SAND2021-12466PE

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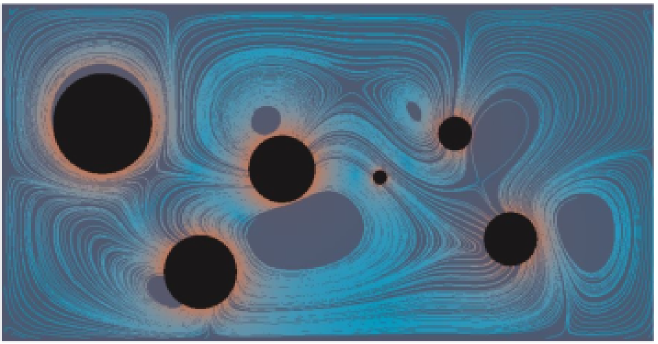

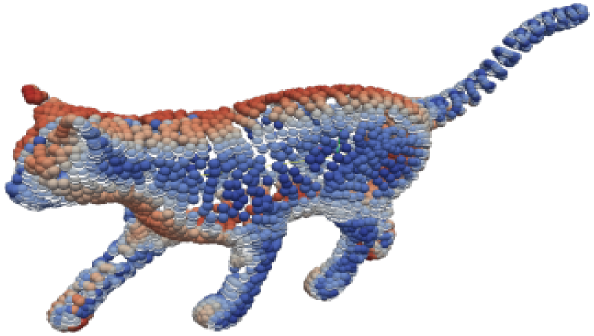

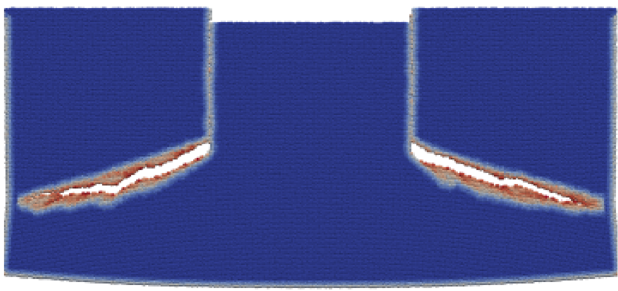

Structure preserving machine learning for data-driven multiscale/multiphysics modeling

CCR Center for Computing Research

Nat Trask
Center for Computing Research
Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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Acknowledgements

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- DOE early career
- Philms (ASCR MMICCs center)
- SNL LDRD
- ASC

Collaborators:

- Graph exterior calculus
  Xiaozhe Hu (Tufts)
- Semiconductor work in 1300
  PIRAMID LDRD
  Huang, X. Gao, S. Reza
- Z-machine + shock physics
  Kris Beckwith, Patrick Knapp
- Combustion Research Facility
  Jackie Chen, MK Lee (8300)
- Subsurface fracture networks
  Jeffrey Hyman (LANL)
- Fracture modeling
  Y. Bazilevs, M. Behzadinsad, J. Foster
  Y. Yu, M. D'Elia
- Bracket dynamics
  P. Stinis (PNNL)
- COMPADRE meshfree work
  P. Kuberry, P. Bochev, M. Perego

Postdocs: Ravi Patel, Mamikon Gulian, Kookjin Lee, Jonas Actor, Marshall Jiang

Staff: Eric Cyr, Mitch Wood, Andy Huang

Please contact for postdoc/collaboration opportunities (natrask@sandia.gov)

Overview

Introduction

Brief overview of our forward simulation work

Objectives

1. Data-driven multiscale finite elements w/ structure preservation
2. High-throughput AI-enabled experimentation for additive manufacturing

Technical Ingredients:

1. Partition of unity networks for approximation
2. Data-driven exterior calculus (DDEC)
3. Data-driven Whitney forms extracting DDEC from POU-nets
4. Geometric dynamical systems for robotics and control

SANDIA

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   Ames, Iowa
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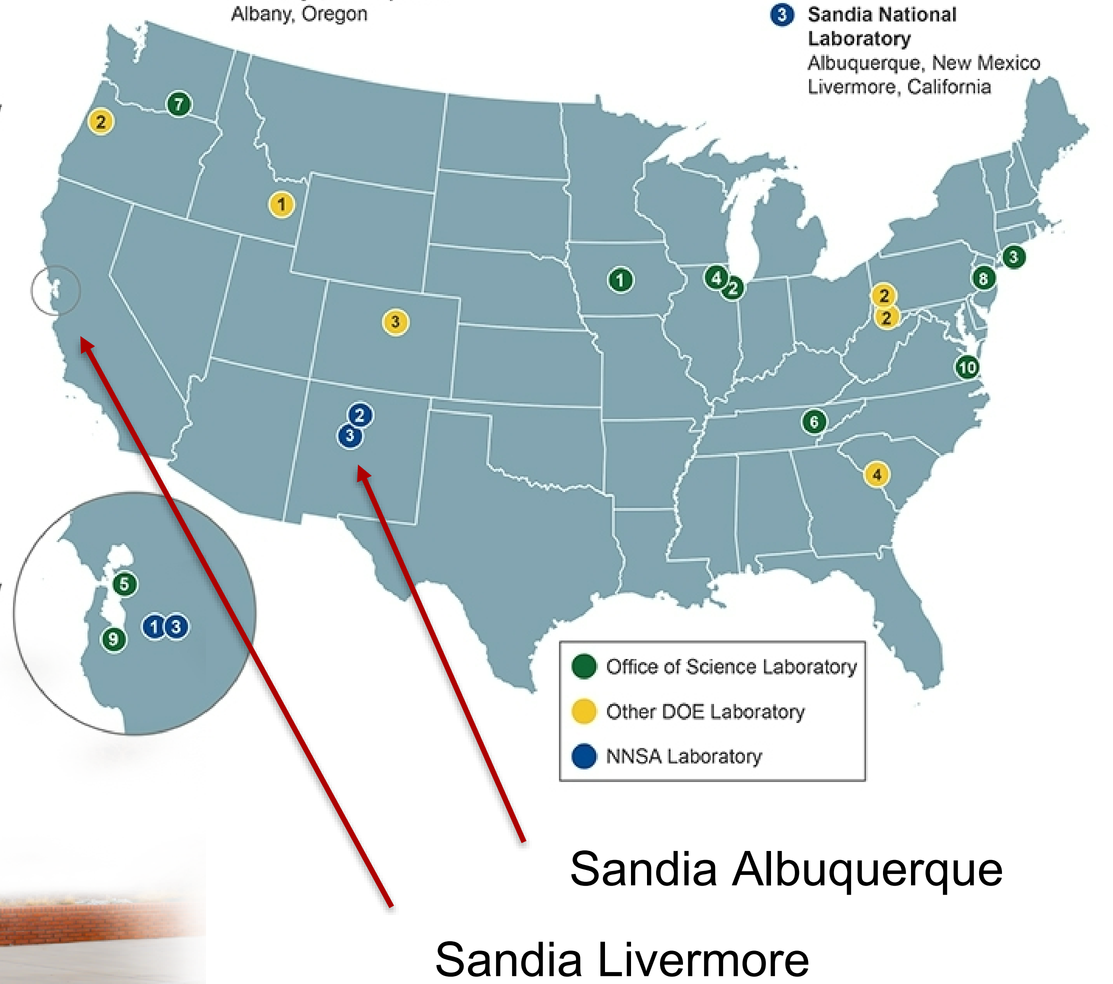
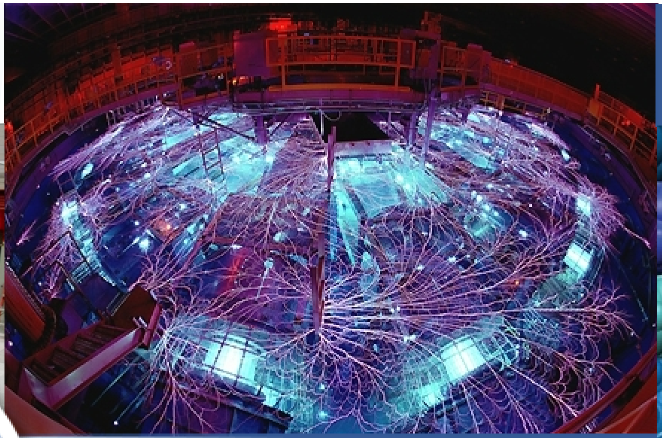


Research foundations within SNL

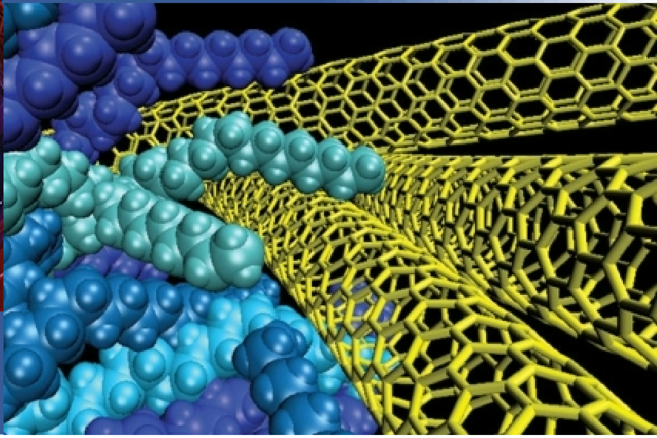
Research foundations drive capability development

Computing & Information Sciences

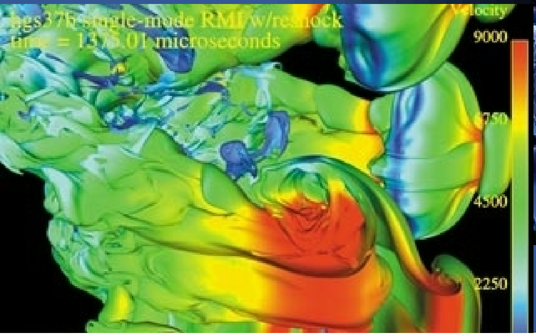
Radiation Effects & High Energy Density Science



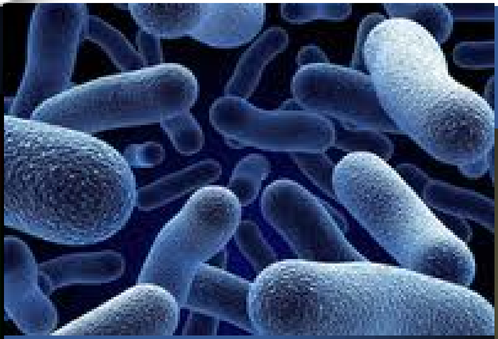
Materials Sciences



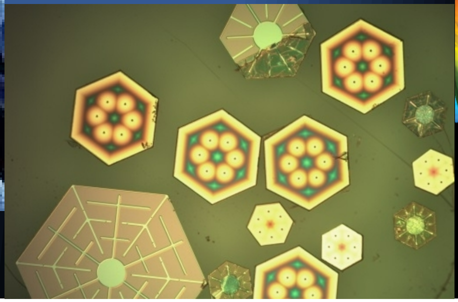
Engineering Sciences



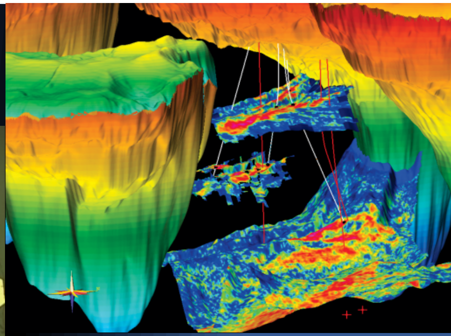
Bioscience



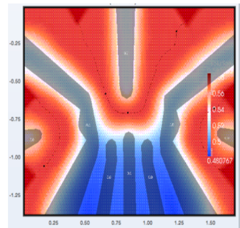
Nanodevices & Microsystems

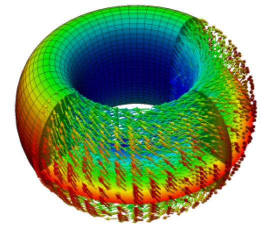


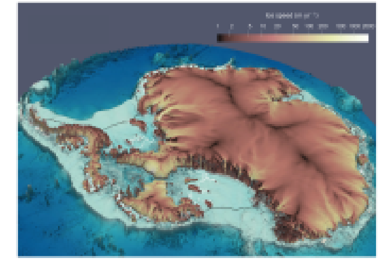
Geoscience



Center for computing research

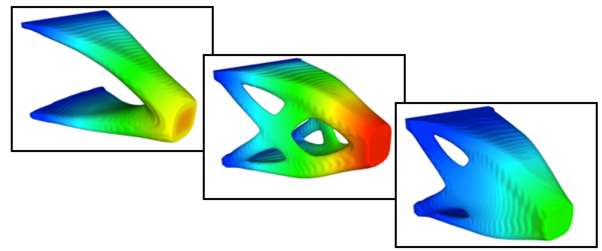


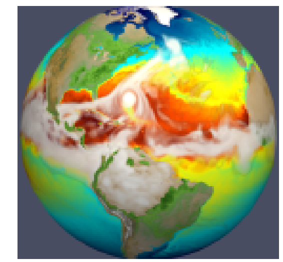




Leading Edge Algorithms and Enabling Technologies

State-of-the-art Computational Science Applications



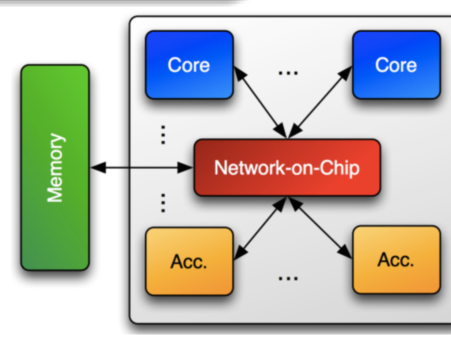


Scalable HPC Architecture and Systems Research

Opportunities for collaboration!

- Graduate student internships
- Postdocs
- Faculty collaborations

Please email: natrask@sandia.gov



Postings: both SciML (applied math/CS) and experimental

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Postdoctoral Appointee - Scientific Machine Learning

Albuquerque, New Mexico
Job ID: 678349

We seek a postdoctoral appointee to apply state-of-the-art scientific machine learning tools to develop data-driven approaches to efficient control and diagnostics of additive manufacturing and electrochemical processes of thin films. The successful candidate will work with a diverse team of modelers, experimentalists and applied mathematicians to develop a machine learning framework for material science problems.

We are committed to nurturing a culture compatible with a broad group of people and perspectives in accordance with the changing makeup of the workforce. In support of this vision, the center actively recruits applicants from diverse groups of backgrounds and fosters an inclusive community.In this role, you will work collaboratively on a multidisciplinary research team conducting fundamental algorithmic research.

On any given day, you may be called on to:

- Conduct leading-edge research in Scientific Machine Learning (SciML), including both physics-informed techniques incorporating engineering/physics models and traditional image analysis of high throughput material science experiments

REQUIRED:

- Possess, or are pursuing, a PhD in mathematics, material science, physics, computer science, or a related engineering or natural science field (conferred within 3 years prior to employment)
- Familiarity with optimization or deep learning, as evidenced by either completion of a graduate class that covered optimization or deep learning or use of optimization or deep learning in a research setting.
- Training in continuum modeling using differential equations, with particular preference for those with training in numerical solution of differential equations for surface physics.

Due to U.S. export-control laws, only U.S. Persons (U.S. citizens, lawful permanent residents, asylees, or refugees) are eligible for consideration.

DESIRED:

- Knowledge or experience of additive manufacturing processes for thin films, including: physical vapor deposition, electroplating, or laser powderbed fusion
- Research experience in numerical optimization for engineering design, particularly with a focus on Bayesian methods and uncertainty quantification
- Expertise in solid mechanics, fluid mechanics, or electrochemistry
- methods, domain decomposition, matrix sketching, or hiearchical matrices
- Experience with Tensorflow/pyTorch, and the application of machine learning (ML) techniques to large datasets

Location: Albuquerque, NM
Full Time, Temporary

What Your Job Will Be Like
Are you interested in research in thin film deposition? We are seeking a motivated postdoctoral appointee to support research in metal thin film deposition as a member of our team of scientists.

On any given day, you may be called on to:

- Plan and perform experiments, install, repair, and maintain diagnostic tools, collect and analyze data with the goal of understanding how process parameters affect film stress, microstructure and performance
- Perform design necessary to support projects or experiments
- Publish professional journal articles and present work at local and national conferences
- Interact and collaborate with other inter-disciplinary research groups within Sandia National Laboratories to develop new research opportunities and projects

Qualifications We Require

- Possess, or are pursuing, a PhD in materials science and engineering, or a related field
- Experience with process research and development
- Experience with vapor deposition processes (sputtering or evaporative deposition)
- Experience with thin film characterization
- Experience with vacuum pumping systems
- Proven track record of publication of results in peer-reviewed journals and presentations at scientific and/ or technical conferences
- Able to acquire and maintain a DOE security clearance

Qualifications We Desire

- Experience with magnetron sputter deposition methods
- Experience with microstructural characterization
- Experience with thin film stress characterization
- Experience with mechanical property characterization
- Experience with high vacuum pumping systems
- Experience with or knowledge of machine learning approaches
- Excellent written and verbal interpersonal skills

Apply online at:
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About Sandia:
Our culture values work-life balance; we offer programs such as flexible work schedules with alternate Fridays off, on-site fitness facilities, and three weeks of vacation. Sandia provides employees with a comprehensive benefits package that includes medical, dental, vision, and a 401(k) with company-match.

Sandia National Laboratories is the nation's premier science and engineering lab for national security and technology innovation. We are a world-class team of scientists, engineers, technologists, post docs, and visiting researchers all focused on cutting-edge technology, ranging from homeland defense, global security, biotechnology, and environmental preservation to energy and combustion research,

Please see also named fellowships: Data science, Hruby, John von Neumann, Truman

Background:

BS/MS in Mechanical Engineering @ Umass

Advisor: David Schmidt

PhD in Applied Math @ Brown

Advisors: Martin Maxey + George Karniadakis

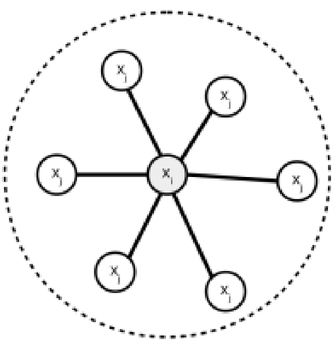
NSF MSPRF Postdoc @ SNL

Advisor: Pavel Bochev

Research focus:

(before ML) Physics-compatible optimization-based multiphysics + multiscale

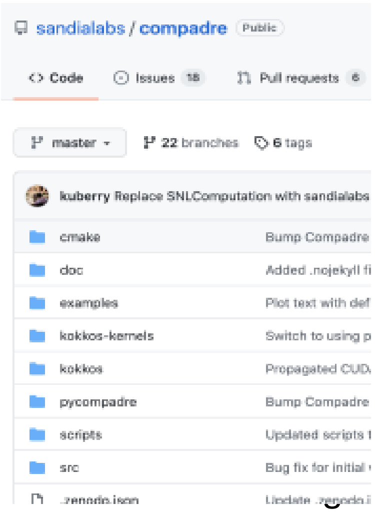
(after ML) Structure preserving data-driven multiphysics + multiscale



$$\tau(u) \approx \tau^h(u)$$

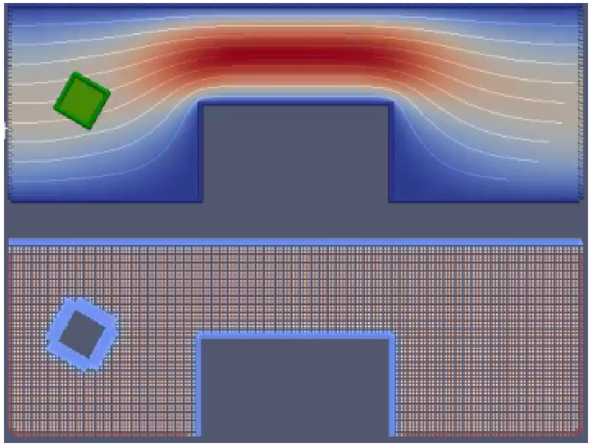
$$p^* = \underset{p \in P}{\mathrm{argmin}} \left(\sum_j \lambda_j(p) - \lambda_j(u) \right)^2 W(\tau, \lambda_j)$$

$$\tau^h(u) := \tau(p^*)$$

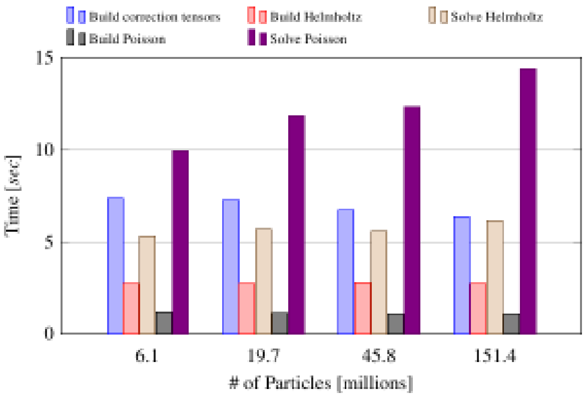


We think a lot about meshing because it's hard!

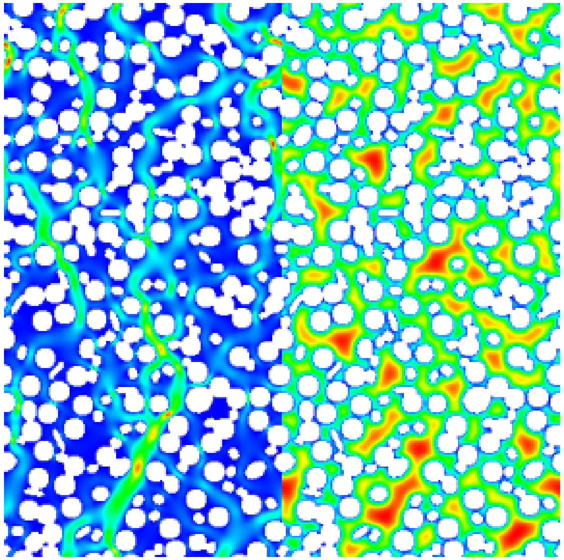
- Meshing is major bottleneck in CAD-to-solution workflow 65% of analyst time
- Developed mimetic meshfree schemes for
  - Treatment of Lagrangian dynamics
  - Automated treatment of pore-scale dynamics
  - Robustness to sliver cells in traditional FEM



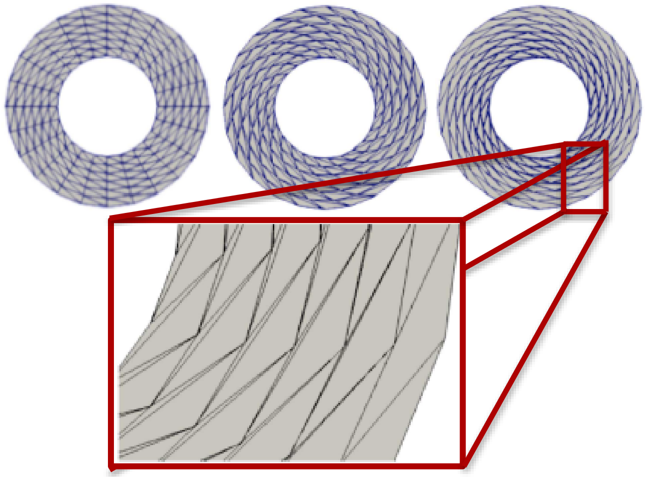
Dense electrophoretic suspensions



Scalable to 500m DOFs



Simulate directly on CT scans



Mesh-hardened FEM on slivers for automatic tet meshing

Accurate multiphysics driven fracture (w/ Y. Bazilevs, J. Foster, Y. Yu)

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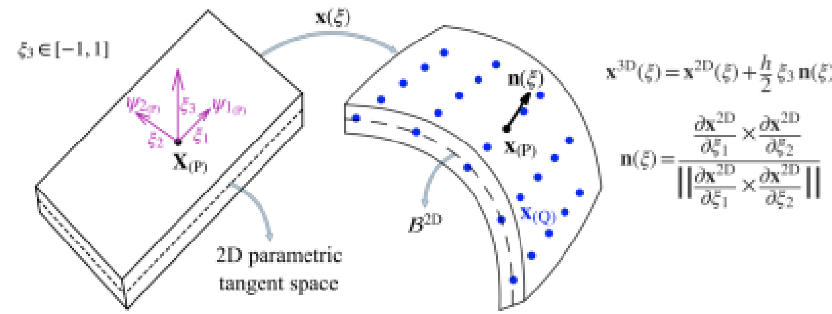
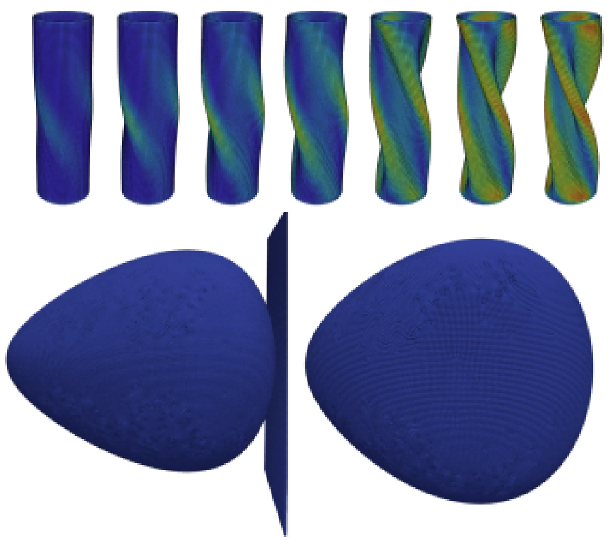
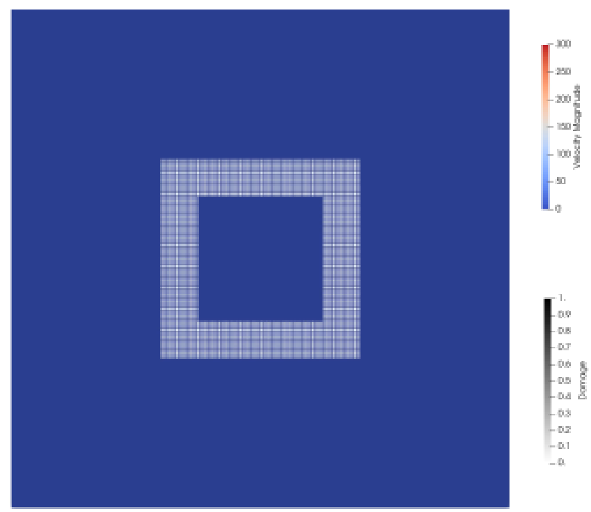
Combining consistent multiphysics discretization with differential geometry estimators allows:

- Construction of high-order shells appropriate for extreme loadings
- Multiphysics coupling for blast-on-structure simulation

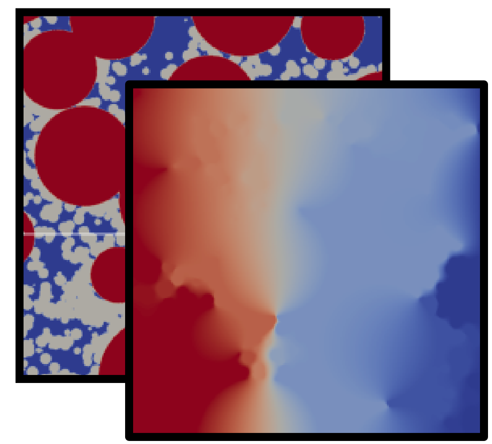




Treatment of brittle/ductile failure while maintaining accuracy competitive with IGA



Coupling to shock codes to handle blast on structure



Multiphysics coupling to simulate lithiation-induced failure in batteries

Sandia National Laboratories

Data-driven modeling at SNL

A survey of some high-consequence applications mandating some guarantees

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-ion battery: lithiation-induced failure driven by transport pathways through microstructure, with fracture altering transport pathways

AI/ML driver:

Can we develop data-driven FEM which encodes subgrid geometric information while **preserving conservation** to treat diffusion pathways?

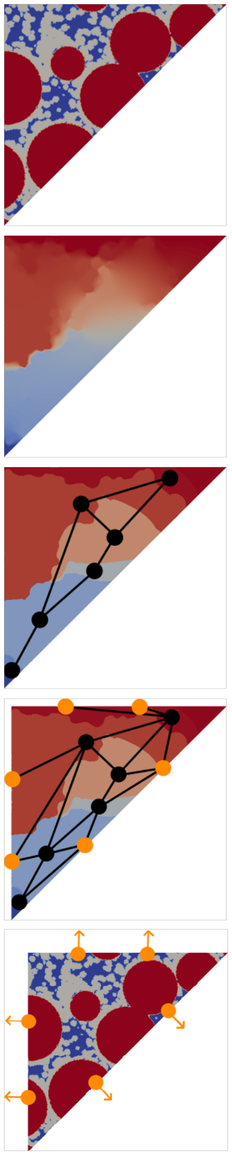
Input
Experimental characterization of voxelized microstructure

Fully resolved high-fidelity training simulation

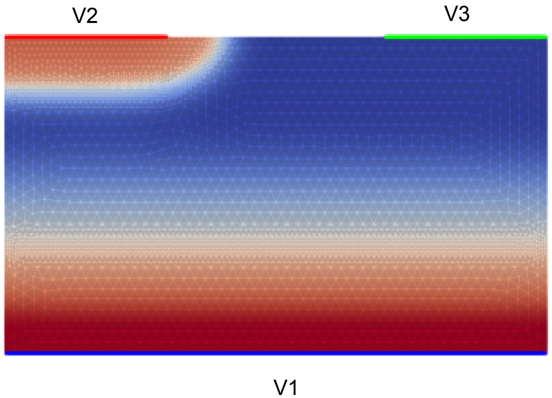
Data-driven partitioning of microstructure solution

Discovery of Dirichlet2Neumann map

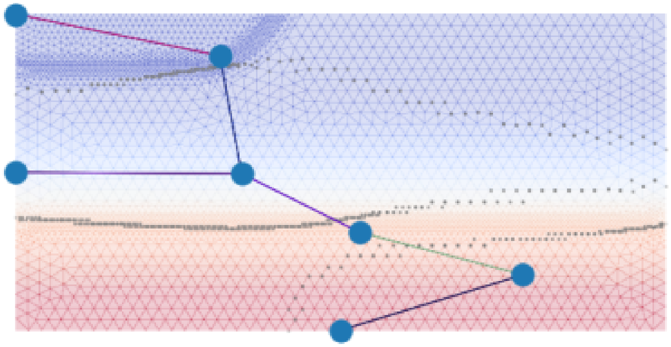
Product
Structure-preserving macro elements encoding microscale response



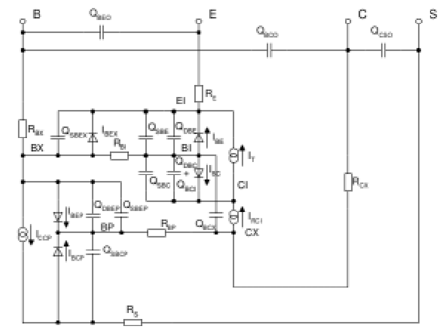
Multiscale E&M: Radiation-hardened semiconductor design



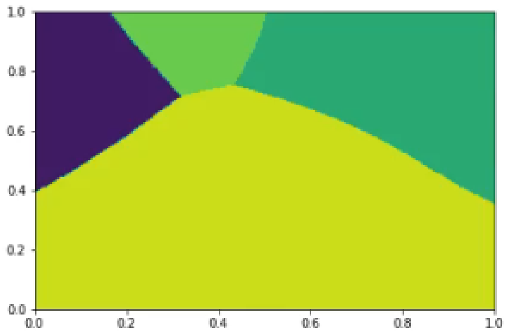
High-fidelity drift-diffusion PDE solution database



Learning data-driven graphical model for voltage-current relation



Result: robust surrogate embedded in production circuit simulator



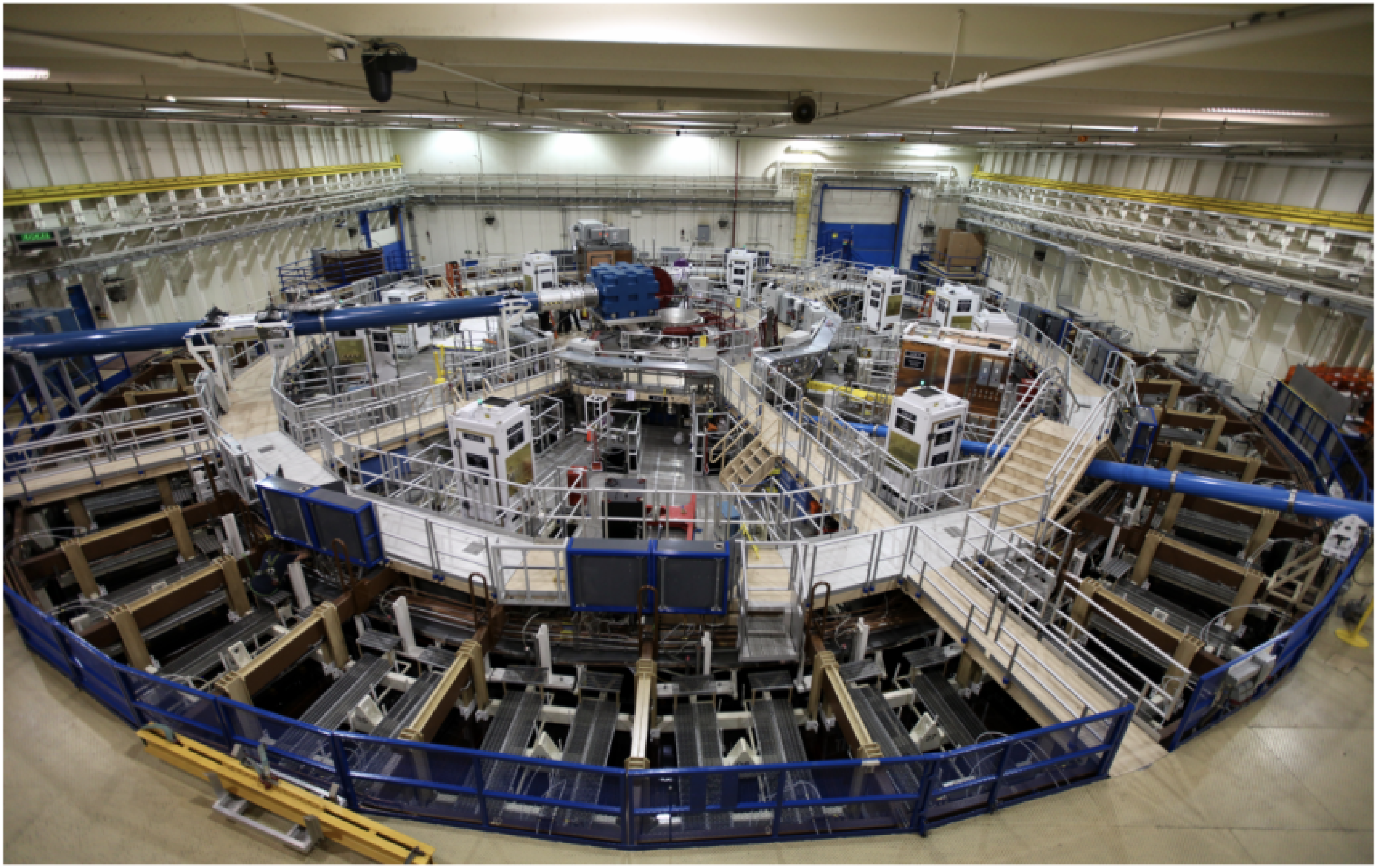
Partitioning into physics-informed subdomains

- For semiconductor devices 1M element simulation (TCAD models) can't scale up to 1B transistors in your phone
- Empirical circuits (compact models) are backbone of system scale design, but can take a decade to develop. After radiation exposure, can't take a decade to recalibrate!

- **AI/ML driver: Use clustering + structure preserving ML to learn a graph surrogate model which can be embedded in a production circuit simulator**

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.

Shock magnetohydrodynamics on Z-machine



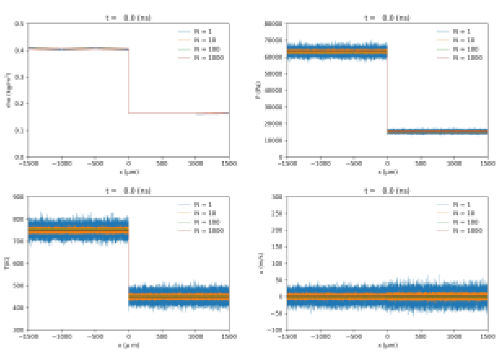
A pulsed power fusion facility for generating extreme environments for short times

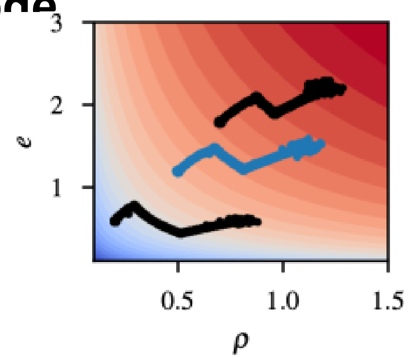
From experiment to data-driven simulation

Discovery of material EOS:
How to extract EOS under extreme conditions from shock response?

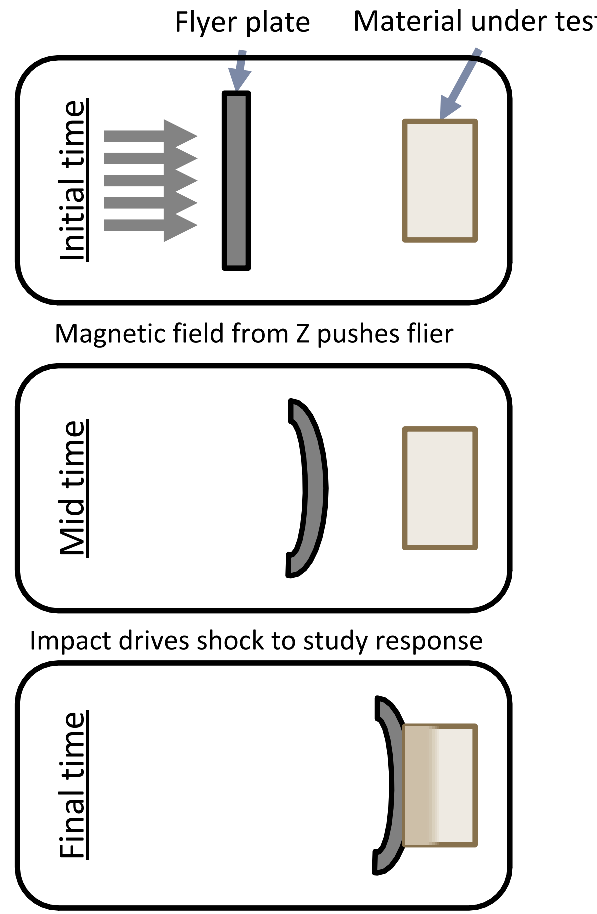
No direct measurements of EOS are available!

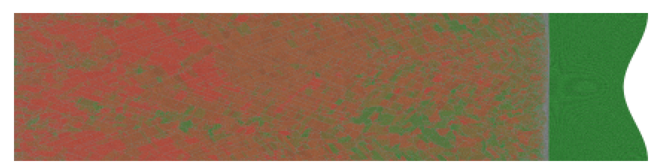
Physics requirements: Need thermodynamic consistency to reliably embed in production ode





Riemann data → **EOS for CFD/MHD**

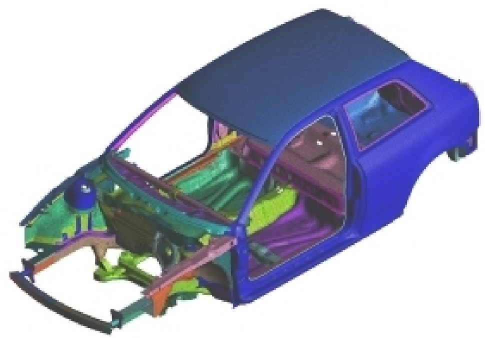


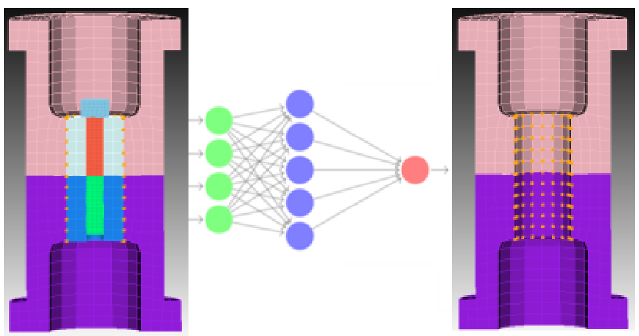


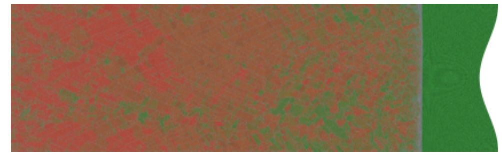
Synthetic data: MD simulations of shocked material

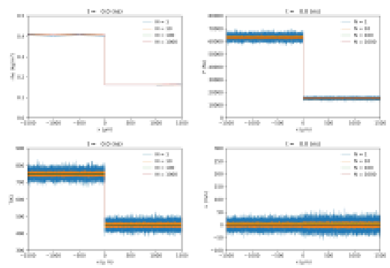
Patel, Ravi G., …, N.Trask, et al. "Thermodynamically consistent physics-informed neural networks for hyperbolic systems." *(to appear in JCP)*

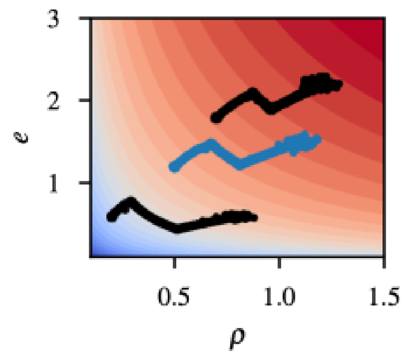
Bridging scales: Embed data-driven components into production code

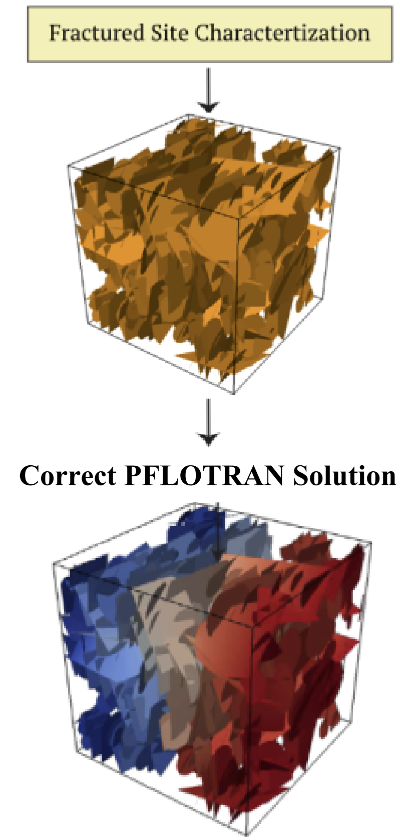












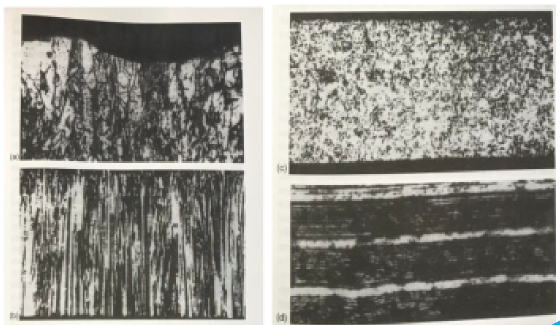
Data-driven fasteners
Replace bolts (1k+ elements) with single data-driven element

Data-driven shock
Discover equation of state from flyer plate data from Z

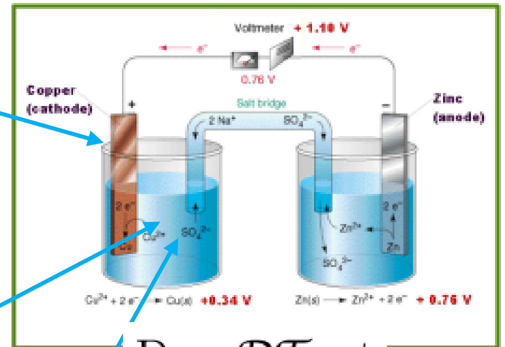
Data-driven subsurface
Calibrate empirical fracture networks to match experimental QOI

With: John Mersch+Eric Parish (left) Patel, Manickam, Wood, Lee, Tomas, Cyr (center), Hyman, Viswanathan (LANL), Huang, Patel (right)

Data-driven digital twins for optimal control of complex systems



Microstructure



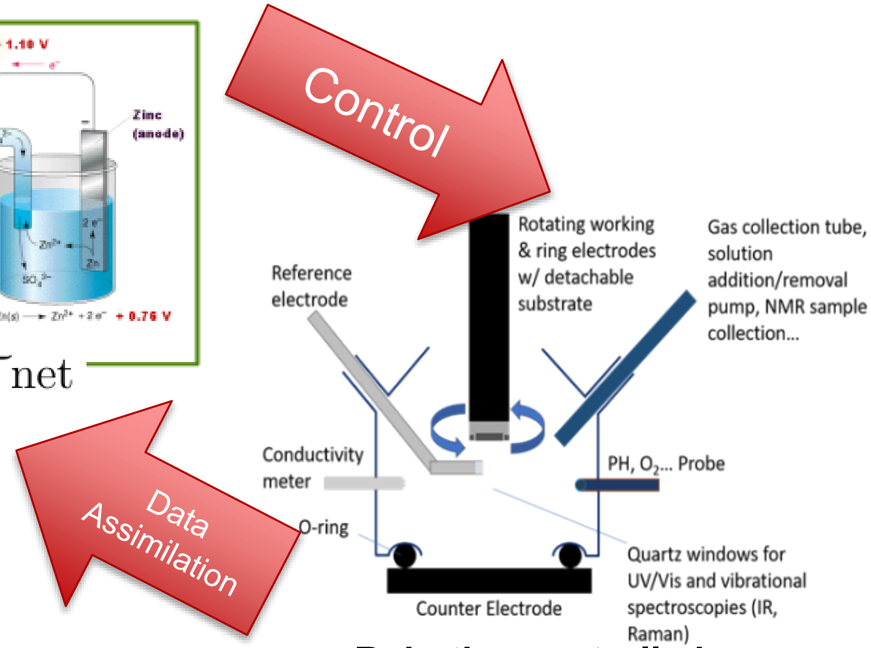
Deep$\mathcal{DT}$net

$$j = i_0 F \left[\exp\left(\frac{\alpha_a F \eta}{RT} \right) - \exp\left(\frac{-\alpha_c F \eta}{RT} \right) \right].$$

Electrochemistry

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} D \left(\frac{z\, c\, F}{R\, T} \frac{\partial V}{\partial x} + \frac{\partial c}{\partial x} \right)$$

Transport



Robotics controlled high-throughput experiments

Problem: How can we provide diagnostics and control for complex systems with high dimensional parameter space, multiscale/multirate/multiphysics phenomena?

New grand challenge LDRD project: Discovery of exploitable fingerprints in data streams coming from high-throughput additive processes in LPBF, electroplating, vapor deposition.

<u>Punchline:</u> AI/ML data-driven models embedded in high-consequence engineering applications require guarantees

(1) How to provide convergence guarantees (AKA "grid refinement")

Designing architectures+optimizers that actually converge

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

Unification of mimetic PDE discretization, algebraic topology and inverse problems

(3) Robustness guarantees for data-driven dynamics in robotics and control

Embedding geometric bracket structure in ML for reliable prediction

CIS RESEARCH FOUNDATION
Research Areas and Strategic Initiatives

Mathematics Algorithms & Simulations

- Mathematical and algorithmic research
- Scalability, performance, credibility
- Multi-scale and multi-physics

Information Sciences & Technology

- Artificial intelligence & machine learning
- Intelligent data collection & retention
- Data-analytics supporting high-consequence decisions

Advanced Computing Systems

- High Performance Computing
- Platform architectures, operating systems, software environments
- Beyond Moore Computing

Cross-Cutting CIS Strategic Initiatives (Initiated in FY20):

Trusted Artificial Intelligence (AI)
Foundation for use of AI technologies and advancements in high-consequence national security applications

Mission Informed Computing Co-Design
Co-design across computing systems, software, operations, algorithms, and applications

Empowering Humans through Computing
Workflows, automation, decision support, and human-data systems

CIS Trusted AI Strategic Crosscut

The ***Trusted AI Strategic Crosscut*** is a new initiative that will coordinate a series of fundamental R&D projects to lay the foundation necessary for Sandia's scientific and national security applications.

AI/ML V&V/UQ/Credibility
Uncertainty propagation and quantification at all stages of the modeling and learning process

Domain-Informed AI/ML
Principled frameworks for incorporating physics, engineering, and/or human expertise into the AI/ML workflow

AI/ML with Limited or Poor-Quality Data
Techniques that enable learning from small, sparse, incomplete, noisy, unknown pedigree, or unlabeled datasets

AI/ML Robustness and Security
Learning techniques that counter adversarial attacks by identifying potential subversions or are resilient to tampering

Mathematical Foundations of AI/ML
Mathematically rigorous approaches to understand high-consequence decisions

<u>Ingredient 1</u>

Probabilistic partition of unity networks

Hybrid architectures combining deep clustering/classification with polynomial regression

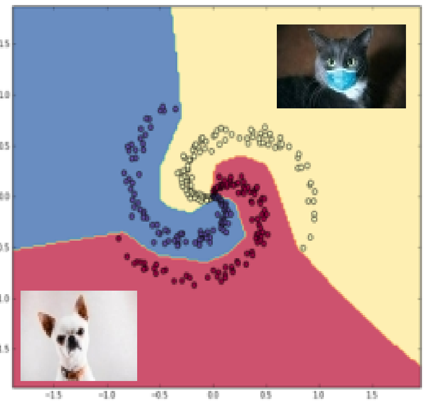
<u>For trusted AI – need architectures which actually converge!</u>

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***

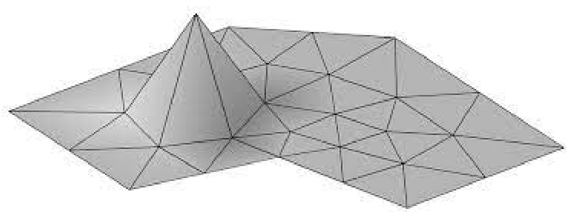
From theory…

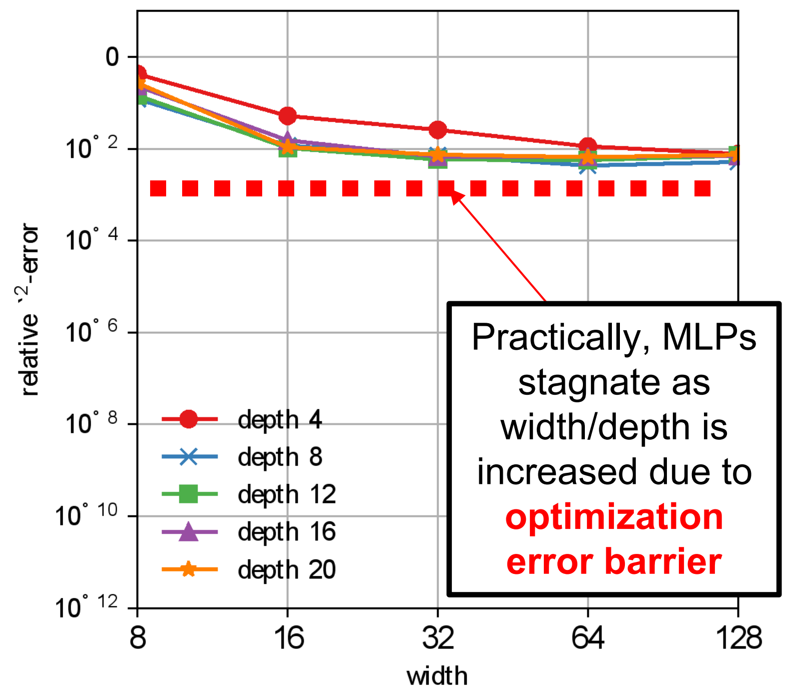
Opschoor et al have established **existence** of neural networks which emulate hp-elements and provide algebraic convergence rates

Emulation of partitions of space



Emulation of monomials on each partition

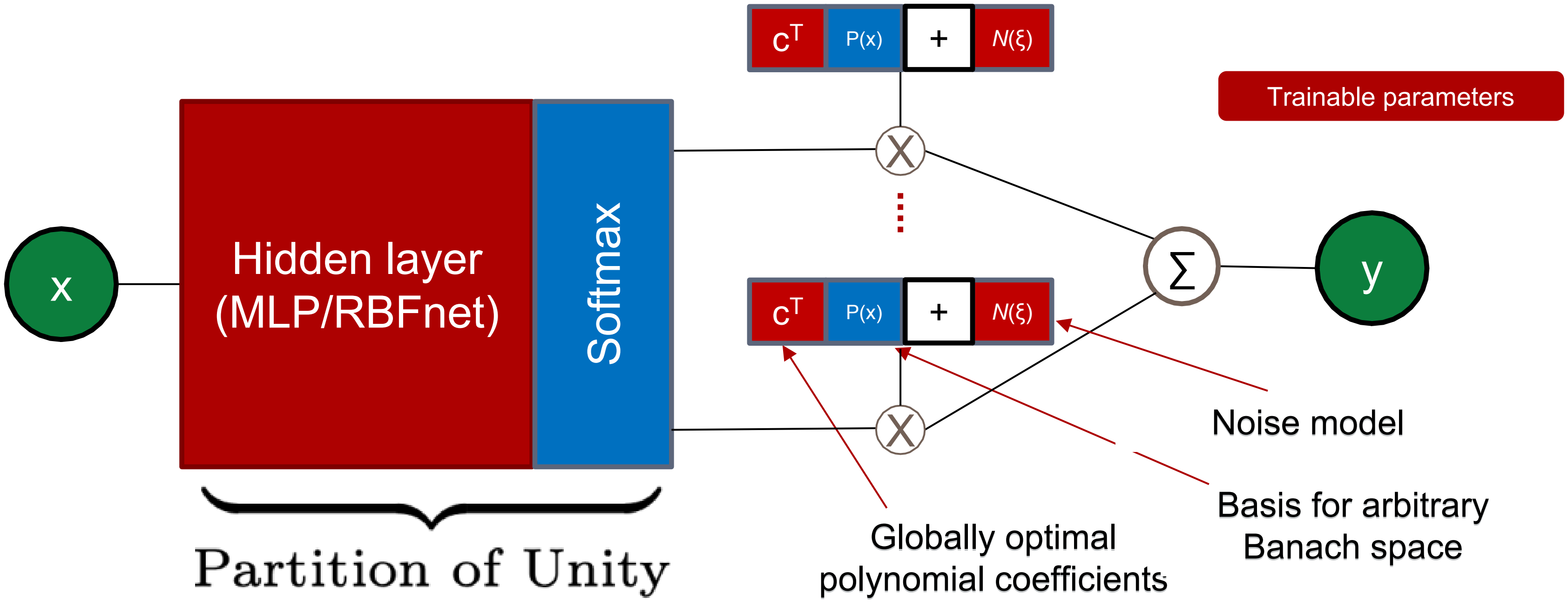




Not realized when training a network with SGD

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

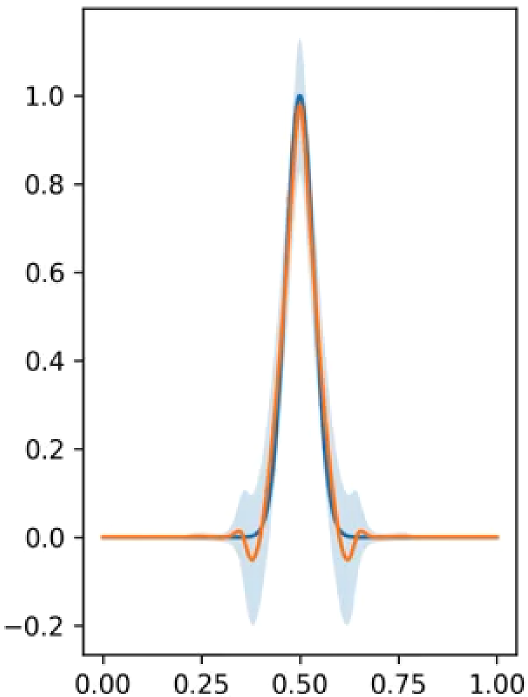


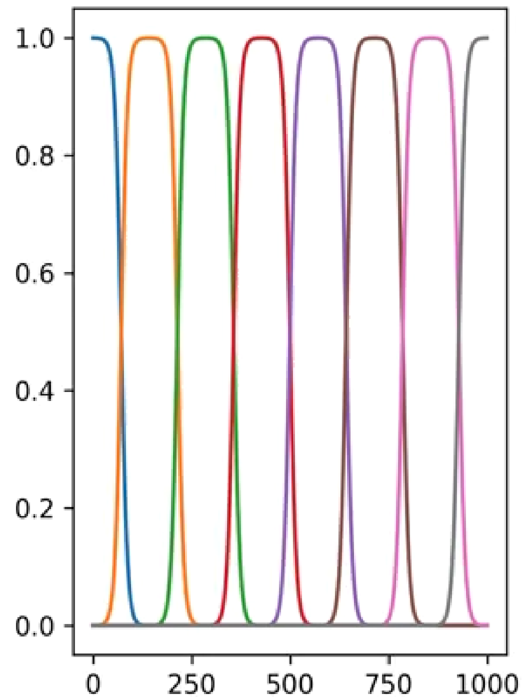
Don't emulate polynomials + partitions – build them in directly!

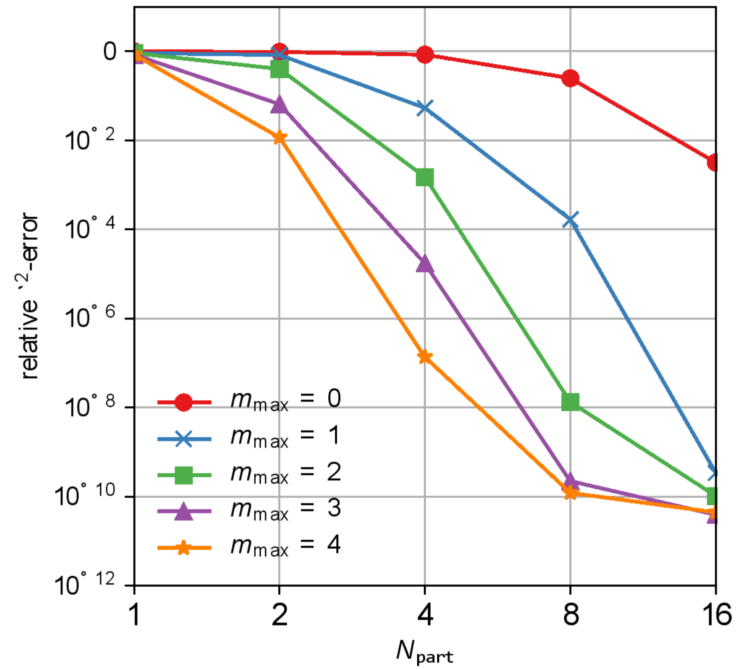
Training:

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

Realization of hp-convergence during training







POUnets demonstrate
algebraic convergence rates
for smooth data

Output:
Piecewise polynomial space with built in error estimator
“Optimal” FEM space **bypassing mesh generation!**

Error estimate: breaking curse of dimensionality

Theorem 1. *Consider an approximant y_{POU} of the form* (1) *with $V = \pi_m(\mathbb{R}^d)$. If $y(\cdot) \in C^{m+1}(\Omega)$ and $\boldsymbol{\xi}^*, \mathbf{c}^*$ solve* (3) *to yield the approximant y^*_{POU}, then*

$$\|y^*_{POU} - y\|^2_{\ell_2(\mathcal{D})} \le C_{m,y} \max_\alpha \operatorname{diam}\left(\operatorname{supp}(\phi^{\boldsymbol{\xi}}_\alpha)\right)^{m+1} \quad (4)$$

where $\|y^*_{POU} - y\|_{\ell_2(\mathcal{D})}$ denotes the root-mean-square norm over the training data pairs in $\mathcal{D}$,

$$\|y^*_{POU} - y\|_{\ell_2(\mathcal{D})} = \sqrt{\frac{1}{N_{data}} \sum_{(\mathbf{x},y)\in\mathcal{D}} \left(y^*_{POU}(\mathbf{x}) - y(\mathbf{x})\right)^2},$$

and

$$C_{m,y} = \|y\|_{C^{m+1}(\Omega)}.$$

Proof. For each α, take $q_\alpha \in \pi_m(\mathbb{R}^d)$ to be the mth order Taylor polynomial of $y(\cdot)$ centered at any point of $\operatorname{supp}(\phi^{\boldsymbol{\xi}}_\alpha)$. Then for all $\mathbf{x} \in \operatorname{supp}(\phi^{\boldsymbol{\xi}}_\alpha)$,

$$|q_\alpha(\mathbf{x}) - y(\mathbf{x})| \le C_{m,y} \operatorname{diam}\left(\operatorname{supp}(\phi^{\boldsymbol{\xi}}_\alpha)\right)^{m+1}. \quad (5)$$

Define the approximant $\widetilde{y}_{POU} = \sum_{\alpha=1}^{N_{part}} \phi^{\boldsymbol{\xi}}_\alpha(\mathbf{x}) q_\alpha(\mathbf{x})$, which is of the form (1) and represented by feasible $(\boldsymbol{\xi}, \mathbf{c})$. Then by definition of y^*_{POU} and (3), we have

$$\begin{aligned}
\|y^*_{POU}(\mathbf{x}) - y(\mathbf{x})\|^2_{\ell_2(\mathcal{D})} &\le \|\widetilde{y}_{POU}(\mathbf{x}) - y(\mathbf{x})\|^2_{\ell_2(\mathcal{D})} \\
&= \left\|\sum_{\alpha=1}^{N_{part}} \phi^{\boldsymbol{\xi}}_\alpha(\mathbf{x}) q_\alpha(\mathbf{x}) - y(\mathbf{x}) \sum_{\alpha=1}^{N_{part}} \phi^{\boldsymbol{\xi}}_\alpha(\mathbf{x})\right\|^2_{\ell_2(\mathcal{D})} \\
&= \left\|\sum_{\alpha=1}^{N_{part}} \phi^{\boldsymbol{\xi}}_\alpha(\mathbf{x}) \left(q_\alpha(\mathbf{x}) - y(\mathbf{x})\right)\right\|^2_{\ell_2(\mathcal{D})}.
\end{aligned}$$

For each $\mathbf{x} = \mathbf{x}_i \in \mathcal{D}$, if $\mathbf{x} \in \operatorname{supp}(\mathcal{D})$, then we apply (5); otherwise, the summand $\phi^{\boldsymbol{\xi}}_\alpha(\mathbf{x}) \left(q_\alpha(\mathbf{x}) - y(\mathbf{x})\right)$ vanishes. So

$$\begin{aligned}
&\|y^*_{POU}(\mathbf{x}) - y(\mathbf{x})\|^2_{\ell_2(\mathcal{D})} \\
&\le \left\|\sum_{\alpha=1}^{N_{part}} C_{m,y} \operatorname{diam}\left(\operatorname{supp}(\phi^{\boldsymbol{\xi}}_\alpha)\right)^{m+1} \phi^{\boldsymbol{\xi}}_\alpha(\mathbf{x})\right\|^2_{\ell_2(\mathcal{D})} \\
&\le C_{m,y} \max_\alpha \operatorname{diam}\left(\operatorname{supp}(\phi^{\boldsymbol{\xi}}_\alpha)\right)^{m+1} \left\|\sum_{\alpha=1}^{N_{part}} \phi^{\boldsymbol{\xi}}_\alpha(\mathbf{x})\right\|^2_{\ell_2(\mathcal{D})} \\
&\le C_{m,y} \max_\alpha \operatorname{diam}\left(\operatorname{supp}(\phi^{\boldsymbol{\xi}}_\alpha)\right)^{m+1}.
\end{aligned}$$

- If reconstructing with polynomials, and **POU with compact support** is found, we realize hp-convergence for smooth functions **independent of dimension**
- **How do we get compact support?**

Lee, Kookjin, et al. "Partition of unity networks: deep hp-approximation." *arXiv preprint arXiv:2101.11256* (2021) AAAI-MLPS

“Toy” problem: data-driven chemical kinetics for combustion

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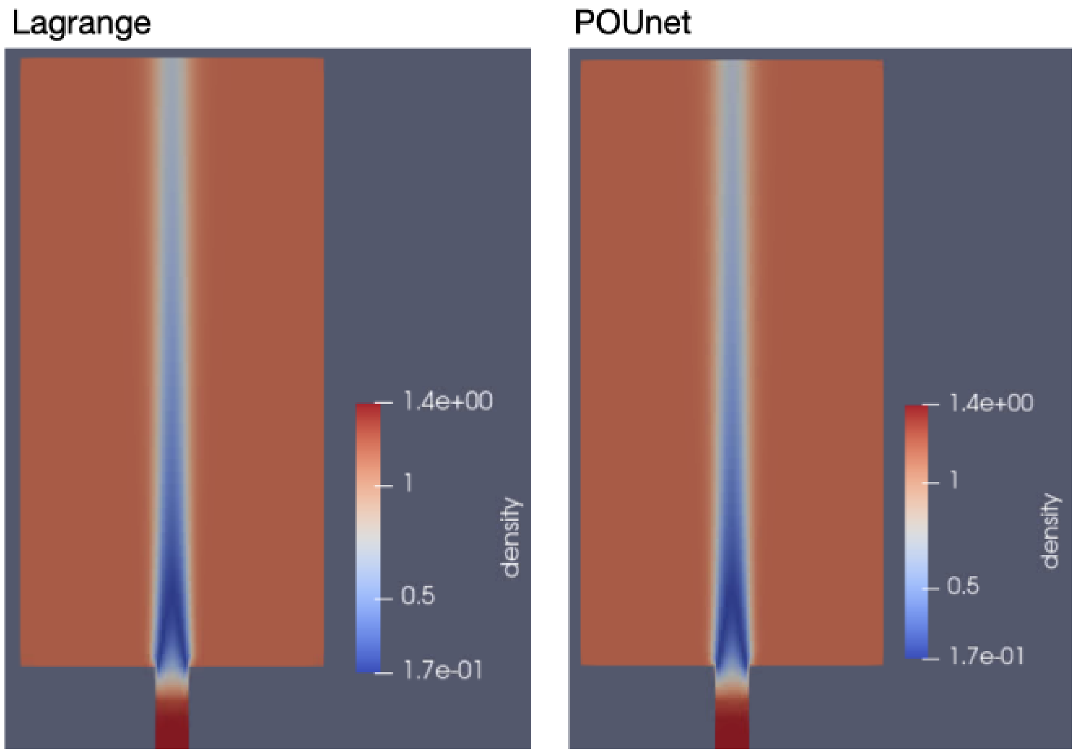
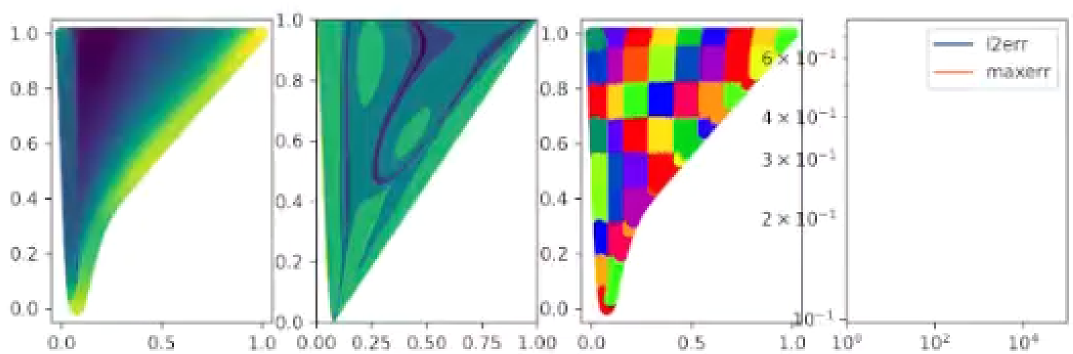




Lookup **Error** **Partitions** **Residuals**

Lookup tables for chemical kinetics suffer from curse-of-dimensionality

- Train a POUnet to replace tables
- Perform inference on trained network in production code

Huge memory savings
- **Before:** 1 GB/specie
- **After:** 500 KB/specie

Impact: Can afford higher dimensional chemistry models

Summer intern project: Elizabeth Armstrong, led by John Newson

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).

Two key ingredients to physics-compatible/mimetic discretization

1: A topological structure

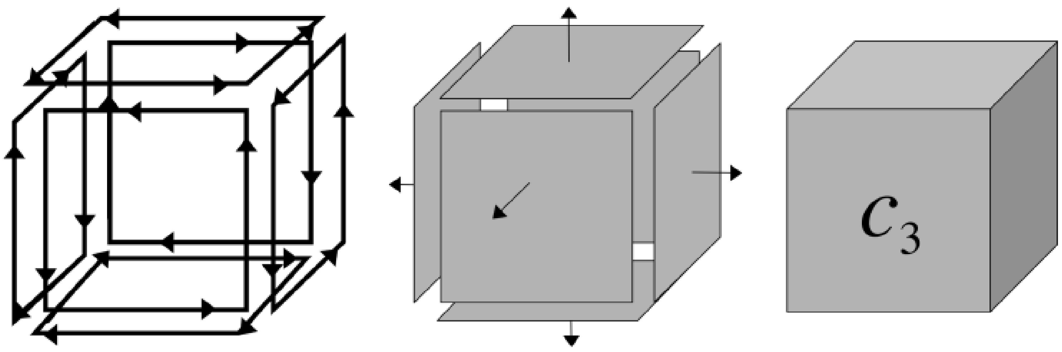
In PDE discretization this is a mesh, with boundary operators linking cells, faces, edges, and nodes

We will use a graph as an inexpensive low-dimensional mesh surrogate

2: Metric information

Measures associated with mesh entities, ensuring discrete exterior derivatives converge to div/grad/curl

Graphs are purely topological with no natural metric, we will use ML to extract metric information from data

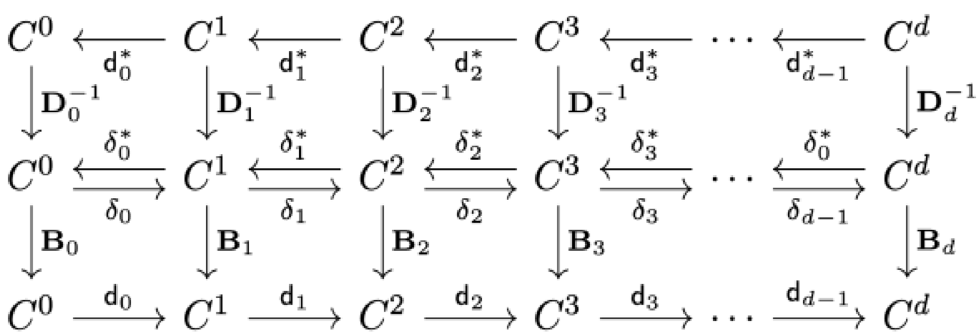


$$0 \leftarrow \partial\partial c_3 \xleftarrow{\partial} \partial c_3 \xleftarrow{\partial} c_3$$

$$\nabla \cdot \mathbf{u} = \frac{1}{\mu(C)} \sum_{f \in \partial C} \int_f \mathbf{u} \cdot d\mathbf{A}$$

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**



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*

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

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

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

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*

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

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

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 w/ metric params

Nonlinear perturbation with DNN params

Output

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

- Stable
- Solvable
- Structure-preserving

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

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

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, preprint on researchgate

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?

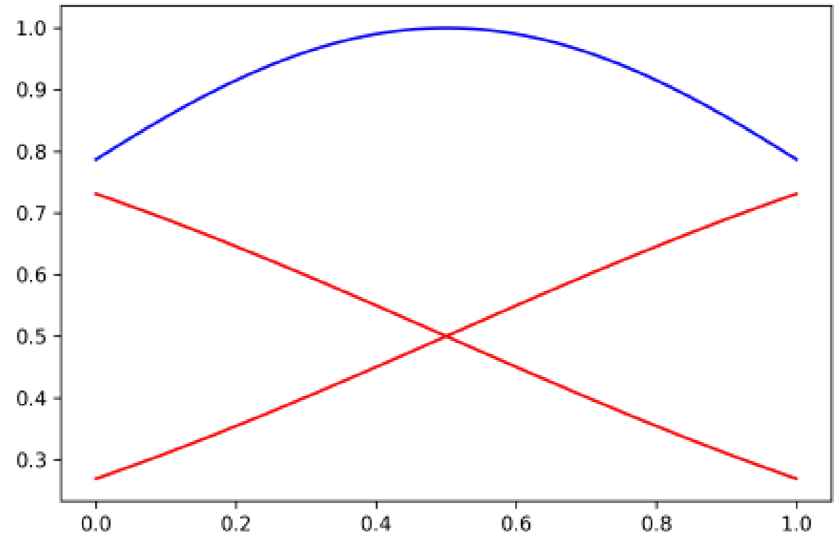
$$\int_c \nabla \cdot \mathbf{u} dx = \int_{f \in \partial c} \mathbf{u} \cdot d\mathbf{A}$$

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

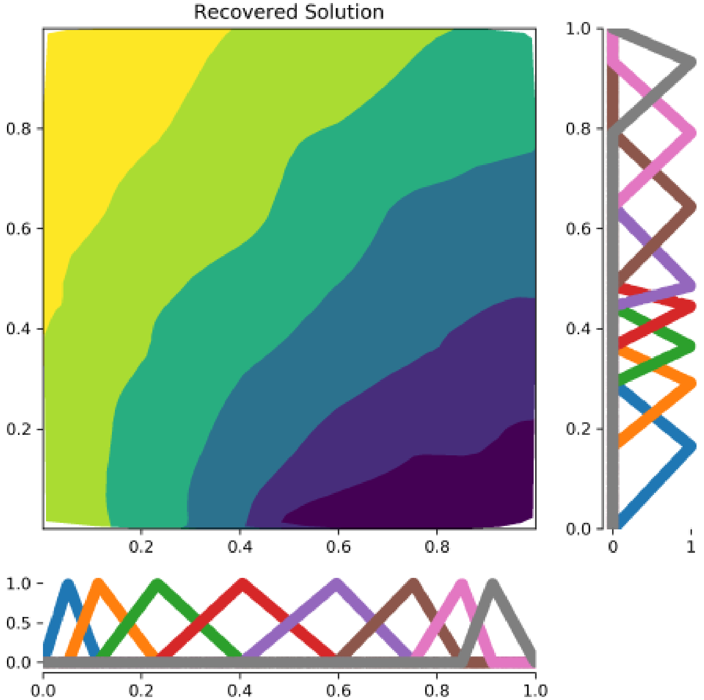
$$\begin{aligned}
\int_\Omega \psi_i \nabla \cdot \mathbf{u} &= -\int_\Omega \nabla \phi_i \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA \\
&= -\sum_j \int_\Omega \phi_j \nabla \phi_i \cdot \mathbf{u} + \int \phi_i \mathbf{u} \cdot dA \\
&= \sum_{j \neq i} \int_\Omega (\phi_i \nabla \phi_j - \phi_j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

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

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

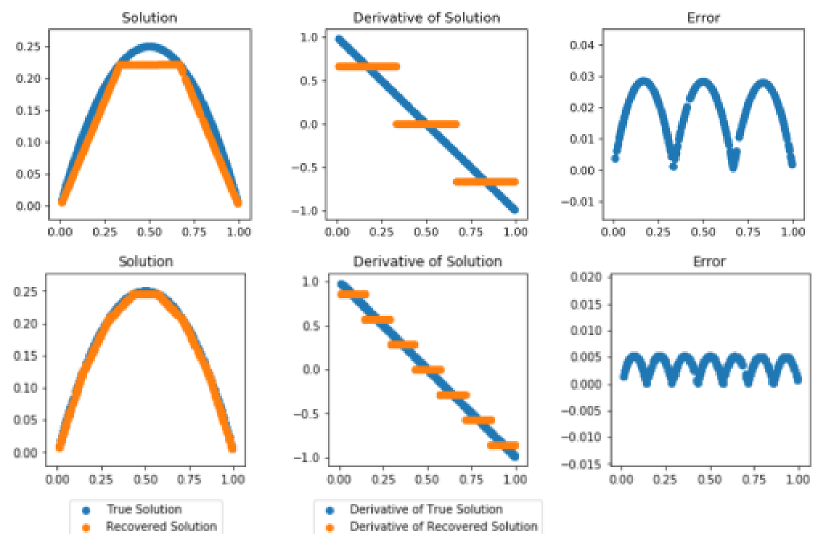
A necessary ingredient: POU allowing exact quadrature

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



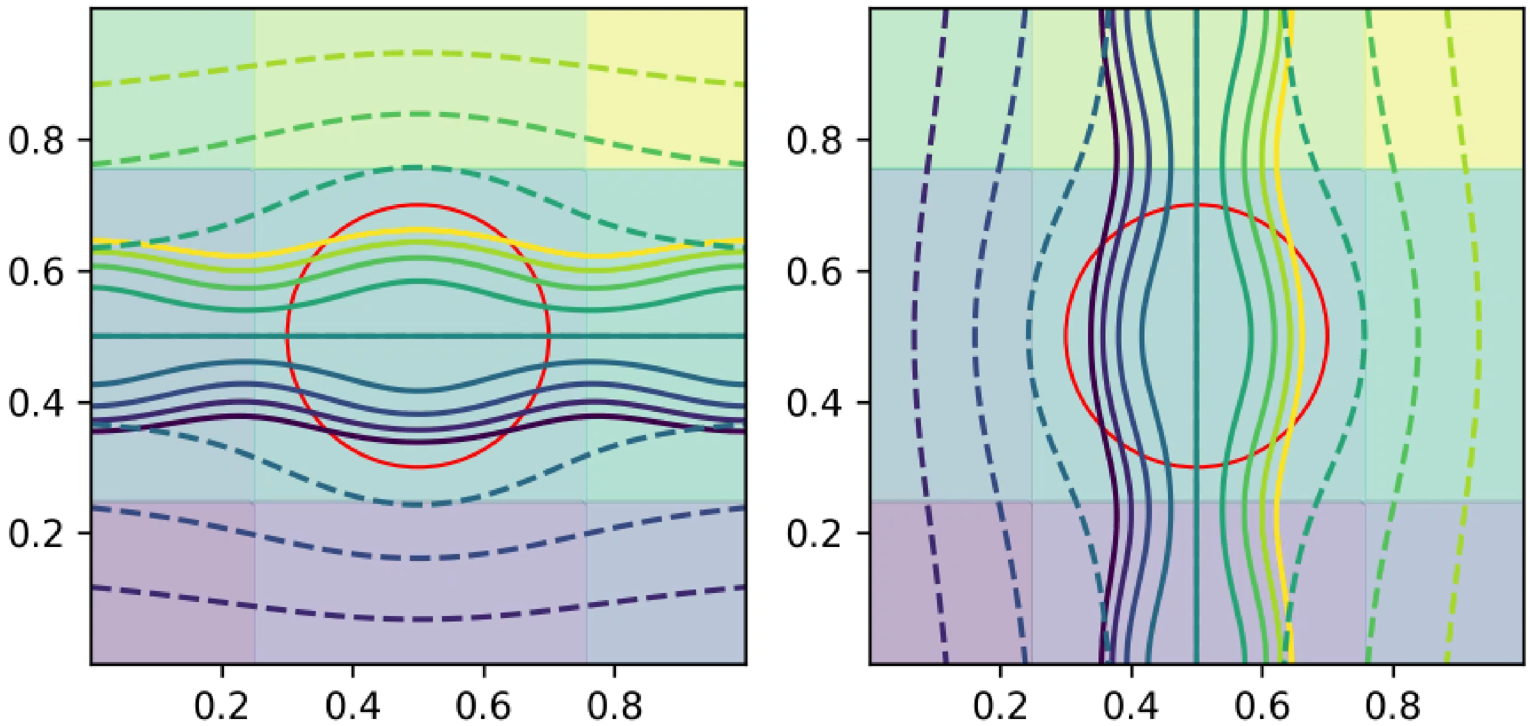
$$
\begin{aligned}
-\Delta u &= 0 && \text{on} && \Omega' = [-1,1] \times [0,1] \\
\partial_n u &= 0 && \text{on} && \Gamma_N = [-1,0] \times \{0\} \\
u &= g(r,\theta) && \text{on} && \Gamma_D = \partial\Omega' \backslash \Gamma_N .
\end{aligned}
$$

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



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



BC + solution → **Training** → Mimetic FEM → **Embedding** → Production code

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

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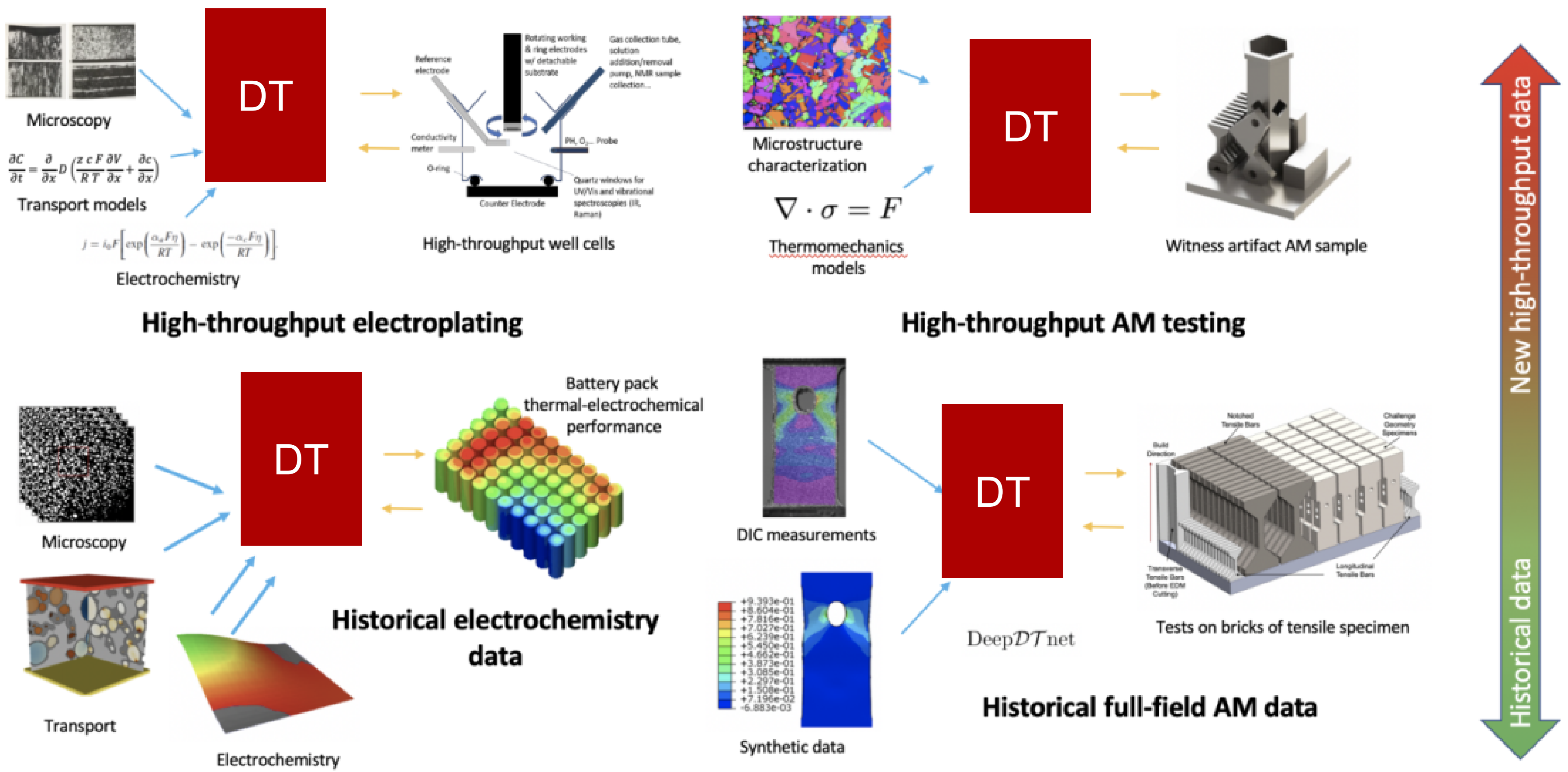
Digital Twins for High-throughput Testing

PDE-based simulation is too expensive for real-time active control.

Need **fast surrogates** to blend **heterogeneous data** amenable to varying degrees of physics-based modeling



Digital Twins for High-throughput Testing

Sandia National Laboratories

Operator regression – replace PDE solves with DNNs trained to lookup parameterized PDE solutions

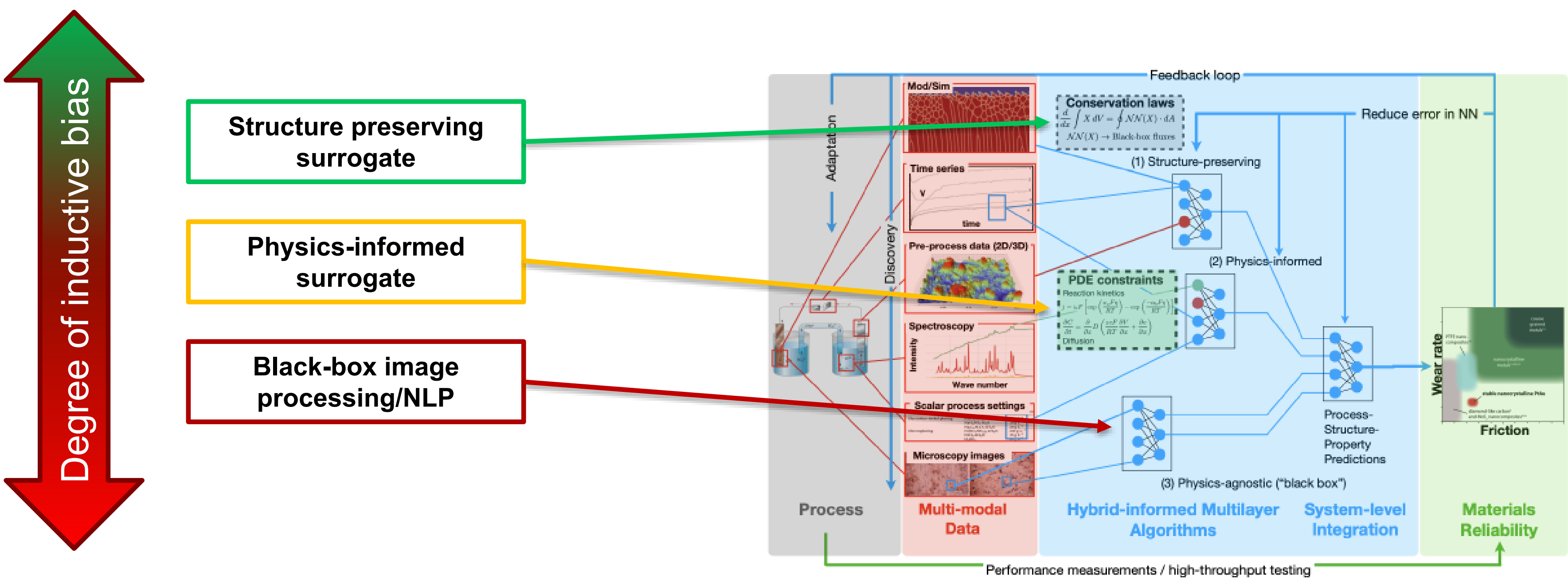
Trask, Nathaniel, et al. "GMLS-Nets: A framework for learning from unstructured data." NeurIPs proceedings (2019)

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)

Learn geometric structure preserving dynamics to support control

Jonas Actor, Andy Huang, Nathaniel Trask. "Polynomial-Spline Neural Networks with Exact Integrals". (under review)

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)



Data-driven dynamical systems for forecasting+control

“Black box” – no required model ⟷ Strong physical priors

Neural ODE (NODE)
Ricky TQ Chen, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud. Neural ordinary differential equations. In *Proceedings of the 32nd International Conference on Neural Information Processing Systems*, pages 6572–6583, 2018.

Universal DiffEq (UDE)
Christopher Rackauckas, Yingbo Ma, Julius Martensen, Collin Warner, Kirill Zubov, Rohit Supekar, Dominic Skinner, Ali Ramadhan, and Alan Edelman. Universal differential equations for scientific machine learning. *arXiv preprint arXiv:2001.04385*, 2020.

Dictionary (e.g SinDy)
Brunton, Steven L., Joshua L. Proctor, and J. Nathan Kutz. "Discovering governing equations from data by sparse identification of nonlinear dynamical systems." *Proceedings of the national academy of sciences* 113.15 (2016): 3932-3937.

$$\frac{d\mathbf{x}}{dt} = \mathcal{N}\mathcal{N}(\mathbf{x};\xi)$$

No modeling required
Bad generalization
Difficult training

$$\frac{d\mathbf{x}}{dt} = F(\mathbf{x};\xi)$$

Need first principles starting point
Good forecasting
Easy to train

Data-driven dynamical systems for forecasting

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"Black box" – no required model | Structure-preserving ML | Strong physical priors

Neural ODE (NODE)
Ricky TQ Chen, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud. Neural ordinary differential equations. In *Proceedings of the 32nd International Conference on Neural Information Processing Systems*, pages 6572–6583, 2018.

Hamiltonian NN
Samuel Greydanus, Misko Dzamba, and Jason Yosinski. Hamiltonian neural networks. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.

Symplectic RNN
Zhengdao Chen, Jianyu Zhang, Martin Arjovsky, and Léon Bottou. Symplectic recurrent neural networks. In *International Conference on Learning Representations*, 2019.

SympNets
Pengzhan Jin, Zhen Zhang, Aiqing Zhu, Yifa Tang, and George Em Karniadakis. Sympnets: Intrinsic structure-preserving symplectic networks for identifying hamiltonian systems. *Neural Networks*, 132:166– 179, 2020.

Lagrangian NN
Miles Cranmer, Sam Greydanus, Stephan Hoyer, Peter Battaglia, David Spergel, and Shirley Ho. La- grangian neural networks. In *ICLR 2020 Workshop on Integration of Deep Neural Models and Differential Equations*, 2020.

Reversible Systems Only!

Universal DiffEq (UDE)
Christopher Rackauckas, Yingbo Ma, Julius Martensen, Collin Warner, Kirill Zubov, Rohit Supekar, Dominic Skinner, Ali Ramadhan, and Alan Edelman. Universal differential equations for scientific machine learning. *arXiv preprint arXiv:2001.04385*, 2020.

Dictionary (e.g SINDy)
Brunton, Steven L., Joshua L. Proctor, and J. Nathan Kutz. "Discovering governing equations from data by sparse identification of nonlinear dynamical systems." *Proceedings of the national academy of sciences* 113.15 (2016): 3932 -3937.

$$\frac{d\mathbf{x}}{dt} = \mathbf{J}_{\theta_1} \nabla_{\mathbf{x}} \mathcal{H}(\mathbf{x};\theta_2)$$

$$\mathbf{J}_{\theta_1} = -\mathbf{J}_{\theta_1}^{\intercal}$$

$$\frac{d\mathcal{H}}{dt} = 0$$

Learn a gradient flow with underlying conserved quantity (Casimir)

Symplectic flow implies conserved phase area = no exploding/vanishing gradients

Better forecasting, accuracy, and stability

Control for robotics (neglecting friction!)

Metriplectic dynamical systems generalize Hamiltonian/Lagrangian dynamics to dissipative systems

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Hamiltonian

$$\frac{d\mathbf{x}}{dt} = \mathbf{J}\,\nabla_{\mathbf{x}}\mathcal{H}(\mathbf{x})$$

$$\mathbf{J} = -\mathbf{J}^{\intercal}$$

$$\frac{d\mathcal{H}}{dt} = 0$$

Port-Hamiltonian

$$\frac{d\mathbf{x}}{dt} = (\mathbf{J} - \mathbf{R})\;\nabla_{\mathbf{x}}\mathcal{H}(\mathbf{x})$$

$$\mathbf{J} = -\mathbf{J}^{\intercal} \qquad \mathbf{R} = \mathbf{R}^{\intercal}$$

$$\frac{d\mathcal{H}}{dt} \leq 0$$

GENERIC

$$\frac{d\mathbf{x}}{dt} = \mathbf{L}\,\nabla_{\mathbf{x}}\mathcal{E}(\mathbf{x}) + \mathbf{M}\,\nabla_{\mathbf{x}}\mathcal{S}(\mathbf{x})$$

$$\mathbf{L} = -\mathbf{L}^{\intercal} \qquad \mathbf{M} = \mathbf{M}^{\intercal}$$

$$\mathbf{L}\,\nabla_{x}\mathcal{S} = \mathbf{M}\,\nabla_{x}\mathcal{E} = 0$$

$$\frac{d\mathcal{E}}{dt} = 0 \qquad \frac{d\mathcal{S}}{dt} \geq 0$$

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \{A, E\} + [A, S]$$

Reversible Irreversible

Guha, Partha. "Metriplectic structure, Leibniz dynamics and dissipative systems." *Journal of Mathematical Analysis and Applications* 326, no. 1 (2007): 121-136

GENERIC: some more details

$$\frac{d\mathbf{x}}{dt} = \mathbf{L}\,\nabla_{\mathbf{x}}\mathcal{E}(\mathbf{x}) + \mathbf{M}\,\nabla_{\mathbf{x}}\mathcal{S}(\mathbf{x})$$

$$\mathbf{L} = -\mathbf{L}^{\intercal} \qquad \mathbf{M} = \mathbf{M}^{\intercal}$$

$$\mathbf{L}\,\nabla_x\mathcal{S} = \mathbf{M}\,\nabla_x\mathcal{E} = 0$$

$$\frac{d\mathcal{E}}{dt} = 0 \qquad \frac{d\mathcal{S}}{dt} \geq 0$$

An algebraic structure for tracking generalized Hamiltonians (Casimirs)

Classically, a model is derived from first principles and one notices GENERIC structure

<u>First law of thermodynamics</u>

$$\begin{aligned}\frac{d\mathcal{E}}{dt} &= \nabla_x\mathcal{E}^{\intercal}\,\frac{d\mathbf{x}}{dt}\\ &= \nabla_x\mathcal{E}^{\intercal}\left(\mathbf{L}\,\nabla_{\mathbf{x}}\mathcal{E}(\mathbf{x}) + \mathbf{M}\,\nabla_{\mathbf{x}}\mathcal{S}(\mathbf{x})\right)\\ &= \nabla_x\mathcal{E}^{\intercal}\,\mathbf{L}\,\nabla_{\mathbf{x}}\mathcal{E}(\mathbf{x}) + \nabla_x\mathcal{S}^{\intercal}\,\mathbf{M}\,\nabla_{\mathbf{x}}\mathcal{E}(\mathbf{x})\\ &= 0\end{aligned}$$

<u>Second law of thermodynamics</u>

$$\begin{aligned}\frac{d\mathcal{S}}{dt} &= \nabla_x\mathcal{S}^{\intercal}\,\frac{d\mathbf{x}}{dt}\\ &= \nabla_x\mathcal{S}^{\intercal}\left(\mathbf{L}\,\nabla_{\mathbf{x}}\mathcal{E}(\mathbf{x}) + \mathbf{M}\,\nabla_{\mathbf{x}}\mathcal{S}(\mathbf{x})\right)\\ &= -\nabla_x\mathcal{E}^{\intercal}\,\mathbf{L}\,\nabla_{\mathbf{x}}\mathcal{S}(\mathbf{x}) + \nabla_x\mathcal{S}^{\intercal}\,\mathbf{M}\,\nabla_{\mathbf{x}}\mathcal{S}(\mathbf{x})\\ &\geq 0\end{aligned}$$

We parameterize algebraic structure and discover dissipative model

Fluctuation dissipation theorem

$$\mathrm{d}\boldsymbol{x}_t = \left(L \frac{\partial E}{\partial \boldsymbol{x}} + M \frac{\partial S}{\partial \boldsymbol{x}} + k_B \frac{\partial}{\partial \boldsymbol{x}} \cdot M \right) \mathrm{d}t + \sqrt{2 k_B M} \mathrm{d}W_t$$

Reversible — Irreversible dissipation — Thermal noise

- **Exact treatment of reversible and irreversible dynamics allows introduction of thermal forcing which *exactly* balances dissipation**
- **Implies existence of long time stationary statistics for equilibrium processes, amenable to large deviations theory**
- **A data-driven alternative to Mori-Zwanzig formalisms. Memory effects are encoded through the evolution of entropy and no need to treat complicated memory effects with integral kernels**

Hans Christian Öttinger, Mark A Peletier, and Alberto Montefusco. A framework of nonequilibrium statistical mechanics. i. role and types of fluctuations. *Journal of Non-Equilibrium Thermodynamics*, 2020.

Toy example: piston driven by two gases

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{p}{m},$$

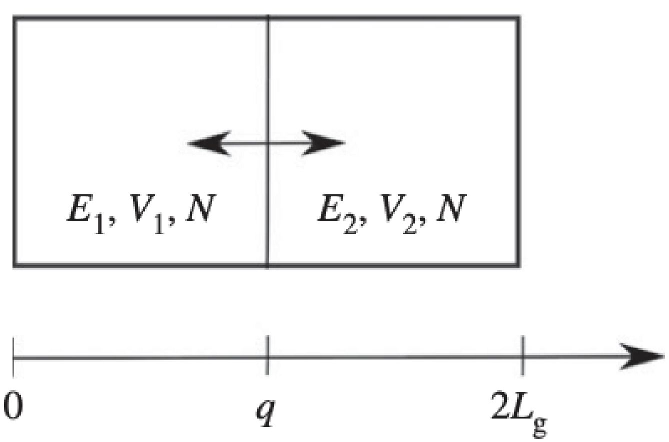
$$\frac{\mathrm{d}S_1}{\mathrm{d}t} = \frac{9N^2k_B^2\alpha}{4E_1}\left(\frac{1}{E_1} - \frac{1}{E_2}\right)$$

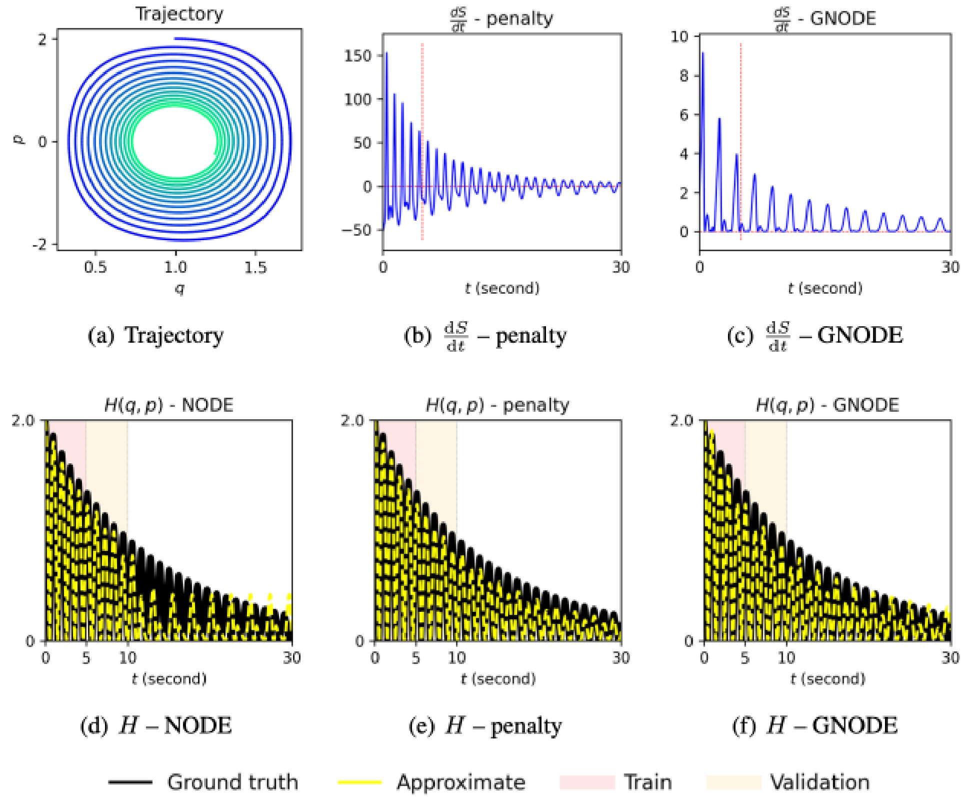
$$\frac{\mathrm{d}p}{\mathrm{d}t} = \frac{2}{3}\left(\frac{E_1}{p} - \frac{E_2}{2L_g - p},\right)$$

$$\frac{\mathrm{d}S_2}{\mathrm{d}t} = -\frac{9N^2k_B^2\alpha}{4E_1}\left(\frac{1}{E_1} - \frac{1}{E_2}\right)$$

$$\frac{S_i}{Nk_B} = \ln\left[\hat{c}V_i(E_i)^{3/2}\right], \quad i = 1, 2$$

$$V_1 = qA_c \quad \text{and} \quad V_2 = (2L_g - q)\,A_c$$





- **Black box neuralODE generalizes poorly**
- **Structure preservation = reliable extrapolation**

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). (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."** ***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)
15. Behzadinasab, M., Moutsanidis, G., Trask, N., Foster, J.T. and Bazilevs, Y., 2021. Coupling of IGA and Peridynamics for Air-Blast Fluid-Structure Interaction Using an Immersed Approach. *Forces in Mechanics*, p.100045.
16. Behzadinasab, M., Alaydin, M., Trask, N. and Bazilevs, Y., 2021. A general-purpose, inelastic, rotation-free Kirchhoff-Love shell formulation for peridynamics. *arXiv preprint arXiv:210*

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)