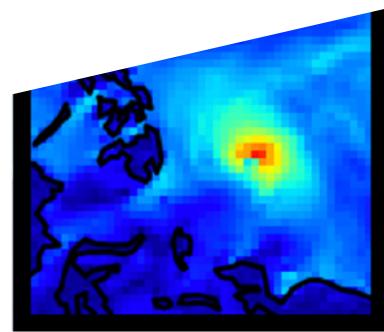
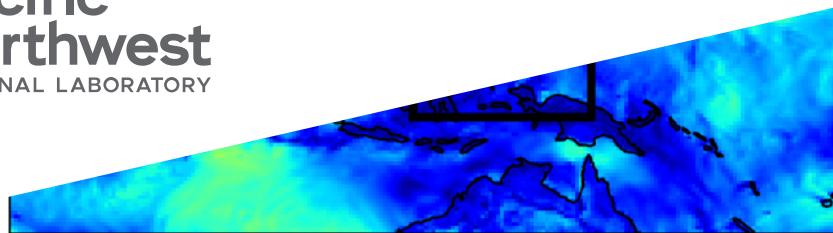
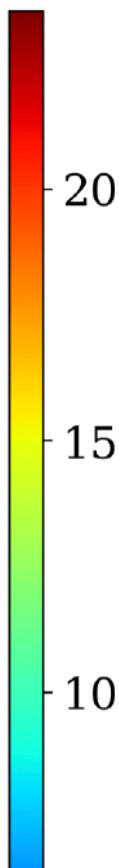
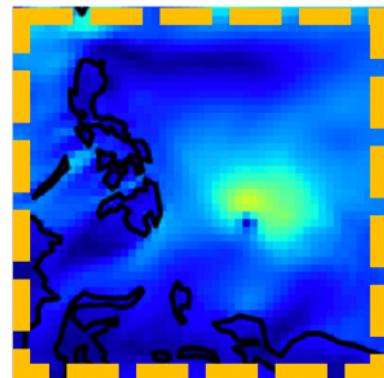
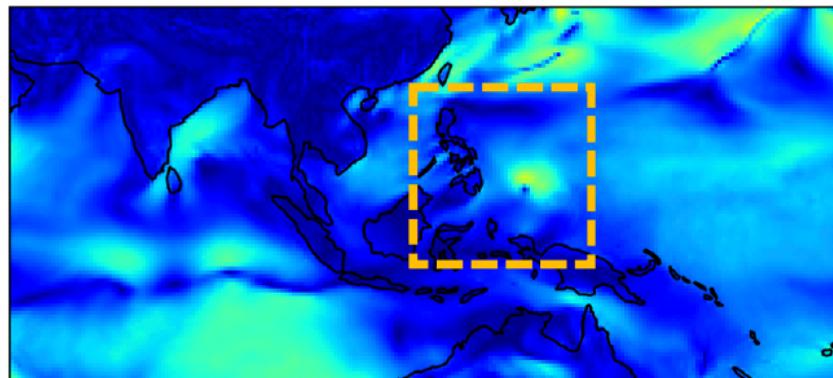




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Neural Operator



SEA-CROGS: Scalable, Efficient and Accelerated Causal Reasoning Operators, Graphs and Spikes for Earth and Embedded Systems

October 2024

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SEA-CROGS: Scalable, Efficient and Accelerated Causal Reasoning Operators, Graphs and Spikes for Earth and Embedded Systems

ANNUAL REPORT

October 2024

Prepared for
the U.S. Department of Energy
under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99354

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SEA-CROGS Progress Report 2022–2024

The SEA-CROGS integrated mathematical and computational activities can be classified into the following three research areas (see fig. 1): (Research Area I) neural operators; (Research Area II) graph neural networks; and (Research Area III) spiking neural networks. These research areas allow co-design of mathematics, algorithmic implementations, and computing hardware to augment foundational understanding and optimal control of complex systems spanning extremely disparate scales, e.g., climate modeling processes, as well as embedded systems and systems-of-systems requiring causal inference, physics-informed modeling, risk-adaptive decision making, and edge computing.

Physics-informed neural networks (PINNs) are a workhorse tool for the project [1], and new work has emphasized crosscutting themes of the mathematics of machine intelligence, causal inference, uncertainty quantification (UQ), and trustworthy physics-informed machine intelligence. In the following sections, we summarize research accomplishments, highlights, and current directions from the first and second years of the project.

1 Research Area I

In this section, we will describe progress in developing a plurality of neural operators that are mathematically rigorous and can be trained robustly by multimodal/multifidelity data.

1.1 Online bias correction machine learning model

We used operator learning to address the model biases in Department of Energy's (DOE's) Energy Exascale Earth System Model (E3SM) [2] by learning the operator \mathcal{G} from \mathcal{U} (before nudge data) to \mathcal{V} (nudging tendency), which reads $\mathcal{G} : \mathcal{U}(x, y, t) \rightarrow \mathcal{V}(x, y, t + \Delta t)$. The trained operator was then integrated with E3SM to form a hybrid model to predict and apply a bias correction for climate simulations. We trained four operator architectures: Autoencoder-based DeepONet [3], U-Net [4], ViTO[5], and Multi-scale Multi-feature UNet (M&M). From these architectures, the M&M architecture has the potential to correct large-scale model biases in short-term climate predictions, as evidenced by the Hurricane Sandy case study (fig. 2a–b). For long-term climate simulations, however, compared with the baseline (CTRL) and nudging (NDGUV), M&M only showed limited improvements in the root mean square errors of most physical qualities, and it had nudging discrepancies (fig. 2c–d). Therefore, further developing the M&M model to improve its performance in correcting long-term climate bias is needed, including the consideration of interactions between additional state variables.

1.2 The conjugate kernel for efficient and accurate training of physics-informed operator networks

Recent work has shown that the empirical neural tangent kernel (NTK) can significantly improve the training of physics-informed (PI) DeepONets. The NTK, however, is costly to calculate, greatly increasing the cost to train such systems. In SEA-CROGS, we studied the performance of the empirical conjugate kernel (CK) [6] for PI-DeepONets, an efficient approximation to the NTK. For PI-DeepONets, we showed that the CK performance is comparable to that of the NTK while significantly reducing the time complexity for training. For example, for

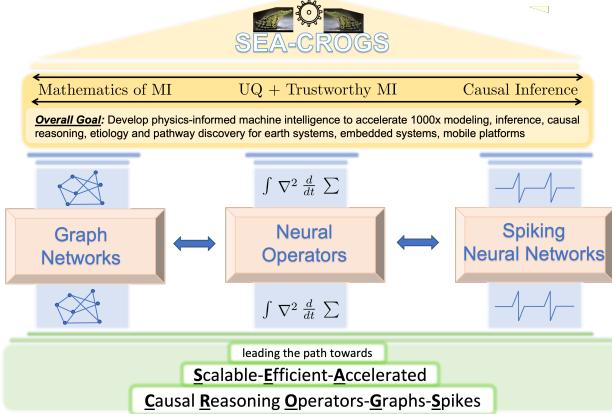


Figure 1: Overview of the SEA-CROGS project. The three mathematical research areas are connected through the cross-cutting research themes.

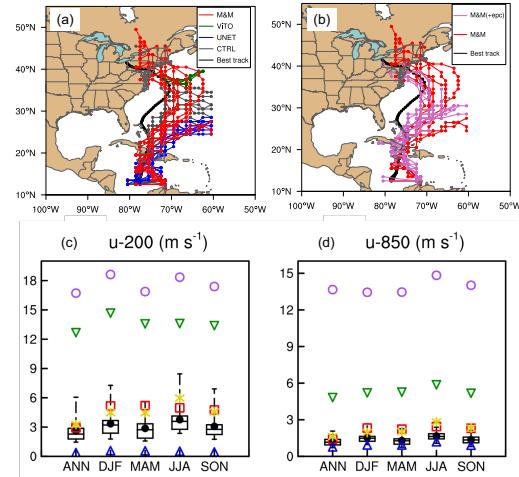


Figure 2: First row: Hurricane Sandy (2012) tracks from (a) E3SM with machine learning bias correction using M&M (red), ViTO (green) and U-Net (blue), compared against observations (best track, black) and free-running E3SM (CTRL, grey); (b) E3SM with M&M architecture trained without (purple) and with (red) an increased number of epochs. Second row: Comparison of root mean square errors of the global spatial distribution derived from a 1-year simulation (2012) in E3SM with free-running (CTRL, red rectangles), UV nudging (NDGUV, blue triangles), U-Net (green triangles), ViTO (purple circles), and M&M (yellow stars) for zonal winds at (c) 200 hPa and (d) 850 hPa pressure levels. The x-axis shows seasonal means for DJF (December–February), MAM (March–May), JJA (June–August), SON (September–November), and the annual mean (ANN).

Burgers' equation with small viscosity $\nu = 0.001$, a PI-DeepONet without the NTK or CK has a mean relative ℓ_2 error of 9.18% [7]. Using the NTK decreases the mean relative error to 2.80% but increases the training time by a factor of 3.8. With the CK, the error increases only slightly to 3.04%, and the training time is only 1.6 times higher than training without the NTK or CK [8].

1.3 Stacking and finite basis DeepONets

PINNs and PI-DeepONets have shown promise for effectively solving equations modeling physical systems. However, these networks can be difficult or impossible to train accurately for some systems of equations. We developed a novel multifidelity framework for stacking PI-DeepONets that uses multifidelity DeepONets [9] to progressively increase the accuracy of a PI-DeepONet [10], shown in fig. 3. Starting from a trained PI-DeepONet, we train a multifidelity PI-DeepONet to learn a correction from the previously trained model. This process can be repeated until the desired accuracy is reached. Through benchmark problems, we showed how stacking improves the accuracy and reduces the required number of trainable parameters. This work was extended to accommodate domain decomposition with finite basis DeepONets at each stacking level to further increase the accuracy of the trained model [11].

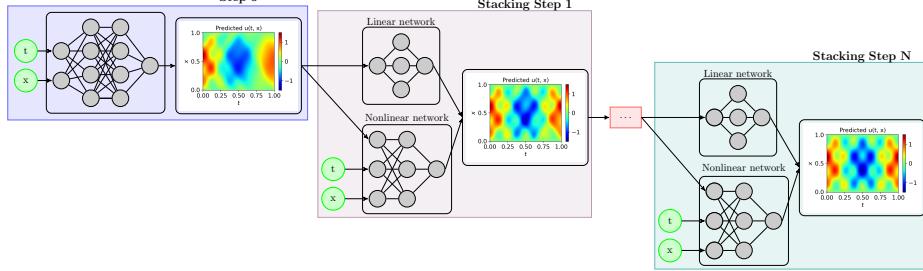


Figure 3: Stacking networks start with a trained PINN or PI-DeepONet, then progressively learn corrections using multifidelity PINNs or DeepONets.

1.4 Identifying the optimal means to mitigate the consequences of anthropogenic climate change through effective forcings

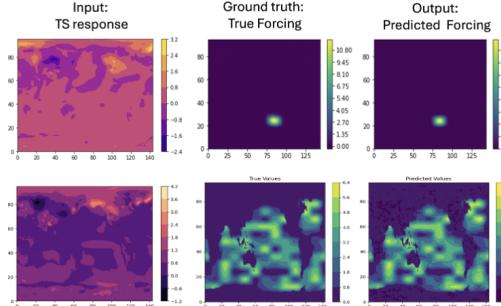


Figure 4: Test prediction of forcing from an M&M model with the linear response of surface temperature as input. The first row shows test results for the model trained with individual forcing and responses, and the second row shows test results for the model trained with the linearly combined forcings and responses.

effects. Both neural operators and graph-based architectures showed good results for these sets. Figure 4 shows plots for a test case not seen during training. To verify the models' effectiveness, the next step is to run a climate solver for the predicted forcing to see if it produces similar responses.

1.5 Feature-adjacent multi-fidelity neural network

The key point in multi-fidelity modeling is how to represent the relationship between the low- and high-fidelity solutions. Note that the low- and high-fidelity solutions are often highly correlated. In general, two objects are considered similar if they share a substantial number of features. Therefore, we can embed this similarity into the multi-fidelity architecture by assuming the low-fidelity and high-fidelity solutions are adjacent by constraining their relative distance in a feature space [12], namely, $\alpha^H = \alpha^L \odot (1 + d_f \lambda)$, where d_f is the relative distance, $\lambda \in [-1, 1]^{N_f}$ is the feature shift (a trainable vector), and α^H and α^L are the coefficients of low- and high-fidelity representations in the feature space spanned by a set of basis functions $f = \{f_i(x)\}_{i=1}^{N_f}$. The feature space is represented with an encoder network, and its mapping to the original solution space is effected through a decoder

network. Figure 5 shows an illustration of the multi-fidelity architecture along with a trivial example. The proposed multi-fidelity approach is validated on forward and inverse problems for steady and unsteady problems described by partial differential equations (PDEs) [12].

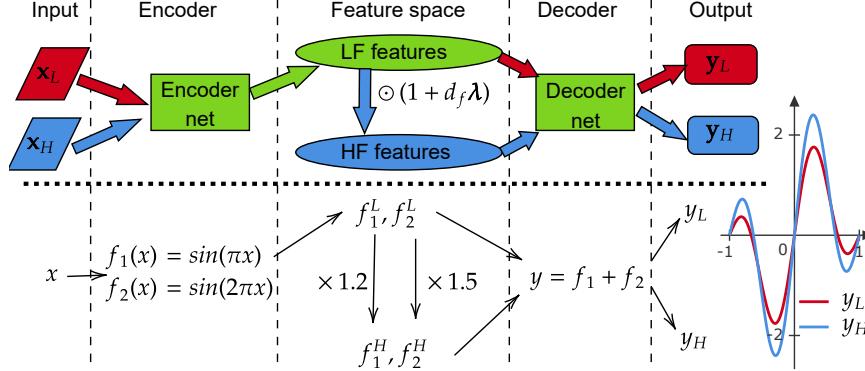


Figure 5: (top) A schematic of the multi-fidelity network architecture and (bottom) a trivial example. In the top part, the green components are shared by the low- and high-fidelity propagation. The red and blue components are used for the low- and high-fidelity propagation, respectively.

1.6 Integrating neural operators with diffusion models improves spectral representation in turbulence modeling

We integrate neural operators with diffusion models to address the spectral limitations of neural operators in surrogate modeling of turbulent flows [13]. While neural operators offer computational efficiency, they exhibit deficiencies in capturing high-frequency flow dynamics, resulting in overly smooth approximations. To overcome this, we condition diffusion models on neural operators to enhance the resolution of turbulent structures. Our approach is validated for different neural operators (FNO [14], MATCHO [15]) on diverse datasets, including a high Reynolds number jet flow simulation [16] and experimental Schlieren velocimetry [17], fig. 6. The proposed method significantly improves the alignment of predicted energy spectra with true distributions compared to neural operators alone. Additionally, proper orthogonal decomposition analysis demonstrates enhanced spectral fidelity in space-time. This work establishes a new paradigm for combining generative models with neural operators to advance surrogate modeling of turbulent systems, and it can be used in other scientific applications that involve microstructure and high-frequency content.

1.7 Self-adaptive weighting and sampling method for physics-informed machine learning

According to NTK theory [18], the residuals of governing equations and boundary conditions decay exponentially during the training dynamics of physics-informed machine learning models. Leveraging this insight, we propose the “inverse residual decay rate” as a quantitative measurement to describe the convergence speed of residuals at individual training points [19]. In our study involving the 1D Poisson equation, we demonstrate that the inefficiency of plain PINNs arises from significant discrepancies in the convergence speeds of residuals across different training points; specifically, the slowest-converging points dominate and hinder the overall solution convergence. To address this issue, we introduce a point-wise adaptive weighting method that balances the residual decay rates across training points. Numerical results demonstrate that our approach of balancing residual decay rates offers several advantages: bounded weights, high prediction accuracy, faster convergence speed, reduced training uncertainty, lower computational cost, and ease of hyperparameter tuning.

However, when attempting to reduce the number of training points to improve computational efficiency while retaining prediction accuracy, we encounter an “overfitting” issue. In experiments with a 1D perturbation equation, we observe that PINNs employing the adaptive weighting method alone suffer from “overfitting” when the number of training points is small. The residuals at the training points become very small, while the residuals at unseen

testing points can be up to 10^4 times larger on average. This observation has motivated us to develop an “adaptive sampling method” to dynamically allocate training points where they are most needed during the training process.

1.8 Hybrid finite element method-PI-DeepOnet coupling for convective fluid transport in porous media with Gaussian sources

It is well-known that when the task is to map a point source (typically represented by a Gaussian) to the solution operator, operator learning frameworks based on standard Gaussian random field sampling often fail. Erdi Kara is developing a method based on dynamically adaptive collocation points to address this issue for both single and multiple Gaussian sources. We have developed an operator learning framework that couples the finite element method (FEM) with a PI-DeepONet to model convective fluid transport in porous media. In this framework, the velocity profile is first obtained by solving Darcy’s law using FEM with adaptive mesh generation. This information is then fed into a transport model, where the mapping from a Gaussian source to the solution profile is learned via PI-DeepONet. With this coupling, the final concentration profile can be predicted for single or multiple point sources represented by Gaussians. Using very limited training data (400 sampled functions), preliminary results are highly promising (see fig. 7).

1.9 Gaussian variational schemes on bounded and unbounded domains

In previous works, we developed Whitney forms based on coarsening of traditional finite element meshes. To solve problems in high dimensions, we developed a new variational scheme using Gaussian radial basis functions in the Whitney form construction [20]. Closed-form expressions for requisite bilinear forms (i.e., mass/stiffness matrices) allow us to pose variational principles without reference to an underlying mesh, avoiding the curse of dimensionality. These models can be swapped in our Whitney form construction or used in their own right as a means of building surrogates.

The scheme minimizes a data reconstruction loss subject to a variational equality constraint, which enforces structure in a traditional conforming Galerkin formulation. We hypothesize that a good surrogate model can be constructed using relatively few Gaussian radial basis functions (GRBFs), particularly when the means and variances are calibrated to match a high-fidelity dataset. Further improvements can be obtained by combining these with deep embeddings. On an infinite domain, the mass and stiffness matrices reduce to polynomial moments of Gaussian distributions, whose closed form we derive by hand. Thus, quantities required to form the discrete operators governing the projected PDE are analytically computed, and we can use them together with nonlinear regressors for fluxes [21] to identify structure-preserving conservation laws consistent with data. We show that this discretization has robust *a priori* error estimates and converges in L -infinity with increasing numbers of RBFs. Ultimately, when solving the underlying equations, the GRBF means and variances are obtained by minimizing the data misfit using a machine learning optimizer such as Adam or L-BFGS. This improves the ability of the GRBF space to approximate the observed data with high fidelity.

To exploit the analytic integrability of the GRBFs, the variational problems must be posed on an infinite domain. We employ a Nietsches trick strategy to enforce boundary conditions on complex geometries via energy penalty. Critically, the principal volumetric component is integrated over an unbounded extension of the domain. This enables applying the same expectation-based expressions developed for the unbounded case when computing the integrals. The remaining penalization terms requiring boundary integrals do not generally have a closed-form expression. However, we show that Monte-Carlo integration is sufficient to retain optimal accuracy. We anticipate that this GRBF approach will be particularly impactful for solving high-dimensional equations like Boltzmann systems posed in \mathbb{R}^6 , where the momentum space is unbounded. Thus, the dimension of the boundary is much lower (3) compared to the “spatial” domain.

The accuracy of this approach is demonstrated on a low-dimensional Poisson problem for both bounded and unbounded domains. Use of equally spaced GRBFs with fixed variance demonstrates the convergence theory. When high-fidelity training data is introduced, minimizing the mismatch through trainable GRBF centers and variances dramatically improves the surrogate quality, achieving a relative mean square error for the unbounded

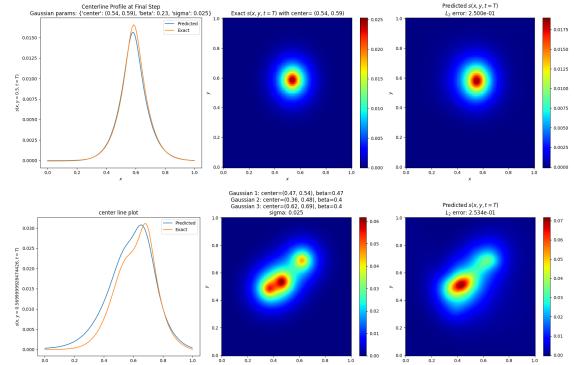


Figure 7: Final concentration profile for a single (top row) and multiple Gaussian (bottom row) sources. Images in the middle are the exact solutions.

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case of 10^{-12} with 32 Gaussians. For the bounded case, 10^{-9} is achieved again for 32 Gaussians. The accuracy reduction in the latter is due to inexact enforcement of the boundary conditions. An additional Poisson problem, posed in 8 dimensions, again shows that a mean square error of 10^{-6} is obtained using 32 Gaussians. A final example extends the Whitney form exterior-calculus approach we proposed in (Actor 2024). This time the GRBFs are used to naturally form space-compatible discretizations. Again, we demonstrate how this approach can be used to support construction of high-quality surrogates with relatively few ($O(10)$) Gaussian basis functions.

1.10 Multimodal disentanglement and causality

We have developed techniques for identifying fingerprints in large datasets using physics and causal learning techniques to identify relevant low-dimensional representations of descriptors or rare events in an unsupervised manner. On one front, we have developed a mathematical framework for performing variational inferences across multimodal datasets, allowing the use of a Gaussian mixture prior to perform clustering to identify correlations between physics-based and physics-agnostic modalities [22]. We have applied this framework to consider material datasets; in work recently published in Materials Today [23], we show how the framework can be used to identify predictive signatures and perform UQ when screening candidate new materials in laser powderbed fusion, physical vapor deposition, or tribology experiments. We published follow-on work [24] extending this framework to identify causal relationships between fingerprints by using differentiable directed acyclic graphs to identify cause/effect relationships between individual fingerprints. In an ongoing collaboration between Sandia National Laboratories (SNL), Caltech, and UPenn, we are employing Owhadi’s hypergraph discovery technique to identify causal relationships between fingerprints via functional relationships.

1.11 Model aggregation

Whether deterministic or stochastic, models can be viewed as functions designed to approximate a specific quantity of interest. We have introduced a data-driven framework that integrates predictions from various models, enhancing overall accuracy by leveraging the individual strengths of each [25]. This non-intrusive, model-agnostic approach treats the contributing models as black boxes and accommodates outputs from diverse methodologies, including machine learning algorithms and traditional numerical solvers. We advocated for a point-wise linear aggregation process. We proposed two methods for optimizing this aggregate: Minimal Error Aggregation (MEA), which minimizes the prediction error, and Minimal Variance Aggregation (MVA), which focuses on reducing variance. While MEA is inherently more accurate when correlations between models and the target quantity are perfectly known, Minimal Empirical Variance Aggregation (MEVA), an empirical version of MVA, consistently outperforms Minimal Empirical Error Aggregation (MEEA), the empirical counterpart of MEA, when these correlations must be estimated from data. The key difference is that MEVA constructs an aggregate by estimating model errors, while MEEA treats the models as features for direct interpolation of the quantity of interest. This makes MEEA more susceptible to overfitting and poor generalization, where the aggregate may underperform individual models during testing. We have demonstrated the versatility and effectiveness of our framework across various applications (fig. 8), including data science and PDEs, illustrating its ability to significantly enhance both robustness and accuracy.

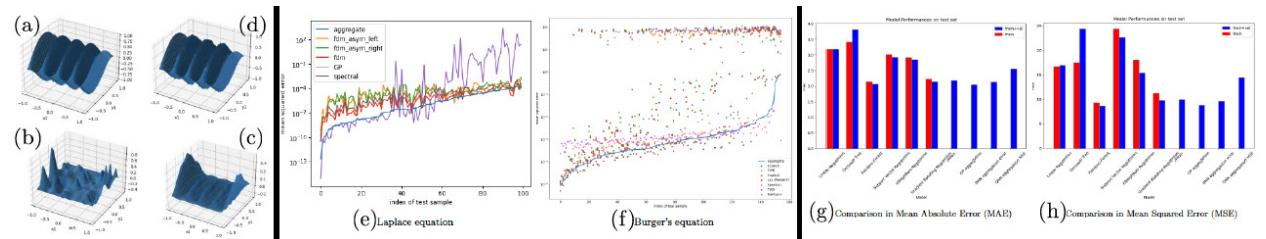


Figure 8: Model aggregation. (a–f) aggregation of PDE solvers. (a) True solution, (b–c) weak solvers, (d) aggregation of weak solvers. (e) Aggregation of distinct solvers for Laplace equation. (f) Aggregation of distinct solvers for the Burgers’ equation. (g–h) Application to the Boston housing dataset (the proposed method, labeled GP aggregation, outperforms individual models).

1.12 Tackling the curse of dimensionality with physics-informed neural networks

This work presents the stochastic dimension gradient descent (SDGD) method to address the curse of dimensionality, which has long hindered computational efforts in solving high-dimensional PDEs. Traditional methods struggle with scalability because the computational cost grows exponentially with the number of dimensions.

SDGD circumvents this by decomposing the PDE residual into dimension-specific components, allowing for random sampling of these dimensional terms during each PINN training iteration. This approach not only reduces the memory footprint but also accelerates convergence, making it feasible to solve PDEs within 100,000 and beyond on a single GPU.

Extensive experiments validate SDGD’s effectiveness across a range of nonlinear PDEs, including complex cases like the Hamilton-Jacobi-Bellman and Schrödinger equations. Compared to traditional methods like stochastic gradient descent over collocation points, SDGD exhibits superior stability and convergence speed, even for highly anisotropic and non-separable solutions. Its mesh-free nature further distinguishes it from other methods, enabling predictions across entire domains without relying on spatial discretization. This allows for efficient solutions to large-scale problems where previous approaches would fail due to out-of-memory errors. The technique thus provides a scalable, general framework for tackling high-dimensional PDEs across physics and engineering fields. Some examples are shown in the Table 1.

	PDE	Metric	100 D	1,000 D	5,000 D	10,000 D	100,000 D
Vanilla PINN	Poisson	Rel. L_2 Error	7.189E-3	5.609E-4	1.768E-3	N.A.	N.A.
	Allen-Cahn	Rel. L_2 Error	7.187E-3	5.617E-4	1.773E-3	N.A.	N.A.
	Sine-Gordon	Rel. L_2 Error	7.192E-3	5.642E-4	1.782E-3	N.A.	N.A.
		Time (Hour)	0.05	4.75	30.54	N.A.	N.A.
		Memory (MB)	1328	4425	56563	> 81252	> 81252
SDGD (Ours)	PDE	Metric	100 D	1,000 D	5,000 D	10,000 D	100,000 D
	Poisson	Rel. L_2 Error	7.189E-3	5.611E-4	1.758E-3	1.850E-3	2.175E-3
	Allen-Cahn	Rel. L_2 Error	7.187E-3	5.615E-4	1.762E-3	1.864E-3	2.178E-3
	Sine-Gordon	Rel. L_2 Error	7.192E-3	5.641E-4	1.795E-3	1.854E-3	2.177E-3
		Time (Hour)	0.05	0.75	1.18	1.5	12
		Memory (MB)	1328	1788	3335	4527	32777

Table 1: Relative L_2 error, time, and memory costs for vanilla PINNs [26] and SDGDs (ours) across different PDEs under various high dimensions. Vanilla PINNs [26] run out of memory for an A100 GPU with 81,252 MB memory in more than 5,000 D, while SDGD scales up to 100,000 D. SDGD errors are similar to those of vanilla PINNs in relatively lower dimensions (100 D, 1,000 D, and 5,000 D) while being much faster and more memory efficient.

2 Research Area II

2.1 Whitney forms: UQ and conditional neural extensions

Previous work in the Center on exterior calculus and Whitney forms [21][27] has been heavily extended.

Conditional neural Whitney forms. Motivated by conditional neural operators in computer vision, we extend Whitney forms so that both the networks prescribing control volumes and the fluxes defined on their interfaces take an additional input $(\psi^0(x; Z), \mathbf{F}(\mathbf{u}; Z))$, where Z can be either a scalar/vector/field-valued parametric dependency in supervised settings, or an exogenous latent variable in unsupervised settings. Much like conditional diffusion models, we are now able to sample a finite element model from the conditional distribution governed by Z . This has important practical implications for constructing digital twins, where Z may amount to sensor data, and we can perform real-time data assimilation to extract structure-preserving physical models. In collaboration with Ani Hsieh at UPenn, we are employing these in the optimal coverage problem to develop control policies for source identification (e.g., oil spills or other contaminants) by swarms of drones [28].

Disentangling aleatoric/epistemic uncertainty via computational graph completion for data-driven exterior calculus and mortar methods. In an ongoing collaboration spanning Caltech, SNL, Stanford, and UPenn, we have integrated the computational graph completion framework developed by Owhadi alongside the data-driven exterior calculus framework developed by Trask. Fast solvers allow us to identify generalized fluxes on graphs using Gaussian processes while guaranteeing structure preservation, which early career students/postdocs (Propp [Stanford], Actor, Walker [SNL]) have developed to study subsurface fracture networks, arterial bloodflow, and semiconductor physics. By exploiting the graph interpretation of Whitney forms, we apply this to quantify the uncertainty of Dirichlet2Neumann maps. The conditional neural field allows modeling of aleatoric uncertainty by performing variational inference to fit stochastic models to Z using either variational autoencoders or latent diffusion models. While this captures aleatoric uncertainty due to stochastic physics, epistemic UQ is necessary to identify the bounds of a trustworthy application for the model. Preliminary work integrating computational

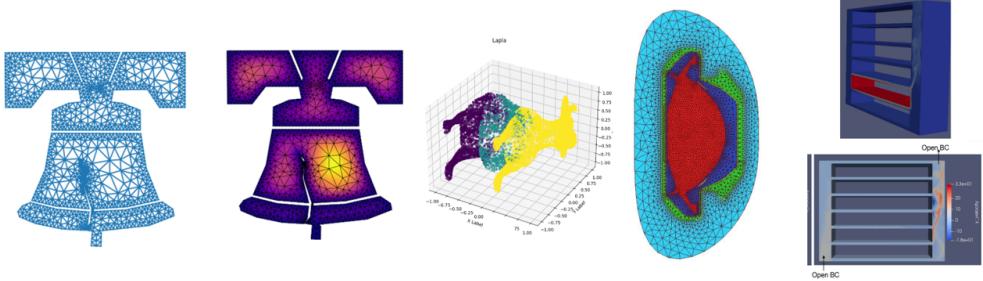


Figure 9: Construction of Whitney forms from complex geometry. From left to right: a triangle/tet-mesh in arbitrary format (1), and we output a nonlinear Whitney form surrogate (2). The process holds in 2- or 3-D (shown here for a cow) (3). In ongoing work with Princeton Plasma Physics Laboratory, we are extending to complex stellarator geometries (4). In ongoing work with SNL, we are building digital twins of battery racks to optimally control thermal runaway (5).

graph completion has shown an ability to fit Gaussian processes to resulting Dirichlet2Neumann maps. In tandem with our recent work on mortar methods [29], this allows us to scalably build models for systems-of-systems with rigorous notions of trust.

Complex geometries and applications. A crucial extension this year identifies that our original construction of Whitney forms in [27] may be recast in a non-invasive manner to construct the network from existing unstructured finite element meshes fig. 9. The core of the method is to parameterize a partition of unity via a convex combination tensor W with trainable positive entries whose rows sum to 1. For conservation law problems, the mass and stiffness matrices required in the variational formulation may be constructed noninvasively similar to projection-based reduced order models (e.g., $M_{WF} = W^T M_{FEM} W$), which are then embedded in a PDE-constrained mixed finite element setting to identify nonlinear conservative fluxes. This forms the basis of important ongoing collaborations—in the StellFoundry SciDAC led by Princeton Plasma Physics Laboratory, Whitney forms are being used as a basis for fusion power stellarator design optimization (Churchill, see [30]). At SNL, the battery design group (Hewson) is using these forms to optimize heat transfer in thermal runaway events, and Cyr has a new Laboratory Directed Research and Development project employing them in SNL-relevant settings. We are in discussions with the CharmNET Mathematical Multifaceted Integrated Capability Center (MMICC) (Lois Chacon) to identify paths for collaboration.

2.2 Geometric structure preservation

In the past year, we have published in NeurIPS on graph attention networks that overcome the over-smoothing phenomenon to achieve state-of-the-art performance in both graph analytics and physics-based tasks [31]. These architectures pose learning in terms of flows governed by reversible and irreversible bracket dynamics, using notions from physics and differential geometry to guarantee that the dynamics of network propagation either conserve energy or free energy, respectively. This is notably the first parameterization of metriplectic dynamics that scales linearly in the number of discretization points, e.g., $O(N)$, where previous works (primarily developed at UPenn, SNL, or Brown) are $O(N^3)$. In other work with standard network architectures where graph structure cannot be exploited, we have developed fully general parameterizations of metriplectic systems that exhibit a reduction in complexity to $O(N^2)$ [32]. In addition to scaling optimally for this level of generality, architectures based on these parametrizations enjoy universal approximation properties as well as a bound on their generalization error in time.

In ongoing work, we have used these techniques to develop data-driven models for coarse-graining physics that scale to arbitrary numbers of degrees of freedom. In Figure 10, we demonstrate an ability to learn stochastic dynamics from a traditional molecular dynamics system while preserving fluctuation-dissipation balance and

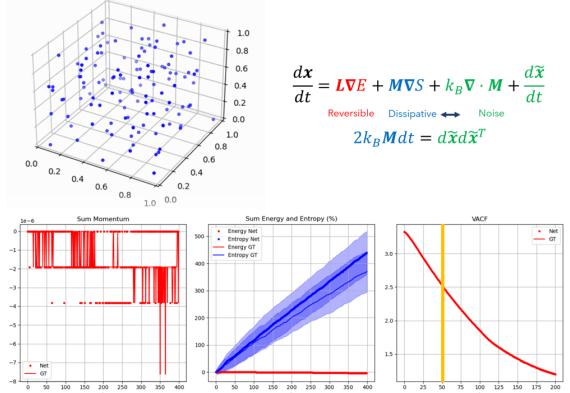


Figure 10: Metriplectic stochastic dynamics fit to ideal gas trajectories. Momentum and energy conservation, non-decreasing entropy production, and fluctuation-dissipation balance are enforced without knowledge of functional form for dynamics, allowing assimilation of complex physics from data and extrapolation. We reproduce velocity autocorrelation using only data before the orange line, as shown here.

thermodynamic consistency. This structure preservation allows reliable performance when forecasting out of distribution. We are currently developing a LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) implementation to allow billion-atom, data-driven particle simulations.

2.3 Graphs enrich transformers

In work accepted to NeurIPS this year, we explore how graph networks can enhance learning in transformer architectures [33]. We have shown that the over-smoothing problem in transformers may be mitigated by reinterpreting self-attention in transformers as a graph filter and redesigning. In exchange for a moderate increase in parameter complexity, we obtain state-of-the-art performance in vision, language, graph analytics, speech, and code classification tasks.

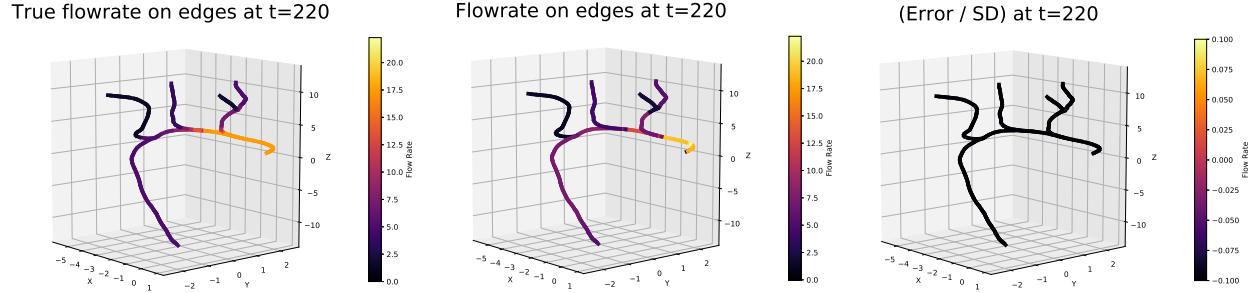


Figure 11: Results for arterial blood-flow dataset. Left: ground truth flow rate on edges. Center: surrogate prediction. Right: Edge-wise error in prediction divided by predicted model standard deviation, demonstrating alignment of model uncertainty and realized error.

2.4 Learning Dirichlet-to-Neumann maps on graphs with Gaussian processes

We present a novel method for learning Dirichlet-to-Neumann maps on graphs using Gaussian processes, focusing on cases where data obeys some conservation constraint from a PDE. We construct a data-driven surrogate model and uncertainty estimates for an entire graph, even when data is only available at a limited subset of the full domain. Our approach combines Gaussian processes and discrete exterior calculus to infer a relationship between node and edge values. In particular, we learn an independent Gaussian process on each edge, mapping nodal values on the endpoints to flux across the edge. We use the graph divergence (derived from the graph incidence matrix) to encode the conservation constraint. By optimizing over the reproducing kernel Hilbert space norm and applying a maximum likelihood estimation penalty on kernel complexity, we ensure that our surrogate model adheres to the relevant conservation law without excessive complexity. We demonstrate the effectiveness of our method on two realistic datasets, highlighting its potential for scientific applications with limited data. In particular, we apply our method to a subsurface discrete fracture network dataset (obeying linear Darcy flow through a graph with numerous cycles and dead-end edges) and an arterial bloodflow dataset (exhibiting highly nonlinear flow on a tree-like graph with many edges in series). In each case, we obtain a surrogate model that provides realistic predictions of dynamics on the full domain despite data only being provided on the boundary. Comparing the error on the test set and the posterior variance reveals that the model effectively predicts where it is trustworthy and where the predictions break down, enabling robust UQ.

2.5 Computational Hypergraph Discovery

We have developed the Computational Hypergraph Discovery (CHD) framework [34]. To describe this framework, observe that most problems within and beyond the scientific domain can be framed into one of the following three levels of function approximation complexity (fig. 12). **Type 1:** Approximate an unknown function given input/output data. **Type 2:** Consider a collection of variables and functions, some of which are unknown, indexed by the nodes and hyperedges of a hypergraph (a generalized graph where edges can connect more than two vertices). Given partial observations of the variables of the hypergraph (satisfying the functional dependencies imposed by its structure), approximate all the unobserved variables and unknown functions. **Type 3:** Expanding on Type 2, if the hypergraph structure itself is unknown, use partial observations of the variables of the hypergraph to discover its structure and approximate its unknown functions. These hypergraphs offer a natural platform for organizing, communicating, and processing computational knowledge. While most scientific problems can be framed as the data-driven discovery of unknown functions in a computational hypergraph whose structure

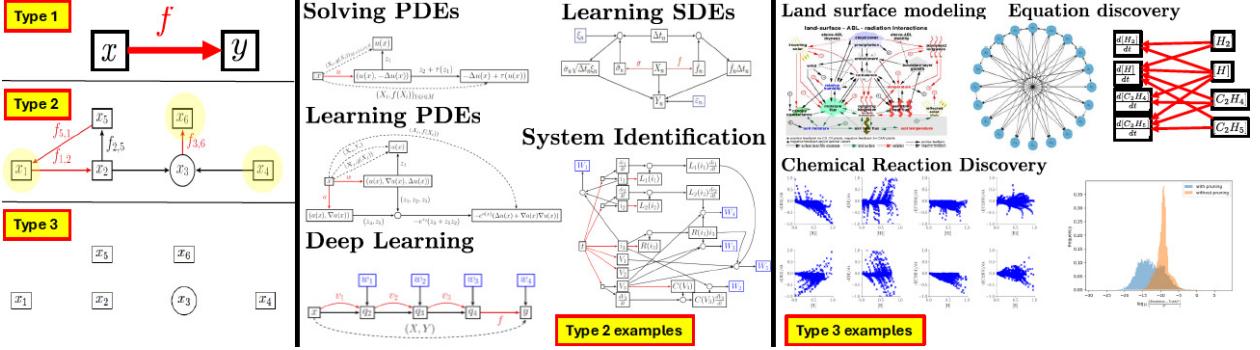


Figure 12: Computational Hypergraph Discovery framework. Middle column: Type 2 problems. Right column: Type 3 problems.

is known (Type 2), many require the data-driven discovery of the structure (connectivity) of the hypergraph itself (Type 3). We have introduced an interpretable Gaussian Process (GP) framework [34] for such (Type 3) problems that does not require randomization of the data, access to or control over its sampling, nor sparsity of the unknown functions in a known or learned basis. Its polynomial complexity, which contrasts sharply with the super-exponential complexity of causal inference methods, is enabled by nonlinear analysis of the variance capabilities of GPs used as a sensing mechanism. Among various applications, we have benchmarked the proposed method for recovering large chemical reaction networks (with more than 1,000 species, see bottom-right column fig. 12). We are currently collaborating with UPenn and SNL to develop this framework toward the discovery of causal-directed acyclic graphs.

2.6 Computational graph completion

In collaboration with SNL, UPenn, and Stanford, we have developed the Computational Graph Completion framework [35] for the data-driven design of graph-based surrogates that have UQ capabilities with applications to data-driven graph exterior calculus. The idea is to learn flux relationships with GPs and use an optimal recovery problem to allow physics enforcement via equality constraints. The method is fast and leads to (1) a hybridizable formulation exposing equality-constrained quadratic problems for unknown internal edge currents and (2) probabilistic digital twins with a tractable posterior encoding of epistemic uncertainty in surrogate models.

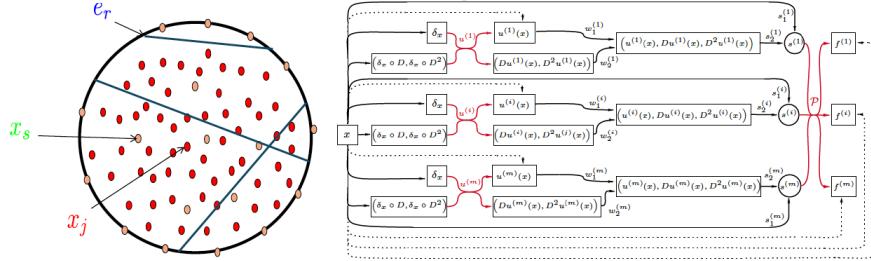


Figure 13: PDE learning. Left: Measurements. Right: The corresponding computational graph.

2.7 Learning PDEs with guarantees

We have introduced a data-efficient kernel/Gaussian Process (GP) method for learning differential equations with rigorous a priori error estimates [36] based on the the Computational Graph Completion framework [35]. The method works for arbitrary nonlinear differential equations. Using the differential equation $\mathcal{P}(x, u(x), Du(x), D^2u(x)) = f(x)$ as an illustration, we considered the problem of learning the unknown function \mathcal{P} defining the structure of the PDE. The data comes in the form of partial linear observation of m source/solution pairs $(f^{(i)}, u^{(i)})$. As an example (see fig. 13, left), these partial linear observations can be the values of $f^{(i)}$ at the red points, the values of $u^{(i)}$ at the green points, and the tomographic integrals of $u^{(i)}$ over the blue segments. Then, recovering the structure \mathcal{P} of the PDE is equivalent to completing the computational graph on the right

column of fig. 13, where the unknown functions are highlighted in red. The solution is to replace those unknown functions with GPs and compute their MAP estimator given available data. The proposed solution comes with convergence and accuracy guarantees and remains efficient in data-scarce regimes.

2.8 Temporal graph embedding based on Mamba

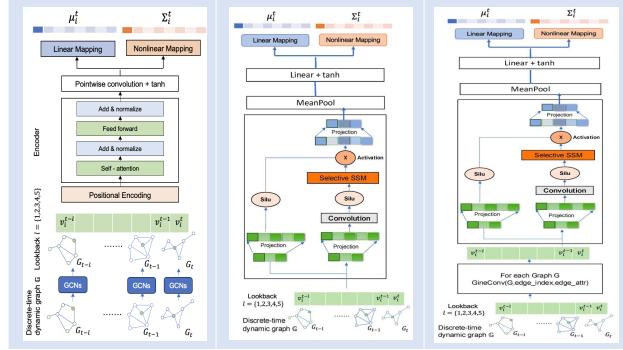


Figure 14: Main architectures of three newly developed spatial-temporal graph embedding approaches, from left to right: TransformerG2G+GCNs, MambaG2G, and MambaG2G+ GINEConv.

transformer-based approaches in link prediction tasks, while offering significant computational efficiency gains on longer sequences. Notably, MambaG2G variants consistently outperform transformer-based models on datasets with high temporal variability such as UCI, Slashdot, Bitcoin, and Reality Mining while maintaining competitive performance on more stable graphs like SBM. We provide insights into the learned temporal dependencies by analyzing attention weights and state matrices, revealing the models’ ability to capture complex temporal patterns. By effectively combining state-space models with graph neural networks, our work addresses key limitations of previous approaches and contributes to the growing body of research on efficient temporal graph representation learning. These findings offer promising directions for scaling dynamic graph embedding to larger, more complex real-world networks, potentially enabling new applications in areas such as social network analysis, financial modeling, and biological system dynamics.

2.9 Graphs4Physics and Physics4Graphs

We developed SympGNNs [37], which are symplectically permutation equivariant graph neural networks that can effectively handle system identification in high-dimensional Hamiltonian systems, as well as node classification. SympGNNs combine symplectic maps with permutation equivariance, a property of graph neural networks. Specifically, we propose two variants of SympGNNs: (1) G-SympGNN and (2) LA-SympGNN, arising from different parameterizations of kinetic and potential energy. We demonstrate the capabilities of SympGNNs on two physical examples: a 40-particle coupled Harmonic oscillator and a 2,000-particle molecular dynamics simulation in a two-dimensional Lennard-Jones potential. Furthermore, we demonstrate the performance of SympGNNs in the node classification task, achieving accuracy comparable to the state of the art. We also empirically show that SympGNNs can overcome the oversmoothing and heterophily problems, two grand challenges in the field of graph neural networks.

We are currently working on developing spherical nonlocal kernel networks to solve the inverse problem of predicting heat flux forcing patterns associated with a given temperature response. With spherical nonlocal kernel networks, we aim to extend the capabilities of the nonlocal kernel network [38] to handle spherical signals by considering a graph that lies on the surface of a sphere. This helps avoid shortcomings such as spherical distortions associated with projecting a spherical signal to a 2D plane. The training data is obtained from q -flux Green’s function experiments [39] utilizing the atmospheric component (Community Atmospheric Model version 5, CAM5) of the Community Earth System Model version 1.1, coupled with a thermodynamic ocean mixed-layer represented by the Community Land Model version 4 and a thermodynamic sea ice component.

Dynamic graph embedding has emerged as a crucial technique for modeling complex time-evolving networks across diverse domains. While transformer-based models have shown promise in capturing long-range dependencies in temporal graph data, they face scalability challenges due to quadratic computational complexity. This study presents a comparative analysis of dynamic graph embedding approaches using transformers and the recently proposed Mamba architecture, a state space model with linear complexity. We introduce three novel models: TransformerG2G with graph convolutional networks, MambaG2G, and MambaG2G with graph isomorphism network edge convolutions. Our experiments on multiple benchmark datasets demonstrate that Mamba-based models achieve comparable or superior performance to

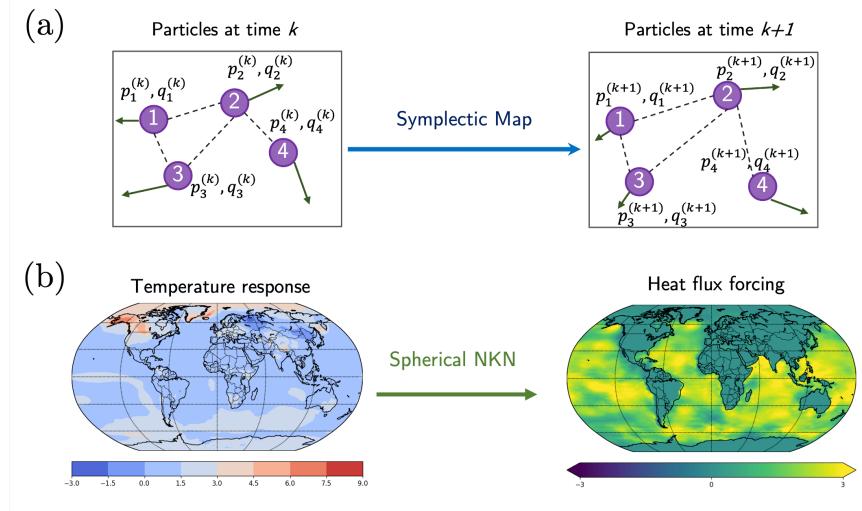


Figure 15: (a) SympGNNS to learn the ‘one-step forward’ solution map. (b) A spherical nonlocal kernel network (NKN) to predict the heat flux forcing corresponding to a given temperature response.

3 Research Area III

In the following sections, we describe our progress in algorithms and hardware architectures toward achieving scalable and energy-efficient spike-based applications.

3.1 Spiking neural networks for scientific machine learning

Spiked neural networks (SNNs) are a new and promising approach to scientific machine learning (SciML), offering energy-efficient computation inspired by biological neural systems. This work employs SNN principles and focuses on their application to solving ordinary differential equations and PDEs [40]. Specifically, we demonstrate that SNNs can be integrated into PINNs and DeepONets, establishing their equivalence to traditional ANNs [41] (fig. 16) and highlighting their inherent stability in long-term simulations of dynamic systems [42]. Additionally, we present empirical results from high-dimensional PDEs processed on neuromorphic hardware, demonstrating the effectiveness of SNNs [43]. These advancements could facilitate solving large-scale scientific and engineering problems with reduced energy consumption on future neuromorphic computers.

3.2 Tensor train decomposition for efficient SNN training

SNNs suffer from memory and computation overhead due to spatiotemporal dynamics and multiple backpropagation computations across timesteps during training. To address this issue, we introduce Tensor Train Decomposition for Spiking Neural Networks (TT-SNN) [44], a method that reduces model size through trainable weight decomposition, resulting in reduced storage, FLOPs (Floating Point Operations Per Second), and latency. In addition, we propose a parallel computation pipeline as an alternative to the typical sequential tensor computation, which can be flexibly integrated into various existing SNN architectures. To the best of our knowledge, this is a first-of-its-kind application of tensor decomposition in SNNs. We validate our method using both static and dynamic datasets, CIFAR10/100 and N-Caltech101, respectively. We also propose a TT-SNN-tailored training accelerator to fully harness the parallelism in TT-SNN. Our results demonstrate substantial reductions in parameter size ($7.98\times$), FLOPs ($9.25\times$), training time (17.7%), and training energy (28.3%) during training for the N-Caltech101 dataset, with negligible accuracy degradation.

3.3 Toward temporal spiking early-exit neural networks

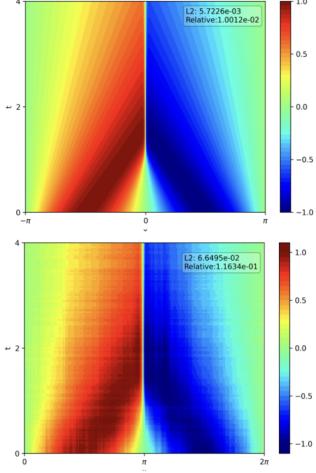


Figure 16: Solution of Burgers’ equation with a separable PINN (artificial neural network [ANN], top) and a converted spiked neural network (bottom). The spiked neural network result has larger errors but is computed much faster than the ANN result.

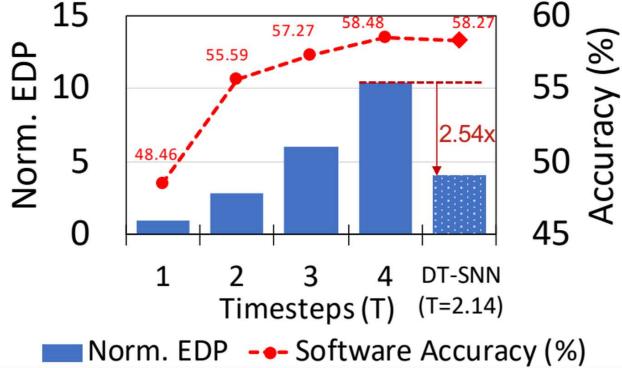


Figure 17: Impact of DT-SNN/SEENN [45] on a spiking hardware accelerator. The Energy-Delay Product (EDPs) are normalized with respect to the value at timestep = 1. We find SEENN yields 2.54 \times reduction in EDP while maintaining iso-accuracy with respect to the SNNs using 4 timesteps.

that SEENN is compatible with both the directly trained SNNs and the ANN-SNN conversion. By dynamically adjusting the number of timesteps, our SEENN achieves a remarkable reduction in the average number of timesteps during inference (fig. 17). For example, our SEENN-II ResNet-19 can achieve 96.1% accuracy with an average of 1.08 timesteps on the CIFAR-10 test dataset.

3.4 Rethinking skip connections in SNNs with time-to-first-spike coding

Time-to-first-spike (TTFS) coding in SNNs offers significant advantages in terms of energy efficiency, closely mimicking the behavior of biological neurons. In a joint collaborative paper between Brown, Pacific Northwest National Laboratory (PNNL), and Yale published in *Frontiers in Neuroscience* [46], we delve into the role of skip connections, a widely used concept in ANNs within the domain of SNNs with TTFS coding. Our focus is on two distinct types of skip connection architectures: (1) addition-based skip connections, and (2) concatenation-based skip connections. We find that addition-based skip connections introduce an additional delay in terms of spike timing. On the other hand, concatenation-based skip connections circumvent this delay but produce time gaps between after-convolution and skip-connection paths, thereby restricting the effective mixing of information from these two paths. To mitigate these issues, we propose a novel approach involving a learnable delay for skip connections in the concatenation-based skip connection architecture. This approach successfully bridges the time gap between the convolutional and skip branches, facilitating improved information mixing. We demonstrate the applicability of TTFS coding on beyond-image-recognition tasks and extend it to scientific machine-learning tasks, broadening the potential uses of SNNs (fig. 18).

3.5 Hardware for spiking neural networks

In [47], we propose Multiplier-less INTeger (MINT) quantization, a uniform quantization scheme that efficiently compresses weights and membrane potentials in SNNs. Unlike previous SNN quantization methods, MINT quantizes memory-intensive membrane potentials to an extremely low precision (2-bit), significantly reducing the memory footprint (fig. 19). MINT also shares the quantization scaling factor between weights and membrane potentials, eliminating the need for multipliers required in conventional uniform quantization. Experimental results show that our method matches the accuracy of full-precision models and other state-of-the-art SNN quantization techniques while surpassing them in memory footprint reduction and hardware cost efficiency at deployment. For example, 2-bit MINT VGG-16 achieves 90.6% accuracy on CIFAR-10, with roughly 93.8% reduction in memory footprint from the full-precision model and 90% reduction in computation energy compared to vanilla uniform quantization at deployment. *This paper received the Best Paper Award nomination.*

SNNs are cost-efficient and deployment-friendly because they process input in both a spatial and temporal manner using binary spikes. However, we observe that the information capacity in SNNs is affected by the number of timesteps, leading to an accuracy-efficiency trade-off. In our NeurIPS 2023 paper [45], we studied fine-grained adjustment of the number of timesteps in SNNs. Specifically, we treat the number of timesteps as a variable conditioned on different input samples to reduce redundant timesteps for certain data. We call our method Spiking Early-Exit Neural Networks (SEENN) or Dynamic Timestep SNN. To determine the appropriate number of timesteps, we propose SEENN-I which uses a confidence score thresholding to filter out the uncertain predictions, and SEENN-II which determines the number of timesteps by reinforcement learning. Moreover, we demonstrate

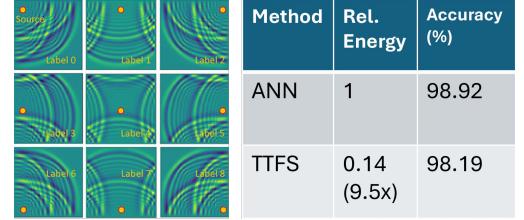


Figure 18: Example of a source localization problem for wave equation solved using a time-to-first-spike (TTFS) SNN algorithm [46]. Each image represents the wave shape at the 100th time step, originating from a wave source located at the center of the respective zone. Energy-efficiency comparison between ANN and our proposed TTFS SNN at inference on the wave equation problem.

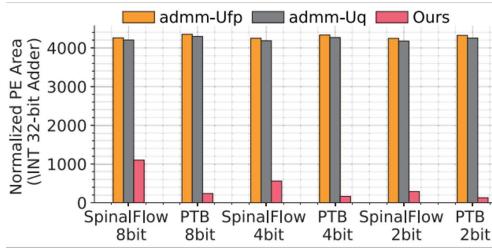


Figure 19: Area comparison between MINT [47] and prior SNN quantization methods using scaling factors. Across different hardware architectures, we find that MINT reduces the area overhead by $> 5\times$.

Hypothesis based pruning, thus guaranteeing the final ticket is optimally utilized when deployed onto the hardware. Experiments indicate that our u-Ticket can guarantee up to 100% hardware utilization, thus reducing up to 76.9% latency and 63.8% energy cost compared to the non-utilization-aware Lottery Ticket Hypothesis method.

In an invited paper in ICASSP 2024 [49], we study two hardware benchmarking platforms for large-scale SNN inference, namely SATA and SpikeSim. SATA is a sparsity-aware systolic-array accelerator, while SpikeSim evaluates SNNs implemented on in-memory computing based analog crossbars. Using these tools, we find that the actual energy-efficiency improvements of recent SNN algorithmic works differ significantly from their estimated values due to various hardware bottlenecks. We identify and address key roadblocks to efficient SNN deployment on hardware, including repeated computations and data movements over timesteps, neuronal module overhead, and vulnerability of SNNs toward crossbar non-idealities.

3.6 Spiking PINNs on Loihi

We demonstrated spiking PINNs on Intel’s Loihi 2 neuromorphic hardware for the first time (Figure 20) [43]. A calibration process was applied to convert the previously trained floating point PINN model to a spiking neural network. Neuron dynamics required by the conversion process were implemented in Loihi 2 microcode. The Loihi 2 architecture only allows for fixed-point calculations.

To accommodate this approach, we designed a conversion procedure to translate the floating point model parameters to the limited fixed-point precision available on Loihi 2 (e.g., the maximum 8 bits of available synaptic weight precision). To extend the precision, we split elements of the synaptic weight matrices into the most-significant byte and least-significant byte. Through this splitting, spikes were applied separately to the high- and low-precision elements and summed. This enabled a 16 bit implementation and permitted an exploration of test energy/time/accuracy trade-offs due to weight precision on real hardware. By evaluating the implementation accuracy, we found that the limited precision only slightly affected the spiking network’s performance. This validated our spiking conversion workflow for translating models to hardware. We also directly measured the energy consumption per inference for the PINN on Loihi 2 and found that, by running multiple copies of the network in parallel, we could achieve around $50 \mu J$ per inference [43]. We presented these results at one of the main neuromorphic computing conferences (NICE) and drew significant interest from both Intel and SpiNNCloud Systems, a maker of another large-scale neuromorphic platform (SpiNNaker). We are conversing with both organizations for scaling PINNs on neuromorphic platforms and for evaluating other SciML models at large scales on these systems.

Pruning for SNNs has emerged as a fundamental methodology for deploying deep SNNs on resource-constrained edge devices. Though the existing pruning methods can provide extremely high weight sparsity for deep SNNs, the high weight sparsity brings a workload imbalance problem. Specifically, the workload imbalance happens when a different number of non-zero weights are assigned to hardware units running in parallel. This results in low hardware utilization and thus imposes longer latency and higher energy costs. In preliminary experiments, we show that sparse SNNs (98% weight sparsity) can suffer as low as 59% utilization. To alleviate the workload imbalance problem, in our recently accepted *IEEE Transactions on Emerging Topics in Computational Intelligence* work [48], we propose u-Ticket, where we monitor and adjust the weight connections of the SNN during Lottery Ticket

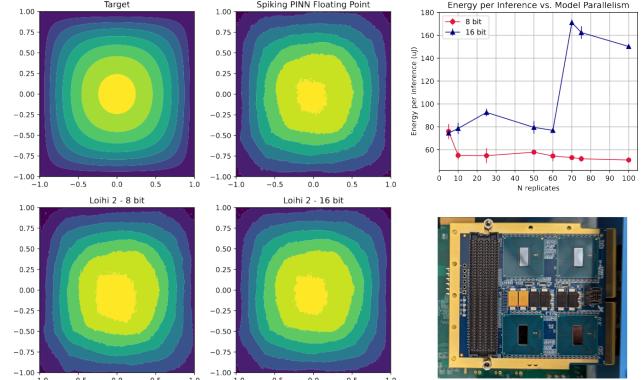


Figure 20: Spiking PINNs on Loihi 2. Left: comparison of Loihi 2 generated inferences (8 bit, bottom left; 16 bit, bottom right) to the floating point spiking PINN (top right) and ground truth solution (top left). Right, top: Energy per inference as a function of the number of simultaneous PINN replicas per chip. The 8 bit model achieves as low as $50 \mu J$ per inference. Right, bottom: four Loihi 2 chips at SNL used in the first spiking PINN demonstration.

We have started converting both separable PINNs and DeepONets for Loihi 2 using our systematic conversion process developed in our first neuromorphic study, which will preserve more accuracy during conversion. Further, in a co-design loop, experience gained from this demonstration is informing the design of new training and conversion procedures for SciML models.

4 Integration, Outreach, and Workforce Development

Because collaboration is a central theme of the MMICCs program, SEA-CROGS is highly integrated internally with publications spanning multiple institutions. External interactions further enhance the dissemination and outreach efforts of the SEA-CROGS project through technology adoption and research collaborations. Figure 21 shows these internal and external collaborations.

4.1 Dissemination

SEA-CROGS team members authored 82 journal articles and peer-reviewed conference papers in the first two years of the project. In addition, SEA-CROGS members have contributed to panels and boards across a wide range of topics designed to increase the participation of students in science, technology, engineering, and mathematics (STEM) fields. Presentations have been made at leading conferences, and a web page (www.pnnl.gov/projects/sea-crogs) for the entire SEA-CROGS project is maintained by PNNL and contains news about the project, a list of publications, and details about software being developed. Many code packages are open source on GitHub, including DeepXDE with over 750,000 downloads so far, as well as NeuralUQ for neural network UQ. The Brown group hosts weekly “Crunch Seminars” recorded and made available on YouTube, www.youtube.com/@CrunchGroup. This provides access for others in the research community. Similar arrangements are made for SEA-CROGS MMICCs Center webinars, and links to the recorded versions are posted on the www.pnnl.gov/projects/sea-crogs website. Finally, Karniadakis organized a workshop held at the Institute for Computational and Experimental Research in Mathematics, Providence RI, March 23–24, 2024 on “The Industrialization of Scientific Machine Learning.”

SEA-CROGS personnel have given numerous invited talks, colloquia, and keynotes listed in appendix A.2.1.

4.2 Workforce development

This project is preparing the next-generation DOE STEM workforce through research training and support of postdoctoral associates, as well as graduate and undergraduate students, in the latest areas of physics-informed machine learning and machine intelligence. Several of our past students and postdoctoral associates have gone on to work at DOE and other national laboratories, making valuable contributions. Others have gone into academia or industry.

Postdoctoral researchers: SEA-CROGS supports a number of postdoctoral associates. As a vehicle to enhance collaboration, we encourage them to spend time at the collaborating labs PNNL and SNL, as well as our university partners at Brown, Caltech, Stanford, etc. SEA-CROGS postdocs have been hired at Brown (Kahana, Bora), Caltech (Yang), UPenn (Kinch, Hernandez), PNNL (Chen), and SNL (Theilman, Voronin).

Caltech postdoc Ricardo Baptista and co-author of CHD joined the University of Toronto as an assistant professor. The first cohort of postdocs at SNL have all been converted to staff (Walker, Actor, Gruber).

Student mentoring: The SEA-CROGS lead principal investigator (Karniadakis) has a long history of mentoring PhD students and postdocs. Currently, over 55 of his mentees are tenure-track professors in universities around the world. He also has a record of placing many of his PhD students in national laboratories. Students at Brown

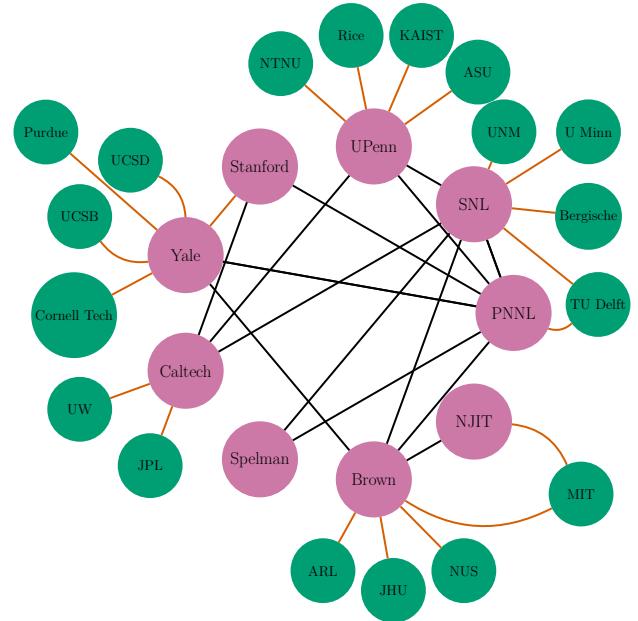


Figure 21: A non-comprehensive schematic illustrating internal (black) and external (orange) collaborations. SEA-CROGS internal participants are represented by pink vertices.

contribute to the weekly Crunch Seminar and regular SEA-CROGS MMICCs Center webinar by interacting with outside speakers or presenting their own research. Together, these opportunities provide training and development not just in their special area of research but also in the broader context of other work in scientific machine learning. Numerous students were recruited to the SEA-CROGS project.

Interns: The CRUNCH group at Brown hosts every year tens of interns from around the world who come to learn PINNs and neural operators, including students from Denmark, Germany, Italy, Uruguay, and Brazil. Caltech hosted Javier Ruiz-Lupon for a Summer Undergraduate Research Fellowship in 2024. Sarah Murphy (PhD student, University of North Carolina, Charlotte), Damien Beecroft (PhD student, University of Washington), and Emily Williams (PhD student, Massachusetts Institute of Technology) were hosted by PNNL as PhD interns in 2023 and 2024 through the National Science Foundation (NSF) Mathematical Sciences Graduate Internship program (Murphy and Beecroft) and the DOE Computational Science Graduate Fellowship program (Williams). The 2023 internships resulted in two publications [11, 10]. At SNL, Actor co-mentored graduate intern Dwyer Deighan through the Predictive Science Academic Alliance Program from the SUNY University at Buffalo in summer 2024. Donghyun Lee (an intern from KAIST, S. Korea) is working with Panda in fall 2024.

Mentorship of underrepresented groups: Panda organized the Institute of Electrical and Electronics Engineers (IEEE) Technical Community on Very Large Scale Integration V Pay it Forward Campaign, which focuses on mentoring and supporting underrepresented groups in the field of very-large-scale integration design and related technologies. Activities included mentorship programs, webinars, and networking opportunities. Additionally, she organized a graduate student panel that was moderated by Semiconductor Research Corporation CEO Dr. Todd Younkin to talk about the challenges, opportunities, and career interests of current PhD graduate students. Howard was selected to join the Association for Women in Mathematics (AWM) Student Chapter Committee to mentor AWM student chapters at universities across the world.

Early STEM exposure: Panda organized a series of artificial intelligence workshops for local middle and high schools in the New Haven community with the Yale Pathways Program and Yale Poorvu Center for Learning, introducing students to fundamental AI concepts and hands-on activities. These workshops aimed to inspire young students and provide them with early exposure to AI technologies, fostering interest in STEM fields. They completed podcasts conducted with three high school students (see <https://tc.computer.org/tcvlsi/events-and-recent-happenings>).

4.3 External collaborations

Universities: The CRUNCH group works with the Massachusetts Institute of Technology, Johns Hopkins University, NUS, and ARL. Yale maintains a number of new collaborations, including at Cornell Tech, Purdue University, UC San Diego, and Stanford University. UPenn maintains new collaborations, including at Rice [50], NTNU in Norway, KAIST in Korea [33], and Arizona State University. SNL maintains collaborations with the University of Minnesota, University of New Mexico, TU Delft (with PNNL [11]), and Bergische Universität Wuppertal.

Industrial and technology adoption: The Brown team is collaborating with Ansys, Simulia/Dassault, Takeda, Phynyx, PredictiveIQ, Cummings, Hypercomp, and Koerber on the topic of physics-informed machine learning. Panda is assisting Intel Labs and IBM Research in developing scalable algorithm-hardware co-design approaches. Caltech collaborates with NASA's Jet Propulsion Laboratory to apply CHD techniques to analyze engineering data from the Endurance Terrestrial Long-Range rover prototype. The Jet Propulsion Laboratory is designing this prototype to demonstrate robust system-level autonomy for a rover capable of high-speed driving over long distances. Trask is assisting a small company (Relogic Research) interested in using Whitney forms to pursue an SBIR. SNL partners with IntelLabs and SpiNNcloud on development of algorithmic technologies in neuromorphic systems (Loihi2 and SpiNNaker2, respectively).

4.4 Policy outreach

Actor was selected for the Society for Industrial and Applied Mathematics' Early Career Public Policy Fellowship for the 2024–2025 term. In this role, Actor works with the society, federal agency program managers, and congressional staffers to advance policy and understanding toward basic research in mathematics and computing, with an emphasis on AI, computing hardware, and digital twins.

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A Presentations and Publications

The SEA-CROGS team measures its success, in part, based on its fundamental contributions to the scientific literature, as well as the generation and dissemination of algorithms and open-source software. A publications list is also available online at <https://www.pnnl.gov/projects/sea-crogs/publications>.

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63. Zhang, Z., Zou, Z., Kuhl, E. & Karniadakis, G. E. Discovering a reaction–diffusion model for Alzheimer’s disease by combining PINNs with symbolic regression. *Computer Methods in Applied Mechanics and Engineering* **419**, 116647 (2024)
64. Zhuang, Q., Yao, C. Z., Zhang, Z. & Karniadakis, G. E. Two-scale Neural Networks for Partial Differential Equations with Small Parameters. *arXiv preprint arXiv:2402.17232* (2024)
65. Zou, Z., Kahana, A., Zhang, E., Turkel, E., Ranade, R., Pathak, J. & Karniadakis, G. E. Large scale scattering using fast solvers based on neural operators. *arXiv preprint arXiv:2405.12380* (2024)
66. Zou, Z., Meng, X. & Karniadakis, G. E. Correcting model misspecification in physics-informed neural networks (PINNs). *Journal of Computational Physics* **505**, 112918 (2024)
67. Zou, Z., Meng, T., Chen, P., Darbon, J. & Karniadakis, G. E. Leveraging viscous Hamilton–Jacobi PDEs for uncertainty quantification in scientific machine learning. *SIAM/ASA Journal on Uncertainty Quantification* **12**, 1165–1191 (2024)

A.1.1 Peer-reviewed conference proceedings

1. Bhattacharjee, A., Moitra, A., Kim, Y., Venkatesha, Y. & Panda, P. *Examining the role and limits of batchnorm optimization to mitigate diverse hardware-noise in in-memory computing* in *Proceedings of the Great Lakes Symposium on VLSI 2023* (2023), 619–624
2. Bhattacharjee, A., Yin, R., Moitra, A. & Panda, P. *Are SNNs Truly Energy-efficient?—A Hardware Perspective* in *ICASSP 2024-2024 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)* (2024), 13311–13315
3. Choi, J., Wi, H., Kim, J., Shin, Y., Lee, K., Trask, N. & Park, N. Graph Convolutions Enrich the Self-Attention in Transformers! *arXiv preprint arXiv:2312.04234* (2023)
4. Chen, P., Meng, T., Zou, Z., Darbon, J. & Karniadakis, G. E. *Leveraging Hamilton-Jacobi PDEs with time-dependent Hamiltonians for continual scientific machine learning* in *6th Annual Learning for Dynamics & Control Conference* (2024), 1–12
5. Galanti, T., Xu, M., Galanti, L. & Poggio, T. Norm-based Generalization Bounds for Compositionally Sparse Neural Networks. *Advances in Neural Information Processing Systems* **36** (2024)
6. Gruber, A., Lee, K., Lim, H., Park, N. & Trask, N. Efficiently Parameterized Neural Metriplectic Systems. *arXiv preprint arXiv:2405.16305* (2024)
7. Gruber, A., Lee, K. & Trask, N. Reversible and irreversible bracket-based dynamics for deep graph neural networks. *Advances in Neural Information Processing Systems* **36** (2024)
8. Howard, A. A., Qadeer, S., Engel, A. W., Tsou, A., Vargas, M., Chiang, T. & Stinis, P. *The conjugate kernel for efficient training of physics-informed deep operator networks* in *ICLR 2024 Workshop on AI4DifferentialEquations In Science* (2024)
9. Lee, D., Yin, R., Kim, Y., Moitra, A., Li, Y. & Panda, P. *TT-SNN: Tensor Train Decomposition for Efficient Spiking Neural Network Training* in *2024 Design, Automation & Test in Europe Conference & Exhibition (DATE)* (2024), 1–6
10. Li, Y., Geller, T., Kim, Y. & Panda, P. Seenn: Towards temporal spiking early exit neural networks. *Advances in Neural Information Processing Systems* **36** (2024)
11. Moitra, A., Yin, R. & Panda, P. *Energy-efficient Hardware Design for Spiking Neural Networks* in *2023 57th Asilomar Conference on Signals, Systems, and Computers* (2023), 543–544
12. Moitra, A., Yin, R. & Panda, P. *Hardware Accelerators for Spiking Neural Networks for Energy-Efficient Edge Computing* in *Proceedings of the Great Lakes Symposium on VLSI 2023* (2023), 137–138
13. Oommen, V., Bora, A., Zhang, Z. & Karniadakis, G. E. Integrating Neural Operators with Diffusion Models Improves Spectral Representation in Turbulence Modeling. *arXiv preprint arXiv:2409.08477* (2024)
14. Theilman, B. H., Zhang, Q., Kahana, A., Cyr, E. C., Trask, N., Aimone, J. B. & Karniadakis, G. E. *Spiking Physics-Informed Neural Networks on Loihi 2* in *2024 Neuro Inspired Computational Elements Conference (NICE)* (2024), 1–6
15. Yin, R., Li, Y., Moitra, A. & Panda, P. *MINT: Multiplier-less INTeger Quantization for Energy Efficient Spiking Neural Networks* in *2024 29th Asia and South Pacific Design Automation Conference (ASP-DAC)* (2024), 830–835

A.2 Conferences and workshops

A.2.1 Invited presentations

- Actor, J. A. "Exterior Calculus in Machine Learned Models". *ICME Seminar at Stanford University*, Palo Alto, CA. January 2024.
- Actor, J. A. "Exterior Calculus for Machine Learned Models". *Applied Mathematics Seminar Series at University of New Mexico*, Albuquerque, NM. September 2024.
- Actor, J. A. "Structure-Preserving Machine Learning via Whitney Forms". *UTEP S. Scott Collis Advanced Modeling and Simulations Seminar*, El Paso, TX. October 2023.
- Batlle, Pau. "Frequentist Confidence Intervals: Refuting the Burrus Conjecture", *Digital Twins for Inverse Problems in Earth Science*, Marseille, France. July 2024.
- Batlle, Pau. "Transparent and Well-Calibrated Uncertainty Quantification for Ill-Posed Inverse Problems", *Center for Advanced Systems Understanding (CASUS) Seminar*, Görlitz, Germany. December 2023.
- Batlle, Pau. "Optimization-Based Frequentist Confidence Intervals for Functionals in Constrained Inverse Problems: Resolving the Burrus Conjecture", *JPL UQ for Remote Sensing Workshop*, September 2023.
- Batlle, Pau. "Frequentist Confidence Intervals: Refuting the Burrus Conjecture", *NASA JPL UQ Seminar*, September 2023.
- Bourdais, Théo. "Computational Hypergraph Discovery", *One World Seminar Series on the Mathematics of Machine Learning*, January 2024.
- Bourdais, Théo. "Computational Hypergraph Discovery", *Digital Twins for Inverse Problems in Earth Science Workshop*, Marseille, France. July 2024.
- Bourdais, Théo. "Computational Hypergraph Discovery", *Differential Equations for Data Science (DEDS2024)*, February 2024.
- Cyr, E.C. Exploiting "time-domain" parallelism to accelerate neural network training and PDE constrained optimization. *Bergische Universität Wuppertal*. August 2024.
- Cyr, E.C. Exploiting "time-domain" parallelism to accelerate neural network training and PDE constrained optimization, *Penn State University*, State College, PA. April 2024.
- Cyr, E.C. Exploiting "time-domain" parallelism to accelerate neural network training and PDE constrained optimization, *University of Pennsylvania*, Philadelphia, PA. April 2024.
- Cyr, E.C. Exploiting "time-domain" parallelism to accelerate neural network training, *BIRS SciML workshop*, Banff, Canada. June 2023.
- Cyr, E.C. Exploiting "time-domain" parallelism to accelerate neural network training and PDE constrained optimization, *CCAM seminar at Purdue*, West Lafayette, IN. April 2023.
- Darcy, Matthieu. "Kernel Methods and PINNs for Rough Partial Differential Equations", *Digital Twins for Inverse Problems in Earth Sciences*, Marseille, France. July 2024.
- Darcy, Matthieu. "Kernel Methods for Rough Partial Differential Equations", *Southern California Applied Mathematics Workshop*, San Diego, CA. April 2024.
- Darcy, Matthieu. "Kernel Methods for Operator Learning", *One World Mathematics of Machine Learning Seminar*, October 2023.
- Darcy, Matthieu. "Kernel Methods are Competitive for Operator Learning", *Argonne National Lab LANS Seminar*, August 2023.
- Darcy, Matthieu. "Kernel Methods are Competitive for Operator Learning", *DataSig Rough Path Interest Group*, May 2023.
- Darcy, Matthieu. "Benchmarking Operator Learning with Simple and Interpretable Kernel Methods", *Workshop on Establishing Benchmarks for Data-Driven Modeling of Physical Systems*, USC, Los Angeles, CA. April 2023.
- Gruber, A. "Learning metriplectic systems and other bracket-based dynamics". *University of Vienna mathematics seminar*, Vienna, Austria. June 2024.
- Gruber, A. "Property-preserving model reduction in bracket-based dynamical systems". *Applied mathematics seminar series at University of New Mexico*, Albuquerque, NM. March 2024.
- Gruber, A. "Data-driven dynamical systems with structural guarantees". *S. Scott Collis advanced modeling and simulations virtual seminar series*, Rio Grande Consortium for Advanced Research on Exascale Simulation. November 2023.

- Gruber, A. "Data-driven dynamical systems with structural guarantees". *Applied mathematics and machine learning seminar at Texas Tech University*, Lubbock, TX. November 2023.
- Gruber, A. "Property-preserving model reduction for conservative and dissipative systems". *Numerical analysis of Galerkin ROMs seminar series*, INRIA Bordeaux, France. October 2023.
- Howard, A.A. "Multifidelity stacking networks for physics-informed training." *Data Sciences for Mesoscale and Macroscale Materials Models*, Chicago, Illinois. May 2024.
- Howard, A.A. "Multifidelity Deep Operator Networks." *Mathematical and Scientific Machine Learning*, Providence, RI. June 2023.
- Howard, A.A. "More of a good thing: multifidelity and stacking networks for physics-informed training." *Portland State University Applied and Computational Mathematics Seminar*, Portland, OR. March 2024.
- Howard, A.A. "More of a good thing: multifidelity and stacking networks for physics-informed training." *Sandia National Laboratory Seminar*, Albuquerque, NM. March 2024.
- Howard, A.A. "Machine learning for Stokes flow: from suspensions to ice sheets." *Advancing fluid and soft-matter dynamics with machine learning and data science*, Madison, WI. June 2024.
- Howard, A.A. "High performance computing for multiphase flows." *Spelman seminar*, Atlanta, GA. September 2023.
- Jalalian, Y. "Forecasting Hamiltonian Dynamics with Computational Graph Completion (CGC)", *International Conference of Differential Equations for Data Science (DEDS)*, February 2023.
- Jalalian, Y. "Data-Efficient Kernel Methods for PDE Identification", *International Conference of Differential Equations for Data Science (DEDS)*, February 2024.
- Karniadakis, G. E. "Interfacing physics-informed neural networks and neural operators for accelerated FEM simulations of multiscale problems", ANSYS, Boston, MA. September 2023.
- Karniadakis, G. E. "From Physics-Informed Machine Learning to Physics-Informed Machine Intelligence: Quo Vadimus?", Georgia Tech, Atlanta, GA. October 2023.
- Karniadakis, G. E. "Interfacing physics-informed neural networks and neural operators for accelerating simulations of multiscale problems", Simulia. December 2023.
- Karniadakis, G. E. "Recent Advances in PINNs and Deep Neural Operators", Stanford University, Stanford, CA. March 2024.
- Karniadakis, G. E. "Physics-Informed Machine Learning: Blending data and physics for fast predictions", Intel. February 2024.
- Karniadakis, G. E. "From Physics-Informed Machine Learning to Physics-Informed Machine Intelligence: Quo Vadimus?", IIT. April 2024.
- Karniadakis, G. E. "Physics-Informed Machine Learning in Engineering and Sciences", University of Central Florida. May 2024.
- Karniadakis, G. E. "From Physics-Informed Machine Learning to Physics-Informed Machine Intelligence: Quo Vadimus?", Purdue University. May 2024.
- Karniadakis, G. E. "Hidden Fluid Mechanics: Learning from any (sparse) data", Society of Engineering Science. August 2024 (GI Taylor Medal).
- Karniadakis, G. E. "Recent Advances in PINNs and Deep Neural Operators". September 2024.
- Lee, Jonghyeon. "Gaussian Processes and the Cole-Hopf Transformation", *Southern California Applied Mathematics Symposium*, San Diego, CA. April 2024.
- Owhadi, H. "Solving/learning PDEs with GPs and Gaussian Process Hydrodynamics", *International Conference on New Trends of Computational and Data Sciences, Caltech*, Pasadena, CA. December 2022.
- Owhadi, H. "Solving/learning PDEs with GPs and Computational Graph Completion", *AI for Science Workshop, Caltech*, Pasadena, CA. February 2023.
- Owhadi, H. "Solving/learning PDEs with GPs and Computational Graph Completion", *Differential Equations for Data Science (DEDS2023)*, February 2023.
- Owhadi, H. "Solving/learning PDEs with GPs and Computational Graph Completion", *Data-driven Modeling of Physical Systems, USC*, Los Angeles, CA. April 2023.
- Owhadi, H. "Kernel Mode Decomposition", *MaSAG Conference*, Rome, Italy. May 2023.
- Owhadi, H. "Solving/learning PDEs with GPs and Computational Graph Completion", *Inaugural CAMDA Conference*, College Station, TX. May 2023.
- Owhadi, H. "Kernel Mode Decomposition", *ECCOMAS-IACM Thematic Conference on Emerging Technologies in Computational Science for Industry*, Sicily, Italy. May 2023.

- Owhadi, H. "Computational Hypergraph Discovery and Completion", *ICERM Workshop: Mathematical and Scientific Machine Learning*, Providence, RI. June 2023.
- Owhadi, H. "Kernel/GP methods for Surrogate Modeling", *Data Science and Machine Learning Summer School*, Emilia Romagna (Italy). June 2023.
- Owhadi, H. "Solving/learning PDEs with GPs and Computational Graph Completion", *Mathematical and Statistical Foundation of Future Data-Driven Engineering*, Isaac Newton Institute for Mathematical Sciences, Cambridge (UK). June 2023.
- Owhadi, H. "Solving/learning PDEs with GPs and Computational Graph Completion", *ICIAM 2023: Machine Learning in Infinite Dimensions*, Tokyo (Japan). August 2023.
- Owhadi, H. "Computational Hypergraph Discovery", *Boeing Applied Mathematics Colloquium Series*, University of Washington, Seattle, WA. November 2023.
- Owhadi, H. "Computational Hypergraph Discovery", *International Workshop on Multiscale Model Reduction and Scientific Machine Learning*, Chinese University of Hong Kong (CUHK), Hong Kong (China). December 2023.
- Owhadi, H. "Co-discovering Graphical Structures and Functional Relationships Within Data: a Gaussian Process framework for Connecting the Dots", *SIAM UQ24*, (Plenary). February 2024.
- Owhadi, H. "Overview of Gaussian Process Techniques for Bridging Scales through Applications to Fluid Dynamics, Rough PDEs, Arbitrary Nonlinear PDEs, and Finding Functional Dependencies and Graphical Structures Within Data", *Workshop on Scale Bridging in Numerical Simulation*, LANL, Los Alamos, NM. April 2024.
- Owhadi, H. "A GP/Kernel Perspective on Digital Twins", *Digital Twins for Inverse Problems in Earth Science*, CIRM, Marseille, France. July 2024.
- Owhadi, H. "Overview of Gaussian Process Techniques for Bridging Scales through Applications to Fluid Dynamics, Rough PDEs, Arbitrary Nonlinear PDEs, and Finding Functional Dependencies and Graphical Structures Within Data", *Workshop on Statistical Aspects of Non-Linear Inverse Problems*, Cambridge (UK). September 2024.
- Owhadi, H. "Overview of Gaussian Process Techniques for Bridging Scales through Applications to Fluid Dynamics, Rough PDEs, Arbitrary Nonlinear PDEs, and Finding Functional Dependencies and Graphical Structures Within Data", *Colloquium at CMOR Department*, Rice University, Houston, TX. October 2024.
- Owhadi, H. "Overview of Gaussian Process Techniques for Bridging Scales through Applications to Fluid Dynamics, Rough PDEs, Arbitrary Nonlinear PDEs, and Finding Functional Dependencies and Graphical Structures Within Data", *UC Riverside Department of Mechanical Engineering Seminar*, Riverside, CA. October 2024.
- Owhadi, H. "Overview of Gaussian Process Techniques for Bridging Scales through Applications to Fluid Dynamics, Rough PDEs, Arbitrary Nonlinear PDEs, and Finding Functional Dependencies and Graphical Structures Within Data", *Yale Foundations of Data Science (FDS) Colloquium*, New Haven, CT. October 2024.
- Panda, P. "A Co-Design Approach to Efficient and Deployable In-Memory Computing". *Design Automation Conference*, SFO, USA. June 2024.
- Panda, P. "Are SNNs truly efficient?- A Hardware Perspective." *ICASSP*, Seoul, S. Korea. April 2024.
- Panda, P. "Neuromorphic Computing for Energy-Efficient Edge Intelligence", *VLSI-DAT*, Hsinchu, Taiwan. April 2024.
- Panda, P. "Hardware-Aware Low-Precision Federated Learning", *DATE*, Valencia, Spain. March 2024.
- Panda, P. "On-device Intelligence with Spiking Neural Networks", *EE Seminar*, Harvard University, Cambridge, MA. March 2024.
- Panda, P. "Energy-Efficient Intelligence with Neuromorphic Computing: From Algorithms to Hardware Design", *ECE Seminar*, Duke University. January 2024.
- Panda, P. "Rethinking AI Algorithm and Hardware Design with Neuromorphic Computing", *VLSID Conference*, Kolkata, India. January 2024.
- Panda, P. "Rethinking AI Algorithm and Hardware Design with Neuromorphic Computing", *ECE Seminar*, UC Santa Barbara, Santa Barbara, CA. October 2023.
- Panda, P. "Edge Intelligence with Neuromorphic Computing: From Algorithms to Hardware Design", *ECE Seminar*, UC Berkeley, Berkeley, CA. November 2023.
- Panda, P. "Computational Needs for Lifelong Learning", *DARPA ERI Summit*. September 2023.
- Propp, A. "Transfer Learning on Multifidelity Data", *Mathematical and Scientific Machine Learning (MSML)*, Providence, RI. June 2023.

- Stinis P. "When big neural networks are not enough" *University of California Santa Cruz, Applied Mathematics Seminar*, Santa Cruz, CA. April 2024.
- Stinis, P. "Multifidelity scientific machine learning" *Michigan State University, Applied Mathematics Seminar*, East Lansing, Michigan. March 2024.
- Stinis, P. "Multifidelity scientific machine learning" *Georgia Institute of Technology, Computational Mathematics Seminar*, Atlanta, GA. November 2023.
- Stinis, P. "Machine-learning custom-made basis functions for partial differential equations" *University of Arizona, Applied Mathematics Colloquium*, Tucson, AZ. March 2023.
- Tartakovsky, D. "Use and Abuse of Machine Learning in Scientific Discovery", *EAISI lecture, Eindhoven Artificial Intelligence Systems Institute*, Eindhoven University of Technology, Eindhoven, Netherlands. March 2024.
- Tartakovsky, D. "Use and Abuse of Machine Learning in Scientific Discovery", *Argyris Lecture 2023*, University of Stuttgart, Stuttgart, Germany. October 2023.

A.2.2 Organized conferences and workshops

- Organized Minisymposium: Panda, P. "SPIKEs", *ICERM 2023 Meeting on Mathematical and Scientific Machine Learning*, Providence, RI. June 2023.
- Organized Minisymposium: Actor, J. A., and Walker, E. A. "Beyond Fingerprinting: AI Approaches to Unearthing Process-Structure-Property Correlations in Additive Manufacturing", *U.S. National Congress on Computational Mechanics*, Albuquerque, NM. July 2023.
- Organized Tutorial: Panda, P. "Hardware and Software Co-Design for Edge AI", *Design Automation Conference 2023*. San Francisco, CA. July 2023.
- Organized Minisymposium: Howard, A. A., and Stinis, P. "Physics-informed machine learning for multiscale materials and engineering systems", *2nd IACM Mechanistic Machine Learning and Digital Engineering for Computational Science Engineering and Technology*, El Paso, TX. September 2023.
- Organized Minisymposium: Actor, J. A., Walker, E. A., et al. "AI/ML Algorithms for Accelerating Material Discovery, Design, and Manufacturing Processes", *2nd IACM Mechanistic Machine Learning and Digital Engineering for Computational Science Engineering and Technology*, El Paso, TX. September 2023.
- Organized Special Session: Panda, P. "Neuromorphic Computing", *Asilomar Conference on Signals, Systems and Computers 2023*. Pacific Grove, CA. October 2023.
- Organized Tutorial and Workshop: Panda, P. and Moitra, A. "Energy-Efficient Intelligence with Neuromorphic Computing: From Algorithms to Hardware Design". *VLSID Conference*, Kolkata, India. January 2024.
- Organized Workshop: D'Elia, M. and Karniadakis, G. "The industrialization of Scientific Machine Learning", *ICERM*, Providence, RI. March 2024.
- Organized Minisymposium: Cyr, E. C., and Smith, D. "Mathematical Advances in Algorithms Design Enabling Emerging Energy Efficient Computing", *SIAM Annual Meeting*, Spokane, WA. July 2024.
- Organized Minisymposium: Howard, A. A., and Stinis, P. "Advances in neural operators and uncertainty quantification for scientific modeling", *SIAM Annual Meeting*, Spokane, WA. July 2024.
- Organized Minisymposium: Actor, J. A., Walker, E. A., et al. "Causal Discovery and Graphical Causal Models", *16th World Congress on Computational Mechanics*, Vancouver, British Columbia (Canada). July 2024.
- Organized Minisymposium: Walker, E. A., Actor, J. A., et al. "Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes", *16th World Congress on Computational Mechanics*, Vancouver, British Columbia (Canada). July 2024.
- Organized Minisymposium: Perego, M., Howard, A. A., and Stinis, P. "Advances in neural operators for modeling mechanics applications", *16th World Congress on Computational Mechanics*, Vancouver, British Columbia (Canada). July 2024.
- Organized Workshop: Owhadi, H. "Digital Twins for Inverse Problems in Earth Science", *CIRM*, Marseille (France). July 2024.
- CMWR Committee: Tartakovsky, D. *The Conference on Computational Methods in Water Resources (CMWR 2024)*, Tucson, AZ. September 2024.

A.2.3 Contributed presentations and posters

- Actor, J. A. "Machine-Learned Finite Element Exterior Calculus for Linear and Nonlinear Problems". *4th Annual Conference on Mathematics of Scientific Machine Learning*, Providence, RI. June 2023.

- Actor, J. A. "Data-Driven Structure Preservation for Scientific Machine Learning". *3rd Sandia Machine Learning and Deep Learning Conference*, Albuquerque, NM. July 2023.
- Actor, J. A. "Machine-Learned Whitney Forms for Structure Preservation". *10th International Conference on Industrial and Applied Mathematics*, Tokyo, Japan. August 2023.
- Actor, J. A. "Data-Driven Reduced Models using Radial Basis Functions". *9th European Congress on Computational Methods in the Applied Sciences*, Lisbon, Portugal. June 2024.
- Actor, J. A. "Data-Driven Variational Reduced Models Using Learned Radial Basis Functions". *Scientific Machine Learning, Emerging Topics*, Trieste, Italy. June 2024.
- Bora, A. "AI for Climate and Extreme Weather Events". *Subra Suresh Symposium at the Frontiers of Technology and Society*, Providence, RI, USA. September 2024.
- Bora, A. "A Hybrid Machine Learning Approach for the Bias Correction of Global Climate Model". *Joint Applied Mathematics and MMICCs Principal Investigators (PI) Meeting*, Albuquerque, NM. January 2024.
- Chen, P. "Leveraging multi-time Hamilton-Jacobi PDEs for certain scientific machine learning problems". *Mathematical and Scientific Machine Learning*, Providence, RI. June 2023.
- Cyr, E. C. "Inference on Neuromorphic Hardware (Loihi2): A Linear Algebra Perspective". *SIAM Annual Meeting*, Spokane, WA. July 2024.
- Cyr, E. C. "Using Biased Gradients to Achieve Parallelism in Neural Network Training". *SIAM Parallel Processing*, Baltimore, MD. March 2024.
- Cyr, E. C. "Reduced Basis Approximations of Parameterized Dynamic PDEs via Neural Networks". *ECOMAS*, Lisbon, Portugal. June 2024.
- Cyr, E. C. "Progress in Layer-Parallel Neural Network Training and Inference". *Copper Mountain Conference on Iterative Methods*, Copper Mountain, CO. April 2024.
- Cyr, E. C. "A 2-Level Domain Decomposition Preconditioner for KKT Systems with Heat-Equation Constraints". *Copper Mountain Conference on Multigrid Methods*, Copper Mountain, CO. April 2023.
- Cyr, E. C. "A Layer-Parallel Approach for Training Deep Neural Networks". *SIAM CSE*, Amsterdam. February 2023.
- Darbon, J. "Leveraging multi-time Hamilton-Jacobi PDEs for certain scientific machine learning problems". *4th AFOSR Monterey Training Workshop on Computational Issues in Nonlinear Control*, Monterey Bay Seaside, CA. May 2023.
- Goswami, S. "On the Geometry Transferability of the Hybrid Iterative Numerical Solver for Differential Equations". *21st Copper Mountain Conference on Multigrid Methods*, Copper Mountain, CO. April 2023.
- Gruber, A. "Learning metriplectic systems from full and partial state information". *Geometric Mechanics Formulations and Structure-Preserving Discretizations Minisymposium at 16th World Congress on Computational Mechanics*, Vancouver, Canada. July 2024.
- Gruber, A. "Learning metriplectic systems and other bracket-based dynamics". *Mathematics for Machine Learning Minisymposium at CMS Summer Meeting*, Saskatoon, Canada. June 2024.
- Gruber, A. "Reversible and irreversible bracket-based dynamics for deep graph neural networks". *NeurIPS 2023*, New Orleans, LA. December 2023.
- Gruber, A. "Data-driven surrogate models for bracket-based dynamical systems". *Data-driven Methods for Circuits and Devices Minisymposium at MMLDE-CSET*, El Paso, TX. September 2023.
- Howard, A. A. "Multifidelity Deep Operator Learning". *2nd ICAM Mechanistic Machine Learning and Digital Engineering for Computational Science Engineering and Technology*, El Paso, TX. September 2023.
- Howard, A. A. "More of a good thing: stacking deep operator networks". *SIAM Annual Meeting*, Spokane, WA. July 2024.
- Howard, A. A. "Uncertainty quantification for multifidelity operator networks". *WCCM*, Vancouver, Canada. July 2024.
- Kahana, A. "Leveraging Large Language Models for Scientific Machine Learning across Domains". *Workshop on The Industrialization of Scientific Machine Learning*, ICERM, Providence, RI. March 2024.
- Kahana, A. "Preconditioning for Large Scale Systems based on the HINTS". *21st Copper Mountain Conference on Multigrid Methods*, Copper Mountain, CO. April 2023.
- Kahana, A. "Using Spiking Neural Networks for Scientific Computations". *Mathematical and Scientific Machine Learning*, Providence, RI. June 2023.
- Kahana, A. "On the Geometry Transferability of the Hybrid Iterative Numerical Solver for Differential Equations". *17th U.S. National Congress on Computational Mechanics*, Albuquerque, NM. July 2023.

- Kahana, A. "Using Spiking Neural Networks for Scientific Computations". *SIAM Conference on Computational Science and Engineering (CSE23)*, Amsterdam, Netherlands. March 2023.
- Kahana, A, Zhang, Q, Karniadakis, G. E., and Stinis, P. "Spiking Neural Network Representation of Partial Differential Equation Evolution Maps". *SIAM Conference on Computational Science and Engineering (CSE23)*, Amsterdam, Netherlands. March 2023.
- Maxey, M. "Mesoscopic simulations of cavitation and vapor bubble development". *American Physical Society, 76th Division of Fluid Dynamics Meeting*, Washington, D.C. November 2023.
- Propp, A. "Graph neural operators for quantification of geometric uncertainty". *World Congress on Computational Mechanics / Pan American Congress on Computational Mechanics (WCCM-PANACM)*, Vancouver, Canada. July 2024.
- Propp, A. "Discovery of Dirichlet-to-Neumann maps on graphs via Gaussian processes". *Scientific Machine Learning: Emerging Topics*, Trieste, Italy. June 2024.
- Propp, A. "Towards costless model selection in contextual bandits: A bias-variance perspective". *Artificial Intelligence and Statistics (AISTATS)*, Barcelona, Spain. May 2024.
- Stinis, P. "Multifidelity scientific machine learning". *SIAM Annual Meeting*, Spokane, WA. July 2024.
- Stinis, P. "Multifidelity scientific machine learning". *North American High Order Methods Conference (NAHOM-Con)*, Hanover, NH. June 2024.
- Stinis, P. "Multifidelity scientific machine learning". *European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS)*, Lisbon, Portugal. June 2024.
- Stinis, P. "Multifidelity scientific machine learning". *American Mathematical Society Central Sectional Meeting*, Milwaukee, WI. April 2024.
- Stinis, P. "When big neural networks are not enough". *ICERM Industrialization of SciML Workshop*, Providence, RI. March 2024.
- Stinis, P. "Spiking Neural Network Representation of Partial Differential Equation Evolution Maps". *SIAM Conference on Computational Science and Engineering (CSE23)*, Amsterdam, Netherlands. March 2023.
- Stinis, P. "Multifidelity scientific machine learning". *Georgia Tech Workshop on Foundation of Scientific AI for Optimization of Complex Systems*, Atlanta, GA. January 2024.
- Stinis, P. "Multifidelity scientific machine learning". *BIRS Scientific Machine Learning Workshop*, Banff, Canada. June 2023.
- Walker, E. A. "Causal disentanglement of multimodal data". *Mathematical and Scientific Machine Learning*, Providence, RI. June 2023.
- Walker, E. A. "A new parametrization of DAGs and causal Markov kernels for scientific feature discovery". *American Causal Inference Conference*, Seattle, WA. May 2024.
- Walker, E. A. "A new parametrization of DAGs and causal Markov kernels for scientific feature discovery". *16th World Congress on Computational Mechanics*, Vancouver, Canada. July 2024.
- Xu, M. "Learning temporal graph embeddings using transformers". *ICIAM Workshop on Mathematics of Geometric Deep Learning, 10th International Congress on Industrial and Applied Mathematics*, Waseda University, Tokyo, Japan. August 2023.
- Xu, M. "Adaptive time-stepping for learning temporal graph embeddings using transformers". *Annual SIAM-NNP Meeting*, NJIT, Newark, NJ. October 2023.
- Xu, M. "Adaptive time-stepping for learning temporal graph embeddings using transformers". Alan Turing Institute, U.K. November 2023.
- Zhang, E. "A Hybrid Iterative Numerical Transferable Solver (HINTS) for PDEs Based on Deep Operator Network and Relaxation Methods". *21st Copper Mountain Conference on Multigrid Methods*, Copper Mountain, CO. April 2023.

A.3 Software released

The SEA-CROGS team has released numerous software packages, listed below. We expand on some of the software pages in this section.

BracketGraphs Code accompanying NeurIPS 2023 paper [31]. Available at
<https://github.com/natrask/BracketGraphs>.

ComputationalHypergraphDiscovery Computational Hypergraph Discovery. Available at
<https://github.com/TheoBourdais/ComputationalHypergraphDiscovery>.

FBKANS Code for implementing finite basis KANs [0]. Available at
<https://github.com/pnnl/neuromancer/tree/feature/fbkans/examples/KANS>.

StackedPINNs Code for implementing stacked PINNs [10]. Available at
https://github.com/pnnl/neuromancer/blob/master/examples/PDEs/Part_5_Pendulum_Stacked.ipynb.

MINT Code accompanying ASPDAC 2024 paper [47]. Available at
<https://github.com/Intelligent-Computing-Lab-Yale/MINT-Quantization>.

SEENN Code accompanying NeurIPS 2023 paper [45]. Available at
<https://github.com/Intelligent-Computing-Lab-Yale/SEENN>.

TTFS Code accompanying Frontiers in Neuroscience 2023 paper [46]. Available at
<https://github.com/Intelligent-Computing-Lab-Yale/SkipResConnection>.

uTicket Code accompanying IEEE TETCI 2024 paper [48]. Available at
<https://github.com/Intelligent-Computing-Lab-Yale/u-Ticket-Pruning>.

A.3.1 DeepXDE: A Deep Learning Library for Solving Differential Equations

DeepXDE is a Python library for PINNs designed to serve both as an education tool to be used in the classroom as well as a research tool for solving problems in computational science and engineering. Specifically, DeepXDE can solve forward problems given initial and boundary conditions, as well as inverse problems given some extra measurements. DeepXDE supports complex-geometry domains based on the technique of constructive solid geometry and enables the user code to be compact, closely resembling the mathematical formulation. More broadly, DeepXDE contributes to the more rapid development of the emerging SciML field.

A.4 Students and postdocs mentored

A.4.1 Students

Brown University: Alan John Varghese (PhD, Engineering) [61, 37], Juan D. Toscano (PhD, Applied Mathematics) [60] and Vivek Oommen (PhD, Engineering) [13] are pursuing PhDs with SEA-CROGS support. Paula Chen (PhD, Applied Mathematics) [54, 55, 56] graduated in May 2023 and is currently at the Naval Air Warfare Center Weapons Division.

Caltech: Théo Bourdais [25, 34], Pau Batlle [51, 52, 53], Matthieu Darcy [51], Yasamin Jalalian, and Jonghyeon Lee. Yifan Chen [57, 53] graduated in 2023 and is currently a Courant Instructor at New York University.

NJIT: Ashish Parmanand Pandey (MSc) and Sarang Patil (PhD).

Spelman: Brianna Severe (undergraduate).

Stanford: Adrienne Propp (PhD, Computational and Mathematical Engineering), Alexander Kiral (PhD, Physics).

UPenn: Handi Zhang. An additional graduate student (Ben Schaeffer) contributes heavily to the project through a synergistic NSF Graduate Research Fellowship Program fellowship.

Yale: Yuhang Li [59, 45], Ruokai Yin [47, 48], Abhiroop Bhattacharjee [63, 49], Donghyun Lee [44], Abhishek Moitra [64, 65] (all PhD students). Youngeun Kim [58, 46] received their PhD in 2024 and has joined Meta Reality Labs as a research scientist.

A.4.2 Postdocs

Brown: Adar Kahana [40, 62], Aniruddha Bora [13, 61]

Caltech: Xianjin Yang

UPenn: Brooks Kinch, Quercus Hernandez

PNNL: Wenqian Chen [19, 12]

Sandia: Bradley Theilman [43], Alexey Voronin

Former postdocs: Caltech postdoc Ricardo Baptista [34] joined the University of Toronto as an assistant professor.

The first cohort of postdocs at SNL have all been converted to staff (Walker [24, 22], Actor [27, 20], and Gruber [32, 31]).

A.5 Recognition, honors, and awards

1. George Karniadakis was awarded the G.I. Taylor Medal “for highly innovative, pioneering, and sustained contributions to computational and theoretical aspects of fluid dynamics” in 2024 by The Society of Engineering Science.
2. George Karniadakis was elected to the National Academy of Engineering in 2022, one of the highest professional honors accorded an engineer.

3. George Karniadakis was named to the 2023 Highly Cited Researchers List by Clarivate Analytics. This list recognizes world-class researchers selected for their exceptional research performance, demonstrated by production of multiple highly cited papers that rank in the top one percent by citations for field and year in Web of Science.
4. Houman Owhadi was awarded the Department of Defense Vannevar Bush Faculty Fellowship (2024).
5. Priya Panda was awarded an NSF CAREER Award for research on “Spiking Neural Networks” (2023).
6. Adrienne Propp was awarded the Stanford University Institute for Computational & Mathematical Engineering (ICME) Student Leadership Award.
7. Priya Panda was awarded the inaugural Purdue Engineering 38 by 38 award (2024).
8. Priya Panda was awarded the DARPA Young Faculty Award for research on “Hardware-Algorithm Co-Design for Edge Applications” (2023).
9. Priya Panda was selected to participate in the German-American Frontiers of Engineering Symposium organized by the National Academy of Engineering and the Alexander Humboldt Foundation in Julich, Germany (2023).
10. The paper from Priya Panda’s group on multiplier-less quantization with spiking networks [47] received the Best Paper Nomination at the ASP-DAC conference (2024).

A.6 Other professional activities

A.6.1 Organizational activities

- Eric C. Cyr is on the Program Committee for the Copper Mountain Conference On Multigrid Methods, ongoing.

A.6.2 Editorial boards

- Eric C. Cyr is an associate editor for the *SIAM Journal on Scientific Computing* and guest edited a SIAM SISC special issue for the 2023 Copper Mountain Conference, 2023.
- George Karniadakis is an associate editor for *Computer Methods in Applied Mechanics and Engineering*, the *Journal of Computational Physics, Biomechanics and Modeling in Mechanobiology*, the *SIAM Journal on Scientific Computing*, *SIAM Review*, and the *SIAM Journal on Uncertainty Quantification*.
- Houman Owhadi is an associate editor of the American Mathematical Society’s *Mathematics of Computation*, *SIAM Journal on Numerical Analysis*, *International Journal for Uncertainty Quantification*, *Journal of Computational Dynamics*, De Gruyter book series on computational science and engineering, the *SIAM/ASA Journal on Uncertainty Quantification*, the American Institute of Mathematical Sciences’ *Foundations of Data Science*, and the *Journal of Machine Learning for Modeling and Computing*.
- Priya Panda is the editor of *Frontiers in Neuroscience, Section: Neuromorphic Engineering*, and an associate editor of *IEEE Transactions on Computer Aided Design of Integrated Circuits & Systems, Area: Emerging Technologies* and *IEEE Transactions on Cognitive and Developmental Systems*. She guest edited a special issue on *Neuro-AI Learning Systems* in *IEEE JETCAS 2023* and served as the editor of an *IEEE JETCAS Special Issue on Dynamical Neuromorphic Computing*.

A.6.3 External student committee service

- Eric C. Cyr served on the student committee for Samuel Adolfo Cruz Alegría, Dissertation Proposal Review Committee (June 2024): “Domain Decomposition Methods for Machine Learning,” Università della Svizzera italiana
- Eric C. Cyr served on the student committee for Corne Verburg, Masters Defense (April 2024): Topic - “Domain Decomposition for Machine Learning Based Segmentation,” TU Delft (Thesis)
- Eric C. Cyr served on the student committee for Gary Saavedra, Masters Defense (March 2023): Topic - “Multilevel Optimization with Dropout for Neural Networks,” University of New Mexico

A.6.4 Diversity service

- Amanda Howard joined the Association for Women in Mathematics Student Chapter Committee
- Adrienne Propp served as a board member / communications chair for Stanford Women in Mathematics, Statistics, and Computational Engineering (WiMSCE).
- Adrienne Propp served as an Enhancing Diversity in Graduate Education Doctoral Fellowship Program (EDGE) mentor for the Stanford EDGE Fellowship.¹
- Adrienne Propp served as a member on the Stanford ICME Student Action Group.²

¹<https://vpge.stanford.edu/fellowships-funding/enhancing-diversity-graduate>

²The Student Action Group consists of ICME student representatives that work alongside ICME Faculty and Staff on matters that concern the institute's educational mission, students' life and the ICME community at large. These include, but are not limited to, curriculum, research rotations, program requirements, qualifying exams, advisor-advisee relations, community events, student support.

B Abbreviations

- AI: artificial intelligence
- ANN: artificial neural network
- CHD: Computational Hypergraph Discovery
- CK: conjugate kernel
- DOE: Department of Energy
- E3SM: Energy Exascale Earth System Model
- FEM: finite element method
- GP: Gaussian process
- GRBF: Gaussian radial basis functions
- ICME: Institute for Computational & Mathematical Engineering
- IEEE: Institute of Electrical and Electronics Engineers
- LRF: linear response function
- MEA: Minimal Error Aggregation
- MEEA: Minimal Empirical Error Aggregation
- MEVA: Minimal Variance Aggregation
- MI: machine intelligence
- MINT: Multiplier-less INTeger
- M&M: Multi-scale Multi-feature UNet
- MMICC: Mathematical Multifaceted Integrated Capability Center
- MVA: Minimal Variance Aggregation
- NTK: neural tangent kernel
- PDE: partial differential equation
- PI: physics-informed
- PINN: physics-informed neural network
- PNNL: Pacific Northwest National Laboratory
- SciML: Scientific machine learning
- SEA-CROGS: Scalable, Efficient and Accelerated Causal Reasoning Operators, Graphs and Spikes for Earth and Embedded Systems
- SEENN: Spiking Early-Exit Neural Network
- SDGD: stochastic dimension gradient descent
- STEM: science, technology, mathematics, and engineering
- SNN: spiked neural network
- SNL: Sandia National Laboratories

- SympGNN: symplectically permutation equivariant graph neural network
- TTFS: time-to-first-spike
- TTSNN: Tensor Train Decomposition for Spiking Neural Networks
- UQ: uncertainty quantification

Pacific Northwest National Laboratory

902 Battelle Boulevard
P.O. Box 999
Richland, WA 99354

1-888-375-PNNL (7665)

www.pnnl.gov