M2dt: Multifaceted Mathematics for Predictive Digital Twins

Data-Driven Coupling and Structure Preservation for Predictive Digital Twins

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Motivation for Coupling

Multi-scale and **multi-physics** problems are ubiquitous and require **rigorous coupling frameworks**

Most existing coupling frameworks are based on traditional discretization methods, i.e., high-fidelity models (HFMs)

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

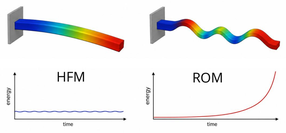
M2DT : MULTIFACETED MATHEMATICS FOR PREDICTIVE DIGITAL TWINS								
DRIVING SCIENTIFIC APPLICATION AREAS								
Advanced materials & manufacturing				Ice/ocean systems				
INTEGRATIVE RESEARCH THRUSTS								
RT1: Dynamically-integrated data assimilation & decisions			RT2: Reduced-order & surrogate modeling			RT3: Mathematics of heterogeneous predictive DTs		
RESEARCH SUB-THRUSTS								
RT1.1 dynamic data assimilation	RT1.2 OED & causal inference	RT1.3 stochastic optimal control	RT2.1 nonlinear dimensionality reduction	RT2.2 structure preserving ROMs	RT2.3 geometric deep learning surrogates	RT3.1 coupled heterogeneous models	RT3.2 decomposition for heterogen. computing	RT3.3 optimal model management
EDUCATION, TRAINING & WORKFORCE DEVELOPMENT								

Motivation for Structure Preservation

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

ROMs in general do NOT automatically inherit these properties!

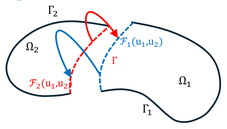
Objective (RT2.2 of M2dt): develop **new structure preserving (SP) model reduction methods** to mirror **properties** of established **compatible discretizations** for HFMs



Interface Flux Surrogates for Coupling

Subdomains are decoupled by using interface flux

$$\dot{u}_i - \nabla \cdot F_i(u_i) = f_i \ \text{ in } \Omega_i$$
$$u_i = \zeta_i \text{ on } \Gamma_i$$
$$\boldsymbol{n} \cdot F_i(u_i) = \lambda \text{ on } \Gamma$$



- Subdomain equations are mixed boundary value problems (BVPs)
- The Dirichlet data ζ_i is given on the Dirichlet boundaries
- The Neumann data λ is the **unknown interface flux that must be estimated**

Approximation of Schur Complement-based Coupling Operators

Generates **approximation** of **Lagrange multiplier-based Schur complement** from Lagrange multiplier-based coupling method-inspired input-output data pairs [8]

(SD)
$$\begin{cases} M_1\dot{\boldsymbol{u}}_1 + G_1^T\boldsymbol{\lambda} = \boldsymbol{f}_1 - K_1\boldsymbol{u}_1 & \text{on } \Omega_1 \\ M_2\dot{\boldsymbol{u}}_2 - G_2^T\boldsymbol{\lambda} = \boldsymbol{f}_2 - K_2\boldsymbol{u}_2 & \text{on } \Omega_2 \\ G_1\boldsymbol{u}_1 - G_2\boldsymbol{u}_2 = \boldsymbol{0} & \text{on } \gamma, \end{cases} \Rightarrow \begin{cases} M_1\dot{\boldsymbol{u}}_1 + G_1^T\boldsymbol{\lambda} = \boldsymbol{f}_1 - K_1\boldsymbol{u}_1 & \text{on } \Omega_1 \\ M_2\dot{\boldsymbol{u}}_2 - G_2^T\boldsymbol{\lambda} = \boldsymbol{f}_2 - K_2\boldsymbol{u}_2 & \text{on } \Omega_2 \\ G_1\dot{\boldsymbol{u}}_1 - G_2\dot{\boldsymbol{u}}_2 = \boldsymbol{0} & \text{on } \gamma, \end{cases}$$

$$S_{SD}\boldsymbol{\lambda} = G_1M_1^{-1}(\boldsymbol{f}_1 - K_1\boldsymbol{u}_1) - G_2M_2^{-1}(\boldsymbol{f}_2 - K_2\boldsymbol{u}_2)$$

(FD) with BDF2
$$\begin{cases} W_1\boldsymbol{u}_1^{n+1} = \Delta t w_0 \boldsymbol{f}_1^{n+1} - \Delta t w_0 G_1^T\boldsymbol{\lambda}^{n+1} + \sum_{j=1}^{s} w_j M_1 \boldsymbol{u}_1^{n+1-j} \\ W_2\boldsymbol{u}_2^{n+1} = \Delta t w_0 \boldsymbol{f}_2^{n+1} + \Delta t w_0 G_2^T\boldsymbol{\lambda}^{n+1} + \sum_{j=1}^{s} w_j M_2 \boldsymbol{u}_2^{n+1-j} \\ G_1\boldsymbol{u}_1^{n+1} - G_2\boldsymbol{u}_2^{n+1} = \boldsymbol{0} \end{cases}$$

$$S_{FD}\boldsymbol{\lambda}^{n+1} = G_1W_1^{-1}\left(\Delta t w_0 \boldsymbol{f}_1^{n+1} + \sum_{j=1}^{s} w_j M_1 \boldsymbol{u}_1^{n+1-j}\right) - G_2W_2^{-1}\left(\Delta t w_0 \boldsymbol{f}_2^{n+1} + \sum_{j=1}^{s} w_j M_2 \boldsymbol{u}_2^{n+1-j}\right)$$

Offline stage:

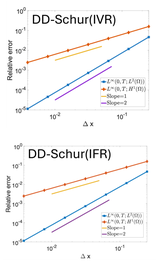
- Use method by Carey* to generate high order flux approximations from coupled solution data
- Solve subdomain problems with homogeneous Neumann boundary conditions (do-nothing)
- Regress $\tilde{S}_{SD}$ or $\tilde{S}_{FD}$ using linear least-squares and input & output data

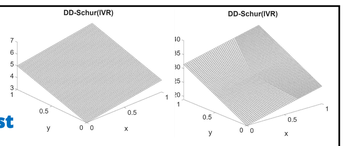
$\lambda = \tilde{S}^{-1} \cdot$ *input data*

Online stage:

- Solve subdomain problems with homogeneous Neumann boundary conditions (do-nothing)
- Solve approximate $\tilde{S}_{SD}$ or $\tilde{S}_{FD}$ approximates against input data, providing an estimate for λ

* G. Carey, S.S. Chow, M.K. Seager, Approximate boundary-flux calculations, ***Comput. Meth. Appl. Mech. Engng***, 50, 167-195



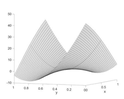


Linear Patch Test Results

Coupling method	Straight interface L^2 error	Straight interface H^1 error	Chevron interface L^2 error	Chevron interface H^1 error
DD-Schur(IFR)	7.41e-15	1.02e-12	1.78e-14	2.40e-12
Traditional IFR	6.48e-15	8.54e-13	7.61e-15	6.34e-13
DD-Schur(IVR)	1.60e-14	2.11e-12	3.27e-14	4.24e-12
Traditional IVR	6.94e-15	9.34e-13	1.75e-14	2.57e-12

Heterogeneous Manufactured Solution (Verification)

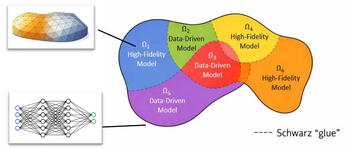
$$u_1 = \frac{\kappa_2}{\kappa_1}\beta\sin(x+y+t) + \frac{a_1\beta}{\kappa_1}\cos(x+y+t)$$
$$u_2 = \beta\sin(x+y+t) + \frac{a_1\beta}{\kappa_1}\cos(x+y+t)$$



Schwarz Alternating Method (SAM) for Coupling

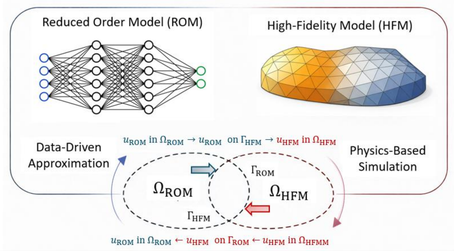
Basic Schwarz alternating method (SAM) scheme for coupling [1-2]

- Decompose $\Omega = \Omega_1 \cup \Omega_2$
- Solve PDE in Ω_2 w/ boundary conditions (BCs) on Γ_2 from just-obtained Ω_1 solution.
- Solve PDE in Ω_1 w/ BCs on Γ_1 from just-obtained Ω_2 solution.
- Iterate until convergence



SAM enables the **seamless plug-and-play coupling** of disparate **meshes**, **solvers**, **time-steppers** and **models** (ROM+HFM) [1-6].

SAM-based ROM-HFM Coupling Workflow



Overlapping Schwarz Alternating Method (O-SAM)

$$\begin{cases} N\left(\boldsymbol{u}_1^{(n+1)}\right) = f, \text{ in } \Omega_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{g}, \text{ on } \partial\Omega_1 \backslash \Gamma_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{u}_2^{(n)} \quad \text{on } \Gamma_1 \end{cases} \qquad \begin{cases} N\left(\boldsymbol{u}_2^{(n+1)}\right) = f, \text{ in } \Omega_2 \\ \boldsymbol{u}_2^{(n+1)} = \boldsymbol{g}, \text{ on } \partial\Omega_2 \backslash \Gamma_2 \\ \boldsymbol{u}_2^{(n+1)} = \boldsymbol{u}_1^{(n+1)} \quad \text{on } \Gamma_2 \end{cases}$$

O-SAM is convergent with **Dirichlet-Dirichlet** boundary conditions (BCs)

Non-Overlapping Schwarz Alternating Method (NO-SAM)

$$\begin{cases} N\left(\boldsymbol{u}_1^{(n+1)}\right) = f, \quad \text{in } \Omega_1 \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{g}, \quad \text{on } \partial\Omega_1 \backslash \Gamma \\ \boldsymbol{u}_1^{(n+1)} = \boldsymbol{\lambda}_{n+1}, \quad \text{on } \Gamma \end{cases} \qquad \begin{cases} N\left(\boldsymbol{u}_2^{(n+1)}\right) = f, \quad \text{in } \Omega_2 \\ \boldsymbol{u}_2^{(n+1)} = \boldsymbol{g}, \quad \text{on } \partial\Omega_2 \backslash \Gamma \\ \nabla\boldsymbol{u}_2^{(n+1)} \cdot \boldsymbol{n} = \nabla\boldsymbol{u}_1^{(n+1)} \cdot \boldsymbol{n}, \text{ on } \Gamma \end{cases}$$

$$\boldsymbol{\lambda}_{n+1} = \theta\boldsymbol{u}_2^{(n)} + (1-\theta)\boldsymbol{\lambda}_n, \text{ on } \Gamma, \text{for } n \geq 1$$

NO-SAM requires **relaxed alternating Dirichlet-Neumann** or **Robin-Robin** BCs

Non-Intrusive ROMs

- Define **ROM model form** in each subdomain:
$$\dot{\hat{q}} + \hat{F}(\hat{q}) = \boldsymbol{0}$$
- **ROM model forms:**
  - Polynomial Operator Inference (POpInf) [4-5]:
$$\hat{F}(\hat{q}) = \hat{A}\hat{q} + \hat{H}(\hat{q}\otimes\hat{q}) + \hat{G}(\hat{q}\otimes\hat{q}\otimes\hat{q})$$
  - Neural Network Operator Interence (NNOpInf) [9]:
$$\hat{F}(\hat{q}) = K(\hat{q}; w)\hat{q}$$
  → enables **structure preservation (SP)**
  - Kernel Manifold ROM (KROM) [7]:
$$\hat{F}(\hat{q}) = \Omega^{\top}k(\hat{q})$$
- **Infer** operators from HFM data by solving regularized **optimization problem**

SAM-based Coupling Algorithm for Non-Intrusive ROMs

Offline stage:

- Create **DD** of Ω into d **subdomains** Ω_i
- Perform a SAM-coupled **all-HFM simulation** on $\cup_i \Omega_i$
- Compute **POD basis** $\boldsymbol{\Phi}_i$ on each Ω_i
- Assume a **functional form** for your ROM in Ω_i, informed by the functional form of the corresponding HFM
  - Transmission conditions enter through **learned source terms** added to the ROM dynamical system

OpInf ROM + Schwarz BCs in Ω_i:
$$\dot{\hat{q}}_i + \hat{A}_i\hat{q}_i + \hat{H}_i(\hat{q}_i \otimes \hat{q}_i) + \underbrace{\hat{B}_i g_i}_{\text{Schwarz Dirichlet BC term}} + \underbrace{\hat{H}_i t_i}_{\text{Schwarz Neumann BC term}} = 0$$

Motivated by **BC** implementation in **FEM**

KROM + Schwarz BCs in Ω_i:
$$\hat{q}_i + \Omega_{q,i}^{\top}k_q(\hat{q}_i) + \underbrace{\Omega_{g,i}^{\top}k_g(g_i)}_{\text{Schwarz Dirichlet BC term}} + \underbrace{\Omega_{t,i}^{\top}k_t(t_i)}_{\text{Schwarz Neumann BC term}} = 0$$

Alternative kernel-based formulation (use linear k_g, k_t)

- Compute ROM operator in each subdomain Ω_i by solving regularized least squares **minimization problem**

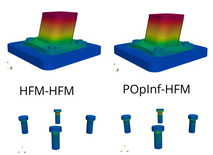
Online stage:

- Apply **Schwarz iteration procedure**, with Schwarz BC transfer via pre-learned boundary contributions

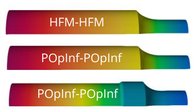
OpInf-OpInf and OpInf-HFM Results [4]

Bolted Joint

All hybrid models **correctly predict** the location of maximum von Mises stress (**failure**) even in **predictive regime**



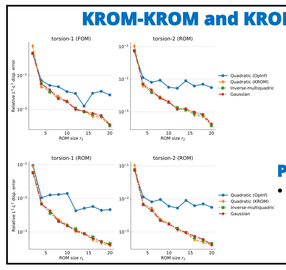
Tension Specimen

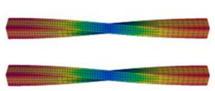


(competing method, Farcas ***et al.***, 2024 gives incorrect solution)

POpInf-POpInf TET10-HEX8 couplings achieve impressive **106× speedup** while maintaining ***O*(0.1%) errors** in **predictive regime**

KROM-KROM and KROM-HFM Results [7]





Top: HFM-HFM, *Bottom:* HFM-KROM, $r_2 = 10$, inverse-multiquadric

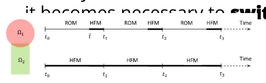
Predictive O-SAM Torsion

- KROMs have lower errors than QOpInf for $r \geq 4$ for both ROM-ROM and HFM-ROM

Towards Adaptive On-the-Fly ROM-HFM Switching

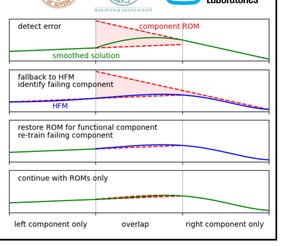
Motivation: ROMs may **fail** at run-time!

- ROMs are generally only as **expressive** as their **training data**
- Non-intrusive ROMs are particularly susceptible to **overfitting** and may not generalize well beyond the training data
- If the system encounters **unforeseen dynamics** at runtime, it becomes necessary to **switch** to the HFM to avoid collapse



ROM-HFM switching workflow:

- **Evaluate** at runtime if a ROM is still accurately predicting the dynamics
- **Switch** failing ROM-components to the HFM
- **Re-train** ROMs on the new data for future predictions



SP Neural Network OpInf ROMs

Goal: create **non-intrusive fully non-linear** OpInf ROMs that enable **structure preservation** (SP).

NN-OpInf

NNOpInf Assumed Form [9]

$$\hat{\hat{u}}(t,\mu) = \sum_{r=1}^{M^*} N_r(\hat{\boldsymbol{u}}, \mu; \theta_r)$$

- NNOpInf parameterizes PDE with **sum** of **neural network (NN) operators**.
- Each NN is **constrained** to satisfy target **problem-specific algebraic structure**

Example SP Parameterizations [9]

Matrix:
$$N_r(\hat{\boldsymbol{u}}, \mu; \theta_r) = \mathbf{A}(\hat{\boldsymbol{u}}, \mu; \theta_r)\hat{\boldsymbol{u}}$$

Symmetrix positive semi-definite (SPSD):
$$N_r(\hat{\boldsymbol{u}}, \mu; \theta_r) = \mathbf{L}(\hat{\boldsymbol{u}}, \mu; \theta_r)\mathbf{L}(\hat{\boldsymbol{u}}, \mu; \theta_r)^T\hat{\boldsymbol{u}}$$

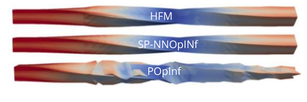
Skew:
$$N_r(\hat{\boldsymbol{u}}, \mu; \theta_r) = (\mathbf{L}(\hat{\boldsymbol{u}}, \mu; \theta_r) - \mathbf{L}(\hat{\boldsymbol{u}}, \mu; \theta_r)^T)\hat{\boldsymbol{u}}$$

Potential:
$$N_r(\hat{\boldsymbol{u}}, \mu; \theta_r) = \nabla_{\hat{\boldsymbol{u}}}\mathcal{L}_\theta(\hat{\boldsymbol{u}}, \mu)$$

SP-NNOpInf Results: 3D Hyperelastic Torsion [9]

HFM has **Lagrangian structure**:
$$\mathbf{M}\ddot{\boldsymbol{u}} = \mathbf{f}(\boldsymbol{u}), \qquad L(\boldsymbol{u}, \dot{\boldsymbol{u}}) = T(\dot{\boldsymbol{u}}) - V(\boldsymbol{u})$$

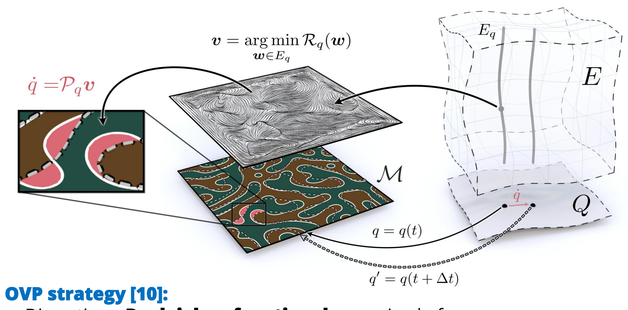
NNOpInf-SPSD-Potential model used:
$$\hat{\mathbf{f}}(\hat{\boldsymbol{u}}, \mu) = \nabla_{\hat{\boldsymbol{u}}}(\hat{\boldsymbol{u}}^T\boldsymbol{L}_\theta((\hat{\boldsymbol{u}}, \mu)\boldsymbol{L}_\theta(\hat{\boldsymbol{u}}, \mu)^T\hat{\boldsymbol{u}})$$



Lagrangian structure-preserving NN-OpInf ROMs maintain **stability** and **robustness** during **future state prediction**

Dynamics Discovery with Onsager's Variational Principle (OVP)

Goal: learn functional-level corrections to dissipation-dominated systems within a **structure-preserving variational integrator**

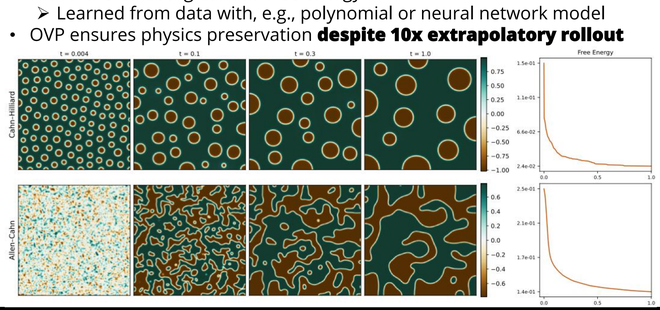


OVP strategy [10]:

- Discretize a **Rayleighan functional** comprised of thermodynamic free energy and dissipation potential
  - OVP at discrete level → variational time-stepping scheme **conserving mass and dissipating free energy by construction**
- Unknown/uncertain terms incorporated into discrete free energy functional and learned from data
  - OVP ensures physics remain preserved **independent of training process**

OVP results [10]:

- Block co-polymer models have uncertain **bulk free energy density** within the Ginzburg-Landau free energy
  - Learned from data with, e.g., polynomial or neural network model
- OVP ensures physics preservation **despite 10x extrapolatory rollout**



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[2] A. Mota, I. Tezaur, G. Phlipot. "The Schwarz alternating method for dynamic solid mechanics", ***Int. J. Numer. Meth. Engng.*** 123 (21) 5036-5071, 2022.

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[4] I. Tezaur, E. Parish, A. Gruber, I. Moore, C. Wentland, A. Mota. "Hybrid coupling with OpInf and the SAM", submitted to ***IJNME***. https://arxiv.org/abs/2511.20687

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[10] A. Gruber, R. Roy-Chowdhury, I. Tezaur, N. Urban. "Flexible and stable dynamics discovery with Onsager's principle", submitted to ***Physica D.*** https://arxiv.org/abs/2606.24106

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