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

M2dt: Multifaceted Mathematics for Predictive Digital Twins
Structure-Preserving Model Order Reduction (SP-MOR)

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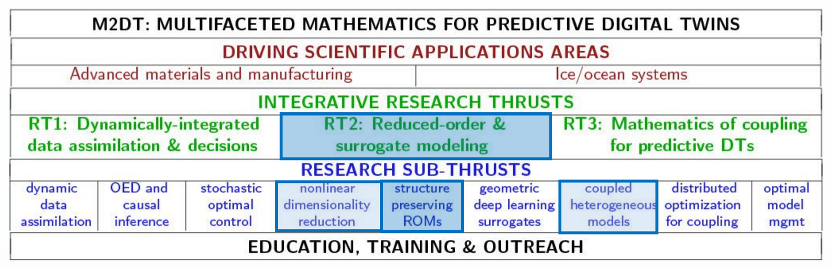
Motivation and Role in M2dt

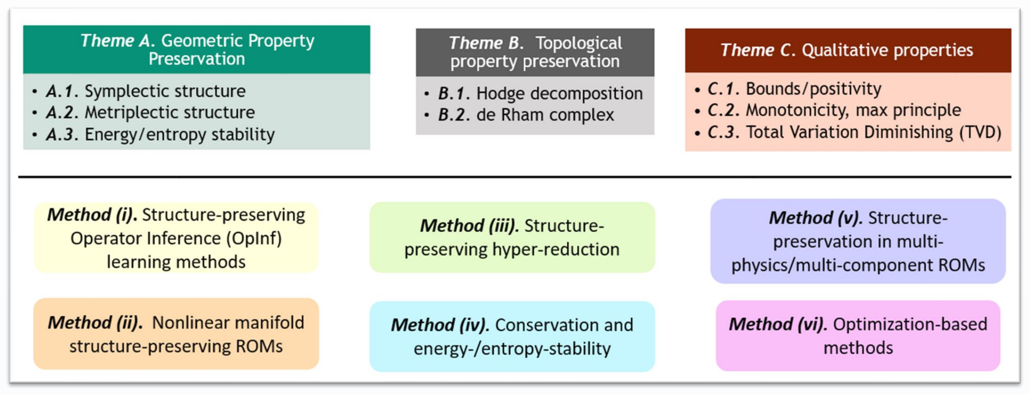
- In order to be **reliable predictive tools** within **digital twin** workflows, reduced order models (ROMs) & surrogates must preserve **key properties** of underlying PDEs

ROMs in general do **NOT** automatically inherit these properties!

Objective (under RT2.2 of M2dt): develop **new property-preserving MOR methods** to mirror the **properties** of established **compatible discretization methods** for FOMs



3 research themes are pursued using the following **6 methods** and their combination:



Geometric Property Preservation: Energy-Stable MOR

Energy-stable dynamical system: $\frac{d\boldsymbol{x}}{dt} + \boldsymbol{f}(\boldsymbol{x},\boldsymbol{\mu}) = \boldsymbol{0}, \quad \frac{1}{2}\frac{d\boldsymbol{x}^2}{dt} \leq 0$

- "Positive-definite" velocity, $\boldsymbol{x}^T\boldsymbol{f}(\boldsymbol{x},\boldsymbol{\mu}) \geq 0$
- Building block of many physical systems
  - Fluid flows, solid dynamics, climate

Traditional MOR approaches are **NOT** automatically **energy-stable** [1].

Positive-definite operator inference (OpInf)

Non-intrusive method for learning "positive-definite" operators

- Extension of classical non-intrusive OpInf [2]
- Learns "positive-definite" operators to build reduced-models endowed with energy stability
- Neural network formulation naturally handles parametric variability and non-polynomial non-linearities
- Relies only on solution snapshots

Technical details: learn a ROM of the form $\frac{d\hat{\boldsymbol{x}}}{dt} = \hat{\mathbf{A}}(\hat{\boldsymbol{x}},\boldsymbol{\mu})\,\hat{\boldsymbol{x}}$

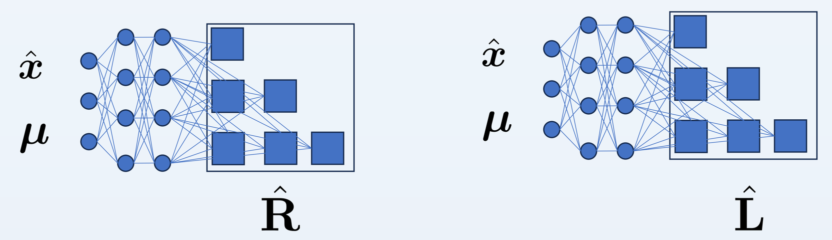
Key idea: construct $-\hat{\mathbf{A}}$ to be positive definite by parametrizing it with a skew-symmetric and a symmetric positive definite (SPD) matrix

$$\hat{\mathbf{A}}(\hat{\boldsymbol{x}},\boldsymbol{\mu}) = \left[\hat{\mathbf{R}}(\hat{\boldsymbol{x}},\boldsymbol{\mu}) - \hat{\mathbf{R}}^T(\hat{\boldsymbol{x}},\boldsymbol{\mu})\right] - \hat{\mathbf{L}}(\hat{\boldsymbol{x}},\boldsymbol{\mu})\,\hat{\mathbf{L}}^T(\hat{\boldsymbol{x}},\boldsymbol{\mu})$$

Skew-symmetric   *SPD*

- Resulting ROMs are provably stable since $\hat{\boldsymbol{x}}^T\hat{\mathbf{A}}\hat{\boldsymbol{x}} \leq 0$

Learning approach: parameterize the operators with neural networks [3-4]



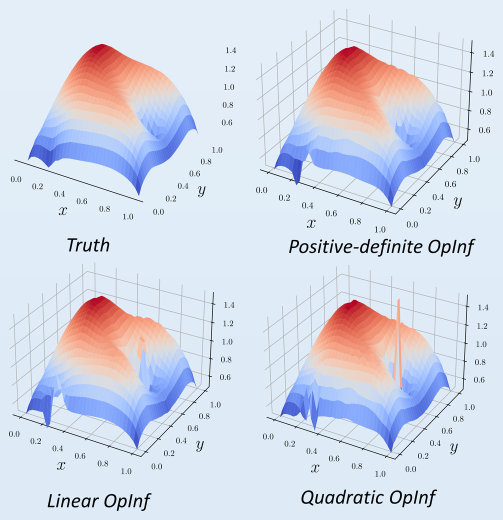
- Gradients are easily computed via back-propagation in modern ML codes
- State-of-the-art training approaches handle over-parameterization
- Parametrized dynamical systems are handled by adding parameters to the network inputs

Example: Shallow ice approximation (future state prediction)

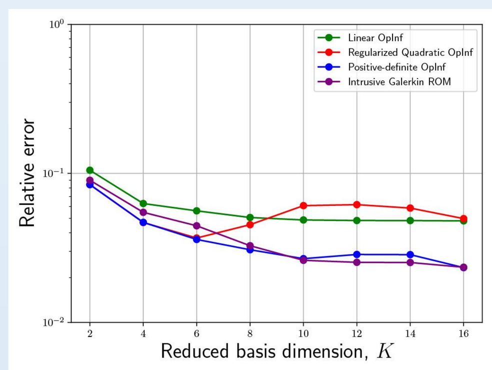
$$\frac{\partial H}{\partial t} + \nabla\cdot\left[-\Gamma H^{n+2}|\nabla s|^{n-1}\nabla s\right] = m \quad \xrightarrow{\text{Spatial discretization}} \quad \frac{d\boldsymbol{x}}{dt} + \boldsymbol{f}(\boldsymbol{x},\boldsymbol{\mu}) = \mathbf{g}$$

"Positive-definite" operator

- Non-polynomial non-linearities
- Compare to classic OpInf methods (linear and quadratic)



- Linear OpInf ROMs not expressive enough
- Quadratic OpInf ROMs go unstable w/o significant regularization
- Linear and Quadratic OpInf ROMs have noticeable artifacts



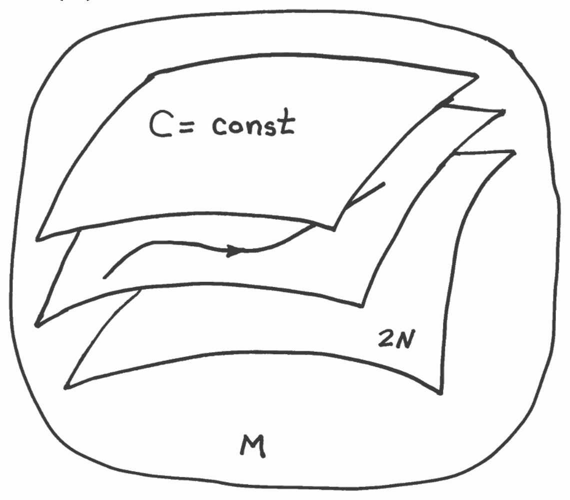
Positive-definite OpInf ROMs are **stable** and **2-3× more accurate** than other ROMs **for all basis dimensions**!

Geometric Property Preservation: Hamiltonian SP-MOR

Hamiltonian system: $\dot{\boldsymbol{x}} = \{\boldsymbol{x}, H(\boldsymbol{x})\} = \boldsymbol{L}(\mathbf{x})\nabla\mathrm{H}(\boldsymbol{x})$

- Scalar potential H
- Skew-symmetric Poisson operator $\boldsymbol{L}^T = -\boldsymbol{L}$

Drawing courtesy of P. J. Morrison.



Guarantees that flow is perpendicular to ∇H and energy is conserved

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

Casimirs C satisfying $\boldsymbol{L}\nabla C = \boldsymbol{0}$ also conserved

- Mass, momentum, etc.

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

Question: *can we design a ROM which respects this structure?*

Canonical and Noncanonical Hamiltonian Operator Inference

Non-intrusive method for learning Hamiltonian ROMs

- Stable by construction
- Converge to intrusive ROMs in the limit of infinite data

For snapshots $\boldsymbol{X} \approx \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$ and $\widetilde{\boldsymbol{M}} = \boldsymbol{U}^T\boldsymbol{M}$, solve:

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

Learning Poisson structure $\hat{\boldsymbol{L}}$ is *noncanonical* inference

- Produces conservative ROM with known quantity H as Hamiltonian

Learning $\boldsymbol{A} = \nabla H$ is *canonical* inference

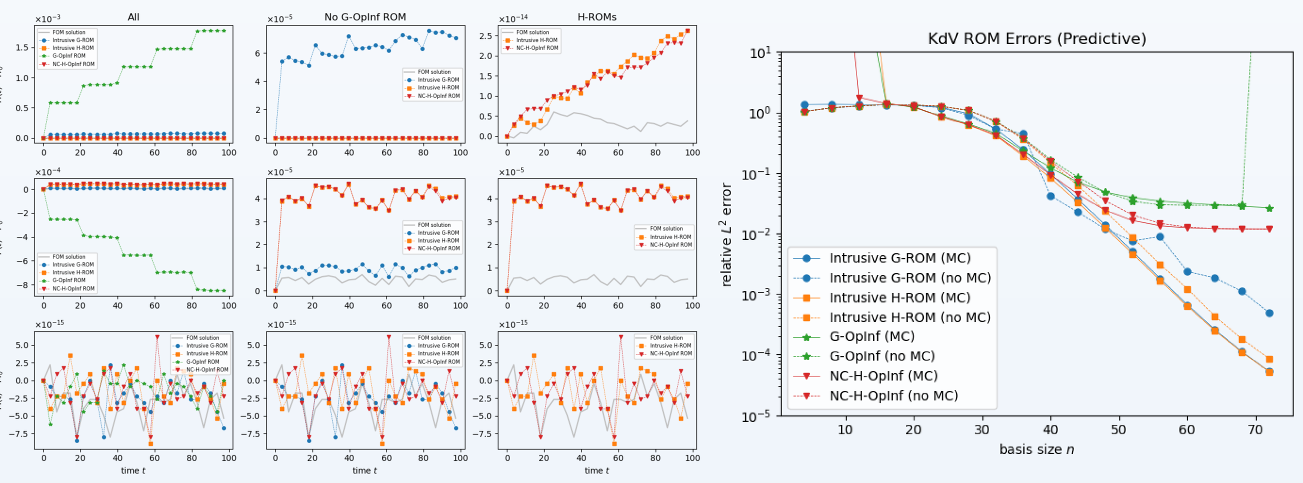
- Produces conservative ROM with known Poisson structure $\boldsymbol{L}$

Unlike **other Hamiltonian SP-MOR methods**, e.g., [5], our approach [6] can handle **canonical** and **non-canonical Hamiltonian systems.**

Example: Korteweg-de Vries (KdV) equation, $x_t = \alpha x x_s + \rho x_s + \gamma x_{sss}$

$$x_t = L\nabla H(x), \quad L = \partial_s, \quad H = \int_0^L \left(\frac{\alpha}{6}x^3 + \frac{\rho}{2}x^2 - \frac{\gamma}{2}x_s^2\right)dx.$$

- We consider the non-canonical form of the KdV equation, which is bi-Hamiltonian



Predicts correct dynamics well outside of training region. Conserves H, C by construction.

Petrov-Galerkin Hamiltonian OpInf for Canonical Systems

State-of-the-art Hamiltonian ROMs require *more* than just Galerkin projection

- Usually Galerkin projection + (formal) least-squares solve
- Additional projection can destroy accuracy. **Can we fix this?**

Canonical systems imply $\boldsymbol{L} = \boldsymbol{J}$ is full rank, so use $\boldsymbol{J}\boldsymbol{U}$ as a test basis! If $\widetilde{\boldsymbol{x}} = \boldsymbol{U}\hat{\boldsymbol{x}}$,

$$\dot{\widetilde{\boldsymbol{x}}} = \boldsymbol{J}\nabla\widehat{H}(\widetilde{\boldsymbol{x}}) \text{ implies } \hat{\boldsymbol{J}}^T\dot{\hat{\boldsymbol{x}}} = \boldsymbol{U}^T\boldsymbol{J}^T\boldsymbol{U}\hat{\boldsymbol{x}} = \boldsymbol{U}^T\boldsymbol{J}^T\boldsymbol{J}\nabla H(\boldsymbol{U}\hat{\boldsymbol{x}}) = \nabla\widehat{H}(\hat{\boldsymbol{x}}).$$

Provably Hamiltonian: energy is conserved.

- Removes the need for an extra column-space projection $\boldsymbol{U}\boldsymbol{U}^T$
- Amenable to non-intrusive OpInf as before. Problem is convex with a global minimum

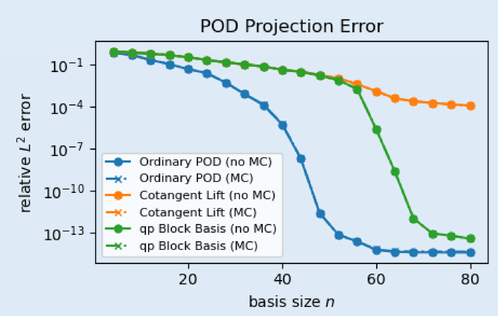
$$\underset{\hat{\boldsymbol{A}}\in\mathbb{R}^{n\times n}}{\arg\min} \left|\hat{\boldsymbol{J}}^{\intercal}\hat{\boldsymbol{X}}_t - \hat{\boldsymbol{A}}\hat{\boldsymbol{X}} - \hat{\nabla}f(\boldsymbol{X})\right|^2, \quad \text{s.t.} \quad \hat{\boldsymbol{A}}^{\intercal} = \hat{\boldsymbol{A}}$$
$$\nabla H(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} + \nabla f(\boldsymbol{x})$$

Error is bounded in reproductive case

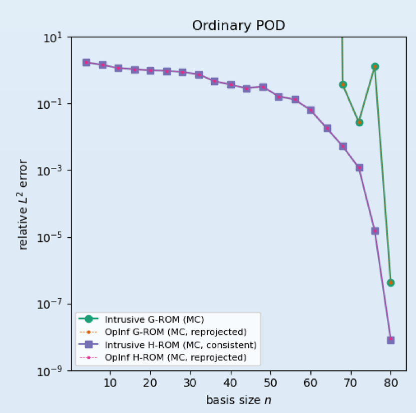
- First term is projection error similar to Galerkin ROM
- Second term is "deviation from symplecticity" error

$$\|\boldsymbol{x} - (\boldsymbol{x}_0 + \boldsymbol{U}\hat{\boldsymbol{x}})\| \leq c\sqrt{\sum_{i>n}\lambda_i} + \bar{c}\,\|\nabla H(\boldsymbol{x})\|\sqrt{\sigma_{\max}\left(\hat{\boldsymbol{J}}^{-\intercal}\hat{\boldsymbol{J}}^{-1} - \boldsymbol{I}\right)}$$

Example: 3D linear elasticity equations



- Galerkin projection only is not enough
- Petrov-Galerkin ROM errors decay smoothly with increasing basis size



Ongoing and Future Work

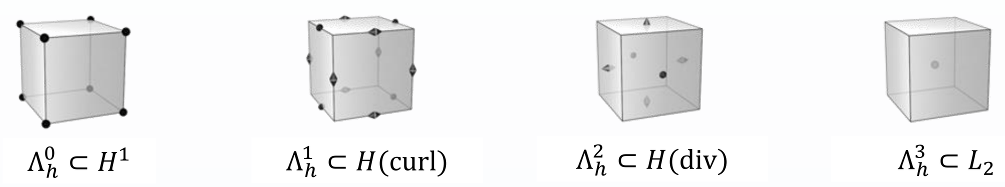
Topological Property Preservation

Finite Element Exterior Calculus (= Single deRham Complex)

$$\Lambda^0 \underset{\delta=-\nabla\cdot}{\overset{d=\nabla}{\rightleftarrows}} \Lambda^1 \underset{\delta=\nabla\times}{\overset{d=\nabla\times}{\rightleftarrows}} \Lambda^2 \underset{\delta=-\nabla}{\overset{d=\nabla\cdot}{\rightleftarrows}} \Lambda^3$$

Integration by parts: $\delta = (-1)^{nk+n+1}\star d\,\star \to \langle\alpha, d\beta\rangle + \langle\delta\alpha,\beta\rangle = \langle\alpha,\beta\rangle_{\partial\Omega}$

Exact sequence: $d\,d = 0.$ **Hodge decomposition:** $\alpha = d\psi + \delta\phi + h.$



The existence of a **discrete Hodge deRham (HdR) complex** is **essential** for constructing **topological structure-preserving** FOM discretizations [7-8].

Question: *can we design ROMs that preserve a discrete HdR complex?*

HdR FOM (General Theory)

$$\begin{array}{ccc} \Lambda^k & \xrightarrow{d} & \Lambda^{k+1} \\ \downarrow \pi^k & & \downarrow \pi^{k+1} \\ \Lambda_h^k & \xrightarrow{d} & \Lambda_h^{k+1} \end{array}$$

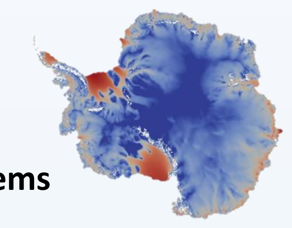
- *Bounded commuting projection operator:* $\pi^k: \Lambda^k \to \Lambda_h^k$ *satisfies* $d\pi^k = \pi^{k+1}d$
- Fundamental object is the inner product $\langle\cdot,\cdot\rangle$, which induces the Hodge star $\star$ and the codifferential $\delta = (-1)^{nk+n+1}\star d\,\star$
- Main examples are **compatible Galerkin methods** [7-8]: finite element exterior calculus (FEEC), mimetic Galerkin differences (MGD), compatible isogeometric methods; mimetic finite differences (MFD)

HdR ROM Idea

$$\begin{array}{ccc} \Lambda_h^k & \xrightarrow{d} & \Lambda_h^{k+1} \\ \downarrow \hat{\pi}^k & & \downarrow \hat{\pi}^{k+1} \\ \hat{\Lambda}_h^k & \xrightarrow{d} & \hat{\Lambda}_h^{k+1} \end{array}$$

- **Idea:** define ROM projection operators $\hat{\pi}^k: \Lambda_h^k \to \widehat{\Lambda}_h^k$ and ROM spaces $\widehat{\Lambda}^k \subset \Lambda^k$ such that this diagram commutes: $d\hat{\pi}^k = \hat{\pi}^{k+1}d$
- This will give a ROM with the same properties as the FOM, e.g., annihilation, integration by parts, Hodge decomposition/cohomology
- Often we are given $\hat{\pi}^k$ and $\widehat{\Lambda}^k$, e.g., from Proper Orthogonal Decomposition/Galerkin projection, so we just need to find commuting $\hat{\pi}^{k+1}$ and corresponding Λ^{k+1}

Other Planned Research Directions



- **Entropy-stable hyper-reduction** for MOR of hyperbolic systems
- **Quadratic Hamiltonian** SP-ROMs
- Development of efficient SP-ROMs for **metriplectic systems** and **systems with dissipation**
- **Optimization-based property** (e.g., bounds, positivity, monotonicity, maximum principle, total variation diminishing, etc.) preservation for ROMs
- Extensions of SP-MOR methods to **multi-physics problems**
- Applications of methods to **M2dt exemplar problems** (ice sheet-ocean interaction, self-assembling block copolymers) and within **OED workflows**

Potential Impact

- This work is **pioneering new property-preserving nonlinear dimension reduction methods** that will support **new classes of compatible ROMs** mirroring the properties of established compatible discretization methods for FOMs
- The three different types of structures are relevant to **numerous problems** in science and engineering, including the M2dt exemplar problems
  - ***Geometric structure***: Hamiltonian, metriplectic, energy-/entropy-stability, etc.
  - ***Topological structure***: HdR complex, cohomology, etc.
  - ***Qualitative properties***: maximum principle, monotonicity, positivity, etc.

Structure preservation is a **pre-requisite** for generating **stable** and **accurate reduced order models** for **predictive digital twins**.

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SAND2023-14990O