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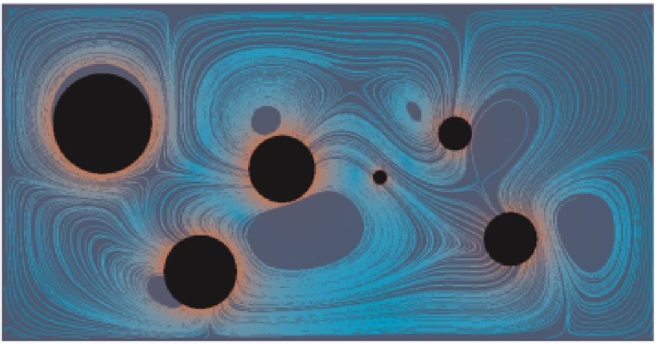

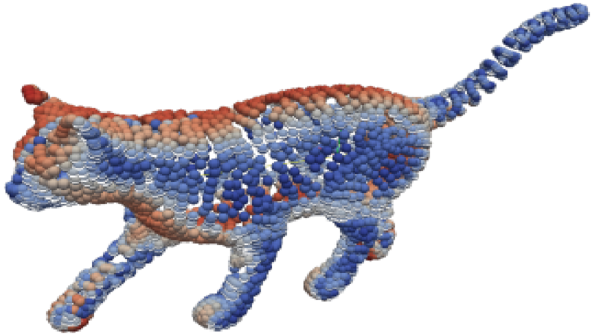

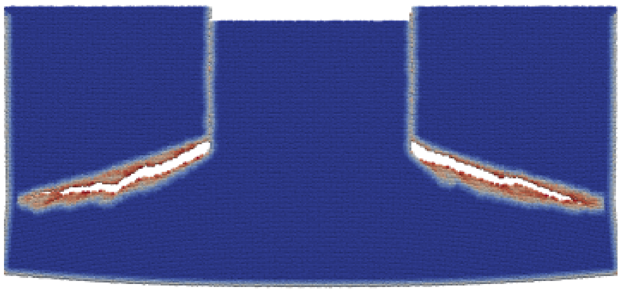

Discovery of Whitney Forms

for construction of structure preserving data-driven models

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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<u>Problem:</u> Applying AI/ML data-driven models in high-consequence engineering applications require guarantees to establish notions of trust

(1) How to provide convergence guarantees

Designing architectures + optimizers that provide notion of “grid convergence” critical for verification and validation

(2) How to build surrogates that guarantee stability, physical realizability + generalizability?

Unification of mimetic PDE discretization, algebraic topology and inverse problems

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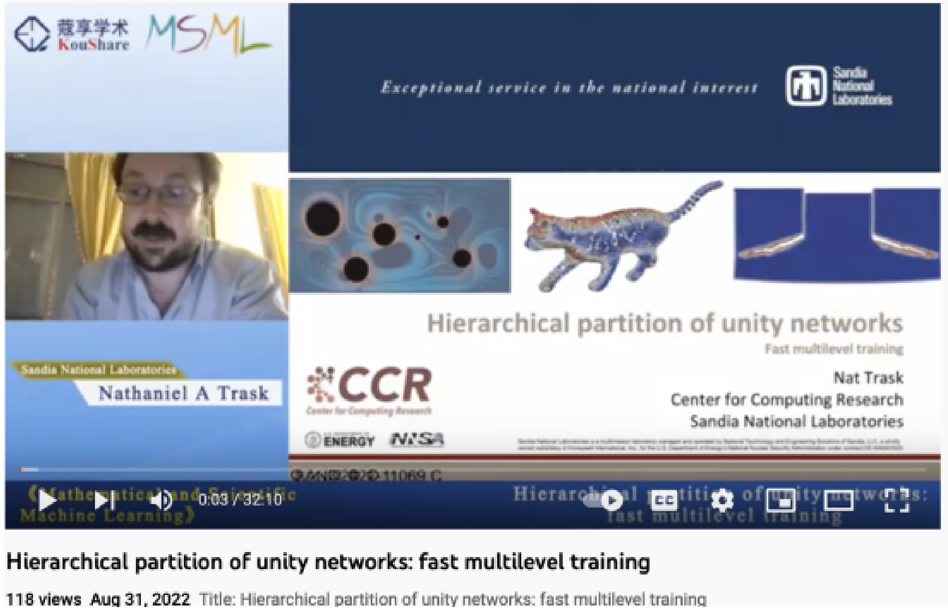
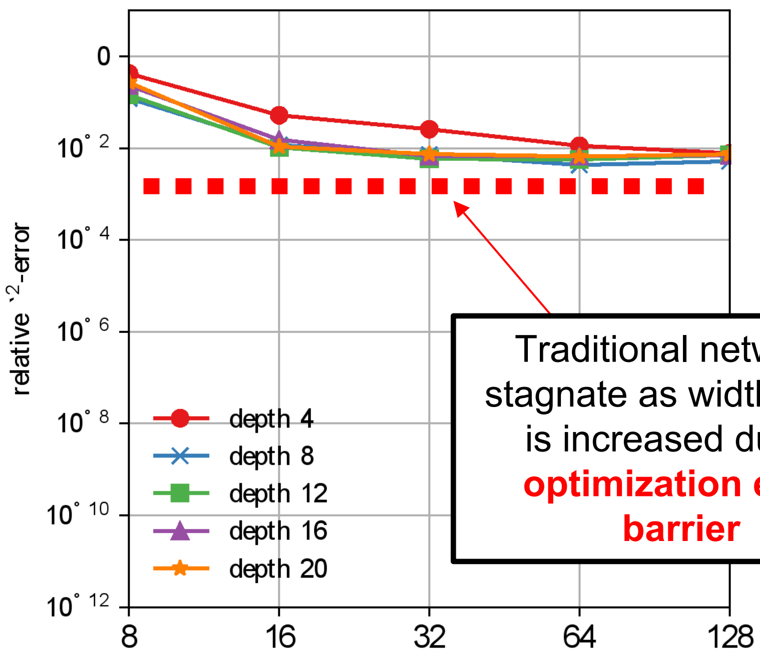
SciML as reliable as traditional FEM

Todays talk will focus on structure preservation, but partition-of-unity turns out to address first issue as well



1. *Cyr, Eric C., et al. "Robust training and initialization of deep neural networks: An adaptive basis viewpoint." Mathematical and Scientific Machine Learning. PMLR, (2020).*
2. *Patel, Ravi G., et al. "A block coordinate descent optimizer for classification problems exploiting convexity." arXiv preprint arXiv:2006.10123 (2020). AAAI-MLPS*
3. *Lee, Kookjin, et al. "Partition of unity networks: deep hp-approximation." arXiv preprint arXiv:2101.11256 (2021) AAAI -MLPS*
4. *Trask, N., Gulian, M. "Probabilistic partition of unity networks: clustering based deep approximation."*
5. ***Trask, Henriksen, Martinez, Cyr "Hierarchical partition of unity networks: fast multilevel training."*** **Accepted to MSML2022, preprint on Researchgate**
6. Armstrong, E., Hansen, M.A., Knaus, R.C., Trask, N.A., Hewson, J.C. and Sutherland, J.C., 2022. Accurate Compression of Tabulated Chemistry Models with Partition of Unity Networks. Combustion Science and Technology, pp.1-18.

How do DNNs work? The problem with universal approximation



Traditional networks stagnate as width/depth is increased due to **optimization error barrier**

Theorem 2. *Let σ be any continuous sigmoidal function. Then finite sums of the form*

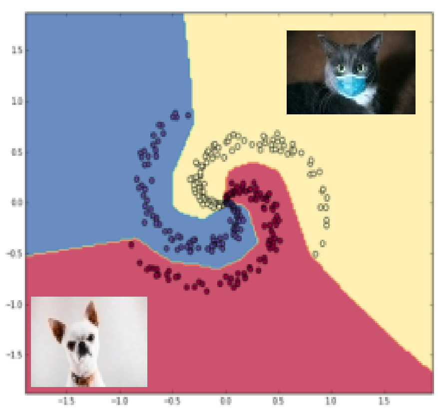
$$G(x) = \sum_{j=1}^{N} \alpha_j \sigma(y_j^T x + \theta_j)$$

are dense in $C(I_n)$. *In other words, given any* $f \in C(I_n)$ *and* $\varepsilon > 0$, *there is a sum,* $G(x)$, *of the above form, for which*

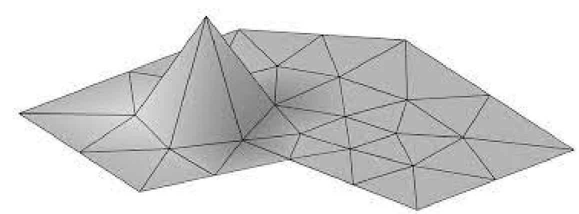
$$|G(x) - f(x)| < \varepsilon \quad \text{for all} \quad x \in I_n.$$

Recent work (Opschoor 2020) establishes more constructive interpretation

Emulation of partition of unity



Emulation of monomials on each partition



Opschoor, J.A., Petersen, P.C. and Schwab, C., 2020. Deep ReLU networks and high-order finite element methods. *Analysis and Applications*, *18*(05), pp.715-770.

Partition of unity

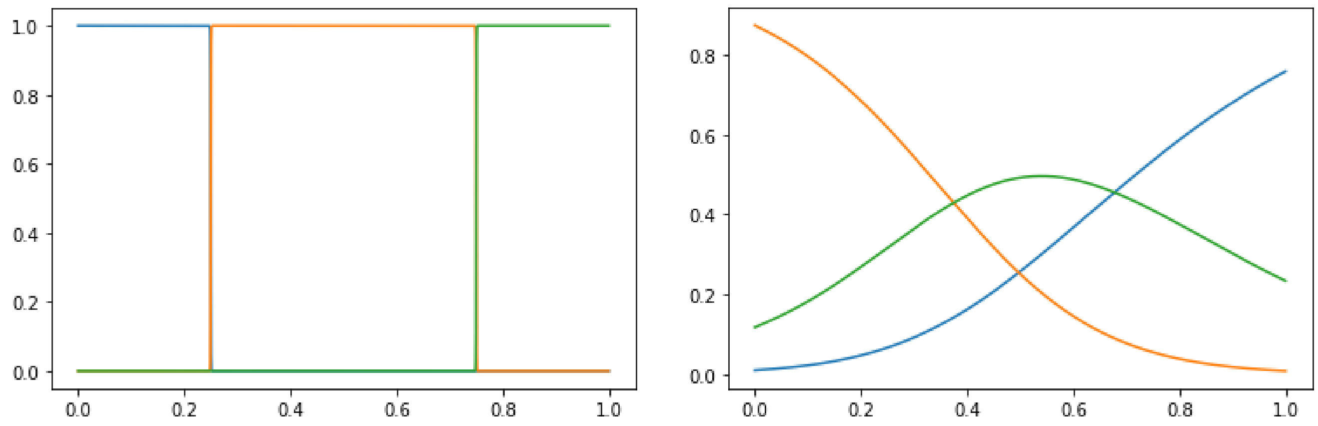
Definition: *Partition of unity (POU)*
A collection of functions $\{\phi_i\}_{i=1,\dots,N}$ satisfying

- $\phi_i > 0$
- $\sum_i \phi_i = 1$

Key role:
Localizing approximation
Identifying charts of atlas

Example:
Consider a partition of $\Omega \subset \mathbb{R}^d$ into disjoint cells $\Omega = \bigcup_i C_i$. Then the indicator functions $\phi_i(x) = \mathbb{1}_{C_i}(x)$ form a POU.

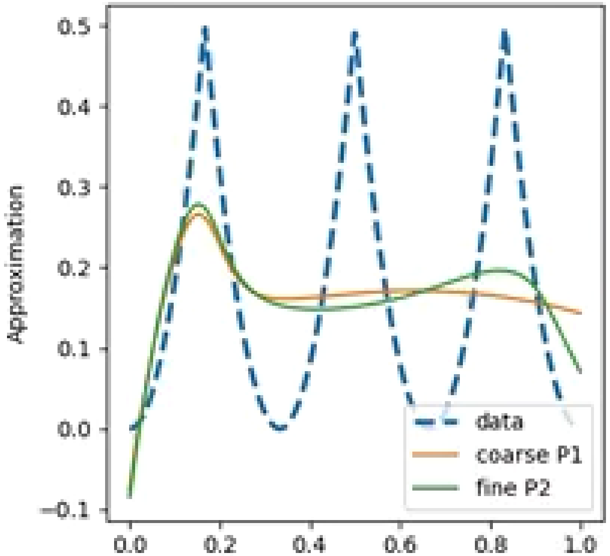
$$\phi_i(x) = \text{softmax} \circ NN(x;\theta)$$

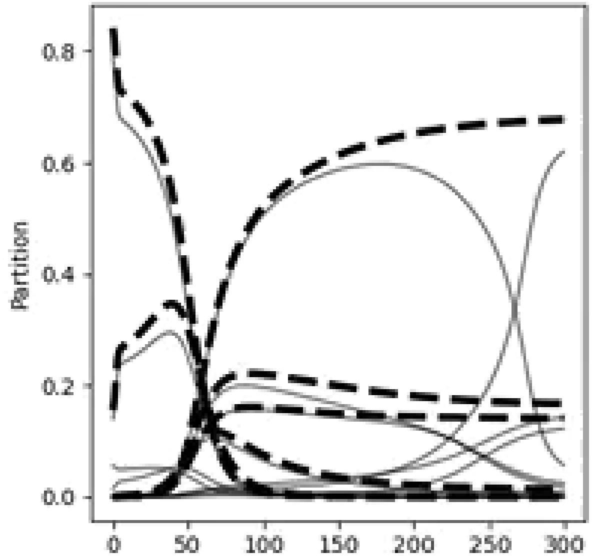


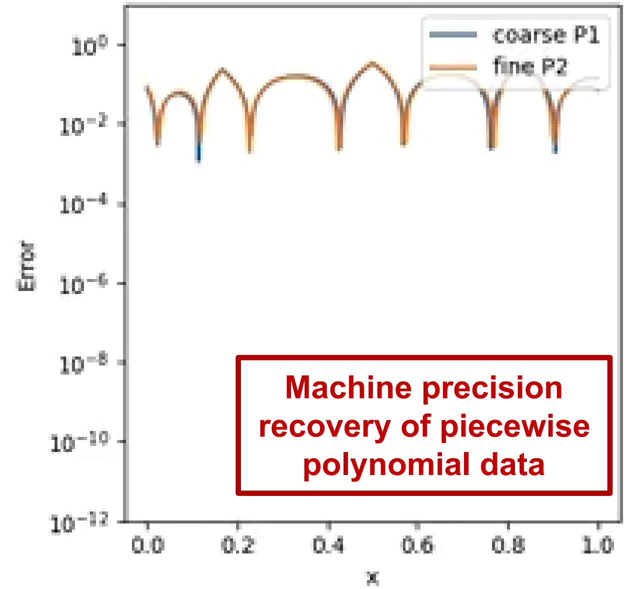
POU corresponding to Cartesian mesh vs learnable POU with non-disjoint support

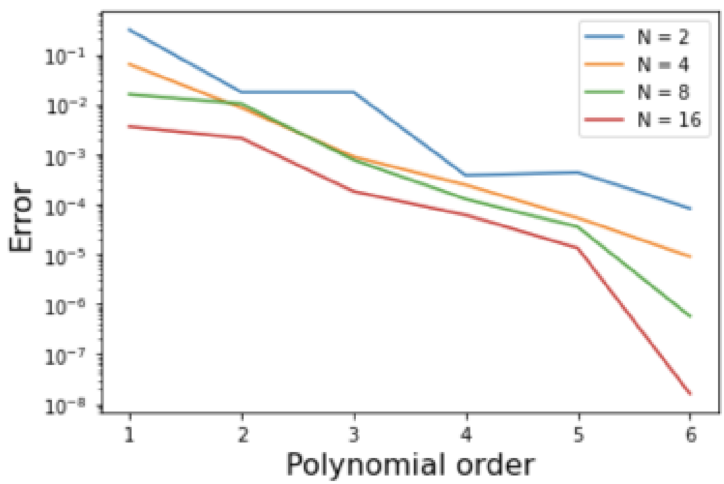
Fast multilevel deep approximation

All results shown for a single set of hyperparameters!









Spectral convergence for smooth data

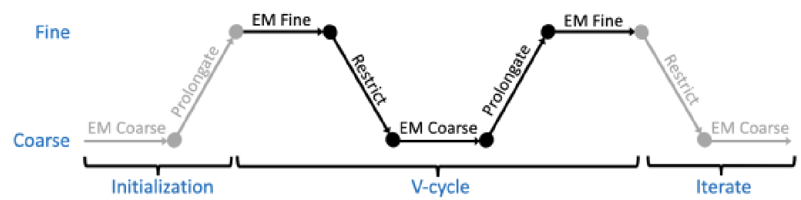


Figure 1: A two-level "V-cycle" for training the hierarchical POU networks. For details in pseudo-code see Algorithm 4.1, where the figure depicts the case $S_{pre} = 0$, $S_{coarse} = 1$ and $S_{post} = 1$.

***Trask, Henriksen, Martinez, Cyr "Hierarchical partition of unity networks: fast multilevel training."* MSML2022**

For physics: Learning primal/dual de Rham complexes

We first briefly recall some definitions and basic results from exterior algebra and differential forms, first introducing the abstract framework before specializing to the finite element exterior calculus (FEEC) setting. A *graded vector space* is a vector space V that can be expressed as $V = \bigoplus_{k=-\infty}^{\infty} V_k$, where V_k are subspaces. Introducing the linear map $\partial_k : V_k \mapsto V_{k-1}$ called the *boundary operator*, with the property $\partial_k \circ \partial_{k+1} = 0$, we define a *chain complex* as follows

$$\cdots \longrightarrow V_{k+1} \xrightarrow{\partial_{k+1}} V_k \xrightarrow{\partial_k} V_{k-1} \longrightarrow \cdots ,$$

where we refer to elements $\Omega \in V_k$ as *chains* and associate with each a real-valued *cochain* $\omega \in V^k$, adopting the convention of using subscripts to denote sets of chains (V_k) and superscripts for sets of cochains (V^k). Given *coboundary* maps $\mathsf{d}^k : \Lambda^k(\Omega) \mapsto \Lambda^{k+1}(\Omega)$ satisfying $\mathsf{d}^k \circ \mathsf{d}^{k-1} = 0$, and *codifferential maps* $d^k : V^k \mapsto V^{k+1}$ satisfying $d^{k-1} \circ d^k = 0$, we finally arrive at the following primal and dual *cochain complexes*.

$$\cdots \longrightarrow V^{k-1} \xrightarrow{\mathsf{d}^{k-1}} V^k \xrightarrow{\mathsf{d}^k} V^{k+1} \longrightarrow \cdots \tag{1}$$

$$\cdots \longleftarrow V^{k-1} \xleftarrow[d^{k-1}]{} V^k \xleftarrow[d^k]{} V^{k+1} \longleftarrow \cdots \tag{2}$$

Example: continuous de Rham complex in 3D

$$0 \longrightarrow H_0(\mathrm{grad}, \Omega) \xrightarrow{\mathrm{grad}} H_0(\mathrm{curl}, \Omega) \xrightarrow{\mathrm{curl}} H_0(\mathrm{div}, \Omega) \xrightarrow{\mathrm{div}} L^2(\Omega) \longrightarrow 0.$$

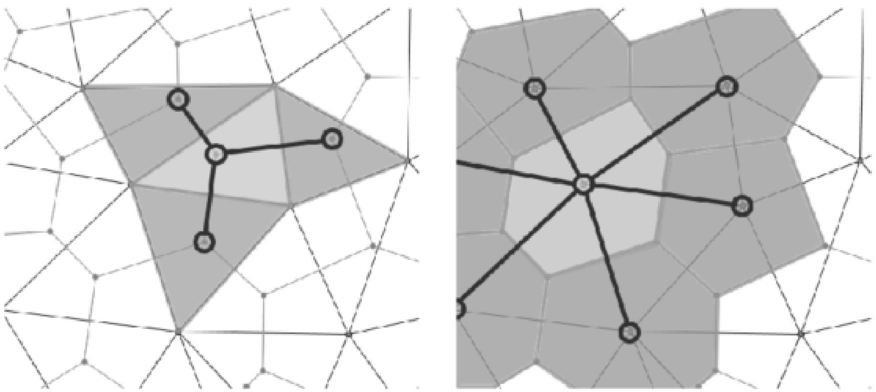
Graph EC, DEC, FEEC… and they're all related

Primal Complex

$$\cdots \longrightarrow V^{k-1} \xrightarrow{\mathrm{d}^{k-1}} V^{k} \xrightarrow{\mathrm{d}^{k}} V^{k+1} \longrightarrow \cdots$$

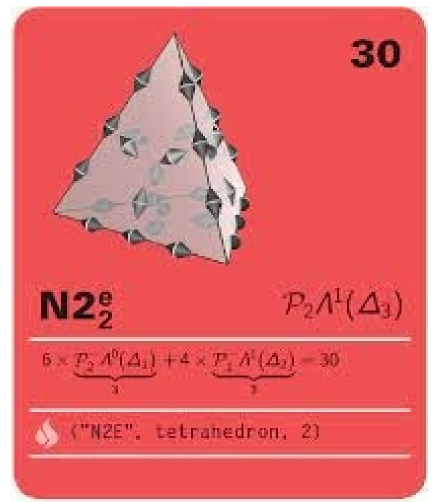
Dual Complex

$$\cdots \longleftarrow V^{k-1} \xleftarrow[d^{k-1}]{} V^{k} \xleftarrow[d^{k}]{} V^{k+1} \longleftarrow \cdots$$



(a) (b)

Discrete exterior calculus: a framework for computer simulation and geometric analysis based on advanced mathematical concepts
•R. Torres, Carlos R. S. Camilo (2016)Computer Science



D. N. Arnold and A. Logg, Periodic Table of the Finite Elements, SIAM News, vol. 47 no. 9, November 2014.

DEC/graph

DOFs on differential forms of primal/dual mesh/graph, using Stokes theorem to derive discrete differential operators

FEEC

Primal FEM space interpolating differential forms, inducing dual space through duality

Previous work with machine learnable graph calculus

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$$
\begin{array}{ccccccccccc}
C^0 & \xleftarrow[\mathsf{d}_0^*]{} & C^1 & \xleftarrow[\mathsf{d}_1^*]{} & C^2 & \xleftarrow[\mathsf{d}_2^*]{} & C^3 & \xleftarrow[\mathsf{d}_3^*]{} & \cdots & \xleftarrow[\mathsf{d}_{d-1}^*]{} & C^d \\
\downarrow \mathbf{D}_0^{-1} & & \downarrow \mathbf{D}_1^{-1} & & \downarrow \mathbf{D}_2^{-1} & & \downarrow \mathbf{D}_3^{-1} & & & & \downarrow \mathbf{D}_d^{-1} \\
C^0 & \overset{\delta_0^*}{\underset{\delta_0}{\leftrightarrows}} & C^1 & \overset{\delta_1^*}{\underset{\delta_1}{\leftrightarrows}} & C^2 & \overset{\delta_2^*}{\underset{\delta_2}{\leftrightarrows}} & C^3 & \overset{\delta_3^*}{\underset{\delta_3}{\leftrightarrows}} & \cdots & \overset{\delta_0^*}{\underset{\delta_{d-1}}{\leftrightarrows}} & C^d \\
\downarrow \mathbf{B}_0 & & \downarrow \mathbf{B}_1 & & \downarrow \mathbf{B}_2 & & \downarrow \mathbf{B}_3 & & & & \downarrow \mathbf{B}_d \\
C^0 & \xrightarrow{\mathsf{d}_0} & C^1 & \xrightarrow{\mathsf{d}_1} & C^2 & \xrightarrow{\mathsf{d}_2} & C^3 & \xrightarrow{\mathsf{d}_3} & \cdots & \xrightarrow{\mathsf{d}_{d-1}} & C^d
\end{array}
$$

$$\mathbf{B}_1\delta_0 = CURL\mathbf{B}_0, \quad \mathbf{B}_2\delta_1 = DIV\mathbf{B}_1,$$

$$\delta_0^*\mathbf{D}_0^{-1} = CURL^*\mathbf{D}_1^{-1}, \quad \mathbf{D}_1^{-1}\delta_1^* = GRAD^*\mathbf{D}_2^{-1}$$

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*

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

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*

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

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

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

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

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

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* $H^k = \ker(\mathsf{d}_k)/\mathrm{im}(\mathsf{d}_{k-1})$.

KEY IDEA:
Augment graph exterior calculus with machine learnable metric information ***B/D*** *which can be used to obtain Hodge Laplacians and fit to data*

"Enforcing exact physics in scientific machine learning: a data-driven exterior calculus on graphs." Trask, et al. JCP 2022

Using DDEC to discover structure preserving surrogates

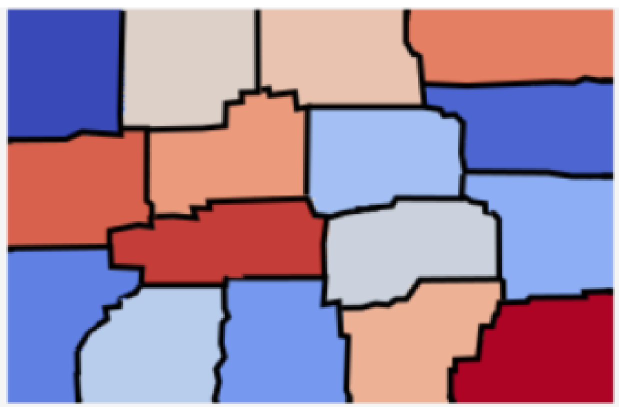
Structure preserving trainable exterior derivatives

$$d_0^\star \mathbf{F} = f$$

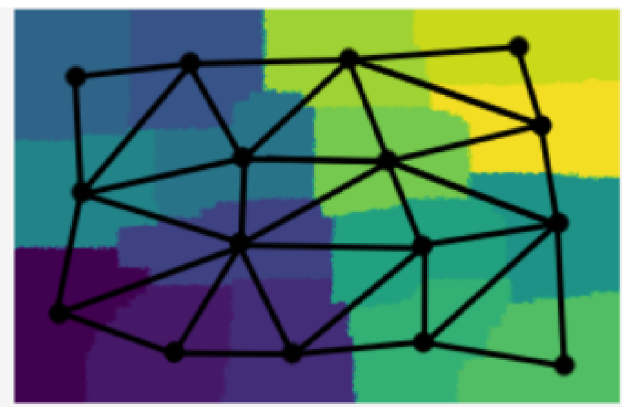
$$\mathbf{F} + \xi d_0 \phi + \mathcal{N}_\eta(\phi) = 0$$

Black box NN flux

High-fidelity PDE solution



Post-process onto a coarsened graph



Average over partitions to obtain training data

General optimization problem

Fluxes: $$\mathbf{w}_{k+1} = \mathsf{d}_k \mathbf{u}_k + \epsilon \mathcal{N}\mathcal{N}(\mathsf{d}_k \mathbf{u}_k; \xi),$$

Conservation: $$\mathsf{d}_{k-1}\ \mathsf{d}^*_{k-1} \mathbf{u}_k + \mathsf{d}^*_k \mathbf{w}_{k+1} = \mathbf{f}_k .$$

$$\Rightarrow \quad a(\mathbf{v}, \mathbf{u}; \mathbf{B}, \mathbf{D}) + N_{\mathbf{v}}[\mathbf{u}; \xi] = b(\mathbf{v})$$

Invertible bilinear form

Nonlinear perturbation

If we can fit the model to data while imposing equality constraint, then during training we restrict to manifold of solvable models preserving physics

$$\underset{\mathbf{B},\mathbf{D},\xi}{\operatorname{argmin}}, ||\mathbf{w} - \mathbf{w}_{\text{data}}||^2$$

$$\text{such that } \mathcal{L}[\mathbf{w}, \mathbf{u}; \mathbf{B}, \mathbf{D}, \xi] = 0$$

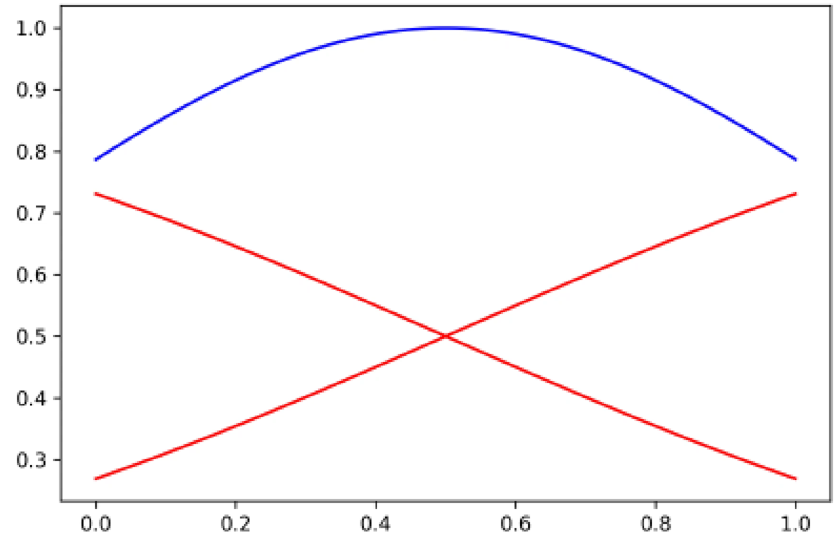
Theorem 3.6. *The equation (24) has at least one solution $\mathbf{u}_k \in \mathbb{V}$ satisfies*

$$\|\mathbf{u}_k\| \leq \frac{\|\mathbf{f}\|}{(C_p - C_N)}. \qquad (26)$$

Can we connect to FEEC to **discover** graph?

Red: POU on cells
Blue: Boundary of POUS

In limit of disjoint partitions, want to recover oriented Dirac distribution



$$\int_c \nabla \cdot \mathbf{u} dx = \int_{f \in \partial c} \mathbf{u} \cdot d\mathbf{A}$$

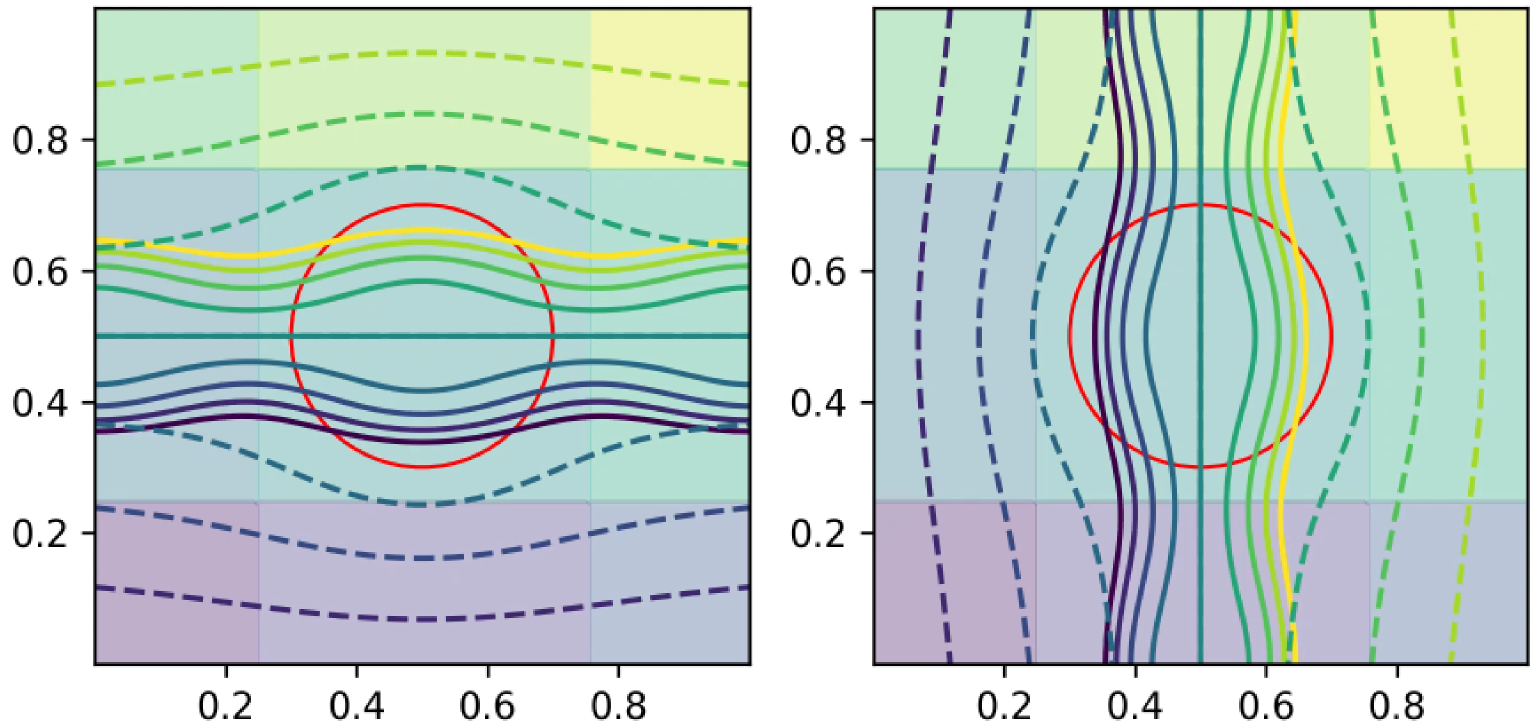
POUs generalize cell

Defining boundary operator provides exterior derivative

IDEA:

Use Whitney forms to learn physically relevant control volumes which best describe physics

Before we get in the weeds – what we're building toward



Obtain a finite element with microstructure embedded in terms of local conservation balances, **bridging geometric and graph perspective**

Whitney forms defining data-driven differential forms

- Let $\psi_i = \phi_i$. Define a function space $V_0 = \{\sum_i c_i \psi_i(x) \,|\, c_i \in \mathbb{R}^{N_0}\}$.
- Integrating by parts we obtain

$$
\begin{aligned}
\int_\Omega \psi_i \nabla \cdot \mathbf{u} &= -\int_\Omega \nabla \phi_i \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA \\
\text{Multiply by } 1 = \textstyle\sum_j \phi_j \qquad &= -\sum_j \int_\Omega \phi_j \nabla \phi_i \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA \\
\text{Add } 0 = \textstyle\sum_j \nabla \phi_j \qquad &= \sum_{j \neq i} \int_\Omega (\phi_i \nabla \phi_j - \phi_j \nabla \phi_i) \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA \\
&= \sum_{j \neq i} \int_\Omega \psi_{ij} \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA
\end{aligned}
$$

where $\psi_{ij} = \phi_i \nabla \phi_j - \phi_j \nabla \phi_i$, and we note that $\psi_{ij} = -\psi_{ji}$.

Compare to: $V_i \nabla \cdot \mathbf{u}_i = \sum_j \mathbf{A}_{ij} \cdot \mathbf{u}_{ij}$

Extensions to de Rham complex on arbitrary manifolds

Replace IBP with Leibniz rule:

$$\int_\Omega (d\omega_k) \wedge \omega_l = (-1)^{k+1} \int_\Omega \omega_k \wedge (d\omega_l) + \int_{\partial\Omega} \operatorname{tr} \omega_k \wedge \operatorname{tr} \omega_l$$

Inductively define Whitney form shape functions by mimicking construction:

$$\psi^k_{j_0 \cdots j_k} = k! \sum_{i=0}^{k} (-1)^i \phi_{j_i} d\phi_{j_0} \wedge \cdots \wedge \widehat{d\phi_{j_i}} \wedge \cdots \wedge d\phi_{j_k}$$

Obtain discrete "differential form" DOFs that induce coboundary operator:

$$U_{j_0 \cdots j_{k+1}} = \int_\omega u \wedge \psi^{k+1}_{j_0 \cdots j_{k+1}}$$

$$D_k(U)_{j_0 \cdots j_k} = (-1)^{n-1} \sum_{j_{k+1} \neq j_0, \cdots, j_k} U_{j_0 \cdots j_{k+1}} + \int \operatorname{tr} u \wedge \operatorname{tr} \psi^k_{j_0 \cdots j_k}$$

Preserve exact sequence property to induce de Rham complex:

$$D_k \circ D_{k-1}(U)_{j_0 \cdots j_{k-1}} = \int_\Omega d(du) \wedge \ \phi^k_{j_0 \cdots j_k} = 0$$

Learning Whitney forms induces a graph complex

Given discrete operators

$$DIV(U)_i := \sum_{j \neq i} U_{ij}, \quad U_{ij} = \int_\Omega \psi_{ij} \cdot \boldsymbol{u}, \ \forall \boldsymbol{u} \in H_0(\text{div})$$

$$CURL(U)_{ij} := \sum_{k \neq i,j} U_{ijk}, \quad U_{ijk} = 2 \int_\Omega \psi_{ijk} \cdot \boldsymbol{u}, \ \forall \boldsymbol{u} \in H_0(\text{curl})$$

$$GRAD(U)_{ijk} := \sum_{l \neq i,j,k} U_{ijkl}, \quad U_{ijkl} = 6 \int_\Omega \psi_{ijkl}\, u, \ \forall u \in H_0(\text{grad})$$

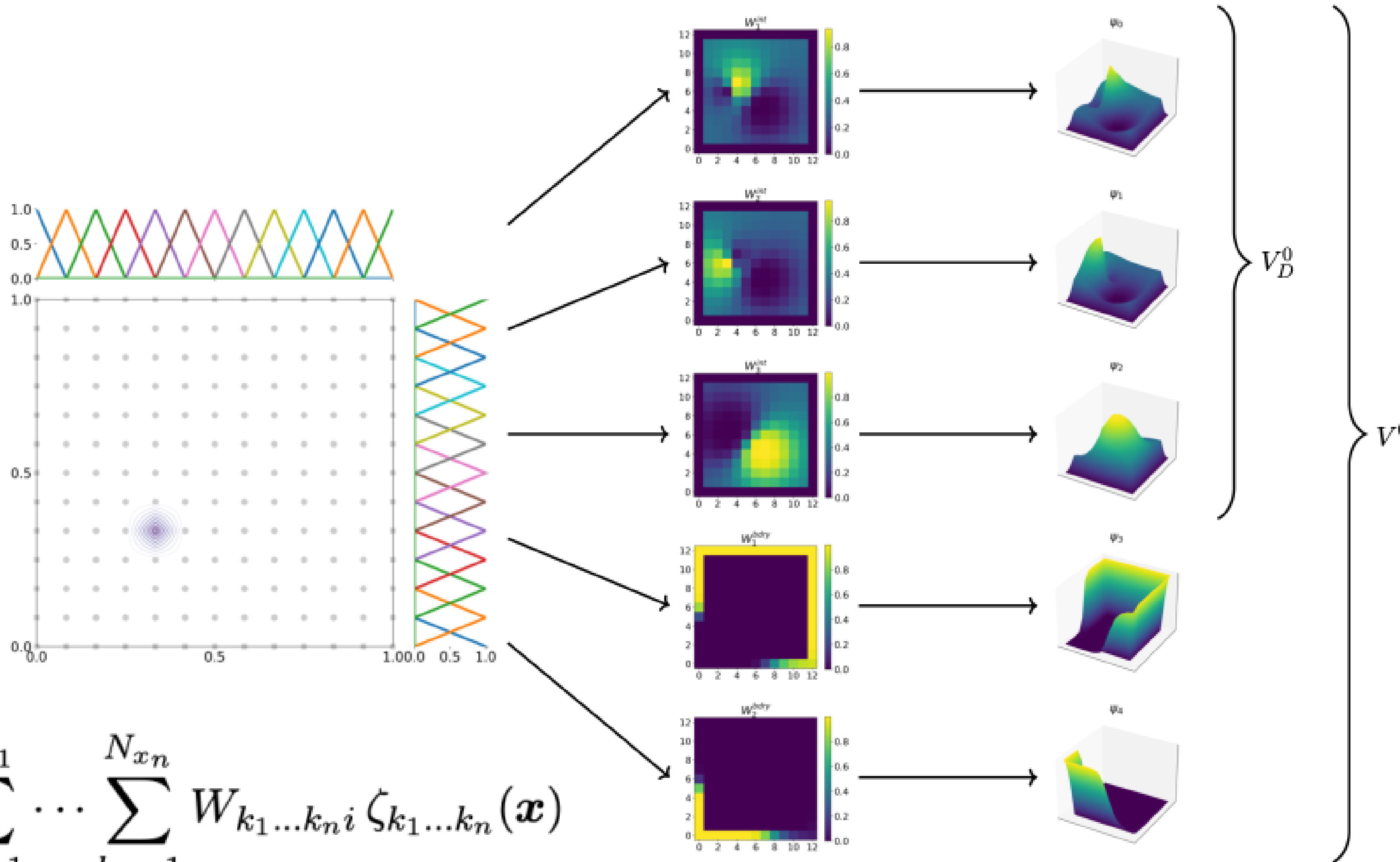
We obtain the expression unifying all 3 perspectives

$$\text{DIV} = \delta_0^T \mathbf{M}_1, \quad \text{CURL} = 2\, \delta_1^T \mathbf{M}_2, \quad \text{GRAD} = 6\, \delta_2^T \mathbf{M}_3$$

Exterior derivative (DEC) — **Graph coboundary** — **FEEC mass matrix**

$$(\mathbf{M}_1)_{(ij),(ab)} = (\psi_{ab}, \psi_{ij}), \ (\mathbf{M}_2)_{(ijk),(abc)} = (\psi_{abc}, \psi_{ijk}), \text{ and } (\mathbf{M}_3)_{(ijkl),(abcd)} = (\psi_{abcd}, \psi_{ijkl})$$

Need POU architecture supporting exact quadrature



$$\phi_i(\boldsymbol{x}) = \sum_{k_1=1}^{N_{x_1}} \cdots \sum_{k_n=1}^{N_{x_n}} W_{k_1 \dots k_n i}\, \zeta_{k_1 \dots k_n}(\boldsymbol{x})$$

$$\mathbf{W}_{(n+1)} = \begin{bmatrix} \mathbf{W}^{\text{int}}_{(n+1)} & 0 \\ 0 & \mathbf{W}^{\text{bdry}}_{(n+1)} \end{bmatrix}$$

Whitney form construction: 0- and 1-forms

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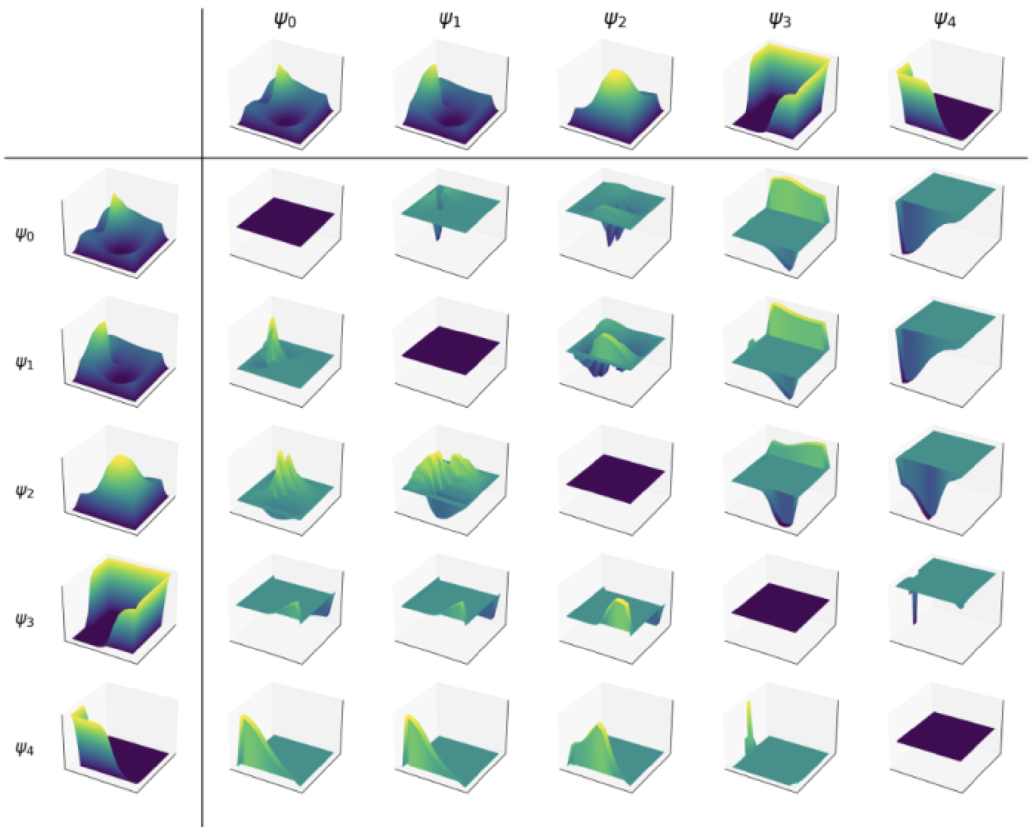
ψ_i

$$(\mathbf{F}, \mathbf{E}) - (\mathsf{d}^0 p_0, \mathbf{E}) = (\mathsf{d}^0 p_D, \mathbf{E})$$
$$-(\mathbf{F}, \mathsf{d}^0 q_0) \qquad = (f, q_0) - (g_N, q_0)_{\Gamma_N}.$$

$$\mathbf{F} = \sum_{i,j} \hat{F}_{ij} \psi_{ij} \qquad \psi_{ij} \in V^1$$
$$p_0 = \sum \hat{p}_i \psi_i \qquad \psi_i \in V^0_D,$$

ψ_j

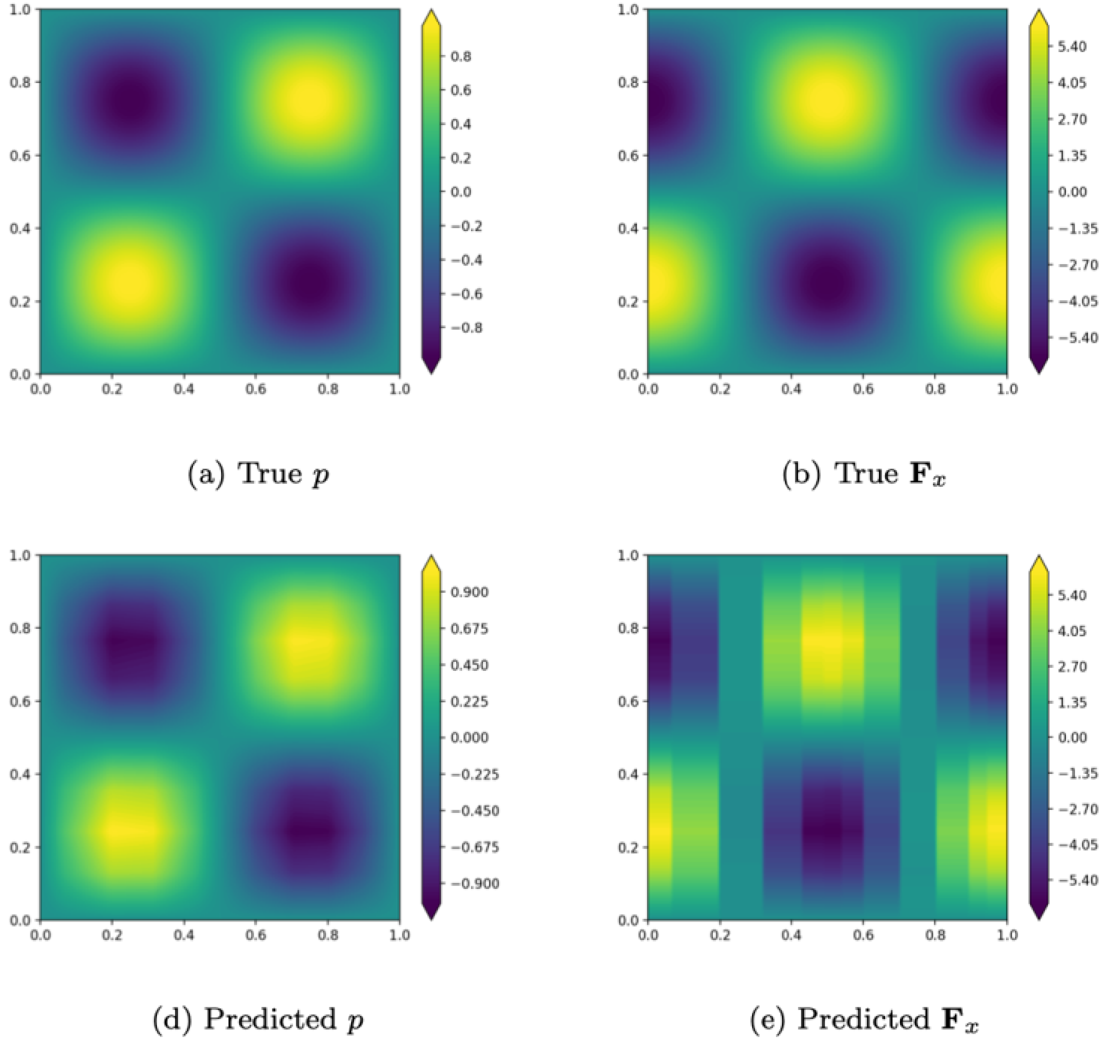


$$\min_{\xi} \left\| p_{\text{data}} - \left(p_D + \sum_i \hat{p}_i \psi_i \right) \right\|_2^2 + \alpha^2 \left\| F_{\text{data}} - \sum_{ij} \hat{F}_{ij} \psi_{ij} \right\|_2^2$$
$$\text{such that} \begin{bmatrix} \mathbf{M}_1 & -\mathbf{M}_1 \mathbf{D}_1^{-1} \delta_0 \mathbf{D}_1 \\ -\mathbf{B}_0^{-1} \delta_0^T \mathbf{B}_1 \mathbf{M}_1 & \mathbf{0} \end{bmatrix} \begin{bmatrix} \widehat{\mathbf{F}} \\ \widehat{\mathbf{p}} \end{bmatrix} = \begin{bmatrix} b_D \\ -b_f - b_N \end{bmatrix}$$

Graph structure (and corresponding relevant control volumes) are encoded via POU parameterization

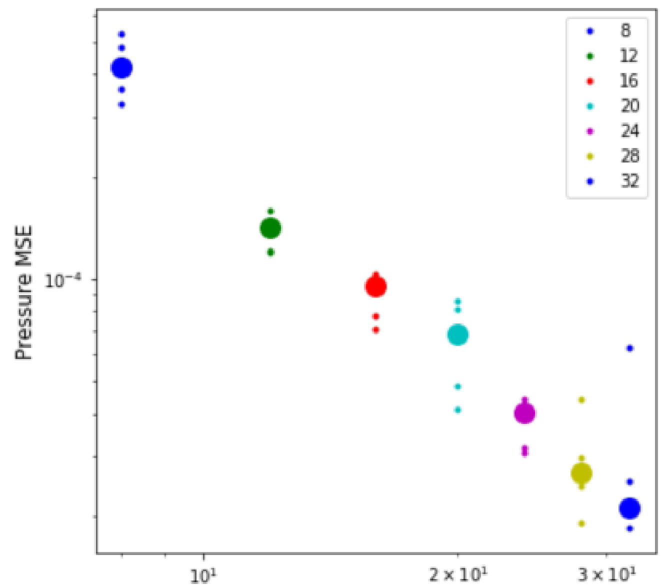
Closed form quadrature allows backprop to find POUs which admit a model consistent to data

Convergence for smooth solutions

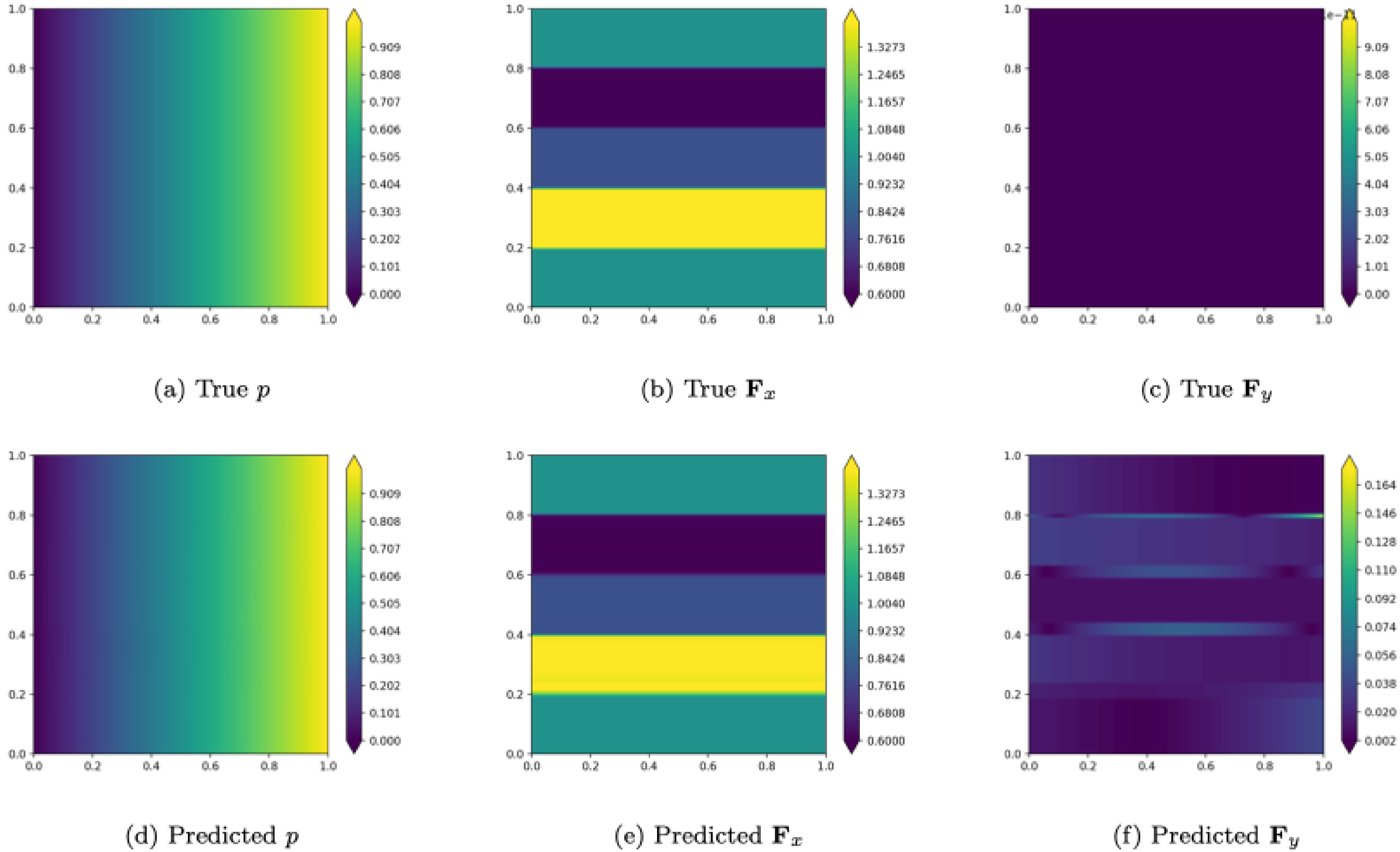


$$\mathbf{F} - \nabla p = 0$$
$$\nabla \cdot \mathbf{F} = -8\pi^2 \sin(2\pi x) \sin(2\pi y)$$
$$p = 0$$
$$\mathbf{F} \cdot \vec{n} = 0$$

$$p(x, y) = \sin(2\pi x) \sin(2\pi y)$$
$$\mathbf{F}(x, y) = \begin{bmatrix} 2\pi \cos(2\pi x) \sin(2\pi y) \\ 2\pi \sin(2\pi x) \cos(2\pi y) \end{bmatrix}$$



5-strip problem: treating material jumps



Digital twin of as-built lithium-ion battery microstructure

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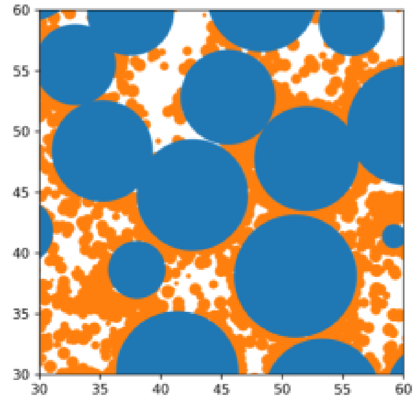
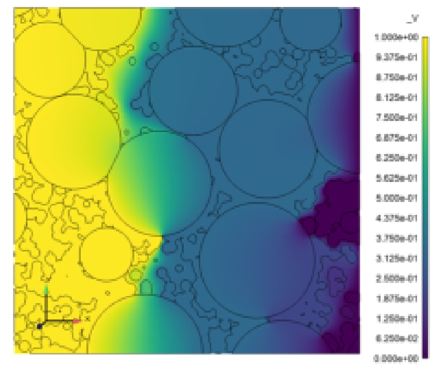
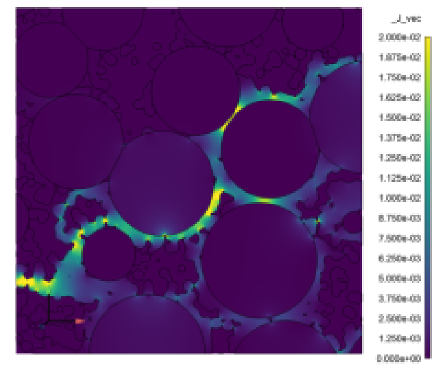


(a) Matrix layout

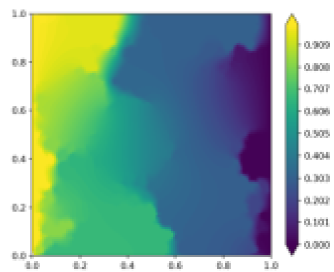


(b) Voltage

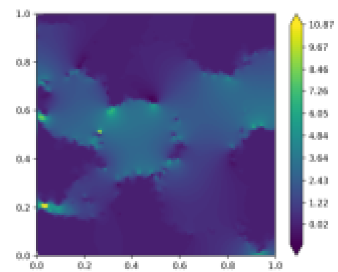


(c) Magnitude of current

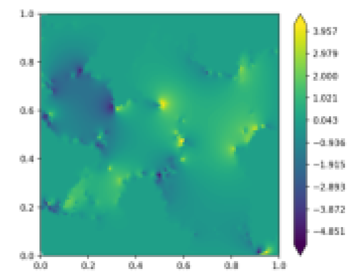
Replace a 5.89M finite element simulation of as-built geometry with 8 data-driven elements w/ ~0.1% error
implemented in production FEM code



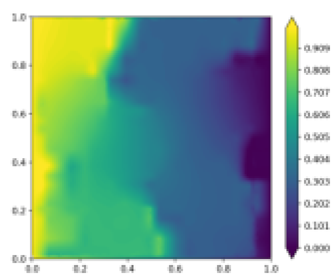
(a) True p



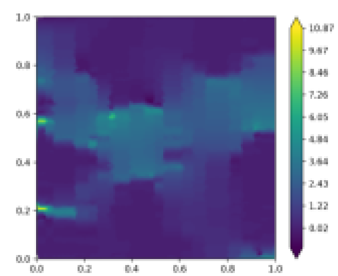
(b) True $\mathbf{F}_x$



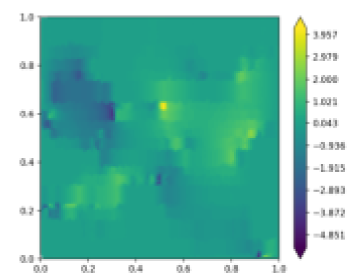
(c) True $\mathbf{F}_y$



(d) Predicted p



(e) Predicted $\mathbf{F}_x$



(f) Predicted $\mathbf{F}_y$

Conclusions and future directions

- POUs provide a path toward:
  - Developing nonparametric hp-convergent approximators
  - Discovering Whitney forms from data
  - Bridging gap geometric description of full-field data and graph models
- Resulting in data-driven models based on control volume
  - Which are conservative and guaranteed stable, even for nonlinear physics
  - Provide a structure-preserving parameterization of Dirichlet2Neumann map
- Future applications
  - Data-driven drift-diffusion equations for semiconductor physics
  - Data-driven modeling of quantum thermo-magnetic materials
  - Data-driven modeling of climate systems

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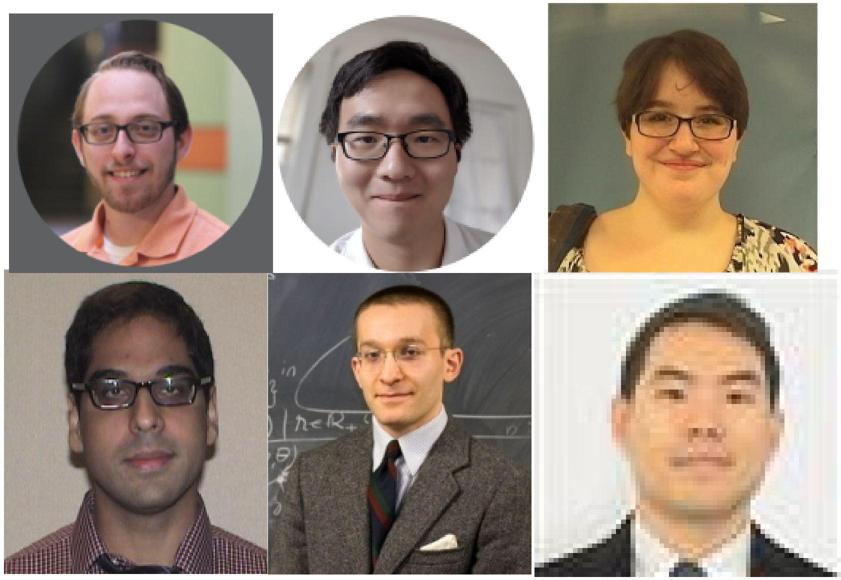

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Relevant publications

1. **Jonas Actor, Andy Huang, Nathaniel Trask. "Polynomial-Spline Neural Networks with Exact Integrals". To appear on arxiv**
2. **Lee, Kookjin, Nathaniel Trask, and Panos Stinis. "Structure-preserving Sparse Identification of Nonlinear Dynamics for Data-driven Modeling." *arXiv preprint arXiv:2109.05364* (2021).**
3. **Trask, Nathaniel, Mamikon Gulian, Andy Huang, and Kookjin Lee. "Probabilistic partition of unity networks: clustering based deep approximation." *arXiv preprint arXiv:2107.03066* (2021).**
4. **Lee, Kookjin, Nathaniel A. Trask, and Panos Stinis. "Machine learning structure preserving brackets for forecasting irreversible processes." *arXiv preprint arXiv:2106.12619* (2021). (accepted to NeurIPS)**
5. You, Huaiqian, et al. "Data-driven learning of nonlocal physics from high-fidelity synthetic data." *Computer Methods in Applied Mechanics and Engineering, AI special issue* (2021)
6. Patel, Ravi G., et al. "A physics-informed operator regression framework for extracting data-driven continuum models." *Computer Methods in Applied Mechanics and Engineering, AI special issue* (2021)
7. **Lee, Kookjin, et al. "Partition of unity networks: deep hp-approximation." *arXiv preprint arXiv:2101.11256* (2021).**
8. **Trask, Nathaniel, Andy Huang, and Xiaozhe Hu. "Enforcing exact physics in scientific machine learning: a data-driven exterior calculus on graphs." *Journal of Computational Physics (2022)***
9. Patel, Ravi G., et al. "Thermodynamically consistent physics-informed neural networks for hyperbolic systems." *arXiv preprint arXiv:2012.05343* (2020).
10. Cyr, Eric C., et al. "Robust training and initialization of deep neural networks: An adaptive basis viewpoint." *Mathematical and Scientific Machine Learning*. PMLR, (2020).
11. Patel, Ravi G., et al. "A block coordinate descent optimizer for classification problems exploiting convexity." *arXiv preprint arXiv:2006.10123* (2020). 2021 AAAI-MLPS Conference
12. Gao, Xujiao, et al. "Physics-Informed Graph Neural Network for Circuit Compact Model Development." *2020 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*. IEEE (2020)
13. Huang, Andy, et al. "Greedy Fiedler Spectral Partitioning for Data-driven Discrete Exterior Calculus." 2021 AAAI-MLPS Conference
14. Trask, Nathaniel, et al. "GMLS-Nets: A framework for learning from unstructured data." NeurIPs proceedings (2019)

Open source software

- GMLS-nets: learning from unstructured data through meshfree approximation (https://github.com/rgp62/gmls-net)
- MOR-Physics: Modal Operator Regression for physics discovery (https://github.com/rgp62/MOR-Physics)