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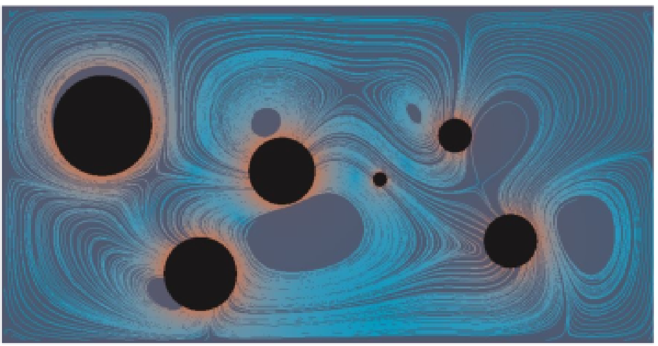

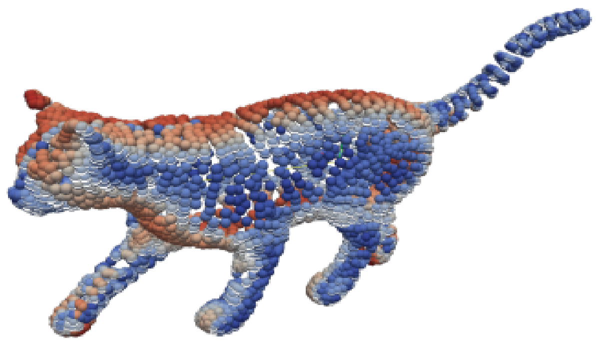

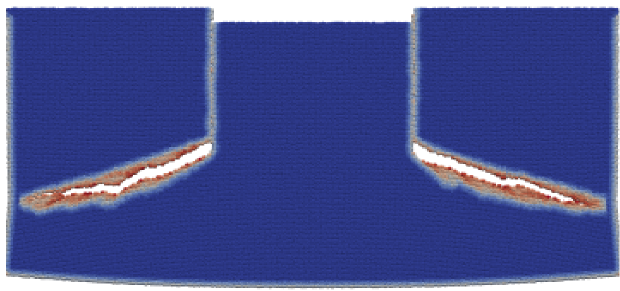

Discovery of structure-preserving finite element spaces for multiscale

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Overview

Objective

Data-driven multiscale finite elements w/ structure preservation

Ingredients:

1. Partition of unity networks for approximation
2. Data-driven exterior calculus (DDEC)
3. **Data-driven Whitney forms extracting DDEC from POU-nets**

Paper on arxiv in the coming month – please email for draft

Embedding microscale physics into continuum FEM

Problem: High-throughput scans of microstructure lead to either expensive resolved simulations or oversimplification of microstructure

CT scans of Li battery: lithiation-induced failure driven by transport pathways through microstructure

AI/ML: Can we develop data-driven FEM which encodes subgrid geometric information while **preserving conservation**

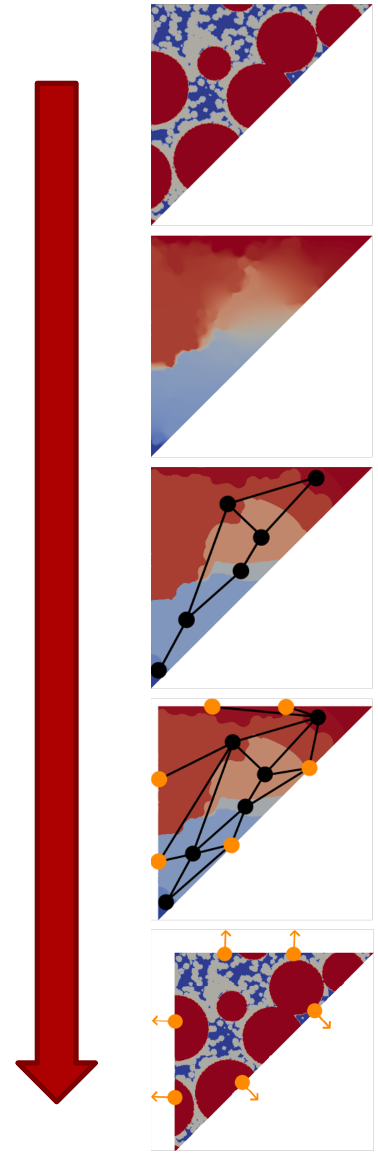
Input
Experimental characterization of voxelized microstructure

Fully resolved high-fidelity training simulation

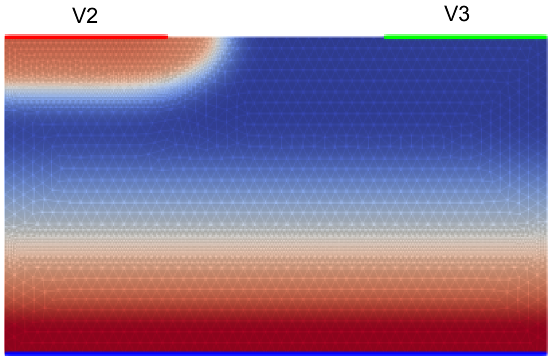
Data-driven partitioning of microstructure solution

Discovery of Dirichlet2Neumann map

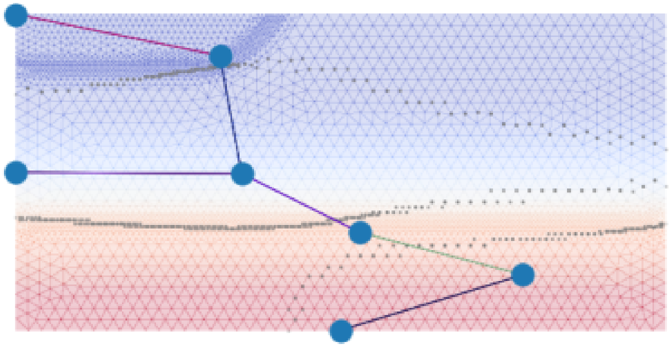
Product
Structure-preserving macro elements encoding microscale response



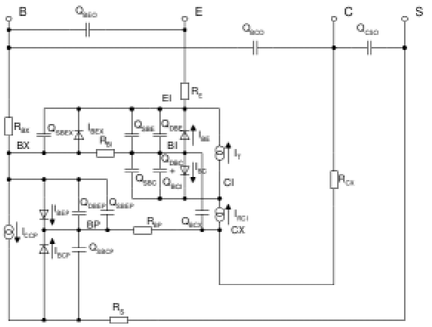
Multiscale E&M: Radiation-hardened semiconductor design



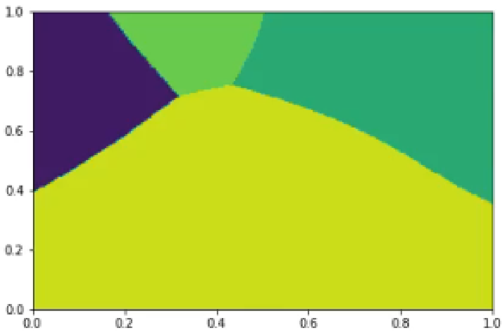
High-fidelity drift-diffusion PDE solution database



Learning data-driven graphical model for voltage-current relation



Result: robust surrogate embedded in production circuit simulator



Partitioning into physics-informed subdomains

- Similar to ROMs – build a database of high-fidelity solns
- Relationship to control volume analysis preserves structure
- Mathematical machinery: data-driven exterior calculus
- **Result:** reduced order electromagnetic models with structure preservation + stability guarantees that can **reliably be scaled up in production circuit simulators**

Gao, X., Huang, A., Trask, N. and Reza, S., Physics-Informed Graph Neural Network for Circuit Compact Model Development. In *2020 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)* (pp. 359-362). IEEE.

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<u>Ingredient 1</u>

Probabilistic partition of unity networks

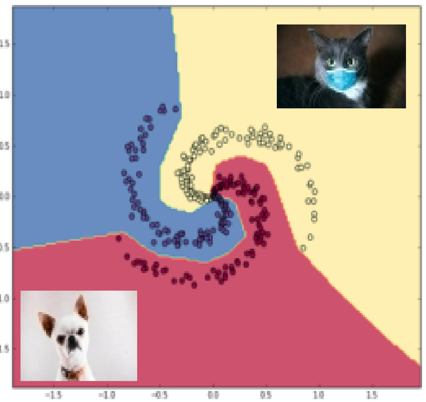
Hybrid architectures combining deep clustering/classification with polynomial regression

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). Accepted to AAAI-MLPS*
3. *Lee, Kookjin, et al. "Partition of unity networks: deep hp-approximation." arXiv preprint arXiv:2101.11256 (2021) accepted to AAAI-MLPS*
4. ***Trask, N., Gulian, M. "Probabilistic partition of unity networks: clustering based deep approximation." under review***

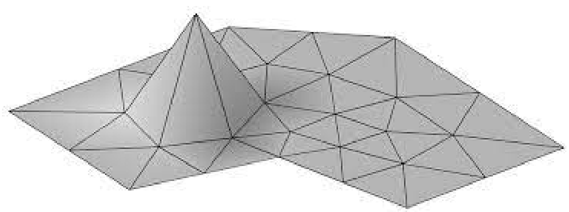
From theory…

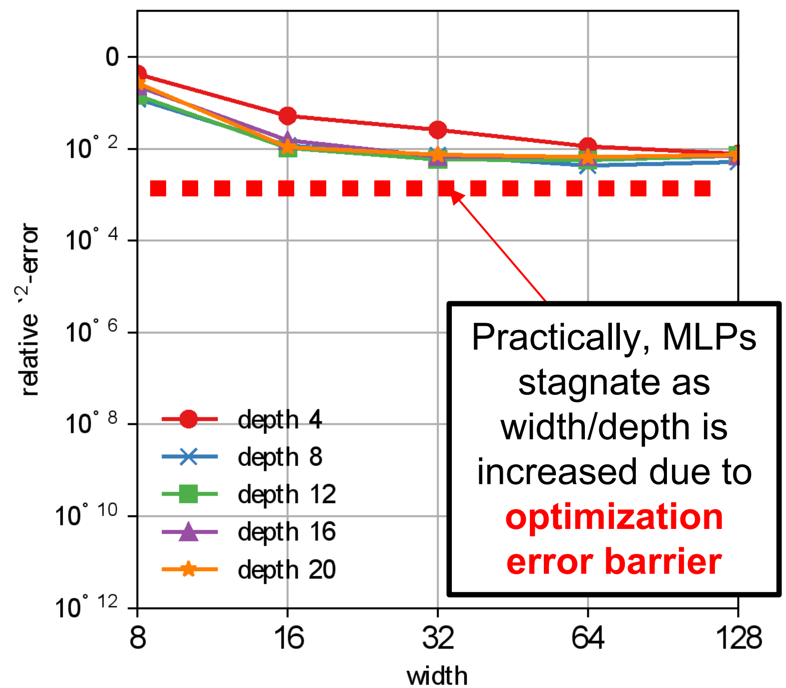
Opschoor et al have established **existence** of neural networks which emulate hp-elements and provide algebraic convergence rates

Emulation of partitions of space



Emulation of monomials on each partition

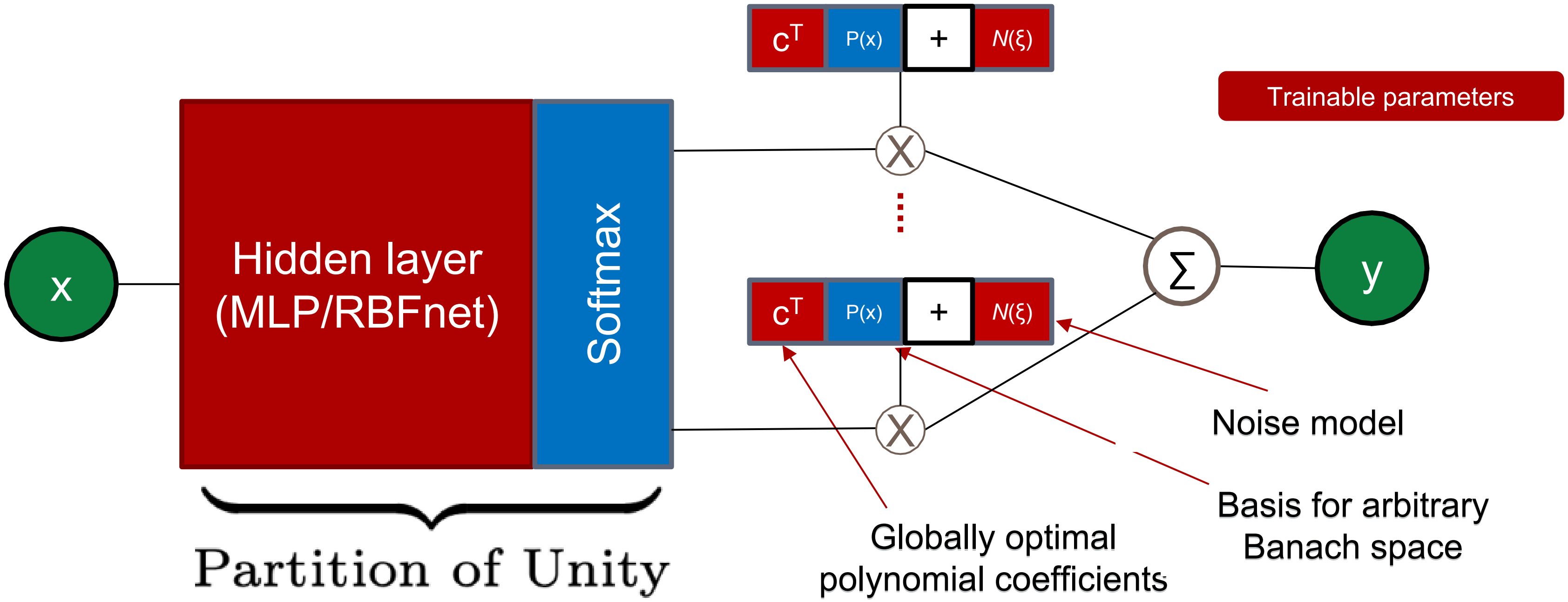




Not realized when training a network with SGD

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.

… to practice: Partition of Unity-Network

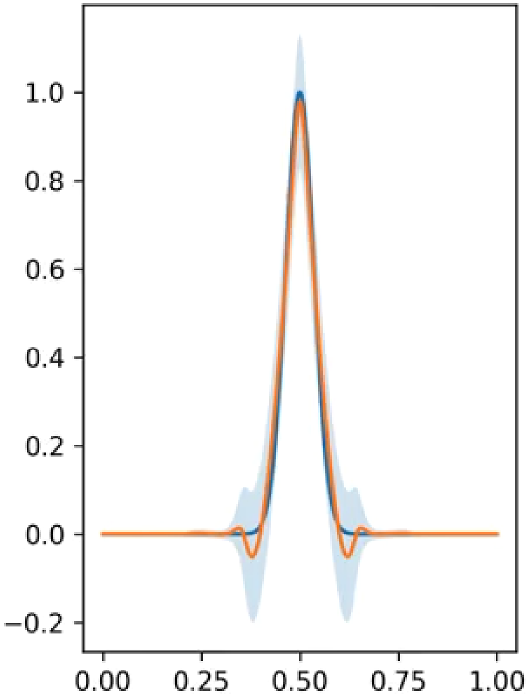


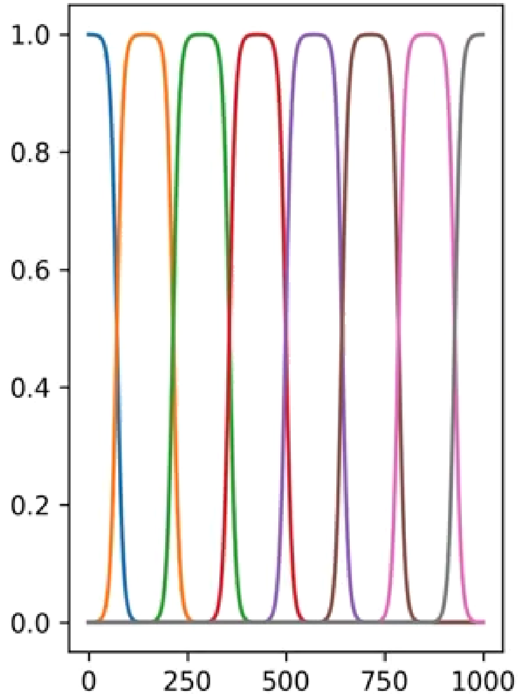
Don't emulate polynomials + partitions – build them in directly!

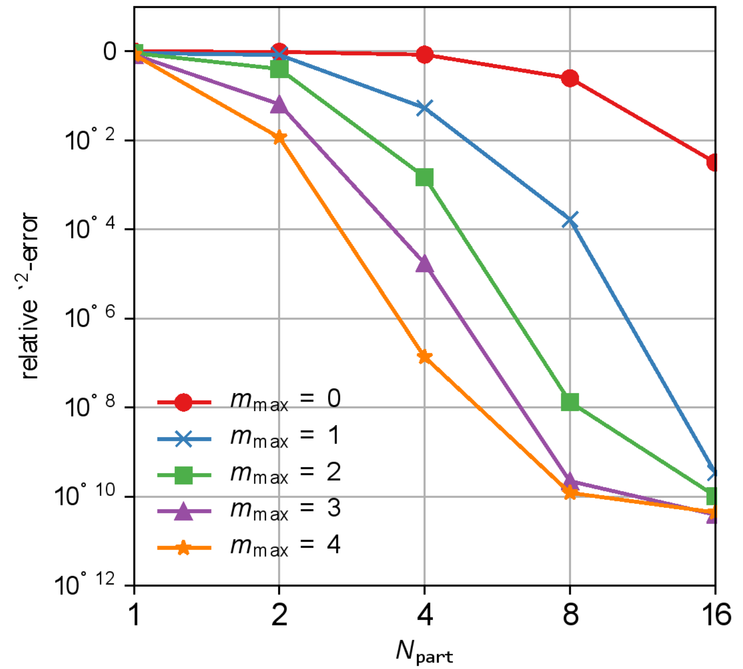
Training:

- Maximum likelihood over dataset
- Closed form expressions for optimal polynomial fit **(embarrassingly parallel!!)**
- SGD to move partitions

Realization of hp-convergence during training







Output:
Piecewise polynomial space with built in error estimator
"Optimal" FEM space

POUnets demonstrate algebraic convergence rates for smooth data

Ingredient 2

Data-driven exterior calculus

Extension of mimetic discretization of PDEs to fit div/grad/curl conservation laws to graph network models

1. Trask, Nathaniel, Andy Huang, and Xiaozhe Hu. "Enforcing exact physics in scientific machine learning: a data-driven exterior calculus on graphs." *arXiv preprint arXiv:2012.11799* (2020).

Machine-learnable graph div/grad/curl that:

- Preserve conservation structure exactly
- Provide **guaranteed solvable** data-driven models
- Handle involution + inf-sup conditions needed for electromagnetics, mechanics, subsurface
- Allow design of **equality-constrained optimizers** that enforce physics to machine **ε**

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

KEY IDEA: Algebraic topology structures provide mathematical tools for designing **guaranteed robustness independent of available data**

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*

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

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

Theorem 0.1. *Assume $\mathcal{NN}$ has Lipschitz constant L_N and that $\mathcal{NN}(0) = 0$. If $\epsilon L_N < 1$, then the model problem has unique solution $\mathbf{u}_k \in \mathbb{V}$ satisfying*

$$\|\mathbf{u}_k\|_a \le \frac{\|\mathbf{f}\|_{-a}}{(1 - \epsilon L_N)}. \tag{1}$$

Trask, Nathaniel, Andy Huang, and Xiaozhe Hu. "Enforcing exact physics in scientific machine learning: a data-driven exterior calculus on graphs." ***arXiv preprint arXiv:2012.11799*** **(2020).**

General optimization problem

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

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

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

Invertible bilinear form w/ metric params

Nonlinear perturbation with DNN params

<u>Output</u>

Without assuming a governing equation, get a variational model guaranteed to be **exactly**:

- Stable
- Solvable
- Structure-preserving

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

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

Ingredient 3

Data-driven Whitney forms extracting DDEC from POU-nets

Extraction of a discrete Stokes theorem from partitions in POU-nets

1. Trask, Nathaniel, Andy Huang, and Xiaozhe Hu. "Enforcing exact physics in scientific machine learning: a data-driven exterior calculus on graphs." *arXiv preprint arXiv:2012.11799* (2020).
2. Jonas Actor, Andy Huang, Nathaniel Trask. “Polynomial-Spline Neural Networks with Exact Integrals”. To appear on arxiv

A Gauss divergence theorem from a POU

Idea: If POU provides automatic differentiable generalization of an indicator function on a cell, can we generalize the Gauss divergence theorem?

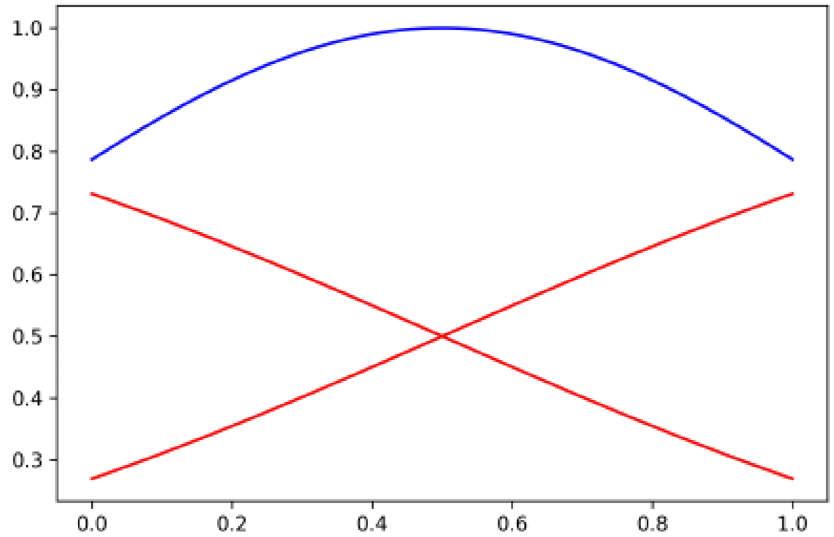
$$\int_c \nabla \cdot \mathbf{u} dx = \int_{f \in \partial c} \mathbf{u} \cdot d\mathbf{A}$$

POUs generalize cell

If we can define a boundary operator, then we obtain a conservative discrete divergence

Red: POU on cells
Blue: Boundary of POUS

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



Whitney forms defining data-driven differential forms

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

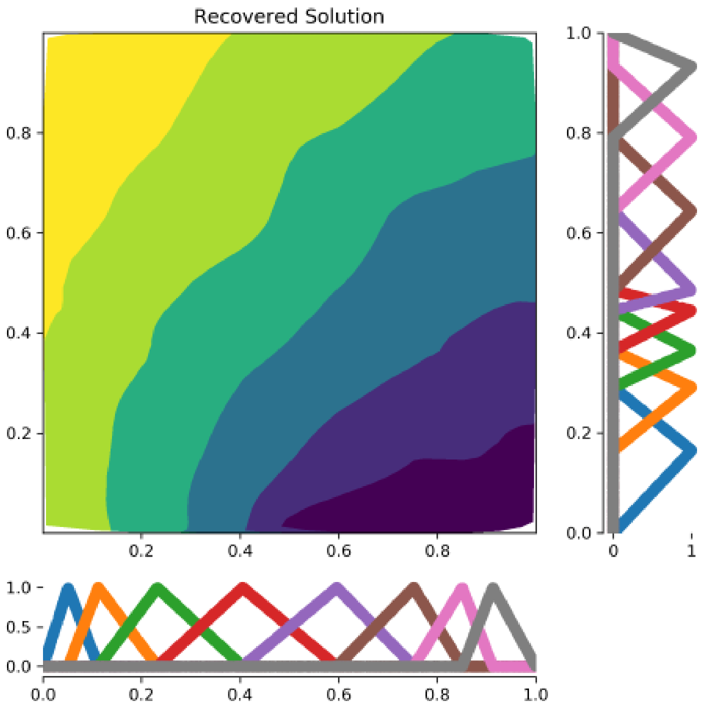
$$\begin{aligned}
\int_\Omega \psi_i \nabla \cdot \mathbf{u} &= - \int_\Omega \nabla \phi_i \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA \\
&= - \sum_j \int_\Omega \phi_j \nabla \phi_i \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA \\
&= \sum_{j \neq i} \int_\Omega \left(\phi_i \nabla \phi_j - \phi_j \nabla \phi_i \right) \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA \\
&= \sum_{j \neq i} \int_\Omega \psi_{ij} \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA
\end{aligned}$$

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

H(grad) Whitney form. Same construction holds in higher dim to obtain de Rham complex on arbitrary manifolds

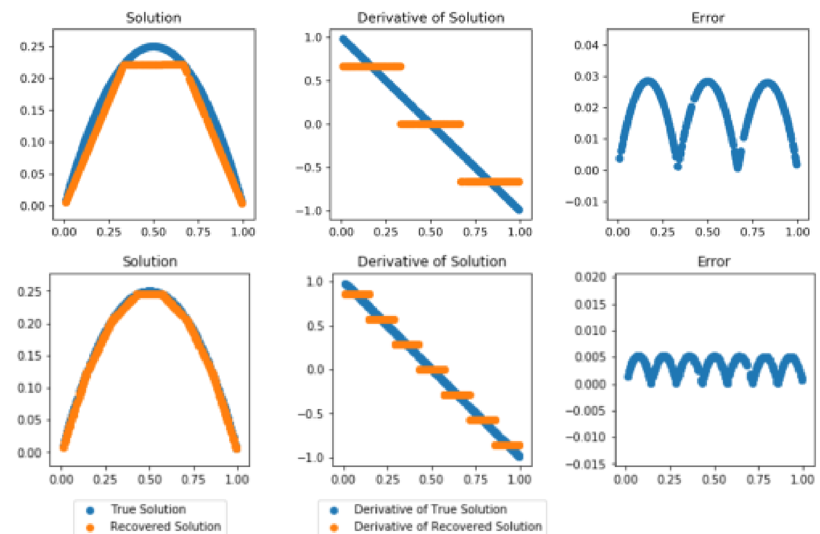
A necessary ingredient: POU allowing exact quadrature

Idea: Beyond this current project, any variational method requires integration of neural networks. Can we design POU-Net with closed form exact quadrature?



$$
\begin{aligned}
-\Delta u &= 0 && \text{on} \quad \Omega' = [-1,1]\times[0,1] \\
\partial_n u &= 0 && \text{on} \quad \Gamma_N = [-1,0]\times\{0\} \\
u &= g(r,\theta) && \text{on} \quad \Gamma_D = \partial\Omega' \backslash \Gamma_N.
\end{aligned}
$$

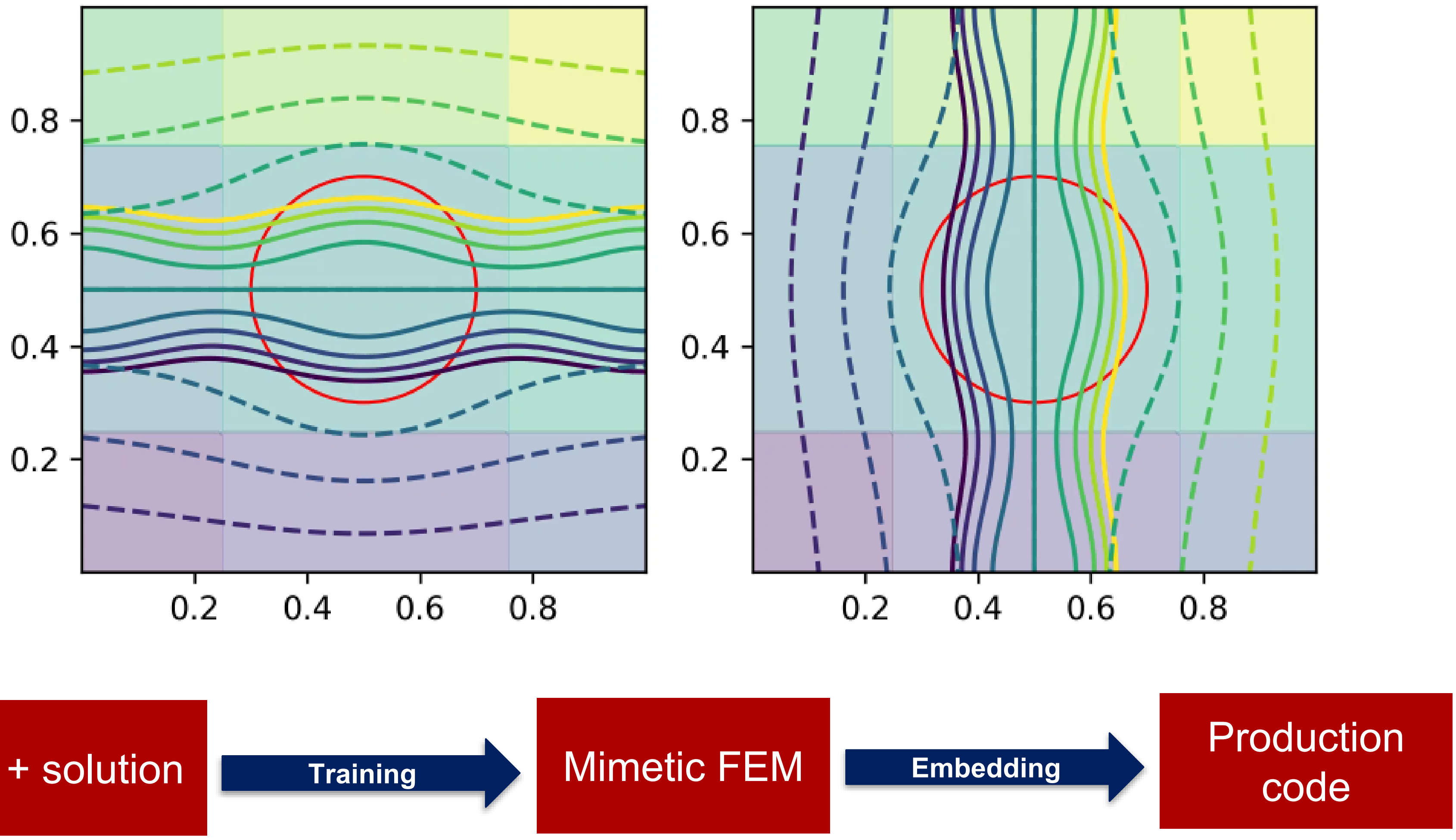
$$
A = \int_{\Omega'} D\Phi D\Phi^T + \beta \int_{\Gamma_D} \Phi\Phi^T, \qquad b = \beta \int_{\Gamma_D} g\Phi.
$$



For example applying to DeepRitz network:

Jonas Actor, Andy Huang, Nathaniel Trask. "Polynomial-Spline Neural Networks with Exact Integrals". To appear on arxiv

Finally: POUs + DDEC = Discovery of multiscale FEM



Obtain a finite element with microstructure embedded in terms of local conservation balances

Highlighted 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).
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." *arXiv preprint arXiv:2012.11799* (2020).**
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)