Digital twins for engineering and scientific discovery

Multimodality, structure-preservation and UQ

Nat Trask
University of Pennsylvania

Penn
University of Pennsylvania

Sandia National Laboratories

SEA-CROGS

What comes next once forward simulation is “free”?

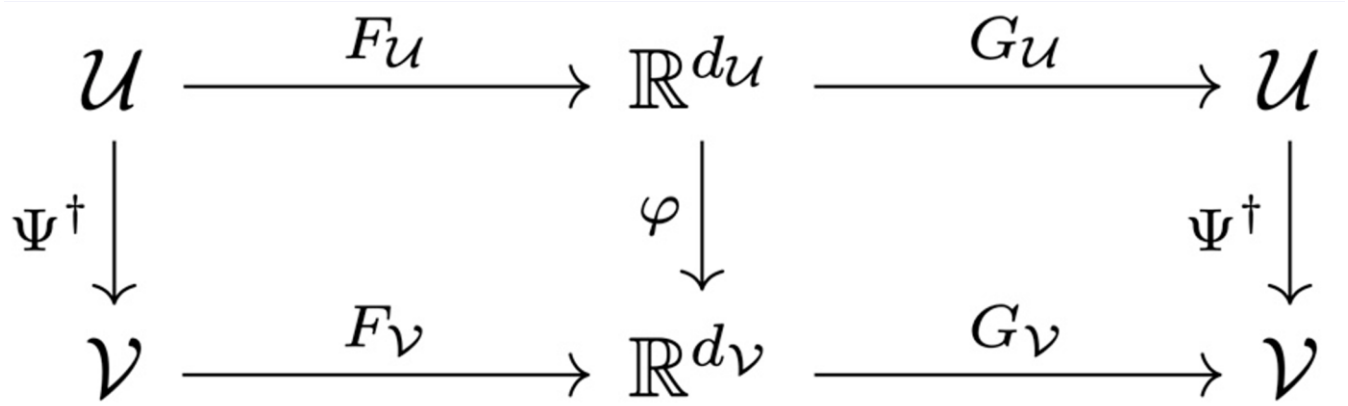
Many operator regression frameworks realize 1000x speedup vs traditional methods

1. Neural operators, DeepONets, foundation models
2. Projection based ROMs

Key algebraic structures

1. Latent finite dimensional representations of domain U and range V
2. Mapping ϕ in reduced space

Limited Physics! Limited guarantees!



Key Idea

Generate examples of function-to-function map that can be used to construct fast data-driven models or surrogates in reduced dimension space

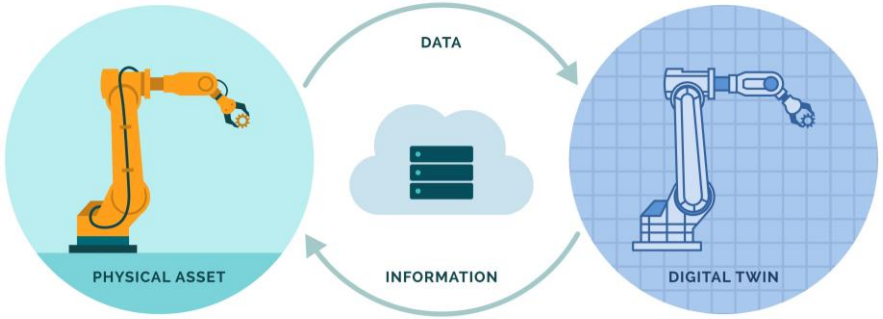
(top) Stuart et al.

Goal 1: Digital Twins of Systems-of-Systems

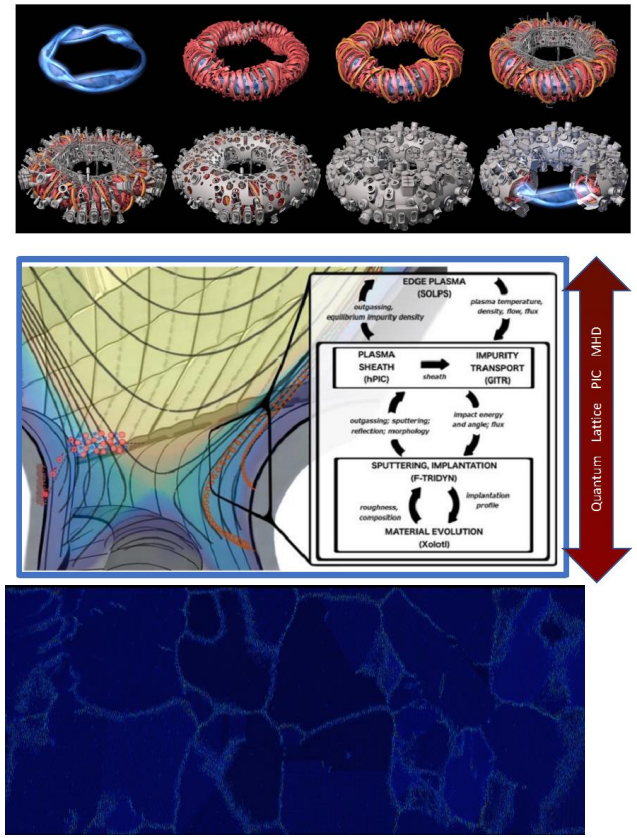
Learn fast FEM models with parametric dependencies on unknown physics to perform real-time prediction and UQ

- Preserve physical structure + realizability
- Guarantee numerical stability under extrapolation
- Disentanglement of aleatoric/epistemic uncertainty
- Support real time inference and data assimilation
- Support causal/mechanistic inference

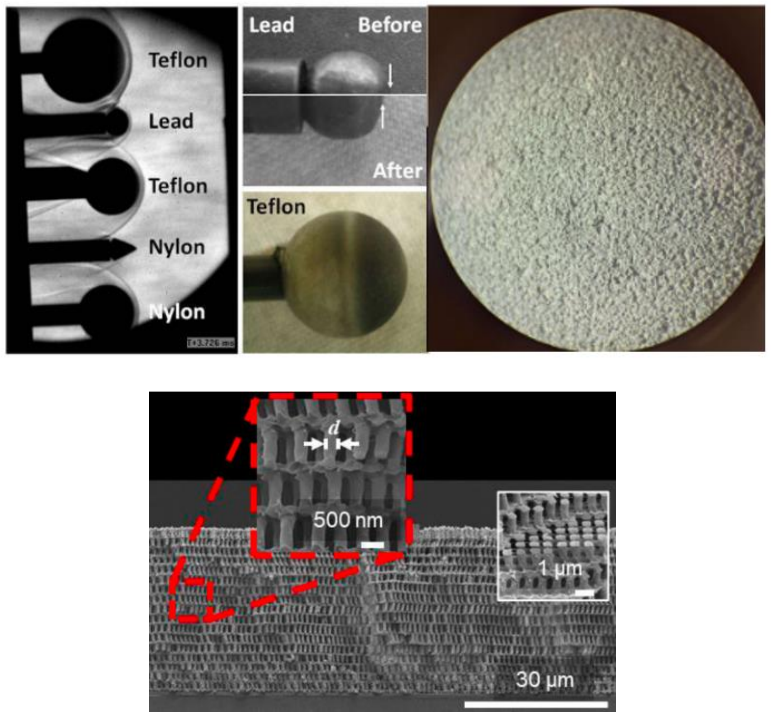
"The size and complexity of many systems being built for government, industry, and the military have reached a threshold where customary methods of analysis, design, implementation, and operation are no longer sufficiently reliable. Many of these large systems are properly described as "systems-of-systems" in that they are composed of many systems" (Dvorak 2005)



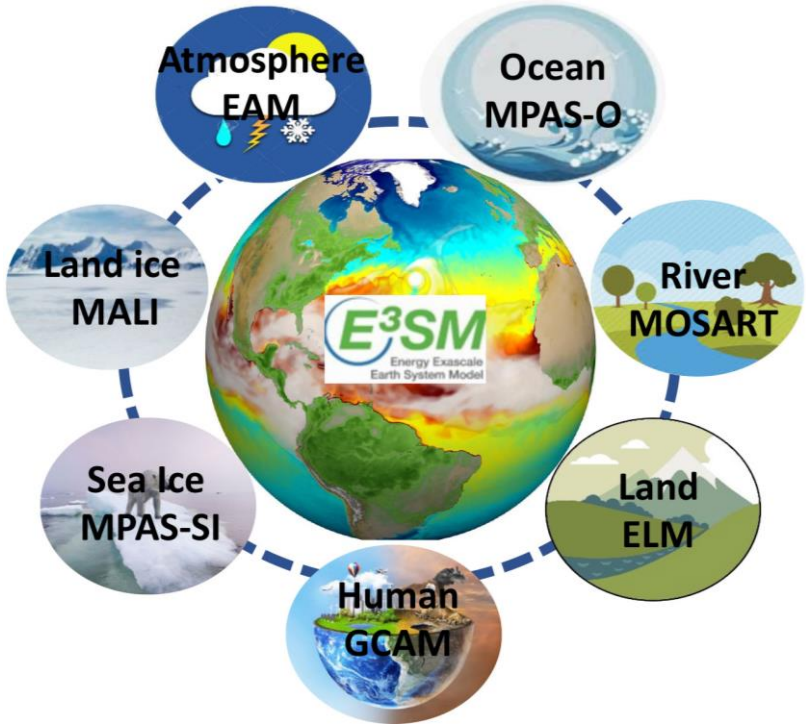
Structure preservation requirements for digital twins



Stellerator shape optimization
Inner loop acceleration to design MCF reactors and ICF targets
Need exact handoff of conserved fluxes, Hugoniot relations, Gauge symmetries



Multimodal hypersonic metamaterials
Non-equilibrium physics in multiscale ablation process with indirect measurements
Need exact mass transfer, non-equilibrium chemistry, fluctuation/dissipation balance

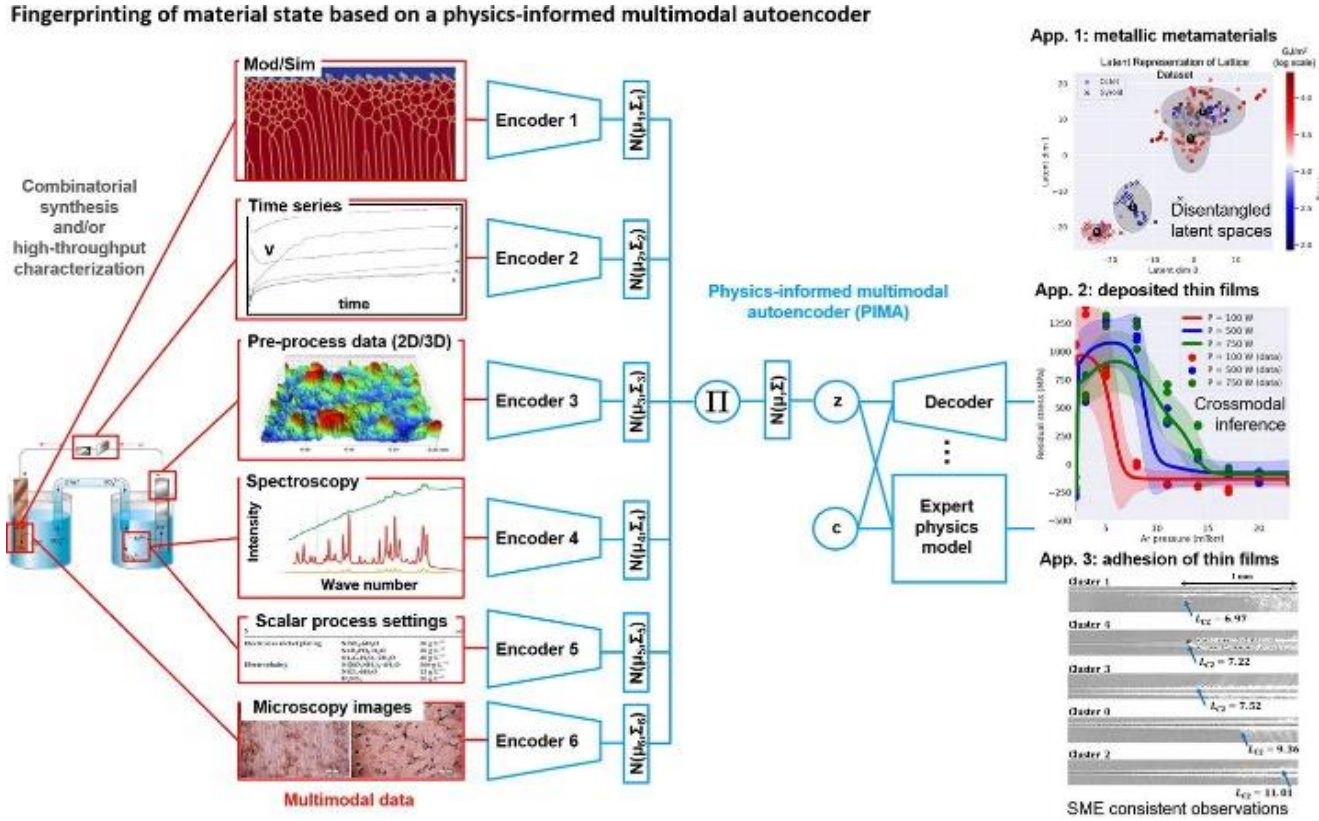


Data assimilation in climate
Causal Fingerprinting in climate attribution for legacy DOE codes
Detect long range "telecasting" across climate subsystems, stably surrogate climate subsystems

Goal 2: Integrated physics in AI-driven scientific discovery

Construct foundation models for material systems able to fuse multimodal data, embed physics and autonomously propose experiments

- Handle sparse, multimodal data
- Integrate physical models encoding mechanistic behavior
- Support Bayesian inference to drive optimal experimental design

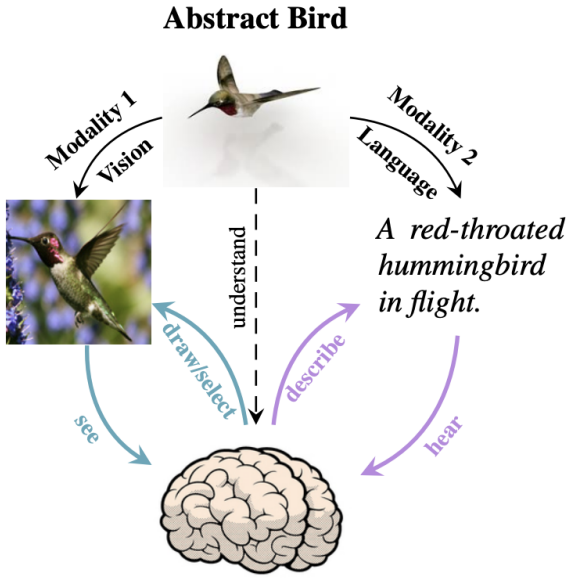


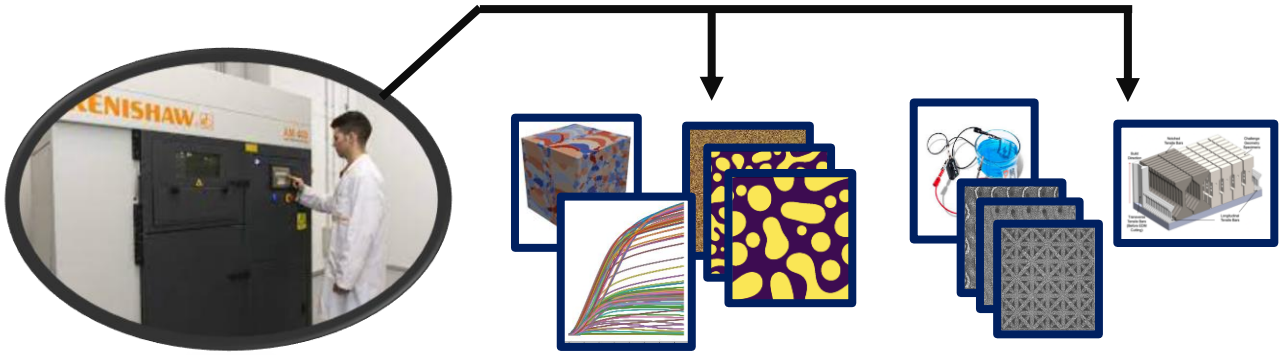
Multimodality and mechanistic causality in materials discovery

"Traditional" Multimodality

Assimilate heterogeneous data sources so they're greater than sum of their parts

e.g. audio + text to generate automatic subtitles





Scientific Multimodality

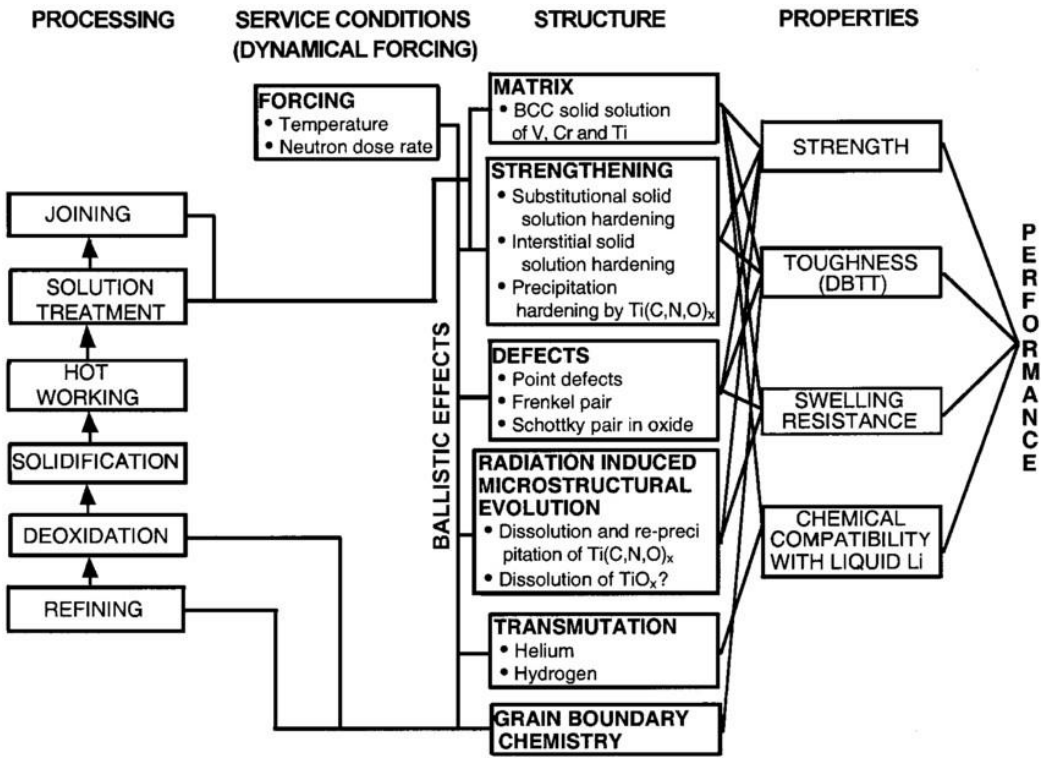
Combining all information available during fabrication and characterization of new materials

Physics-amenable modalities

Field measurements
Simulated data

Physics-agnostic modalities

Microscopy, spectra, audio



When people say AI (as opposed to ML) often they envision interpretable reasoning and cause/effect exposing scientific mechanisms

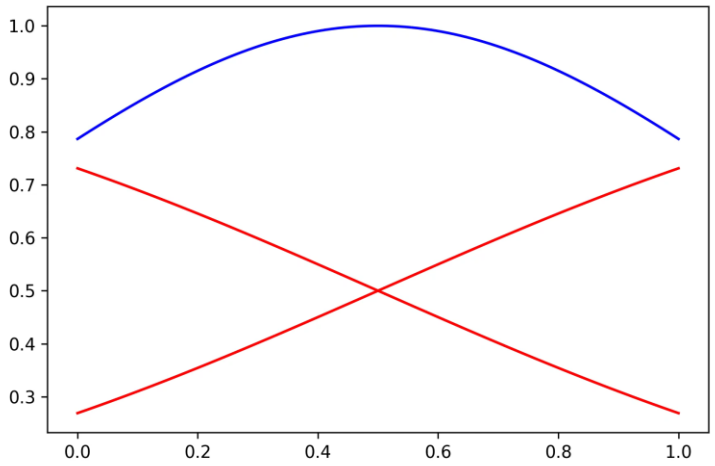
(e.g. Olson Diagram)

Shi, Y., Siddharth, N., Paige, B. and Torr, P.H., 2019. Variational mixture-of-experts autoencoders for multi-modal deep generative models. *arXiv preprint arXiv:1911.03393*.

Goal 1:
Digital Twins of
Systems-of-Systems

Learn fast FEM models with parametric dependencies on unknown physics to perform real-time prediction and UQ

Structure preserving neural operators via finite element exterior calculus



$$\mathcal{W}_i = \lambda_i$$

$$\mathcal{W}_{ij} = \lambda_i \nabla \lambda_j - \lambda_j \nabla \lambda_i$$

Neural Whitney forms
Differentiable architecture parameterizing control volumes and their boundaries

$$\mathrm{d}_{k-1}\ \mathrm{d}^*_{k-1}\mathbf{u}_k + \mathrm{d}^*_k \mathbf{w}_{k+1} = \mathbf{f}_k$$

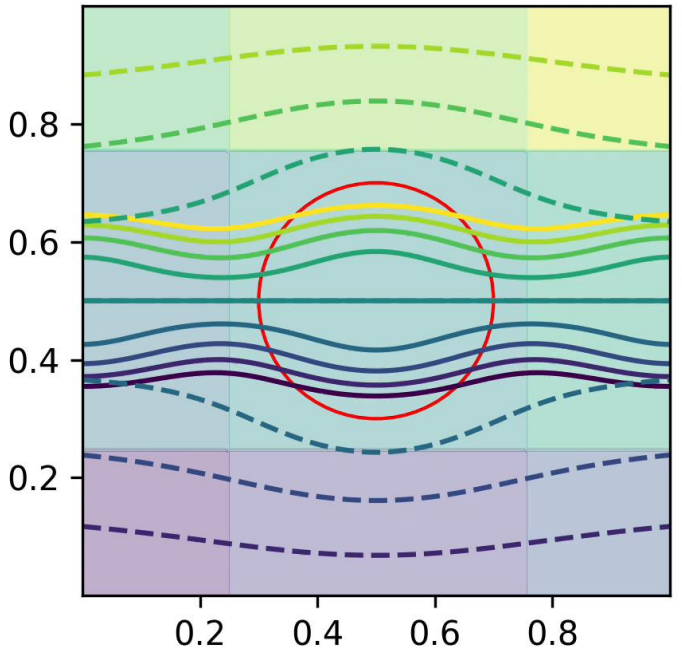
Conservation balance
Exact physics treatment

$$\mathbf{w}_{k+1} = d_k \mathbf{u}_k + \mathcal{N}[d_k \mathbf{u}_k; \theta]$$

Black-box generalized fluxes
Diffusion stabilized nonlinearity w/ uncertainty

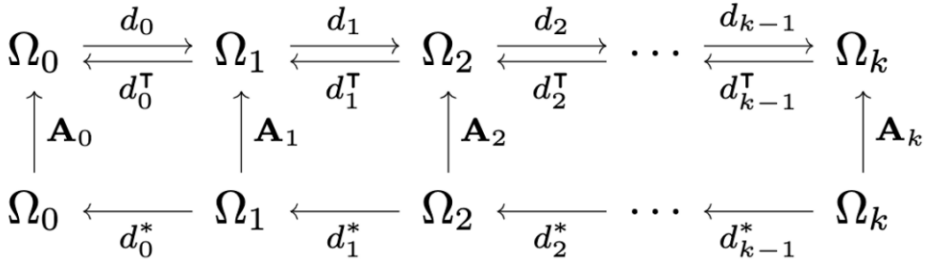
$$\begin{array}{ccccccccc}
\Omega_0 & \underset{d_0^\intercal}{\overset{d_0}{\rightleftarrows}} & \Omega_1 & \underset{d_1^\intercal}{\overset{d_1}{\rightleftarrows}} & \Omega_2 & \underset{d_2^\intercal}{\overset{d_2}{\rightleftarrows}} & \cdots & \underset{d_{k-1}^\intercal}{\overset{d_{k-1}}{\rightleftarrows}} & \Omega_k \\
\uparrow \mathbf{A}_0 & & \uparrow \mathbf{A}_1 & & \uparrow \mathbf{A}_2 & & & & \uparrow \mathbf{A}_k \\
\Omega_0 & \underset{d_0^*}{\longleftarrow} & \Omega_1 & \underset{d_1^*}{\longleftarrow} & \Omega_2 & \underset{d_2^*}{\longleftarrow} & \cdots & \underset{d_{k-1}^*}{\longleftarrow} & \Omega_k
\end{array}$$

Exact structure preservation
Machine learnable de Rham complex which provides downstream stability theory



Data-driven FEM
Simultaneously identify control volumes and integral balance laws whose solution matches (sparse) data

Result: Combinatorial Hodge + Lax Milgram theory for elliptic operators



Combinatorial Hodge Laplacian

$$\Delta_k = d_{k-1} d_{k-1}^* + d_k^* d_k$$

Obtain standard results from traditional finite element analysis:

- *Preserve exact sequence property*
- *Hodge decomposition*
- *Poincare inequality*
- *Lax-Milgram stability theory*
- *Conservation structure*

Theorem 3.1. *The discrete derivatives* d_k *in* (11) *form an exact sequence if the simplicial complex is exact, and in particular* $\mathsf{d}_{k+1} \circ \mathsf{d}_k = 0$. *In* $\mathbb{R}^3$, *we have* $CURL_h \circ GRAD_h = DIV_h \circ CURL_h = 0$.

Theorem 3.2. *The discrete derivatives* d_k^* *in* (11) *form an exact sequence of the simplicial complex is exact, and in particular* $\mathsf{d}_k^* \circ \mathsf{d}_{k+1}^* = 0$. *In* $\mathbb{R}^3$, $DIV_h^* \circ CURL_h^* = CURL_h^* \circ GRAD_h^* = 0$.

Theorem 3.3 (Hodge Decomposition). *For* C^k, *the following decomposition holds*

$$C^k = \mathrm{im}(\mathsf{d}_{k-1}) \bigoplus\nolimits_k \ker(\Delta_k) \bigoplus\nolimits_k \mathrm{im}(\mathsf{d}_k^*), \tag{17}$$

where $\bigoplus_k$ *means the orthogonality with respect to the* $(\cdot,\cdot)_{\mathbf{D}_k\mathbf{B}_k^{-1}}$*-inner product.*

Theorem 3.4 (Poincaré inequality). *For each* k, *there exists a constant* $c_{P,k}$ *such that*

$$\|\mathbf{z}_k\|_{\mathbf{D}_k\mathbf{B}_k^{-1}} \leq c_{P,k} \|\mathsf{d}_k \mathbf{z}_k\|_{\mathbf{D}_{k+1}\mathbf{B}_{k+1}^{-1}}, \quad \mathbf{z}_k \in \mathrm{im}(\mathsf{d}_k^*),$$

and another constant $c_{P,k}^*$ *such that*

$$\|\mathbf{z}_k\|_{\mathbf{D}_k\mathbf{B}_k^{-1}} \leq c_{P,k}^* \|\mathsf{d}_{k-1}^* \mathbf{z}_k\|_{\mathbf{D}_{k-1}\mathbf{B}_{k-1}^{-1}}, \quad \mathbf{z}_k \in \mathrm{im}(\mathsf{d}_{k-1}).$$

Thus, for $\mathbf{u}_k \in C^k$, *we have*

$$\inf_{\mathbf{h}_k \in \ker(\Delta_k)} \|\mathbf{u}_k - \mathbf{h}_k\|_{\mathbf{D}_k\mathbf{B}_k^{-1}} \leq C \left(\|\mathsf{d}_k \mathbf{u}_k\|_{\mathbf{D}_{k+1}\mathbf{B}_{k+1}^{-1}} + \|\mathsf{d}_{k-1}^* \mathbf{u}_k\|_{\mathbf{D}_{k-1}\mathbf{B}_{k-1}^{-1}} \right),$$

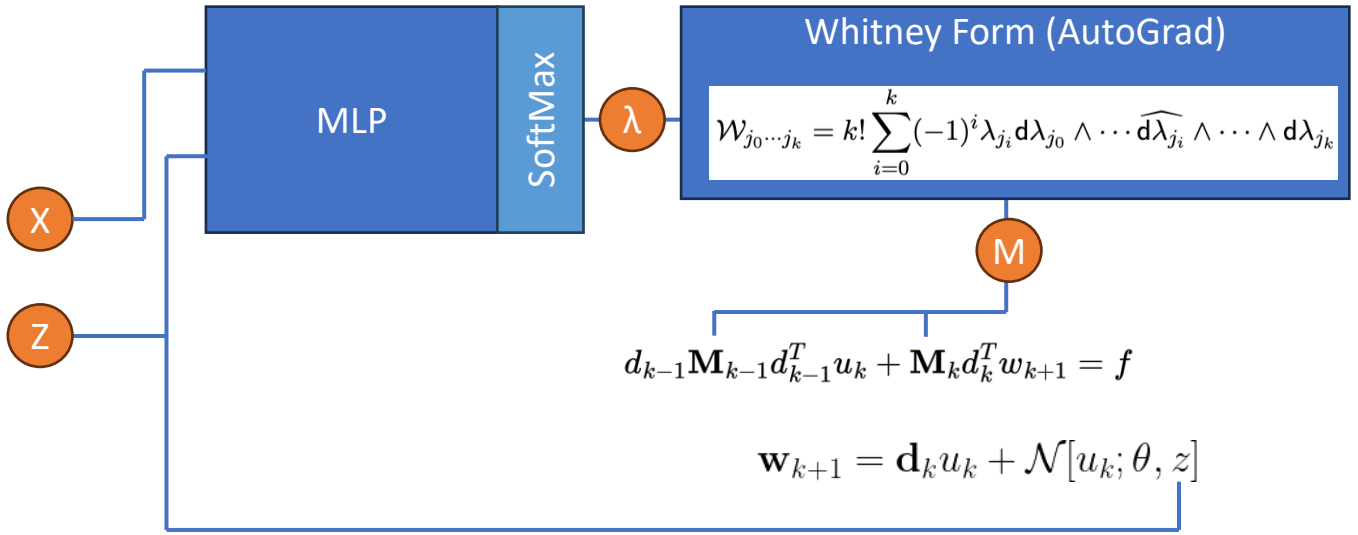
where constant $C > 0$ *only depends on* $c_{P,k}$ *and* $c_{P,k}^*$.

Theorem 3.5 (Invertibility of Hodge Laplacian). *The* k^{th}*-order Hodge Laplacian* Δ_k *is positive-semidefinite, with the dimension of its null-space equal to the dimension of the corresponding homology* $H^k = \ker(\mathsf{d}_k)/\mathrm{im}(\mathsf{d}_{k-1})$.

Trask, N., Huang, A. and Hu, X., 2022. Enforcing exact physics in scientific machine learning: a data-driven exterior calculus on graphs. *Journal of Computational Physics*, *456*, p.110969.

Real-time digital twins via conditional neural Whitney forms

Paper to be released end of Jan



Massive strides in *conditional generative modeling*, generating images conditioned on a prompt (above)

We extend the idea to sample from the space of finite element models conditioned on an input Z (sensor readings, parameterized geometry, or a latent variable) 1000x faster than standard FEM model

$$\underset{\mathbf{A},\theta}{\operatorname{argmin}}||\mathbf{u}-\mathbf{u}_{data}||^2+\epsilon^2||\mathbf{w}-\mathbf{w}_{data}||^2$$
$$\text{such that } a(\mathbf{u},\mathbf{v};\mathbf{A})+N_{\mathbf{v}}[\mathbf{u};\theta]=b(\mathbf{v}) \quad \forall\mathbf{v}$$

Actor, J.A., Hu, X., Huang, A., Roberts, S.A. and Trask, N., 2024. Data-driven Whitney forms for structure-preserving control volume analysis. *Journal of Computational Physics*, *496*, p.112520.

Left taken from: Synthesizing Coherent Story with Auto-Regressive Latent Diffusion Models
Xichen Pan[1], Pengda Qin[2], Yuhong Li[2], Hui Xue[2], Wenhu Chen

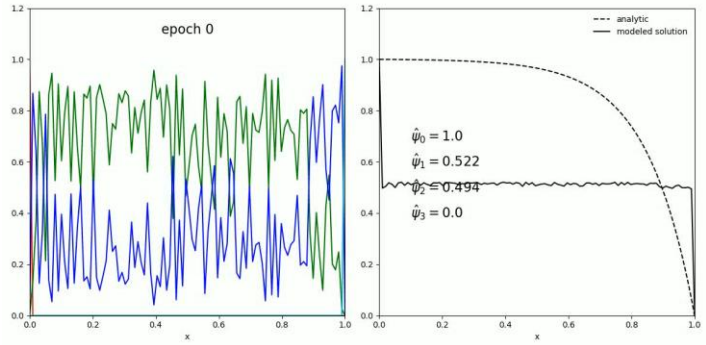
Supervised conditioning: parametric families of data-driven FEM models

Singularly perturbed advection-diffusion

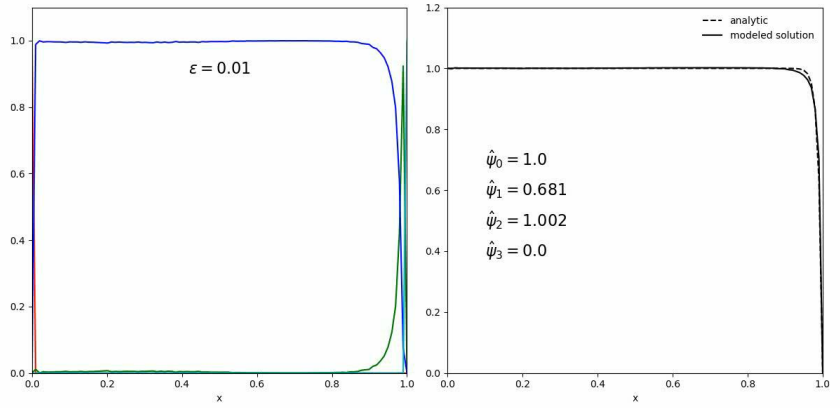
$$\partial_x u + \frac{1}{Pe}\partial_{xx} u = f$$

Condition on Peclet number

$$\mathrm{Pe} = \frac{\text{advective transport rate}}{\text{diffusive transport rate}}$$

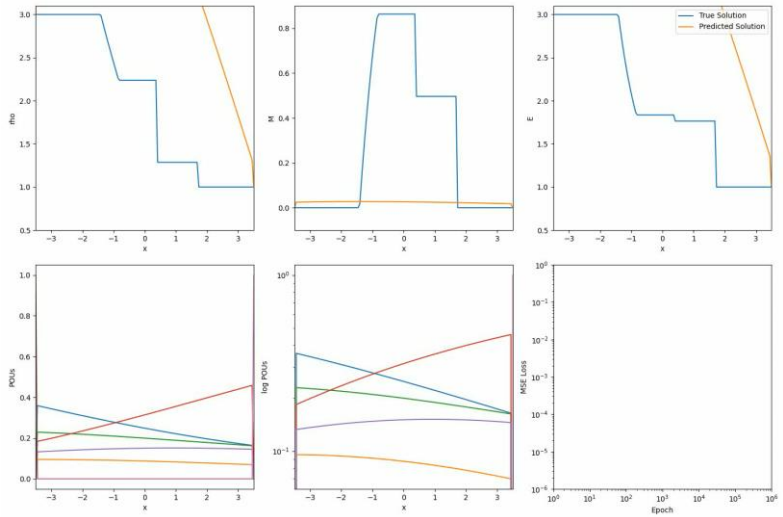


Unsupervised fitting of subdomains to boundary layers

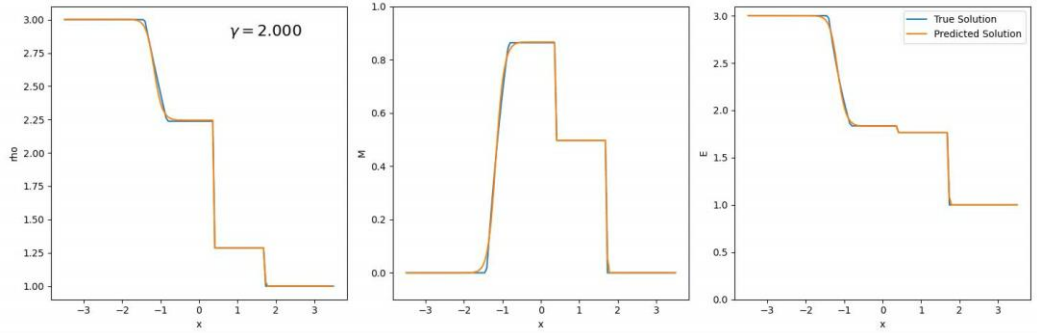


Conditioning of subdomains on Peclet #

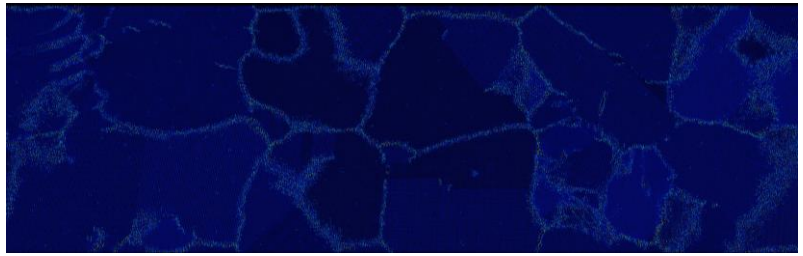
Unsupervised fitting of control volumes to strong and weak shock boundaries in spacetime



Conditioning on constitutive equation yields a family of shock models for different materials



Support fitting of data-driven Riemann solvers to upscale MD data

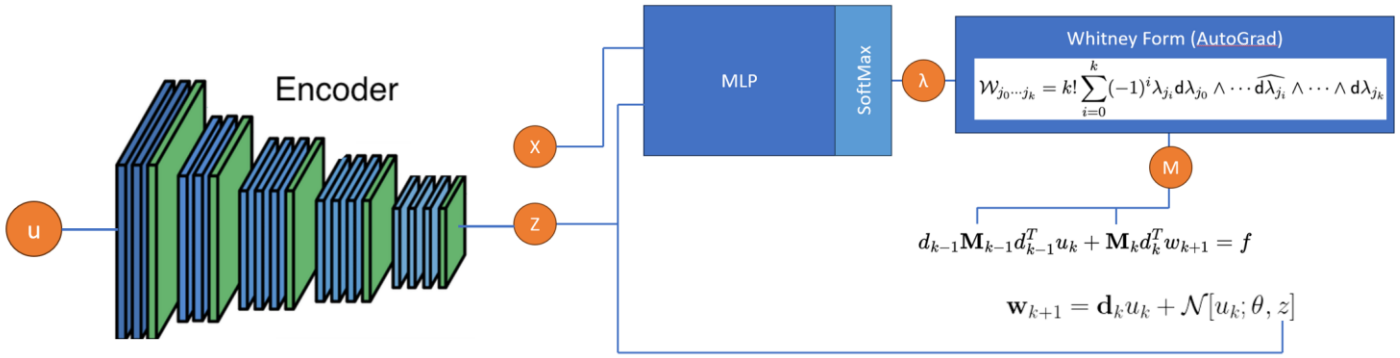


Unsupervised conditioning: identification of exogenous physics

$$\partial_x u + \frac{1}{Pe}\partial_{xx} u = f$$

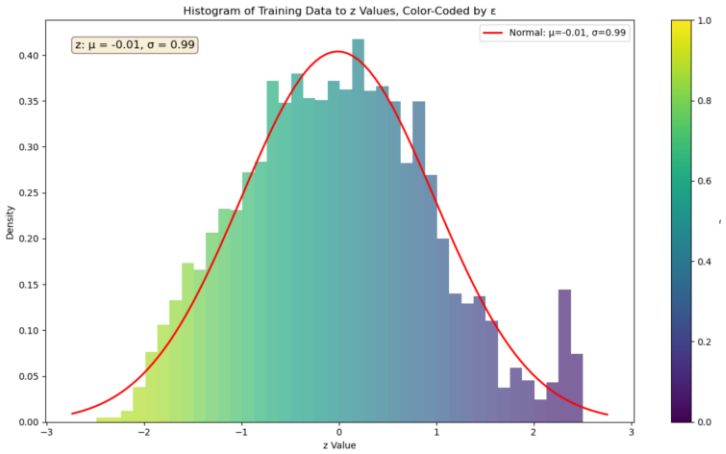
$$\mathrm{Pe} = \frac{\text{advective transport rate}}{\text{diffusive transport rate}}$$

$$Pe \sim \mathcal{N}(\mu, \sigma^2)$$

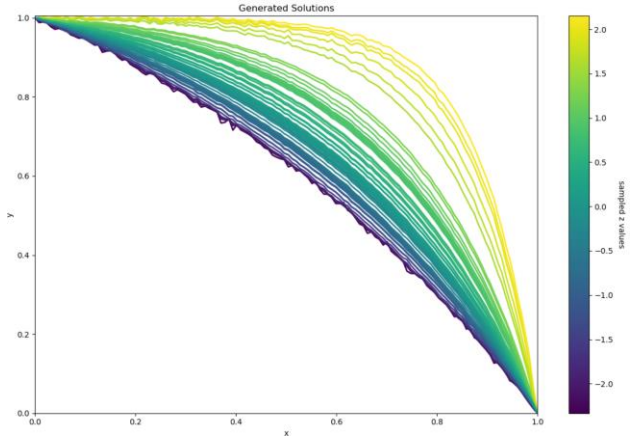


$$\mathcal{L} = -\mathbb{E}[\log p(u|x,z)] + \mathcal{KL}(p(z)||q(z|u,x)) + \lambda^\intercal \left(\mathbf{d}_0^\intercal \mathbf{M}_1 \mathbf{d}_0 u + \mathbf{d}_0^\intercal \mathbf{M}_1 \mathcal{N}(u; z, \theta) - b\right)$$

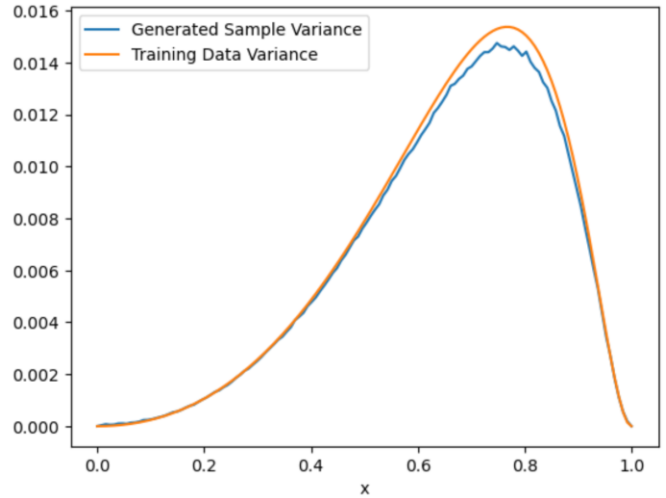
Reconstruction **Prior Penalty** **Physics constraint**



Latent variable maps directly to Peclet number

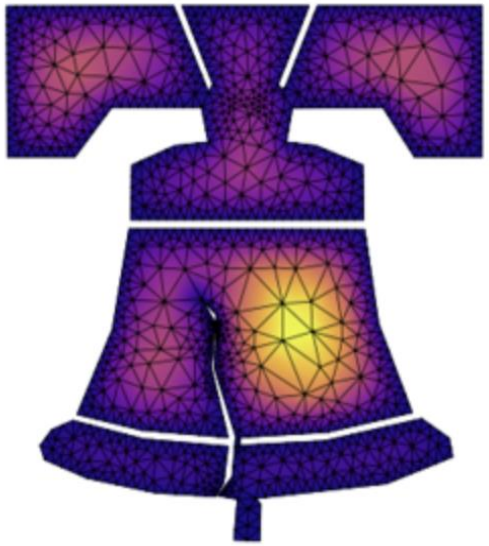


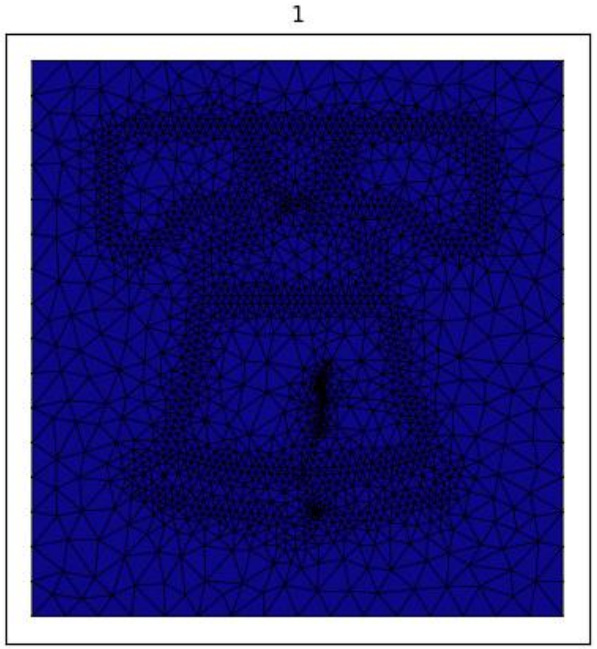
Generative model guaranteed to preserve physical structure



Uncertainty from sampling prior accurately matches data distribution

Exact structure preservation for complex geometries



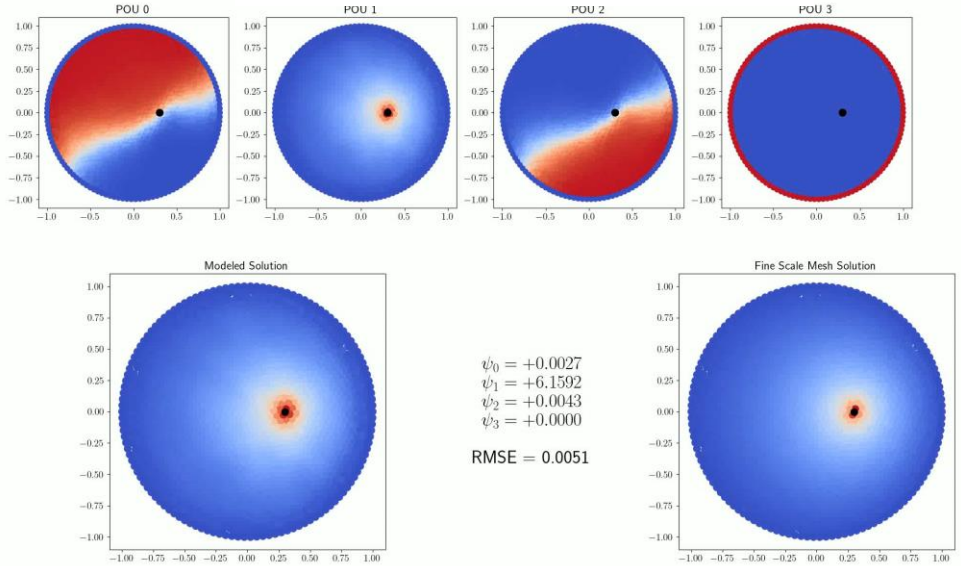


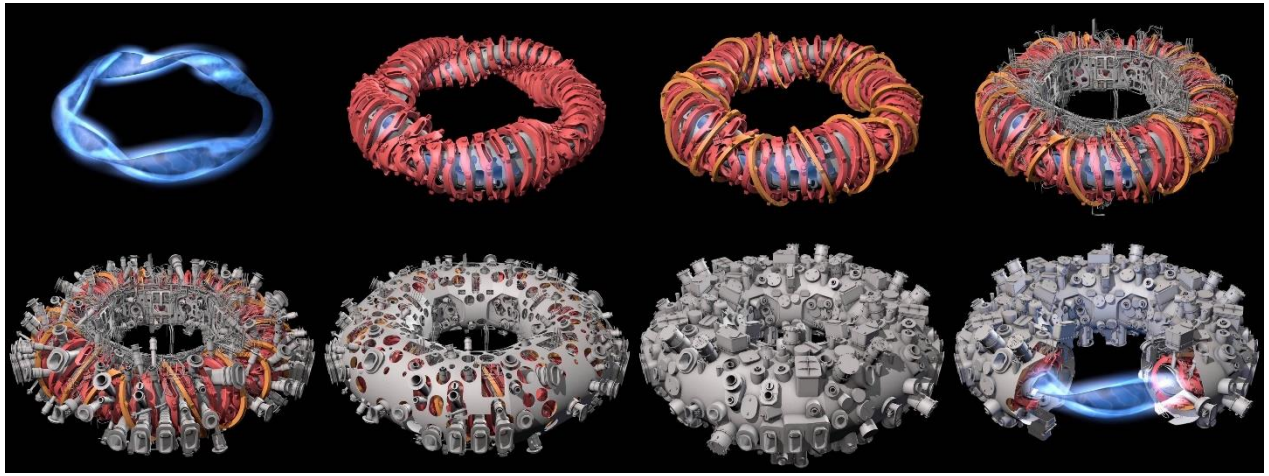
Conditioning on material properties

$$\nabla \cdot E = \delta(x - \mathbf{z})$$

$$E + \nabla\phi = 0$$

Conditioning on point charge location



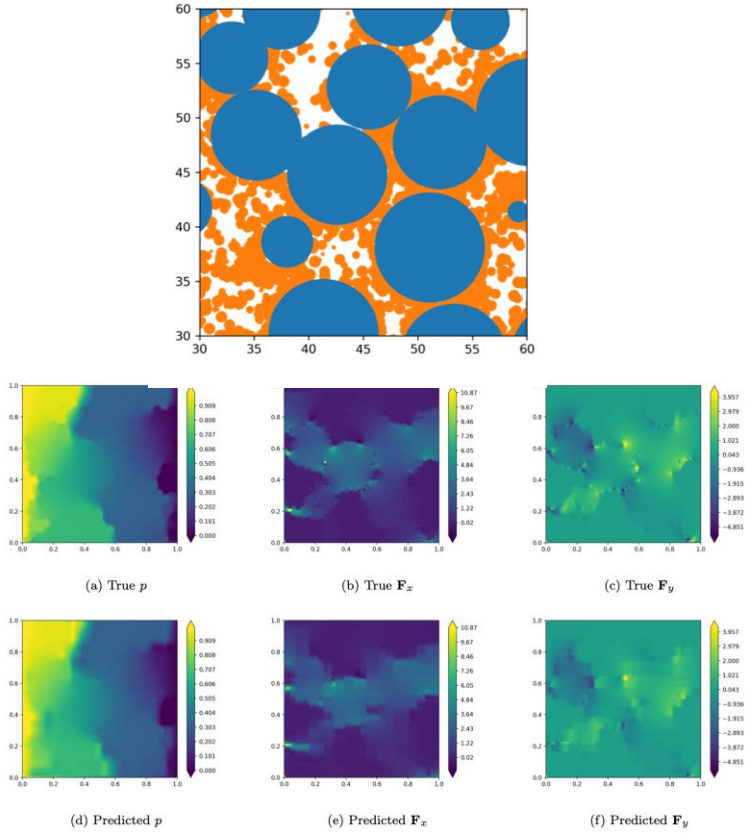


Complex geometries: implementations in FENICS to treat models on arbitrary polyhedral meshes without invasive code modifications

Structure-preserving source identification: identify sources compatible with *exact* charge balance

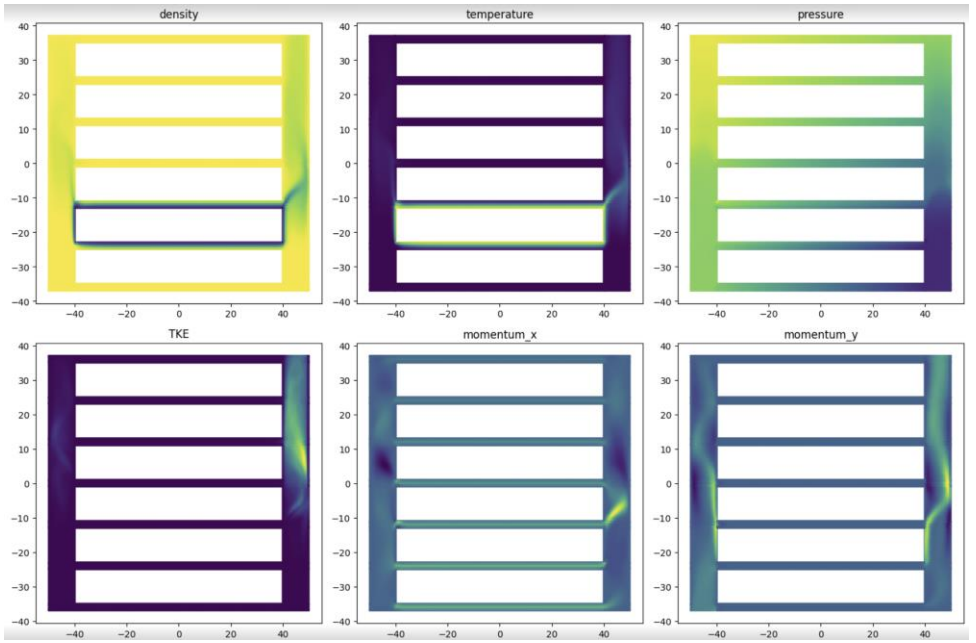
Extensions to physics-critical systems: Digital twins of stellerators and inertial confinement fusion targets require exact handoffs of

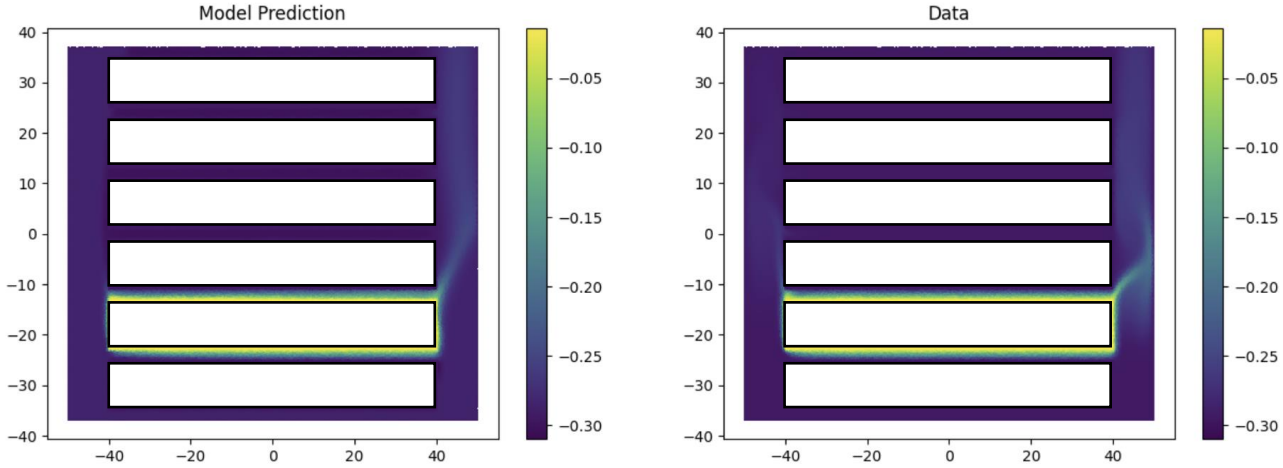
Li-ion battery digital twin bridging material to engineering scale



Heat BC

Material prop.





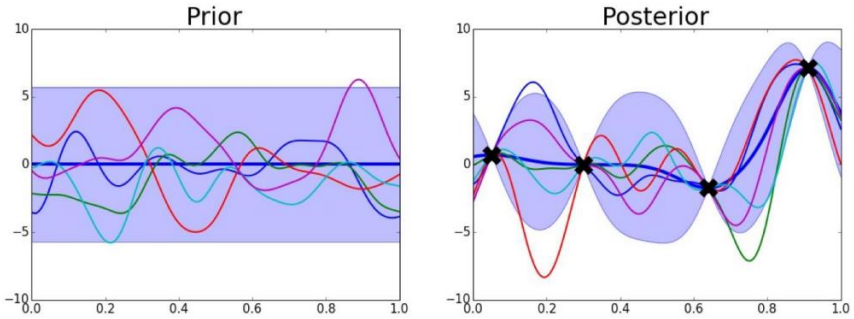
Microstructure: Replace a ~6M finite element simulation of as-built geometry with 8 data-driven elements w/ ~0.1% error

Battery pack: Replace ~1M element LES w/ 6 elements reproducing Reynolds average field quantities and providing exact heat flux

Structure preservation allows bi-directional and modular coupling across scales from mesoscale (microns) to server rooms macroscale (meters)

Beyond BayesOpt – Active learning with DTs

$$y = f(\boldsymbol{x}) + \epsilon \qquad f \sim \mathcal{GP}(0, k(\boldsymbol{x}, \boldsymbol{x}'; \boldsymbol{\theta}))$$



Training via maximizing the marginal likelihood

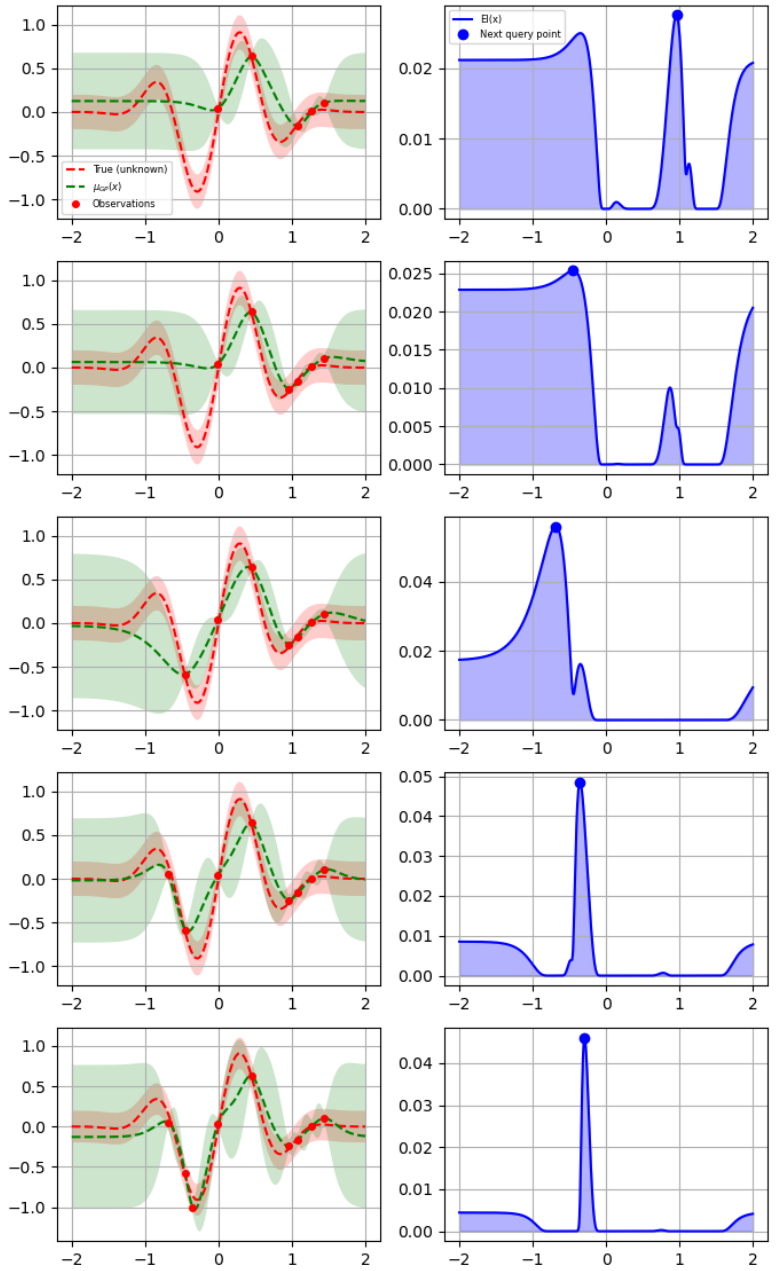
$$\log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) = -\frac{1}{2}\log|\boldsymbol{K} + \sigma_\epsilon^2 \boldsymbol{I}| - \frac{1}{2}\boldsymbol{y}^T(\boldsymbol{K} + \sigma_\epsilon^2 \boldsymbol{I})^{-1}\boldsymbol{y} - \frac{N}{2}\log 2\pi$$

Prediction via conditioning on available data

$$p(f_*|\boldsymbol{y}, \boldsymbol{X}, \boldsymbol{x}_*) = \mathcal{N}(f_*|\mu_*, \sigma_*^2),$$
$$\mu_*(\boldsymbol{x}_*) = \boldsymbol{k}_{*N}(\boldsymbol{K} + \sigma_\epsilon^2 \boldsymbol{I})^{-1}\boldsymbol{y},$$
$$\sigma_*^2(\boldsymbol{x}_*) = \boldsymbol{k}_{**} - \boldsymbol{k}_{*N}(\boldsymbol{K} + \sigma_\epsilon^2 \boldsymbol{I})^{-1}\boldsymbol{k}_{N*},$$

The good: closed form expressions for posterior distributions that can easily be used to design acquisition functions in active learning.

The bad: Poor scaling leads to typical tractability only for moderately low-dimension scalar to scalar maps, with limited ability to embed physics.



Enforcing physics via the optimal recovery problem [Owhadi 2022]

Let $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a symmetric positive definite bivariate kernel, and let $\mathcal{H}_K = \text{span}\{K(\cdot, x_i)\}$ be the induced RKHS space with accompanying RKHS norm $\|\cdot\|_K$. The **optimal recovery problem** consists of finding $f \in \mathcal{H}_K : \mathbf{X} \subset \mathcal{X} \mapsto \mathbf{Y} \subset \mathbb{R}$.

$$\min_{f \in \mathcal{H}_K} \|f\|_K^2 + \frac{1}{\epsilon} \|f(\mathbf{X}) - \mathbf{Y}\|_2^2 .$$

Expanding in terms of linear algebra

$$V^* = \arg\min_{V \in \mathbf{R}^N} V^T K(\mathbf{X}, \mathbf{X}) V + \frac{1}{\epsilon} \|K(\mathbf{X}, \mathbf{X}) V - \mathbf{Y}\|_2^2 .$$

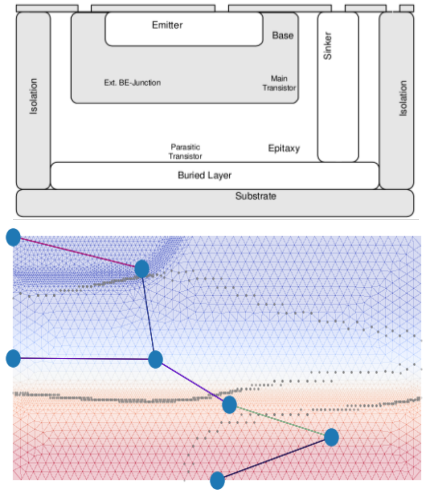
We recover in expectation the traditional Gaussian process posterior

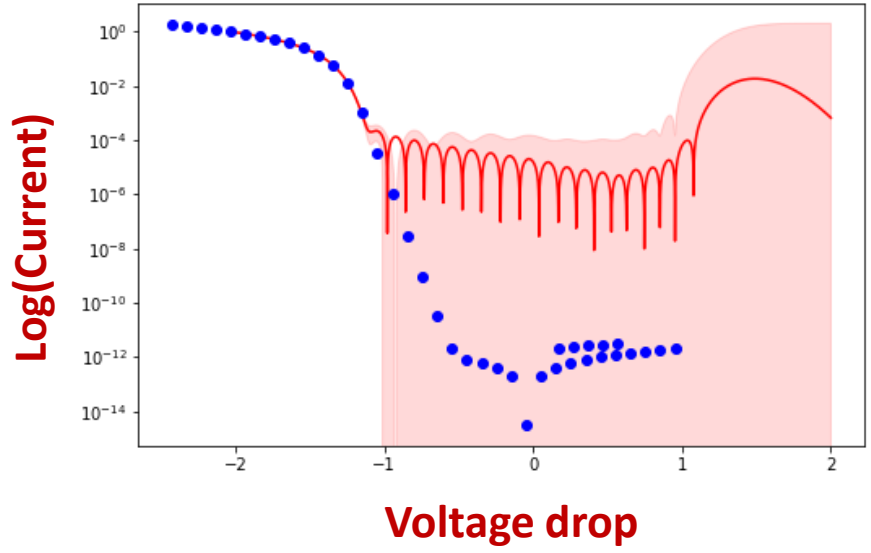
$$f^*(\cdot) = K(\cdot, \mathbf{X})(\mathbf{K} + \epsilon I)^{-1}\mathbf{Y}.$$

Reframe control volume fluxes as constrained GPs

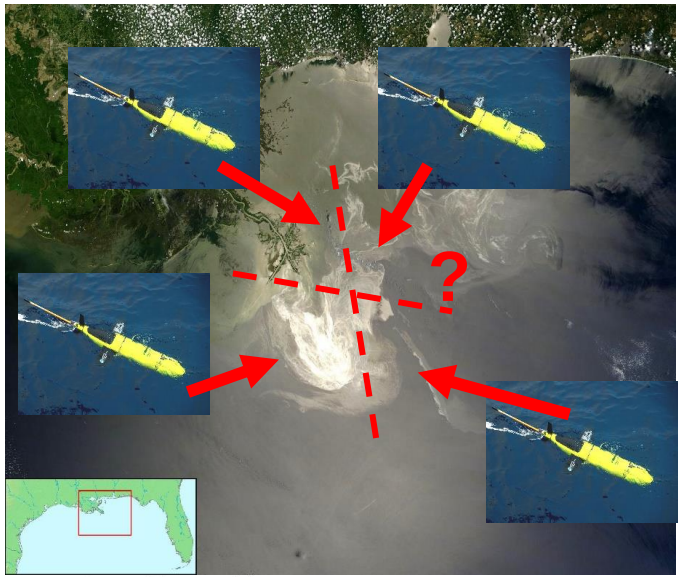
$$\min_{\theta, \mathbf{u}_{\text{un}}} \min_{\mathbf{F}_{\text{un}}} \sum_{e \in \mathcal{E}} \mathbf{F}_e^T (K_e(\delta_0 \mathbf{u}_e, \delta_0 \mathbf{u}_e) + \epsilon I)^{-1} \mathbf{F}_e + \log\det(K_e(\delta_0 \mathbf{u}_e, \delta_0 \mathbf{u}_e) + \epsilon I)$$

$$\text{s.t. } \mathbf{d}_k^\intercal \mathbf{F} = 0$$





Feeding the DT beast: real time data assimilation and the optimal coverage problem



Deepwater Horizon, 2010
NASA/GSFC, MODIS

Minimize: Sensor degradation

$$\mathcal{H}(P,\mathcal{W}) = \sum_{i=1}^{n} \int_{W_i} f(\|q - p_i\|)\phi(q)dq \qquad (1)$$

Sensor location

Dominance region Importance

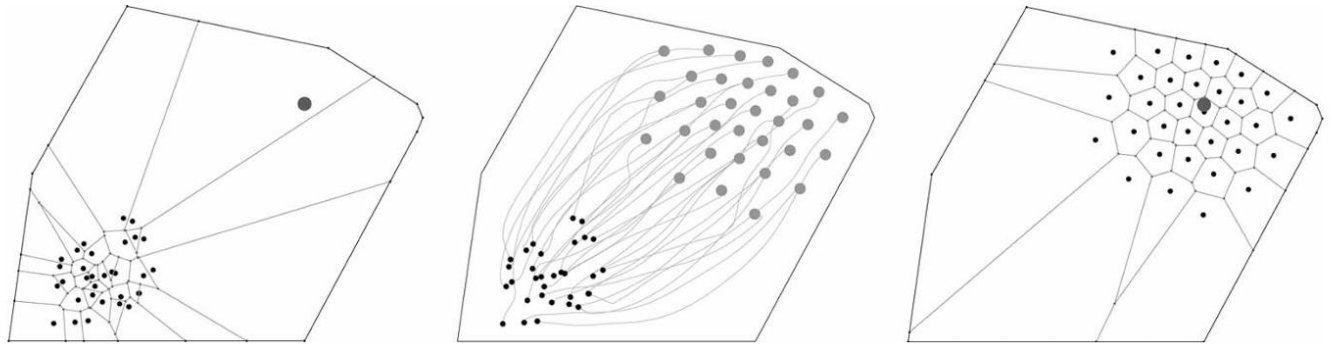
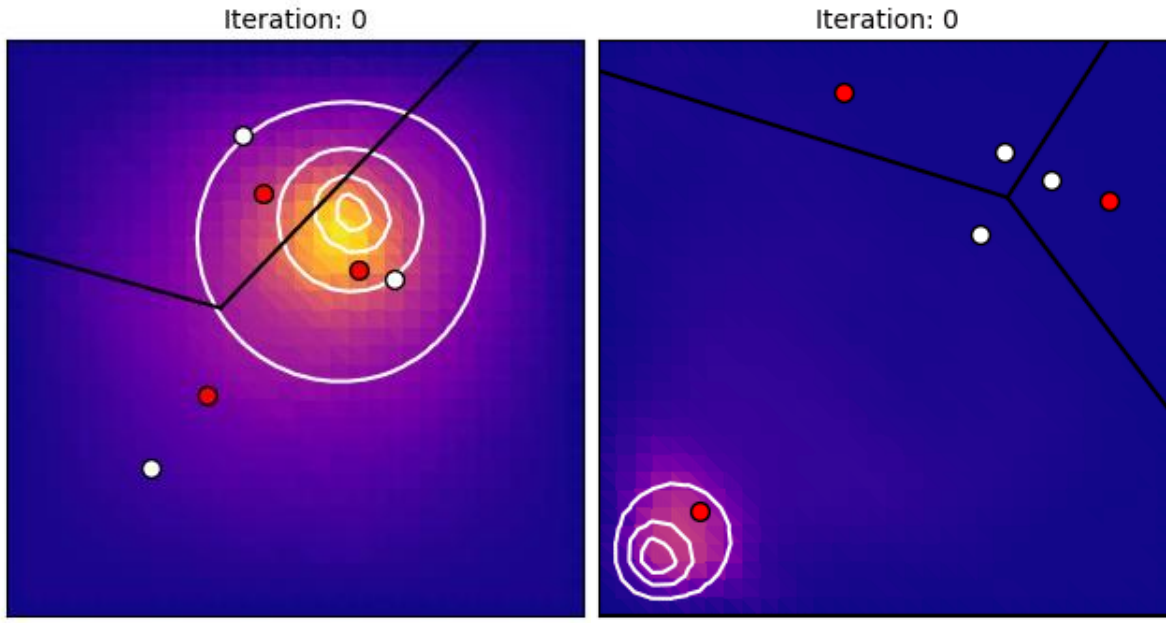


Fig. 3. Lloyd continuous-time algorithm for 32 agents on a convex polygonal environment, with the Gaussian density function of Fig. 1. The control gain in (6) is $k_{\text{prop}} = 1$ for all the vehicles. The left (respectively, right) figure illustrates the initial (respectively, final) locations and Voronoi partition. The central figure illustrates the gradient descent flow.

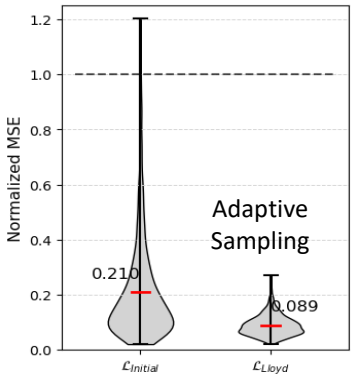
Can lightweight digital twins be embedded on distributed sensor platforms to guide collection of data in near-real time?

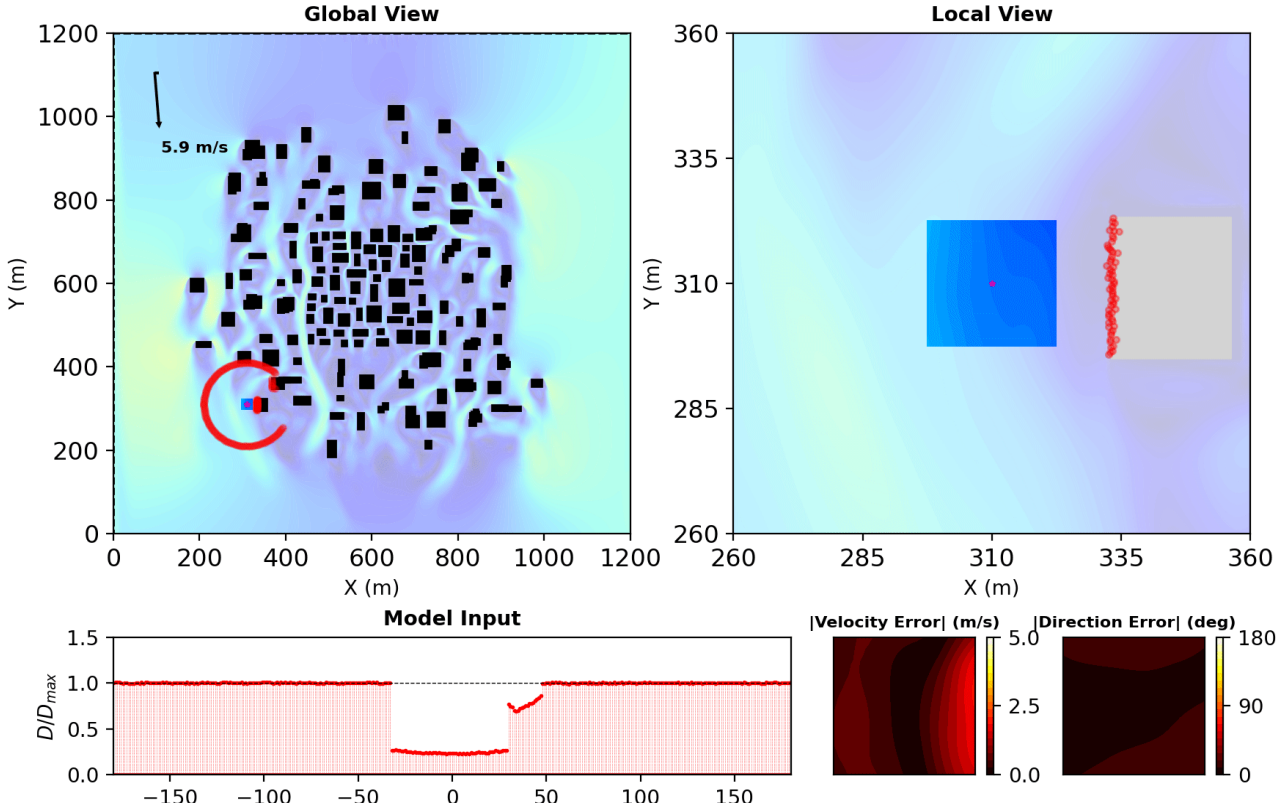
Feeding the DT beast: real time data assimilation and the optimal coverage problem



Left: Static source
Right: Moving source

White points: sensors
Red points: weighted centroid
Heatmap: CNWF solution based on sensor data
Contour: true FEM solution





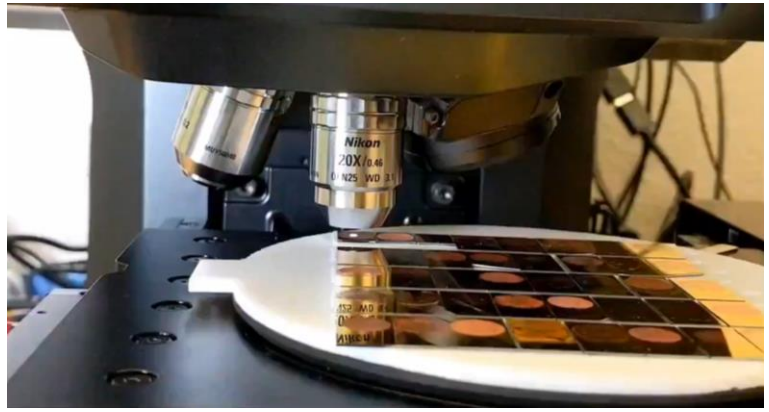
Left: Control scheme to identify physical model for source location for a stationary *(left)* and moving *(right)* source.

Right: Collaboration with robotics group at Upenn (Hsieh, Kumar) to sense physics based digital twins in an urban environment

Goal 2:
Integrating physics into AI-driven scientific discovery

Construct foundation models for material systems able to fuse multimodal data, embed physics and autonomously propose experiments

Sparse data in material discovery: high-throughput experiments and multimodality



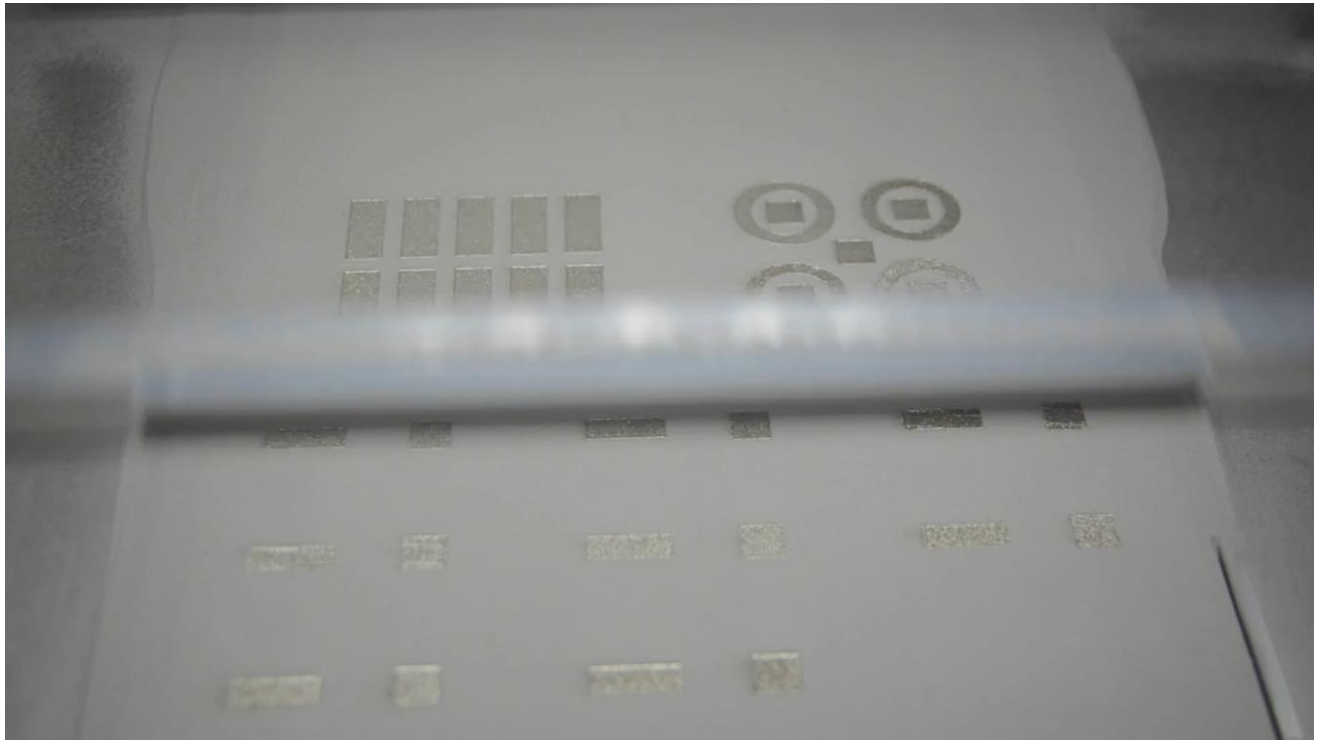
Even with high-throughput, data is small!

Conventional campaigns target a handful of bespoke experiments

High-throughput collect hundreds – far from the billions of datapoints in LLMS!

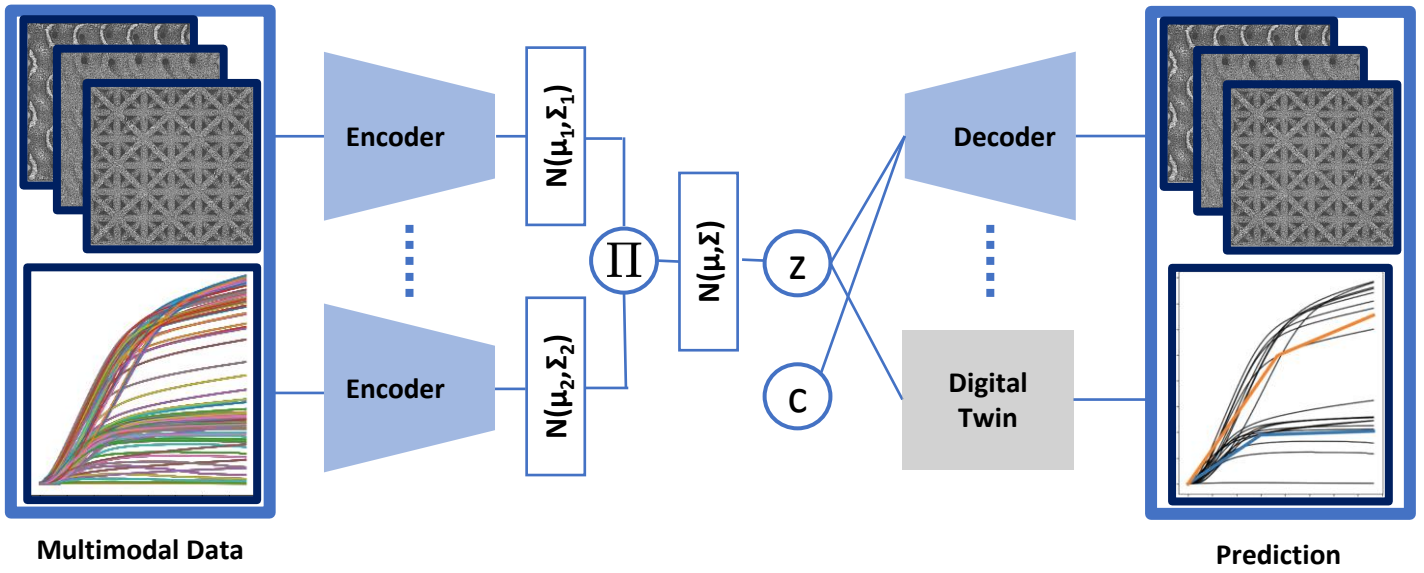
Can we compensate with multimodality?

AI-enabled thin film design:
Laser powderbed fusion
Physical vapor deposition
Electroplating

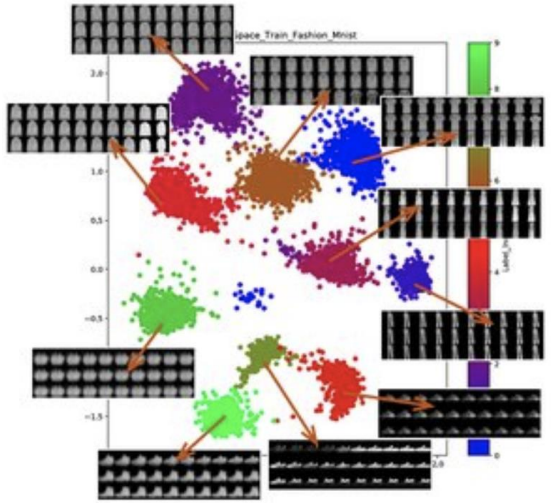


Process parameters: laser power, speed, path, powder composition
High-fidelity characterization: microscopy, XRF, XRD, TEM, SEM
Low-fidelity signals: light, sound, images, profilometry

Physics-informed multimodal autoencoder (PIMA)



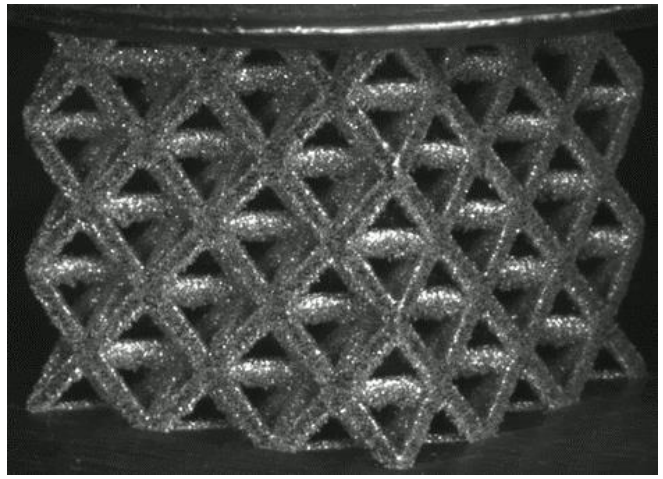
Informal Idea:
We discover a shared latent representation of data providing a Rosetta stone across modalities w/ uncertainty estimation

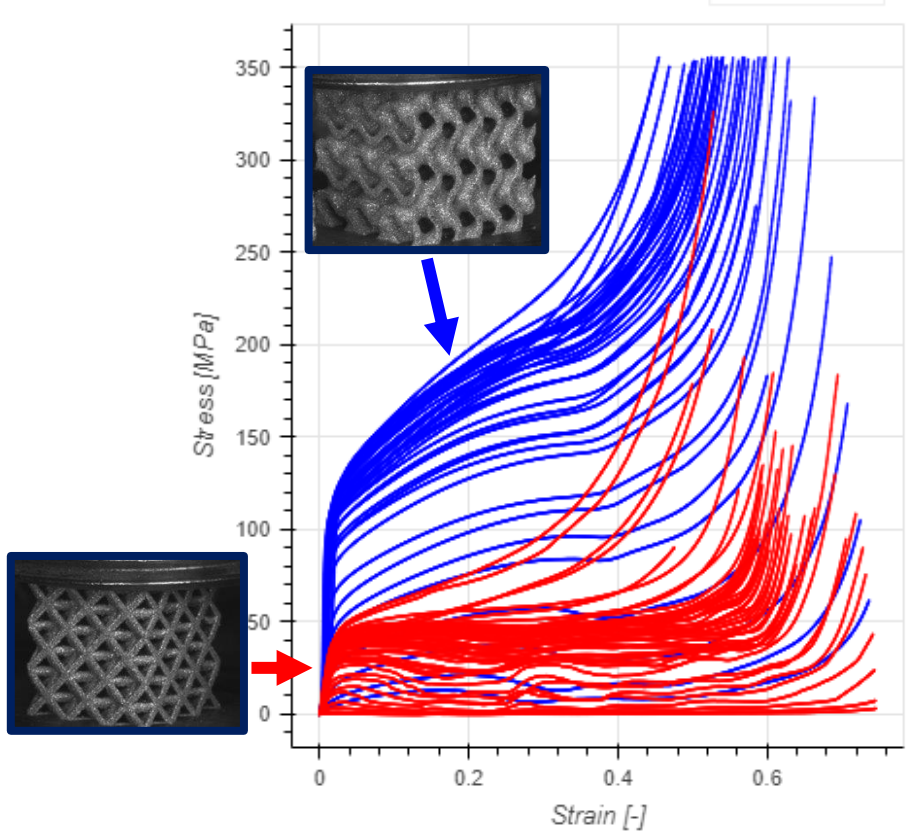


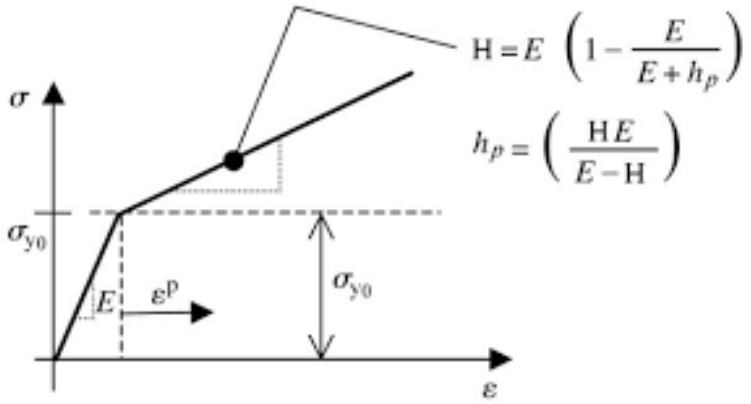
Details:

- Gaussian product distribution gives deep posterior embedding for each modality
- Gaussian mixture prior in latent space identifies populations in data across modalities
- *Closed form expressions* for ELBO – no Monte Carlo
- Supports Bayesian inference across modalities
- Fast training with EM

A simple multimodal dataset: images+uniaxial tension of metal additive lattices







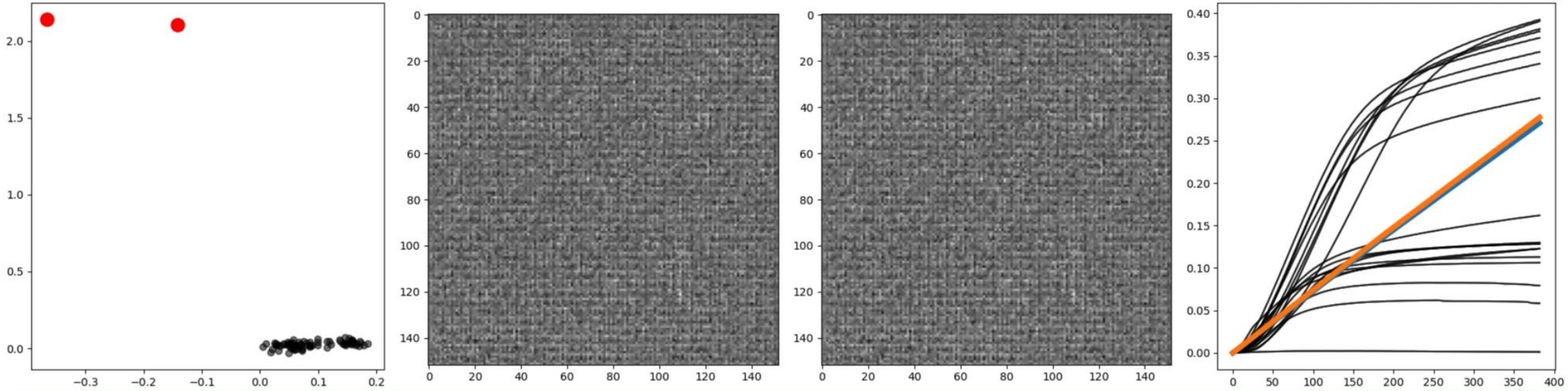
For historical lattice compression dataset:

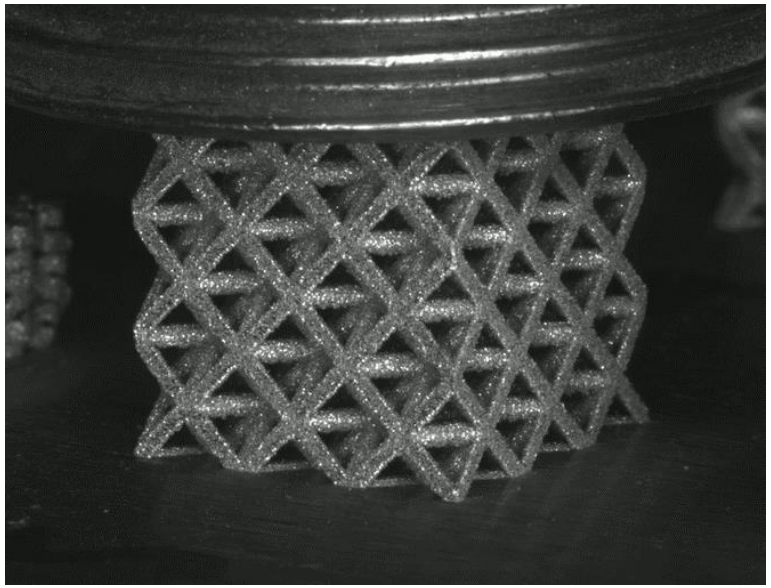
Modality 1: Images of microstructure prior to deformation

Modality 2: Uniaxial stress strain curve

Expert physics model: simple linear strain hardening model

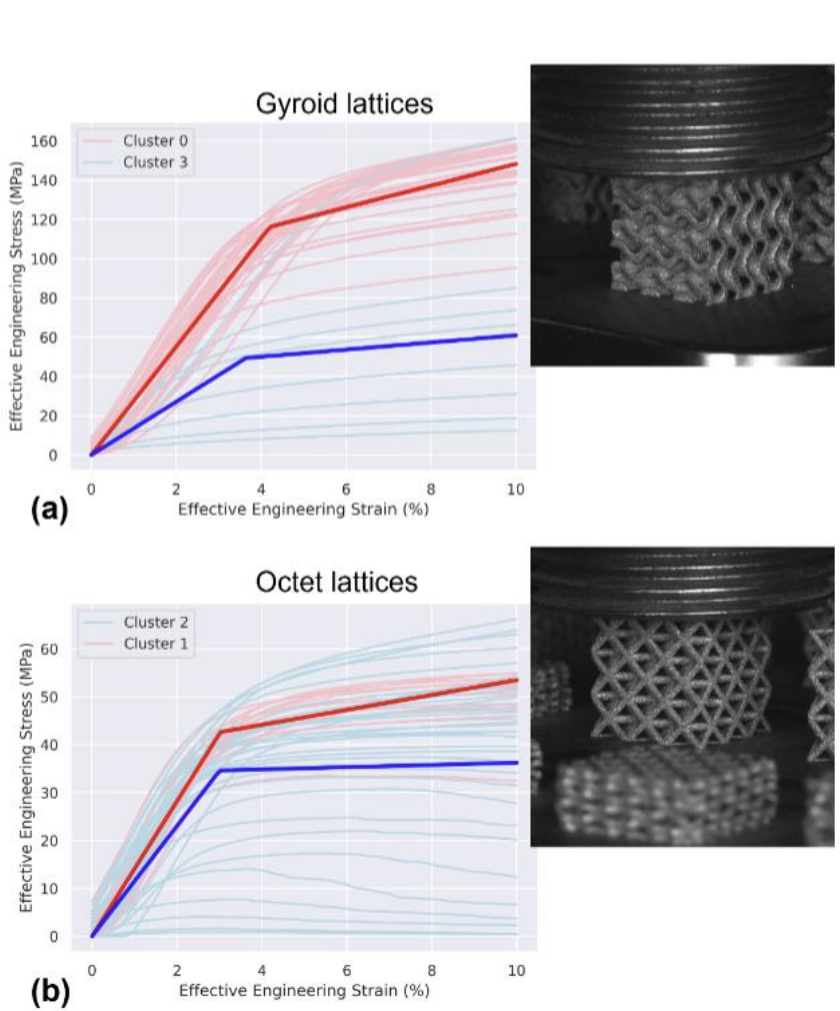
Example 1: Disentangling latent representations with physics

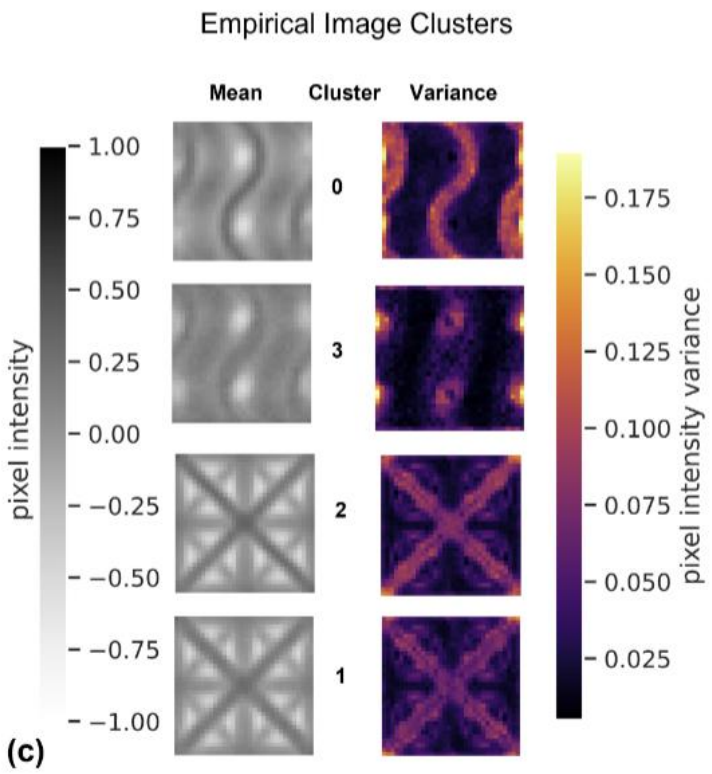


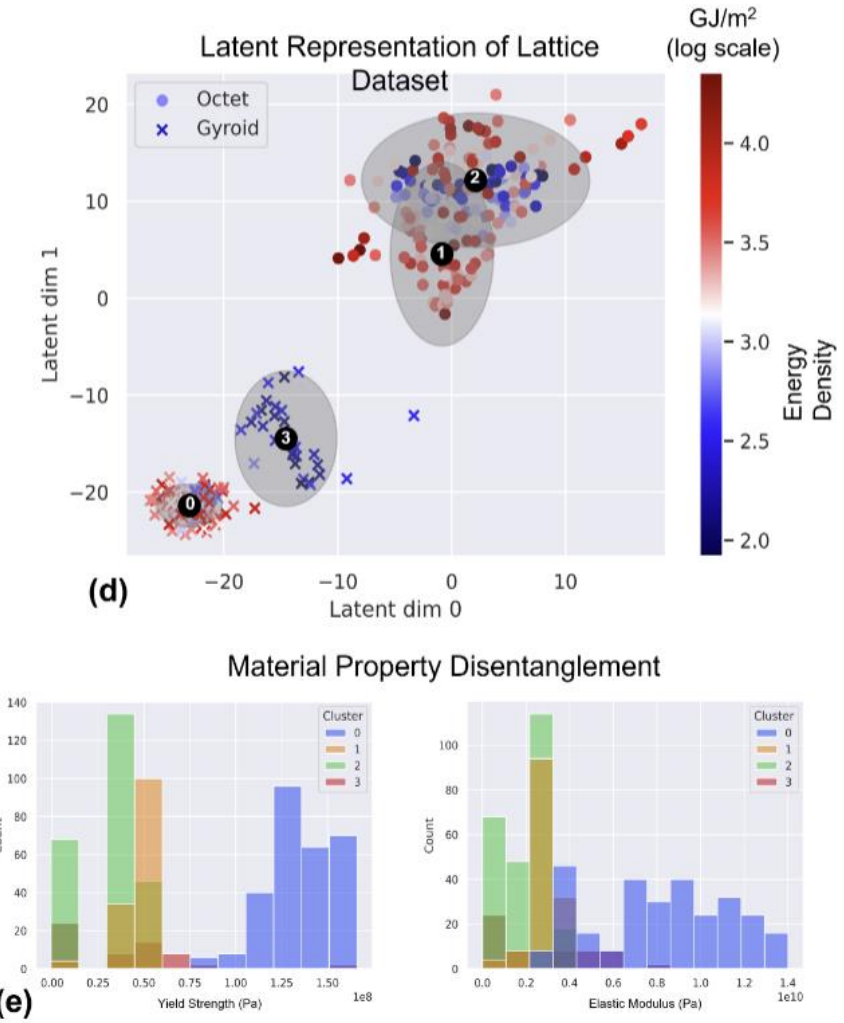


1. Images of lattices and stress/strain curves are disentangled in latent space
2. Once disentangled, images are calibrated to clusters
3. Once disentangled, expert models calibrate into two populations
4. **Impact:** Low-throughput uniaxial testing replaced w/ high-throughput imaging

Disentangling latent representations with physics



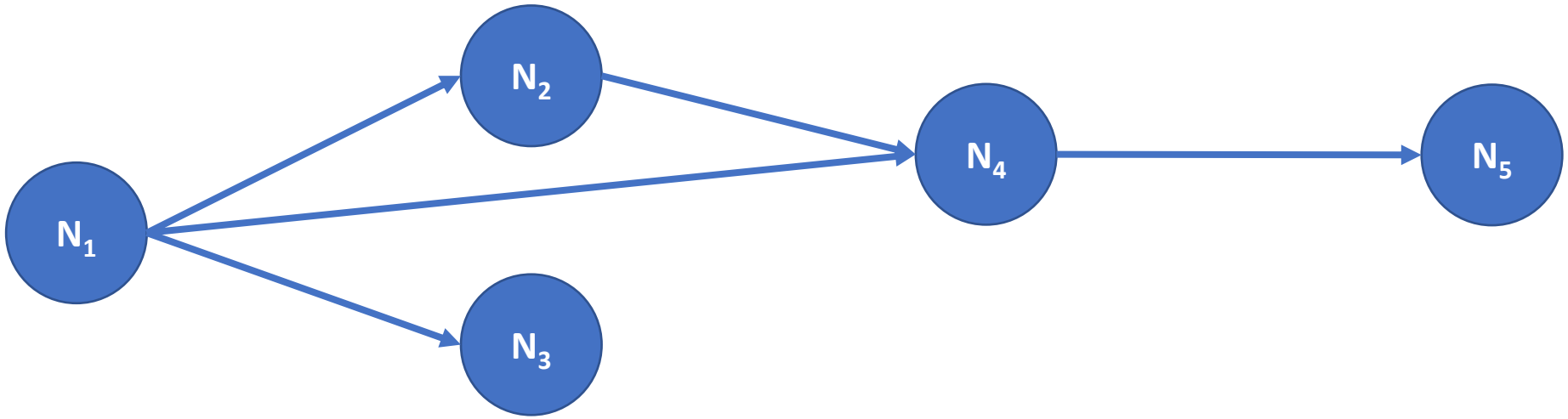




Physical model reveals qualitative regimes of performance, other modalities facilitate hypothesis generation for explainability

Trask, N., Martinez, C., Shilt, T., Walker, E., Lee, K., Garland, A., ... & Boyce, B. L. (2024). Unsupervised physics-informed disentanglement of multimodal materials data. *Materials Today*, *80*, 286-296.

Directed Acyclic Graphs encode causal relationships



Why DAGs?

- Preclude cyclic reasoning
- Suggest dependency structure
- Have causal interpretation

Structural Causal Decomposition

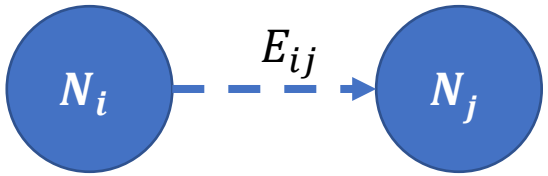
$$p(N) = \prod_{\ell} p(N_\ell | Pa(N_\ell))$$

Idea: replace categorical distribution Gaussian mixture prior with SCD

Causality: can use DAG-structured priors to reveal causal relationships?

$$E_{ij} = ReLU\left(tanh\frac{(B \cdot \mathcal{G}\xi)_{ij}}{\beta}\right)$$

E: directed adjacency matrix. $E_{ij} = p(N_i \to N_j)$
B: trainable metric (nonnegative)
$\mathcal{G}$: graph gradient operator
ξ: trainable node scores



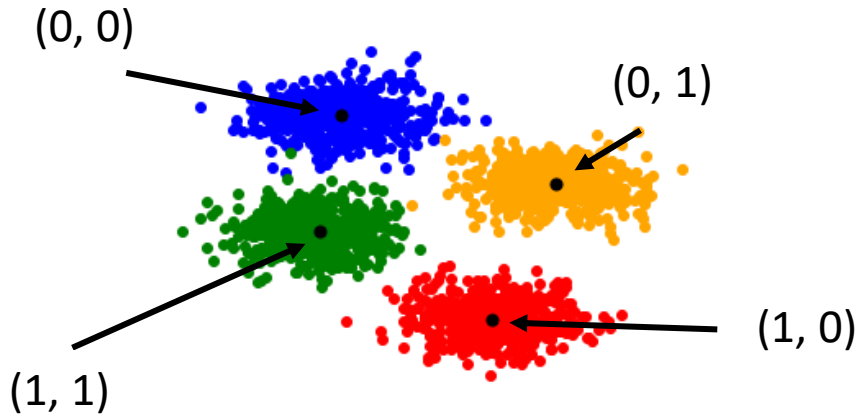
Theorem: $\lim_{\beta \to 0} E$ defines a DAG and can recover any DAG.

Proof sketch: $Curl \circ Grad = 0$, so E is curl-free and induces a DAG. Graph gradient recovers complete DAGs, and B allows recovery for any sub-DAG.

$$\text{ELBO} = \mathbb{E}_{q(Z,C|X)}\left[\log \frac{p(X,Z,C)}{q(Z,C|X)}\right]$$

X: input data
Z: latent space
C: Categorical for Gaussian Mixture

$$p(C) = p(N) = \prod_{\ell} p(N_\ell | Pa(N_\ell))$$

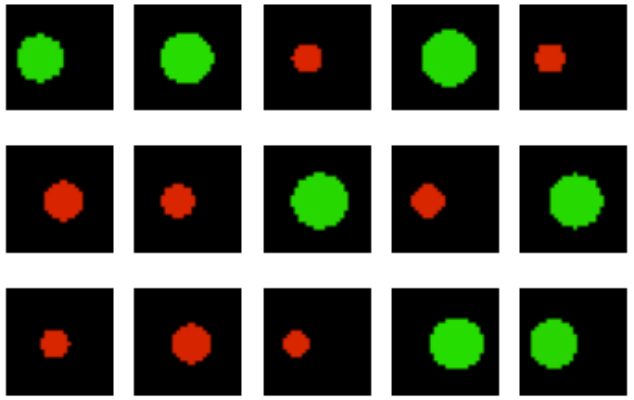


$$p(0,1) = p(N_i = 0)p\left(N_j = 1 \middle| N_i = 0\right)$$

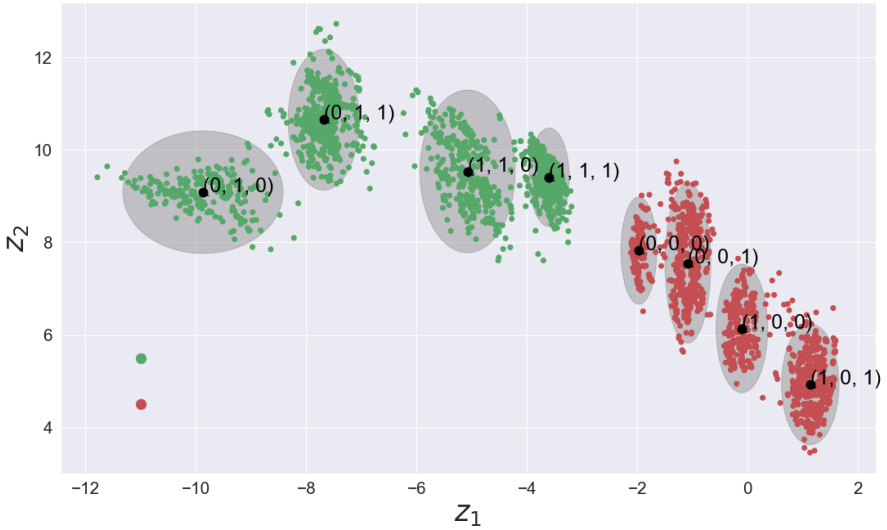
Causality: some synthetic toy results

Synthetic Circles Dataset

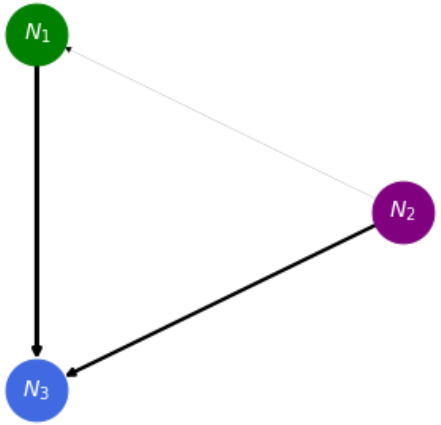
features: color, size, and shift



Results



Learned latent space



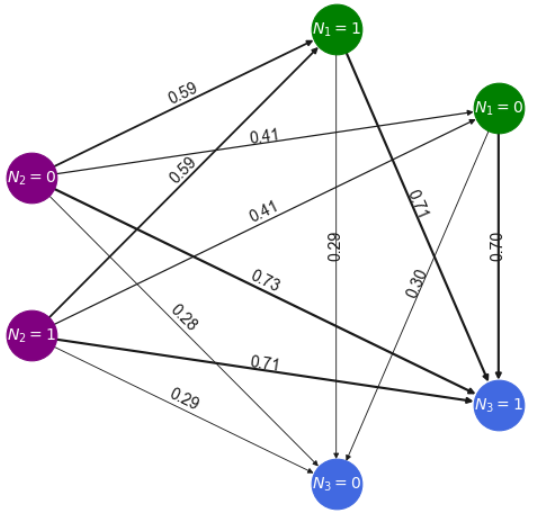
Obtain an embedding that shows that circle size (N1) and circle color (N2) determine the position of the circle (N3), without establishing a priori that N1-3 are features

E. Walker et al, “Flow-based parametrizations for DAG and feature discovery in scientific multimodal data”, Frontiers in Mechanical Engineering, 9/23/2024

Analysis

N_1: Size
N_2: Color
N_3: Shift

$$p(N) = p(N_2)p(N_1|N_2)p(N_3|N_1, N_2)$$



Edge weights are
$p(N_i = n\,|N_j = m)$

Acknowledgements & References

Structure preservation in digital twins

- Gruber, Anthony, Kookjin Lee, and Nathaniel Trask. "Reversible and irreversible bracket-based dynamics for deep graph neural networks." *Advances in Neural Information Processing Systems* 36 (2024).
- Jiang, S., Actor, J., Roberts, S. and Trask, N., 2024. A structure-preserving domain decomposition method for data-driven modeling. *arXiv preprint arXiv:2406.05571*. (accepted to special issue)
- Actor, J.A., Hu, X., Huang, A., Roberts, S.A. and Trask, N., 2024. Data-driven Whitney forms for structure-preserving control volume analysis. *Journal of Computational Physics*, *496*, p.112520.
- Trask, N., Huang, A. and Hu, X., 2022. Enforcing exact physics in scientific machine learning: a data-driven exterior calculus on graphs. *Journal of Computational Physics*, *456*, p.110969.

Multimodal and causal scientific discovery

- Trask, N., Martinez, C., Shilt, T., Walker, E., Lee, K., Garland, A., Adams, D.P., Curry, J.F., Dugger, M.T., Larson, S.R. and Boyce, B.L., 2024. Unsupervised physics-informed disentanglement of multimodal materials data. *Materials Today*, *80*, pp.286-296.
- Walker, Elise, Jonas A. Actor, Carianne Martinez, and Nathaniel Trask. "Causal disentanglement of multimodal data." *arXiv preprint arXiv:2310.18471* (2023).
- Walker, Elise, et al. "Flow-based parameterization for DAG and feature discovery in scientific multimodal data." *Frontiers in Mechanical Engineering* 10 (2024): 1408649.
- Walker, E., Trask, N., Martinez, C., Lee, K., Actor, J.A., Saha, S., Shilt, T., Vizoso, D., Dingreville, R. and Boyce, B.L., 2025. Unsupervised physics-informed disentanglement of multimodal data. *Foundations of Data Science*, *7*(1), pp.418-445.
- Boyce, Brad, et al. *BeyondFingerprinting: AI-guided discovery of robust materials & processes*. No. SAND2024-11708. Sandia National Lab.(SNL-NM), Albuquerque, NM (United States), 2024.

Collaborators

- **UPenn:** Brooks Kinch, Paris Perdikaris, Ben Schaffer, Ani Hsieh, Vijay Kumar, Spencer Folk
- **Tufts:** Xiaozhe Hu
- **SNL:** Andy Huang, Jonas Actor, Marshall Jiang, Anthony Gruber, Eric Cyr
- **PNNL:** Panos Stinis
- **PPPL:** Michael Churchill, Nate Ferraro
- **Caltech:** Houman Owhadi
- **Stanford:** Daniel Tartakovsky, Adrienne Propp
- **Boston University:** Emma Lejeune
- **USF:** Ivan Oleynik

SEA-CROGS

https://www.pnnl.gov/projects/sea-crogs