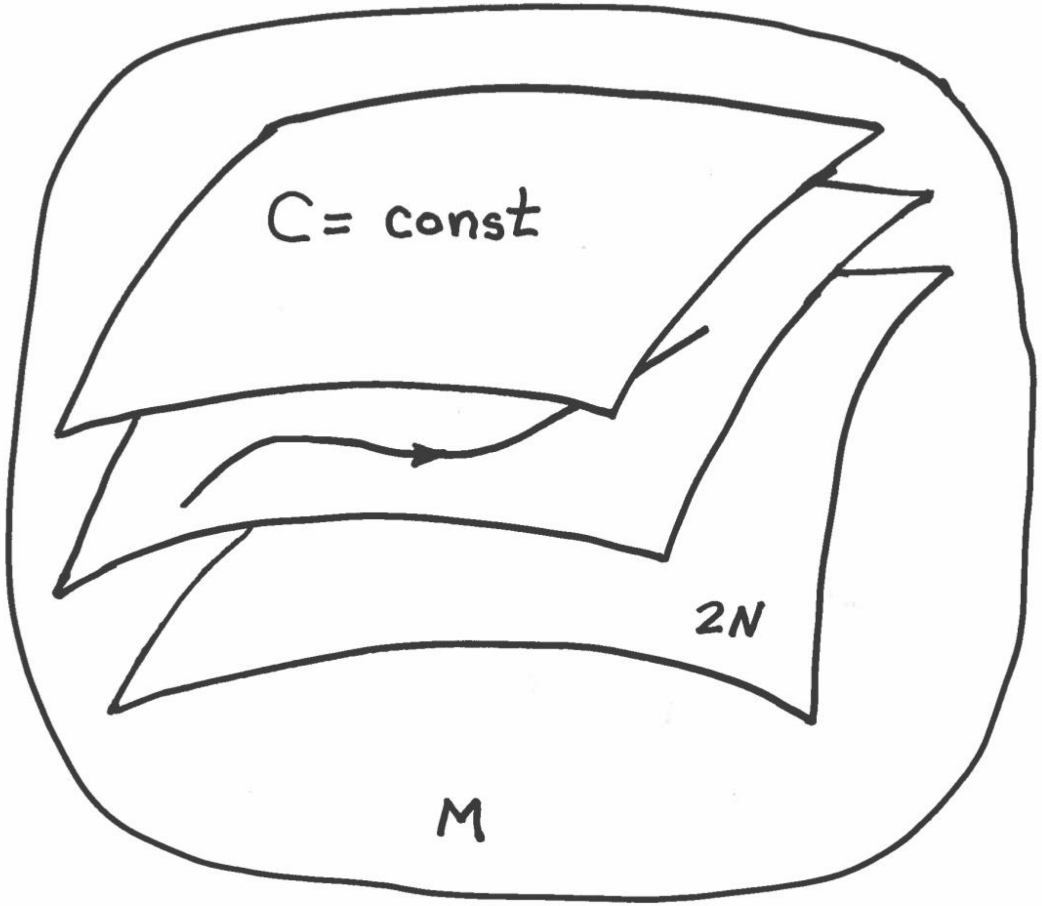


Illustration courtesy of P. J. Morrison

Hamiltonian Operator Inference (H-OpInf)

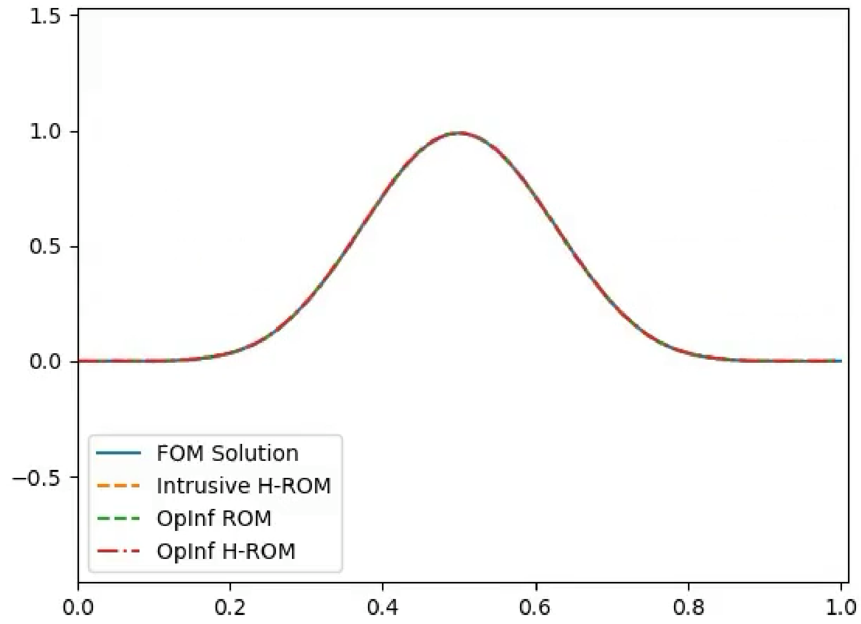
- Naïve Galerkin ROM: $\dot{\hat{\boldsymbol{x}}} = \boldsymbol{U}^T \boldsymbol{L} \nabla H(\boldsymbol{U}\hat{\boldsymbol{x}})$
  - ➢ Data matrix $\boldsymbol{X} \approx \boldsymbol{U\Sigma}\mathbf{V}^{\mathrm{T}}$
  - ➢ POD approximation $\tilde{\boldsymbol{x}} = \boldsymbol{U}\hat{\boldsymbol{x}}$
- Not Hamiltonian! $(\boldsymbol{L}^T\boldsymbol{U})^T = \boldsymbol{U}^T\boldsymbol{L} \neq -\boldsymbol{L}^T\boldsymbol{U}$
  - ➢ (energy not conserved)
- Not symplectic!
  - ➢ (no Jacobi identity)

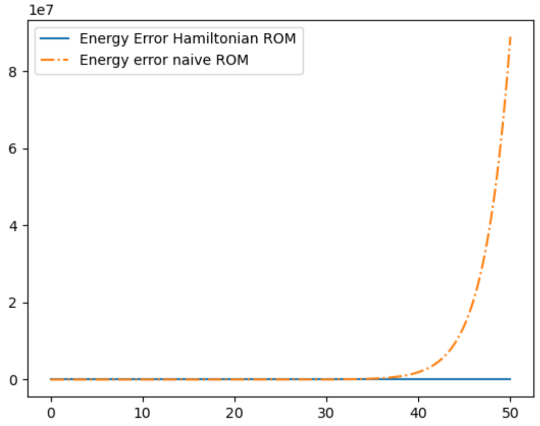
- Conversely, Hamiltonian ROM satisfies both*
  - ➢ Solve overdetermined system $\boldsymbol{U}^T\boldsymbol{L} = \hat{\boldsymbol{L}}\boldsymbol{U}^T$.
  - ➢ Evolution equation:

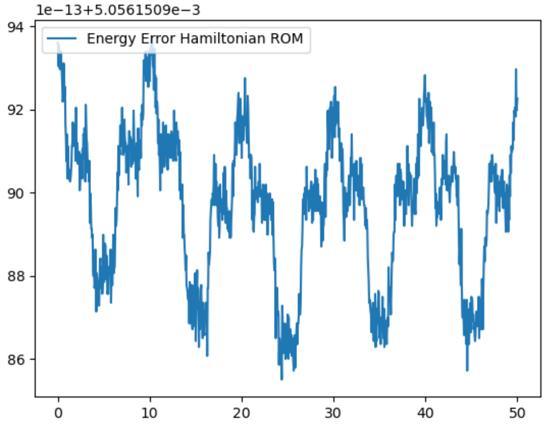
$$\dot{\hat{\boldsymbol{x}}} = \hat{\boldsymbol{L}}\nabla\hat{H}(\hat{\boldsymbol{x}}) = \boldsymbol{U}^T\boldsymbol{L}(\boldsymbol{U}\hat{\boldsymbol{x}})\boldsymbol{U}\boldsymbol{U}^T\nabla H(\boldsymbol{U}\hat{\boldsymbol{x}})$$

  - ➢ Closed orbits are preserved.

* When $\boldsymbol{L}$ is $\boldsymbol{x}$-independent







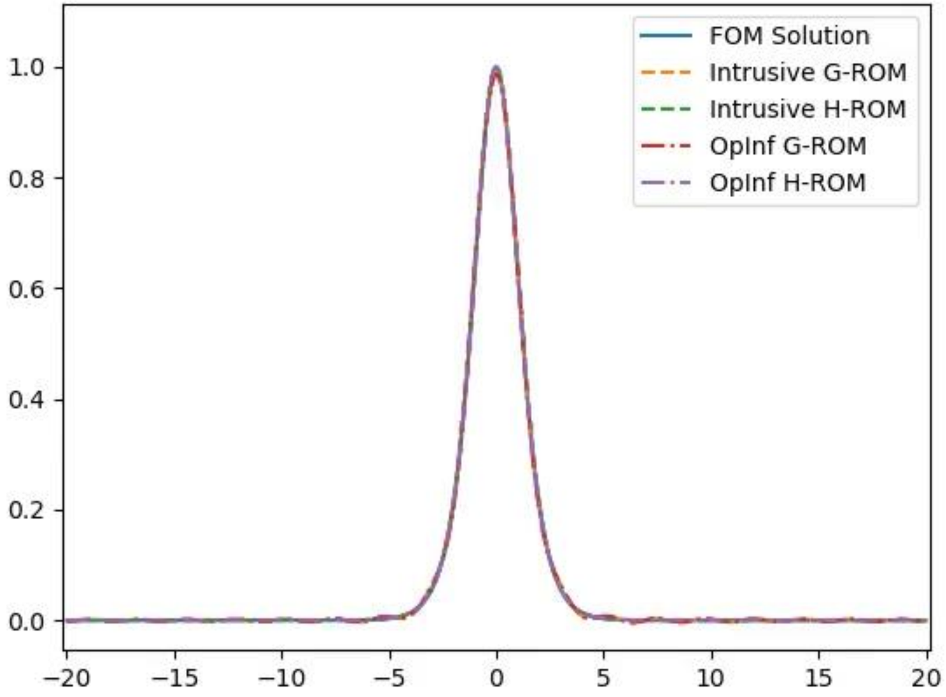
Hamiltonian Operator Inference (H-OpInf)

- Non-intrusive case: operator inference
  - Solve a minimization for RO operators $\hat{\boldsymbol{L}}, \hat{\boldsymbol{A}}$:

$$\underset{\hat{\boldsymbol{A}} \text{ or } \hat{\boldsymbol{L}}}{argmin} \left|\hat{\boldsymbol{X}}_t - \hat{\boldsymbol{L}}\hat{\boldsymbol{A}}\hat{\boldsymbol{X}}\right|^2, \qquad \hat{\boldsymbol{L}}^T = -\hat{\boldsymbol{L}},\ \hat{\boldsymbol{A}}^T = \hat{\boldsymbol{A}}.$$

- Reduces to a single linear solve.
- Converges to intrusive ROM in the limit of infinite data.
- If $\boldsymbol{L}$ is known, this is "canonical inference".
  - Extends previous work (H. Sharma, B. Kramer, Z. Wang, 2022)
    - To arbitrary basis $\boldsymbol{U}$
    - To arbitrary $\nabla H(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} + \nabla f(x)$
- If $\boldsymbol{A}$ is known, this is noncanonical inference.
  - Poisson structure is learned instead.

Model Problem 1: 1D Korteweg-De Vries (KdV) equation



Hamiltonian Operator Inference (H-OpInf)

Albany-LCM[1]

Model Problem 2: 3D transient solid mechanics[1]

- Noticed mixed results for larger, 3D problems.
  - ➢ Linear elasticity with material parameters of steel:

$$\rho \ddot{\boldsymbol{q}} = \nabla \cdot \boldsymbol{\sigma} = \nabla \cdot \left(\lambda \operatorname{tr}(\boldsymbol{\epsilon}) \boldsymbol{I} + 2\mu \boldsymbol{\epsilon}\right)$$

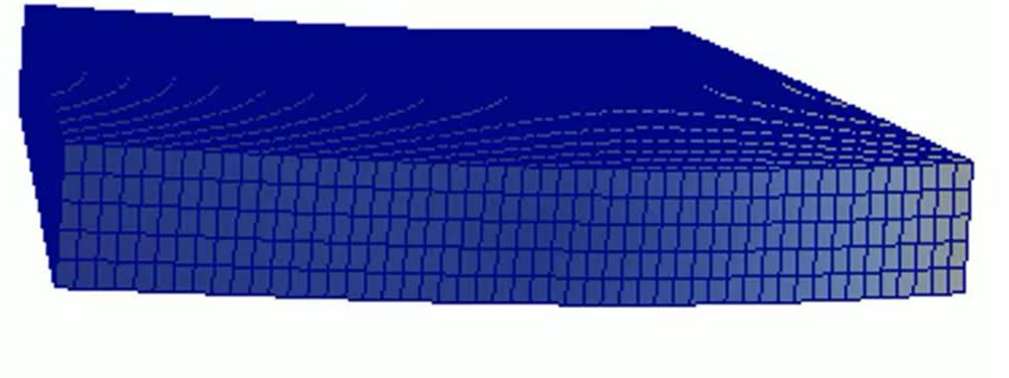
$$\boldsymbol{\epsilon} = \frac{1}{2}\left(\nabla \boldsymbol{q} + (\nabla \boldsymbol{q})^{\intercal}\right)$$

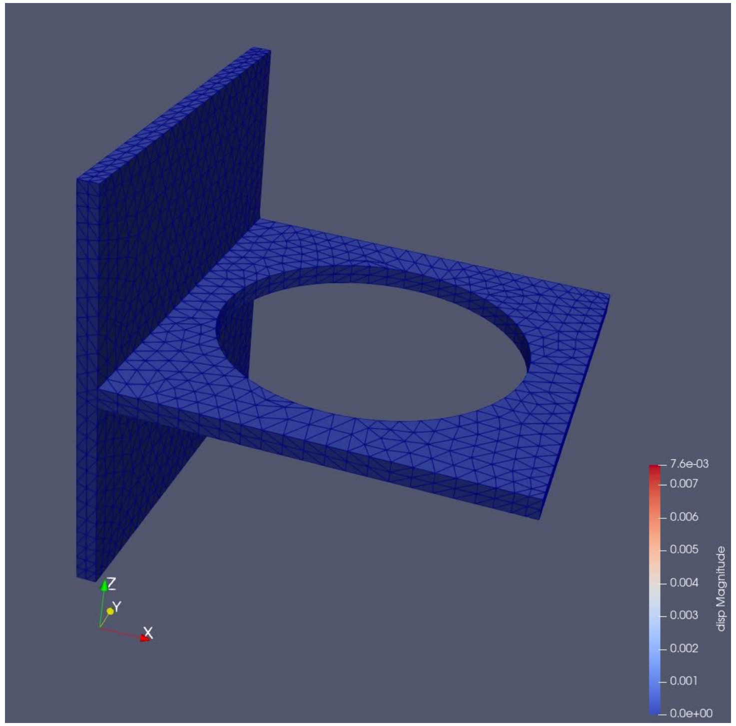
$$H\left(\boldsymbol{q}, \dot{\boldsymbol{q}}\right) = \frac{1}{2}\int_{\Omega}\left(\rho\left|\dot{\boldsymbol{q}}\right|^{2} + \lambda \operatorname{tr}\left(\boldsymbol{\epsilon}\right)^{2} + 2\mu\left|\boldsymbol{\epsilon}\right|^{2}\right) dV$$

- After discretization, system looks like[2]:

$$\begin{pmatrix} \dot{\hat{\boldsymbol{q}}} \\ \dot{\hat{\boldsymbol{p}}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} & \boldsymbol{I} \\ -\boldsymbol{I} & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \widehat{\boldsymbol{K}} & \boldsymbol{0} \\ \boldsymbol{0} & \widehat{\boldsymbol{M}^{-1}} \end{pmatrix} \begin{pmatrix} \hat{\boldsymbol{q}} \\ \hat{\boldsymbol{p}} \end{pmatrix},$$

$$\widehat{\boldsymbol{M}^{-1}} = \boldsymbol{U}^{T}\boldsymbol{M}^{-1}\boldsymbol{U}, \qquad \widehat{\boldsymbol{K}} = \boldsymbol{U}^{T}\boldsymbol{K}\boldsymbol{U}.$$



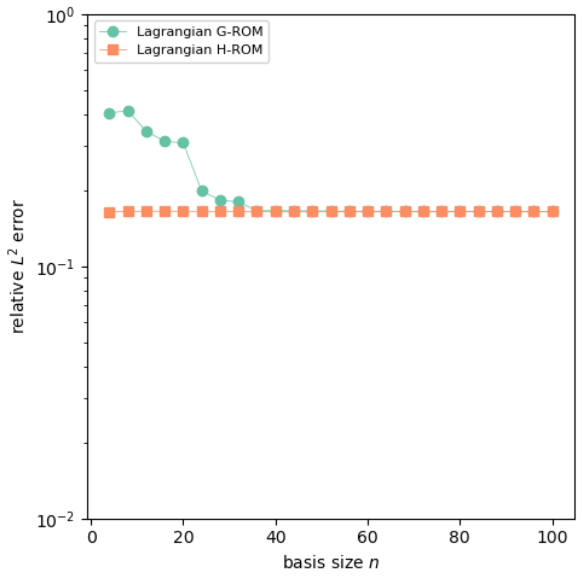


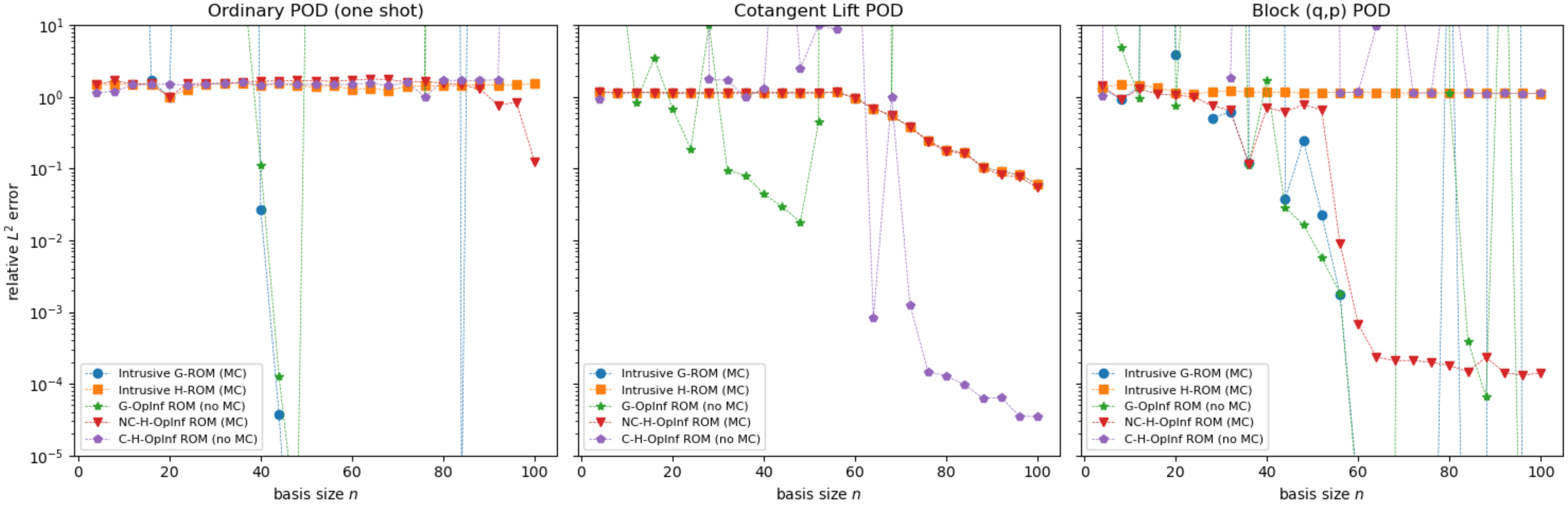
[1]Albany-LCM HPC code: https://github.com/sandialabs/LCM. [2]Data/matrices: https://github.com/sandialabs/HamiltonianOpInf.

Hamiltonian Operator Inference (H-OpInf)

Model Problem 2: 3D transient solid mechanics

- Neither Hamiltonian nor Galerkin ROM worked well.
  - ➢ Lagrangian ROM* and equivalent Hamiltonian ROM were stable, but not much better.
    - ❖ *Galerkin projection from Lagrangian FOM.
- Opinf solutions do not match intrusive due to closure error.
  - ➢ (actually beneficial in this case)





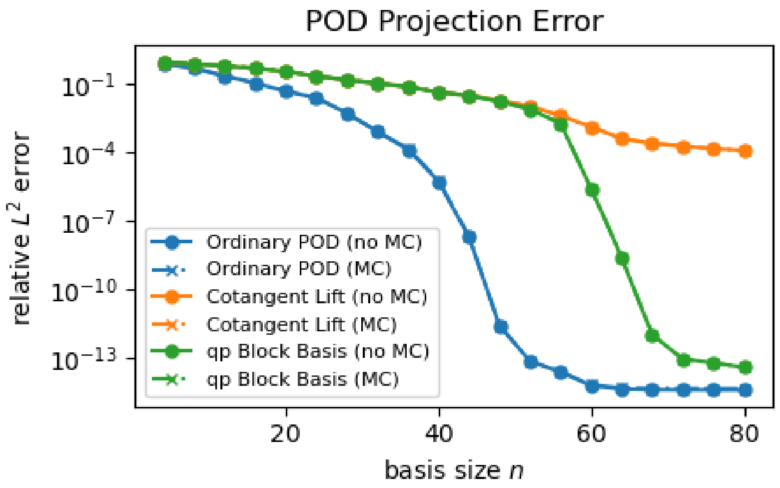
Hamiltonian Operator Inference (H-OpInf)

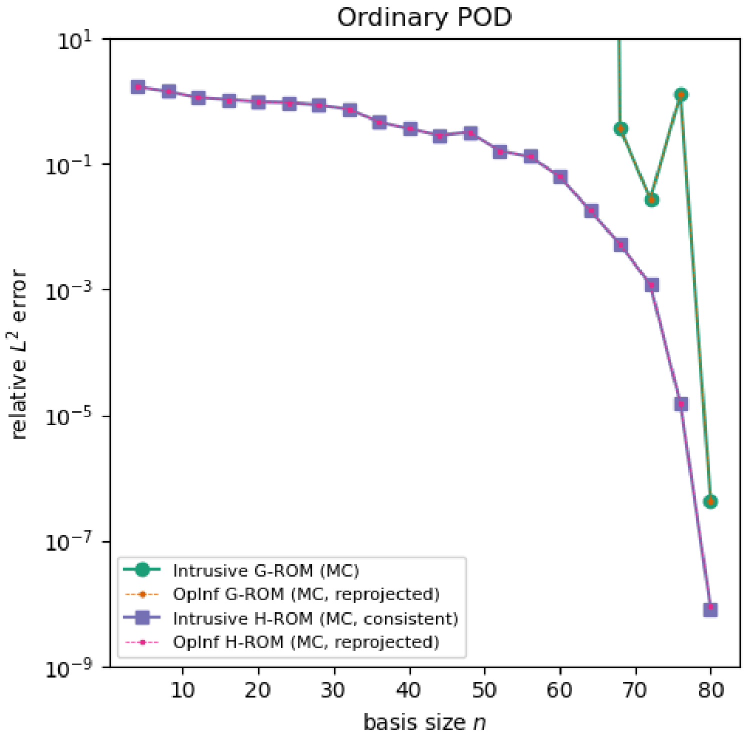
Model Problem 2: 3D transient solid mechanics

- Projection errors are reasonable.
  - ➢ A good ROM should be possible.
- Latest thinking uses a Petrov-Galerkin (PG) projection:
  - ➢ Linear elasticity has a canonical Hamiltonian form
    - ❖ So, $\boldsymbol{JU}$ is a valid test basis, implying:

$$\hat{\boldsymbol{J}}^T\hat{\boldsymbol{x}} = \boldsymbol{U}^T\boldsymbol{J}^T\boldsymbol{U}\hat{\boldsymbol{x}} = \boldsymbol{U}^T\boldsymbol{J}^T\boldsymbol{J}\nabla H(\boldsymbol{U}\hat{\boldsymbol{x}}) = \nabla\hat{H}(\hat{\boldsymbol{x}})$$

- Provably Hamiltonian: energy/symplecticity are conserved.
- Removes the need for an extra column-space projection $\boldsymbol{UU}^{\mathrm{T}}$.
  - ➢ Improved accuracy without harming generalizability.
- Can show that error (in reproductive case) is balanced between:
  - ➢ POD projection error $|(\mathbf{I} - \boldsymbol{UU}^T)\boldsymbol{x}|$
  - ➢ Max eigenvalue of $\hat{\boldsymbol{J}}^T\hat{\boldsymbol{J}} - \boldsymbol{I}$



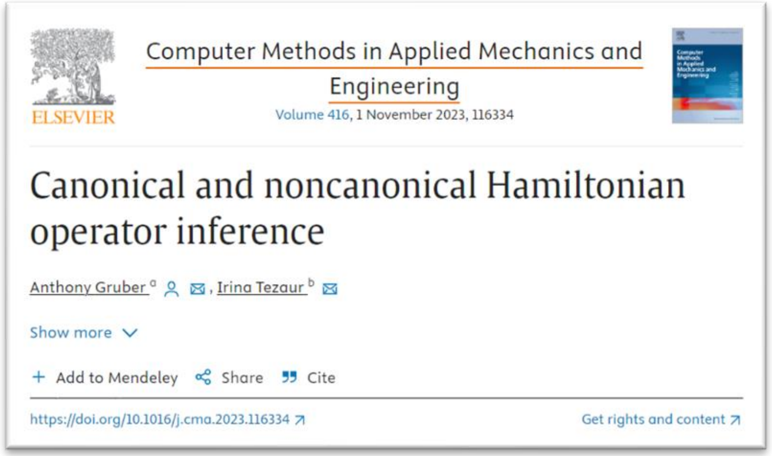


Hamiltonian Operator Inference (H-OpInf)

Takeaways:

- Structure-preservation is necessary but not sufficient for good predictive accuracy.
- The best Hamiltonian ROM balances projection error and symplecticity error.
  - ➢ Explains why "cotangent lift" basis is best when projection error is low.
- More work to do to extend to noncanonical systems.
  - ➢ PG projection **not** full rank…

For details on new H-OpInf ROM approach, see:


Computer Methods in Applied Mechanics and Engineering
Volume 416, 1 November 2023, 116334

Canonical and noncanonical Hamiltonian operator inference

Anthony Gruber [a], Irina Tezaur [b]

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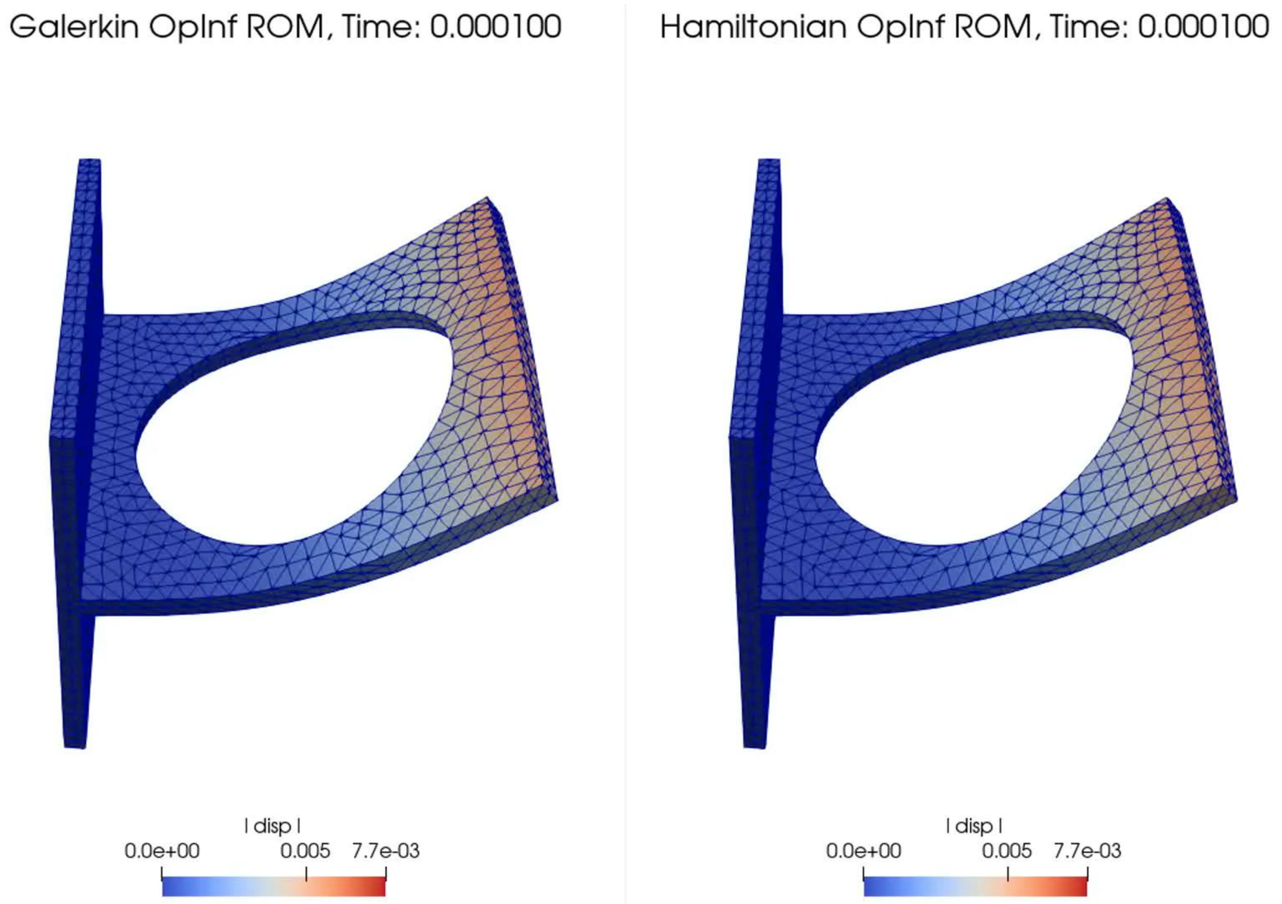


Need to ***understand structure present in exemplars*** to see if similar techniques are useful there.

Progress in relation to project plan milestones

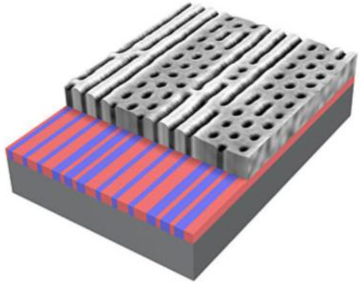
- ☺ Created set of **model problems** to develop RT3.1 and RT2.2 methods on
  - 😐 *Still need to better define **connections** to driving testbeds*
- ☺ Defined **research roadmap** for various tasks (see Pavel & Chris's talk)
  - 😐 *Interested in improving **cross-institution collaboration** and **integration across subthrusts***
  - ☺ ***Opportunity:*** collaboration on **nonlinear manifold ROMs** (RT2.1) and use of ROMs to **enable OED/optimal control** (RT1)
- ☺ Developed ROM formulations that preserve **Hamiltonian** and **energy-/entropy-stability structure**
  - 😐 *Discussing and defining **structure relevant to exemplars** would be worthwhile*
- ☺ Formulated ROM formulations that preserve **topological structure** (see Pavel & Chris's talk)
- ☺ ***Ahead of schedule*: developed monolithic** and **iterative DD-based** ROM-ROM and ROM-FOM **coupling methods**
- ☺ **3 proceedings papers** and **5 journal articles** partially or fully funded by M2dt have been **published** during FY23, with others submitted/in review and in preparation.
- ☺ **16 conference/workshop/seminar talks** were given on M2dt work during FY23 (U Reno, SIAM CS&E, ARIA ROM Workshop, CoDA, CFC, INI workshop, COUPLED, USNCCM, MMLDE-CSET, NA G-ROMs seminar, etc.). Abstracts are being submitted for FY24 presentations.

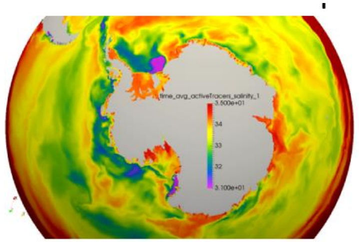
Start of Backup Slides

Motivation for reduced order & surrogate modeling

Despite improved algorithms and powerful supercomputers, **“high-fidelity” models** are often too expensive for use in a design or analysis setting.

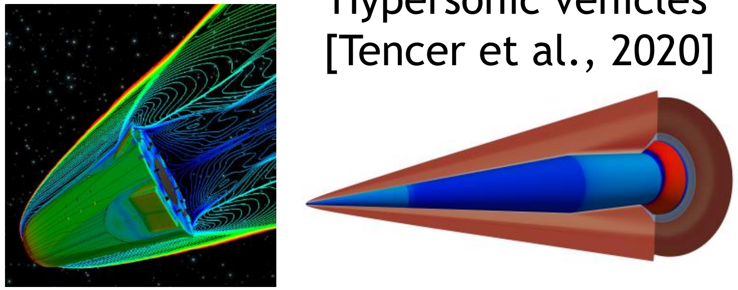
- **Testbed 1: self-assembling block copolymer thin films in nanomaterials.** material design involves multi-component compositions and is extremely high-dimensional; optimal experimental design & optimal control under uncertainty requires reduced order models (ROMs).



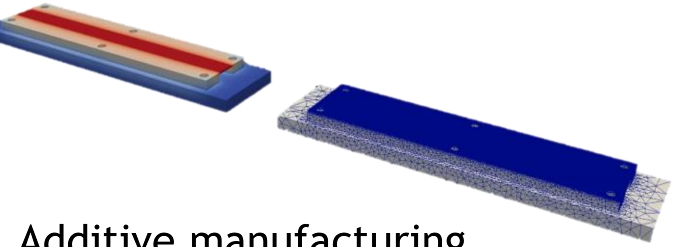


- **Testbed 2: ice-ocean coupling.** decadal-century scale simulations can require millions of CPU-hours; high-fidelity simulations are too costly for UQ; Bayesian inference of high-dimensional parameter fields is intractable

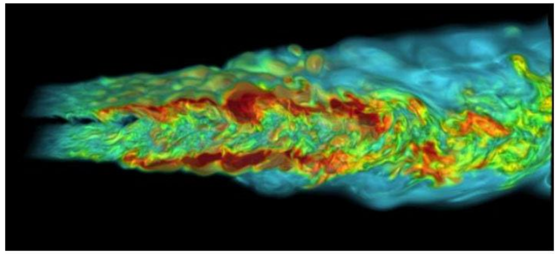
- Numerous other **DOE DT application areas** require **reduced order & surrogate modeling**, e.g.,



Hypersonic vehicles
[Tencer et al., 2020]



Additive manufacturing
[Shephard et al., 2019]



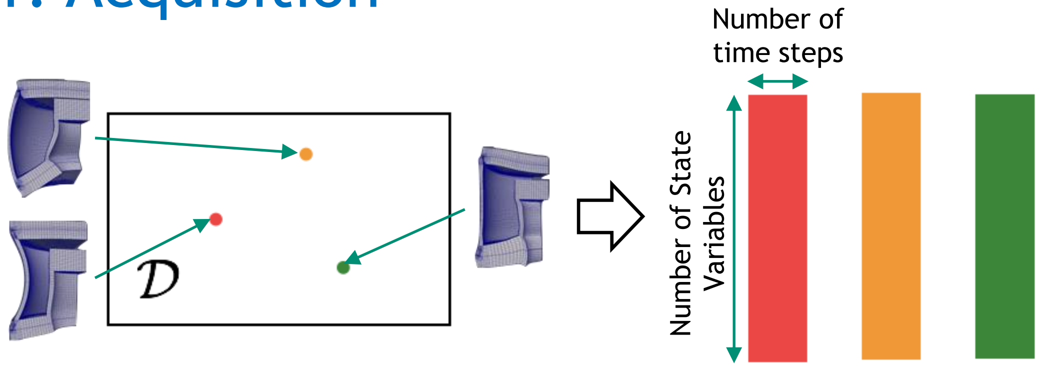
Turbulent reacting flows
[Chan et al., 2017]

...

Approaches to reduced order: Projection-Based Model Order Reduction (MOR)

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

1. Acquisition

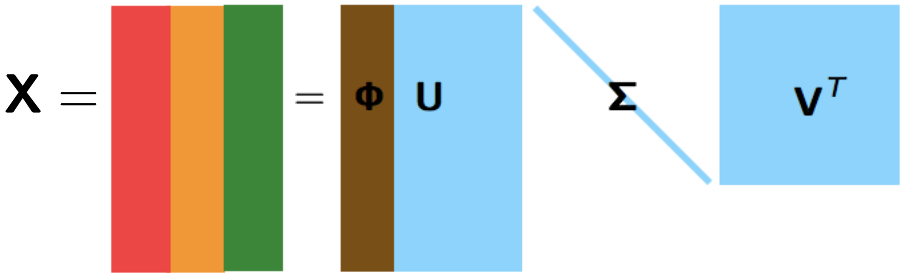


Solve ODE at different design points

Save solution data

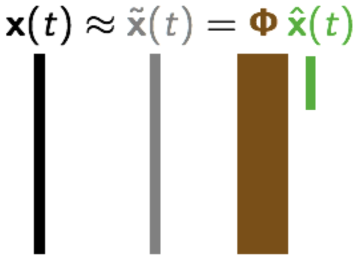
2. Learning

Unsupervised Learning of Reduced Basis (via Proper Orthogonal Decomposition, Nonlinear Manifold Learning, …):



3. Projection-Based Reduction

Reduce the number of unknowns

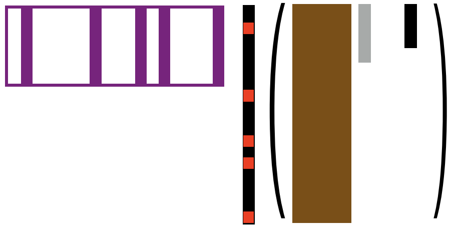


Perform Galerkin projection

$$\boldsymbol{\Phi}^T \boldsymbol{\Phi} \frac{d^2 \hat{\boldsymbol{x}}}{dt^2} = \boldsymbol{\Phi}^T \boldsymbol{f}(\boldsymbol{\Phi}\hat{\boldsymbol{x}}, t; \boldsymbol{\mu})$$

Hyper-reduce nonlinear terms

$$\boldsymbol{f}(\boldsymbol{\Phi}\hat{\boldsymbol{x}}, t; \boldsymbol{\mu}) \approx \boldsymbol{A} \quad \boldsymbol{f}_{\mathrm{int}}(\boldsymbol{\Phi}\hat{\boldsymbol{x}})$$



Hyper-reduction/sample mesh

Approaches to reduced order modeling: Non-intrusive Operator Inference (OpInf)

Non-intrusive Operator Inference (OpInf) blends the perspectives of **projection-based MOR** and **machine learning.**

1. A **physics-based model**
   Typically described by PDEs or ODEs
2. Lens of **projection** to define the form of a structure-preserving low-dimensional model

Define the **structure of the reduced model**

$$\dot{\hat{\mathbf{x}}} = \widehat{\mathbf{A}}\hat{\mathbf{x}} + \widehat{\mathbf{B}}\mathbf{u} + \widehat{\mathbf{H}}(\hat{\mathbf{x}} \otimes \hat{\mathbf{x}})$$

Non-intrusive learning by inferring reduced operators from simulation data [Peherstorfer & W., 2016]

snapshots generated from projected simulation data

low-dimensional operators define the reduced model as a dynamical system

$$\min_{\widehat{\mathbf{A}},\widehat{\mathbf{B}},\widehat{\mathbf{H}}} \left\| \widehat{\mathbf{X}}^\top \widehat{\mathbf{A}}^\top + \left(\widehat{\mathbf{X}} \odot \widehat{\mathbf{X}}\right)^\top \widehat{\mathbf{H}}^\top + \mathbf{U}^\top \widehat{\mathbf{B}}^\top - \dot{\widehat{\mathbf{X}}}^\top \right\|_F^2$$

minimum residual formulation leads to linear least squares

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**