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

Speakers: Irina Tezaur and Anthony Gruber
Sandia National Laboratories

M2dt Project All-Hands Meeting
Wednesday, October 25, 2023
### Research thrust organization

#### Part 1 of talk (RT3.1)  
Irina Tezaur

#### Part 2 of talk (RT2.2)  
Anthony Gruber

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**DRIVING SCIENTIFIC APPLICATION AREA: PREDICTIVE DIGITAL TWINS**

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<th>Testbed 2: Coupled ice shelf-ocean cavity testbed</th>
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<td>Alexander &amp; Biros</td>
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**INTEGRATIVE RESEARCH THRUSTS**

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<th>Reduced-order &amp; surrogate modeling</th>
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<td>Marzouk &amp; Leyffer</td>
<td>Ghattas &amp; Tezaur</td>
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**RESEARCH SUB-THRUSTS**

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<th>dynamic data assimilation</th>
<th>OED and causal inference</th>
<th>stochastic optimal control</th>
<th>nonlinear dimensionality reduction</th>
<th>structure preserving ROMs</th>
<th>geometric deep learning surrogates</th>
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**EDUCATION, TRAINING & OUTREACH**

| Leyffer & Willcox |

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**ROM = reduced order model**

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\[ \int M^2 dt \]
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

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Collaborations within M2dt

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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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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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This talk
Schwarz alternating method for domain decomposition (DD)

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

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

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**Basic Schwarz Algorithm**

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

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

---

**Overlapping 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

<table>
<thead>
<tr>
<th><strong>As a</strong> Preconditioner <strong>for the Linearized System</strong></th>
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<td>AS A <strong>SOLVER</strong> FOR THE COUPLED FULLY NONLINEAR PROBLEM</td>
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![Image of Drake](image_url)
• 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.

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\(^1\) Mota et al. 2017; Mota et al. 2022.  
\(^2\) [https://github.com/sandialabs/LCM](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** \(i_{\text{Dir}}\)

- **Method I** in [Gunzburger et al. 2007] is employed
  
  \[ u(t) \approx \bar{u} + \Phi \hat{u}(t), \quad v(t) \approx \bar{v} + \Phi \hat{v}(t), \quad a(t) \approx \bar{a} + \Phi \hat{a}(t) \]

  - POD modes made to satisfy homogeneous DBCs: \( \Phi(i_{\text{Dir}}, :) = 0 \)
  - BCs imposed by modifying \( \bar{u}, \bar{v}, \bar{a}: \bar{u}(i_{\text{Dir}}) \leftarrow \chi_u, \bar{v}(i_{\text{Dir}}) \leftarrow \chi_v, \bar{a}(i_{\text{Dir}}) \leftarrow \chi_a \)

**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 \( \Omega = \bigcup_i \Omega_i \)
- **Future work**: generate snapshots/bases separately in each \( \Omega_i \) [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 $\Omega_1 = [0, 0.6]$ and $\Omega_2 = [0.6, 1.0]$
- (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 solution exhibits **spurious oscillations** whereas coupled FOM-HROM solution is **smooth and oscillation-free**!
Numerical results

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

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

**Figure 1:** Solution of \( u \) component at various times

**Figure 2:** 1D cross-sections of solution \( u \) for FOM-HROM-HROM-HROM coupling

- **FOM-HROM couplings** of POD/LSPG ROMs w/ ECSW hyper-reduction, FOM in “hardest” subdomain \( \Omega_1 \)
- **Prediction** across parameters \( \mu_1 \) and \( \mu_2 \)
- **Schwarz** converges in 3 iterations per time-step

**Figure 3:** 4 overlapping subdomain DD

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

<table>
<thead>
<tr>
<th>Subdomains</th>
<th>99% SV Energy</th>
</tr>
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<tbody>
<tr>
<td>( \Omega_1 )</td>
<td>–</td>
</tr>
<tr>
<td>( \Omega_2 )</td>
<td>120</td>
</tr>
<tr>
<td>( \Omega_3 )</td>
<td>60</td>
</tr>
<tr>
<td>( \Omega_4 )</td>
<td>66</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
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</table>

Errors \( O(0.1\%) \), 2.26× speedup over all-FOM coupling
Numerical results

Model Problem 3: Riemann problem for 2D Euler equations

\[
\begin{align*}
\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{bmatrix} &+ \frac{\partial}{\partial x} \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (E + p)u \end{bmatrix} + \frac{\partial}{\partial y} \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (E + p)v \end{bmatrix} = 0 \\
p &= (\gamma - 1) \left( \rho E - \frac{1}{2} \rho (u^2 + v^2) \right)
\end{align*}
\]

- 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*

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

* https://github.com/Pressio/pressio-demoapps
Model problem: time-dependent advection-diffusion problem on $\Omega = \Omega_1 \cup \Omega_2$ with $\Omega_1 \cap \Omega_2 = \emptyset$

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

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

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

- **Continuity of states**: $c_1(x,t) - c_2(x,t) = 0$
- **Continuity of total flux**: $F_1(x,t) \cdot n_\Gamma = F_1(x,t) \cdot n_\Gamma$

$\Rightarrow$ Imposed weakly using Lagrange multiplier (LM) $\lambda$

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

\[
\begin{pmatrix}
M_1 & 0 & G_1^T \\
0 & M_2 & -G_2^T \\
G_1 & -G_2 & 0
\end{pmatrix}
\begin{pmatrix}
\dot{c}_1 \\
\dot{c}_2 \\
\lambda
\end{pmatrix} =
\begin{pmatrix}
f_1 - K_1 c_1 \\
f_2 - K_2 c_2 \\
0
\end{pmatrix}
\]  

(2)

- \( M_i \): mass matrices
- \( K_i := D_i + A_i \): stiffness matrices, where \( D_i \) and \( A_i \) are matrices for diffusive and advective terms, respectively
- \( G_i \): constraints matrices enforcing constraints in weak sense

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

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

(3)

Equations decouple if using explicit or IMEX time-integration!

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

- Pick explicit or IMEX time-integration scheme for \( \Omega_1 \) and \( \Omega_2 \)
- Approximate LM space as trace of FE space on \( \Omega_1 \) or \( \Omega_2 \)
- Compute matrices \( M_i, K_i, G_i \) and vectors \( f_i \)
- For each timestep \( t^n \):
  - Solve Schur complement system (4) for the LM \( \lambda^n \)
  - Update the state variables \( c_i^n \) by advancing (3) in time

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

(4)

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

Time integration schemes and time-steps in \( \Omega_1 \) and \( \Omega_2 \) can be different!
“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)

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

$$c_{i,0}(t) \approx \tilde{c}_{i,0}(t) := \bar{c}_{i,0} + \Phi_{i,0}\hat{c}_{i,0}(t), \quad c_{i,\Gamma}(t) \approx \tilde{c}_{i,\Gamma}(t) := \bar{c}_{i,\Gamma} + \Phi_{i,\Gamma}\hat{c}_{i,\Gamma}(t)$$

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

$$\begin{pmatrix}
\bar{G}_1 \\
\bar{G}_2
\end{pmatrix}
\begin{pmatrix}
\hat{c}_{1,\Gamma} \\
\hat{c}_{2,\Gamma}
\end{pmatrix}
= 
\begin{pmatrix}
\bar{G}_1 \\
\bar{G}_2
\end{pmatrix}
\begin{pmatrix}
\hat{s}_{1,\Gamma} \\
\hat{s}_{2,\Gamma}
\end{pmatrix}$$

Define $\tilde{M}_{i,jk} := \Phi_{i,j}^T M_{i,jk} \Phi_{i,k}, \quad \tilde{G}_i := \Phi_{i,LM} G_{i,\Gamma}, \quad \tilde{P}_i := \tilde{M}_{i,\Gamma} - \tilde{M}_{i,\Gamma 0} \tilde{M}_{i,0}^{-1} \tilde{M}_{i,\Gamma 0}$ for $\{j, k\} \in \{0, \Gamma\}$ and solve:

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

Advance the following systems forward in time:

$$\begin{pmatrix}
\tilde{M}_{i,\Gamma} & \tilde{M}_{i,0} \\
\tilde{M}_{i,\Gamma 0} & \tilde{M}_{i,\Gamma}
\end{pmatrix}
\begin{pmatrix}
\hat{c}_{i,\Gamma} \\
\hat{c}_{i,0}
\end{pmatrix}
= 
\begin{pmatrix}
\hat{s}_{i,\Gamma} \\
\hat{s}_{i,0}
\end{pmatrix}$$

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/ \( \Gamma \) 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

• 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!

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

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].
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**.

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<th>Theme C. Qualitative properties</th>
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<td>• B.2. de Rham complex</td>
<td>• C.2. Monotonicity, max principle</td>
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<td>• A.3. Energy/entropy stability</td>
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<td>• C.3. Total Variation Diminishing (TVD)</td>
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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
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- **Method (v).** Structure-preserving multi-physics/multi-component ROMs
- **Method (vi).** Optimization-based methods

**Deep dive in this talk**

(for discussion of other themes/methods, see next talk by Pavel)
Hamiltonian Operator Inference (H-OpInf)

- Hamiltonian systems $\dot{x} = \{x, H(x)\} = L(x)\nabla H(x)$ are archetypically **conservative**.
  - Governed by scalar potential $H$ and skew-symmetric matrix operator $L$.

- $L$ defines (potentially degenerate) **Poisson bracket** $\{F, G\} = \nabla F \cdot L \nabla G$.
  - Satisfies Jacobi identity:
    $$\{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\} = 0.$$

- Guarantees that flow is perpendicular to $\nabla H$ and **energy is conserved**.
  $$\dot{H}(x) = \dot{x} \cdot \nabla H = L \nabla H \cdot \nabla H = -L \nabla H \cdot \nabla H = 0.$$

**Examples:** Incompressible Euler, Maxwell, shallow water, Monge-Ampere, sine-Gordon, nonlinear Schrodinger, ...
Hamiltonian Operator Inference (H-OpInf)

- Naïve Galerkin ROM: \( \dot{\tilde{x}} = U^T L \nabla H(U\tilde{x}) \)
  - Data matrix \( X \approx U\Sigma V^T \)
  - POD approximation \( \tilde{x} = U\tilde{x} \)

- Not Hamiltonian! \((L^T U)^T = U^T L \neq -L^T U\)
  - (energy not conserved)

- Not symplectic!
  - (no Jacobi identity)

- Conversely, Hamiltonian ROM satisfies both*
  - Solve overdetermined system \( U^T L = \tilde{L} U^T \).
  - Evolution equation:
    \[
    \dot{\tilde{x}} = \tilde{L} \nabla H(\tilde{x}) = U^T L(U\tilde{x}) UU^T \nabla H(U\tilde{x})
    \]
  - Closed orbits are preserved.

* When \( L \) is \( x \)-independent
Hamiltonian Operator Inference (H-OpInf)

- Non-intrusive case: operator inference
  - Solve a minimization for RO operators $\hat{L}, \hat{A}$:
    \[
    \arg\min_{\hat{A} \text{ or } \hat{L}} |\hat{X}_t - \hat{L}\hat{A}\hat{X}|^2, \quad \hat{L}^T = -\hat{L}, \quad \hat{A}^T = \hat{A}.
    \]

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

Model Problem 1: 1D Korteweg-De Vries (KdV) equation
Model Problem 2: 3D transient solid mechanics

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

\[
\rho \ddot{\mathbf{q}} = \nabla \cdot \mathbf{\sigma} = \nabla \cdot (\lambda \text{tr}(\varepsilon) \mathbf{I} + 2\mu \varepsilon)
\]
\[
\varepsilon = \frac{1}{2} \left( \nabla \mathbf{q} + (\nabla \mathbf{q})^T \right)
\]

\[
H(q, \dot{q}) = \frac{1}{2} \int_{\Omega} \left( \rho |\dot{q}|^2 + \lambda \text{tr}(\varepsilon)^2 + 2\mu |\varepsilon|^2 \right) dV
\]

- After discretization, system looks like:

\[
\begin{pmatrix}
\hat{\mathbf{q}} \\
\hat{\mathbf{p}}
\end{pmatrix} =
\begin{pmatrix}
\mathbf{0} & \mathbf{I} \\
-\mathbf{I} & \mathbf{0}
\end{pmatrix}
\begin{pmatrix}
\hat{\mathbf{K}} \\
\mathbf{0}
\end{pmatrix}
\begin{pmatrix}
\mathbf{0} \\
\mathbf{M}^{-1}
\end{pmatrix}
\begin{pmatrix}
\hat{\mathbf{q}} \\
\hat{\mathbf{p}}
\end{pmatrix},
\]

\[
\mathbf{M}^{-1} = \mathbf{U}^T \mathbf{M}^{-1} \mathbf{U}, \quad \hat{\mathbf{K}} = \mathbf{U}^T \mathbf{K} \mathbf{U}.
\]

\footnote{Albany-LCM HPC code: \url{https://github.com/sandialabs/LCM}. Data/matrices: \url{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)
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, $JU$ is a valid test basis, implying:
    $\hat{J}^T \hat{x} = U^T J^T U \hat{x} = U^T J^T J \nabla H(U \hat{x}) = \nabla \hat{H}(\hat{x})$

- Provably Hamiltonian: energy/symplecticity are conserved.
- Removes the need for an extra column-space projection $UU^T$.
  - Improved accuracy without harming generalizability.

- Can show that error (in reproductive case) is balanced between:
  - POD projection error $| (I - UU^T)x |$
  - Max eigenvalue of $\hat{J}^T \hat{J} - I$
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:

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): \( \frac{dx}{dt} = f(x, t; \mu) \)

1. Acquisition

Solve ODE at different design points

Number of time steps

Number of State Variables

Save solution data

2. Learning

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

\[ X = \Phi U \Sigma V^T \]

3. Projection-Based Reduction

Reduce the number of unknowns

\[ x(t) \approx \tilde{x}(t) = \Phi \tilde{x}(t) \]

Perform Galerkin projection

\[ \Phi^T \Phi \frac{d^2 \tilde{x}}{dt^2} = \Phi^T f(\Phi \tilde{x}, t; \mu) \]

Hyper-reduce nonlinear terms

\[ f(\Phi \tilde{x}, t; \mu) \approx A f_{int}(\Phi \tilde{x}) \]

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
\[
\hat{x} = \hat{A}\hat{x} + \hat{B}u + \hat{H}(\hat{x} \otimes \hat{x})
\]

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