

GRAPH-BASED OPERATOR LEARNING FROM LIMITED DATA ON IRREGULAR DOMAINS

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ABSTRACT

Operator learning seeks to approximate mappings from input functions to output solutions, particularly in the context of partial differential equations (PDEs). While recent advances such as DeepONet and Fourier Neural Operator (FNO) have demonstrated strong performance, they often rely on regular grid discretizations, limiting their applicability to complex or irregular domains. In this work, we propose a **Graph-based Operator Learning with Attention (GOLA)** framework that addresses this limitation by constructing graphs from irregularly sampled spatial points and leveraging attention-enhanced Graph Neural Networks (GNNs) to model spatial dependencies with global information. To improve the expressive capacity, we introduce a Fourier-based encoder that projects input functions into a frequency space using learnable complex coefficients, allowing for flexible embeddings even with sparse or nonuniform samples. We evaluated our approach across a range of 2D PDEs, including Darcy Flow, Advection, Eikonal, and Nonlinear Diffusion, under varying sampling densities. Our method consistently outperforms baselines, particularly in data-scarce regimes, demonstrating strong generalization and efficiency on irregular domains.

1 INTRODUCTION

Learning mappings between function spaces is a fundamental task in computational physics and scientific machine learning, especially for approximating solution operators of partial differential equations (PDEs). Operator learning offers a paradigm shift by learning the solution operator directly from data, enabling fast, mesh-free predictions across varying input conditions. Despite their success, existing operator learning models such as DeepONet (Lu et al., 2019) and Fourier Neural Operator (FNO) (Li et al., 2020a) exhibit notable limitations that restrict their applicability in more general settings. A key shortcoming lies in their reliance on regular, uniform grid discretizations. FNO, for instance, requires inputs to be defined on fixed Cartesian grids to leverage fast Fourier transforms efficiently. This assumption limits their flexibility and generalization ability when applied to problems defined on complex geometries, irregular meshes, or unstructured domains, which are common in real-world physical systems. Furthermore, these models often struggle with sparse or non-uniformly sampled data, leading to degraded performance and increased computational cost when adapting to more realistic, heterogeneous scenarios.

To address these limitations, we propose a **Graph-based Operator Learning with Attention (GOLA)** framework that leverages Graph Neural Networks (GNNs) to learn PDE solution operators over irregular spatial domains. By constructing graphs from sampled spatial coordinates and encoding local geometric and functional dependencies through message passing, the model naturally adapts to non-Euclidean geometries. To enhance global expressivity, we further incorporate attention-based mechanisms that can capture long-range dependencies more effectively and a Fourier-based encoder that projects input functions into a frequency domain using learnable complex-valued bases. Our model exhibits superior data efficiency and generalization, achieving smaller prediction errors with fewer training samples and demonstrating robustness under domain shifts.

The main contributions of this work are as follows:

- We introduce GOLA, a unified architecture combining spectral encoding and attention-enhanced GNNs for operator learning on irregular domains.

- We propose a learnable Fourier encoder that projects input functions into a frequency domain tailored for spatial graphs.
- Through extensive experiments, we demonstrate that GOLA generalizes across PDE types, sample densities, and resolution shifts, achieving state-of-the-art performance in challenging data-scarce regimes.

2 RELATED WORK

There are many latest research about graph and attention methods in scientific machine learning (Xiao et al., 2024), (Kissas et al., 2022), (Boullé and Townsend, 2024), (Xu et al., 2024), (Jin and Gu, 2023), (Cuomo et al., 2022) (Kovachki et al., 2024), (Nelsen and Stuart, 2024), (Battle et al., 2023).

Graph neural networks for scientific machine learning. (Battaglia et al., 2018) applies shared functions over nodes and edges, captures relational inductive biases and generalizes across different physical scenarios. (Bar-Sinai et al., 2019) learns data-driven discretization schemes for solving PDEs by training a neural network to predict spatial derivatives directly from local stencils. By replacing hand-crafted finite difference rules with learned operators, it adapts discretizations to the underlying data for improved accuracy and generalization. (Sanchez-Gonzalez et al., 2020) predicts future physical states by performing message passing over the mesh graph, capturing both local and global dynamics without relying on explicit numerical solvers. Graph Kernel Networks (GKNs) (Li et al., 2020b) directly approximates continuous mappings between infinite-dimensional function spaces by utilizing graph kernel convolution layers. PDE-GCN (Wang et al., 2022) represents partial differential equations on arbitrary graphs by combining spectral graph convolution with PDE-specific inductive biases. It learns to predict physical dynamics directly on graph-structured domains, enabling generalization across varying geometries and discretizations. The Message Passing Neural PDE Solver (Brandstetter et al., 2022) formulates spatiotemporal PDE dynamics by applying learned message passing updates on graph representations of the solution domain. Physics-Informed Transformer (PIT) (Dos Santos et al., 2023) embeds physical priors into the Transformer architecture to model PDE surrogate solutions. It leverages self-attention to capture long-range dependencies and integrates PDE residuals as soft constraints during training to improve generalization. GraphCast (Lam et al., 2024) learns the Earth’s atmosphere as a spatiotemporal graph and uses a graph neural network to iteratively forecast future weather states based on past observations. It performs message passing over the graph to capture spatial correlations and temporal dynamics, enabling accurate medium-range forecasts.

Attention-based methods for scientific machine learning. U-Netformer (Liu et al., 2022) proposes a hybrid neural architecture that combines the U-Net’s hierarchical encoder-decoder structure with transformer-based attention modules to capture both local and global dependencies in PDE solution spaces. Tokenformer (Zhou et al., 2023) reformulates PDE solving as a token mixing problem by representing input fields as tokens and applying self-attention across them to model spatial correlations. Adaptive Fourier Neural Operators (AFNO) (Guibas et al., 2021) are an efficient token-mixing mechanism for vision transformers that perform resolution-independent global convolution in the Fourier domain—enhanced by block-diagonal channel mixing, adaptive weight sharing, and frequency sparsification—to deliver quasi-linear complexity and superior performance over traditional self-attention on high-resolution image tasks. Our proposed GOLA combines the local relational strengths of attention-enhanced GNNs and the global spectral capabilities of Fourier-based encoding. This hybrid approach has shown notable improvements in generalization and data efficiency, particularly under challenging data-scarce conditions on irregular domains.

3 METHODOLOGY

3.1 PROBLEM FORMULATION

Consider the general form of a PDE

$$\mathcal{N}[u](\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} \in \Omega \times [0, \infty) \quad (1)$$

where $\mathbf{x}$ denotes a compact representation of the spatial and temporal coordinates, Ω is the spatial domain, and $[0, \infty)$ is the temporal domain. $\mathcal{N}$ is a differential operator, $u(\mathbf{x})$ is the unknown solution,

and $f(\mathbf{x})$ is a given source term. The objective is to learn the solution operator $\mathcal{G} : \mathcal{F} \rightarrow \mathcal{U}$, where $\mathcal{F}$ and $\mathcal{U}$ are Banach spaces. We assume access to a training dataset $\mathcal{D} = \{(f_n, u_n)\}_{n=1}^N$, consisting of multiple input-output function pairs, where each $f_n(\cdot)$ and $u_n(\cdot)$ is represented by discrete samples over a finite set of points.

While existing approaches such as DeepONet and FNO have demonstrated strong performance, they typically rely on structured, grid-based discretizations of the domain. This assumption limits their applicability to unstructured meshes, complex geometries, and adaptively sampled domains. To overcome this limitation, we employ GNNs for operator learning by representing the domain as a graph. This allows for modeling on arbitrary domains and sampling patterns. Once trained, the operator learning model can efficiently predict the solution u for a new instance of the input f at random locations.

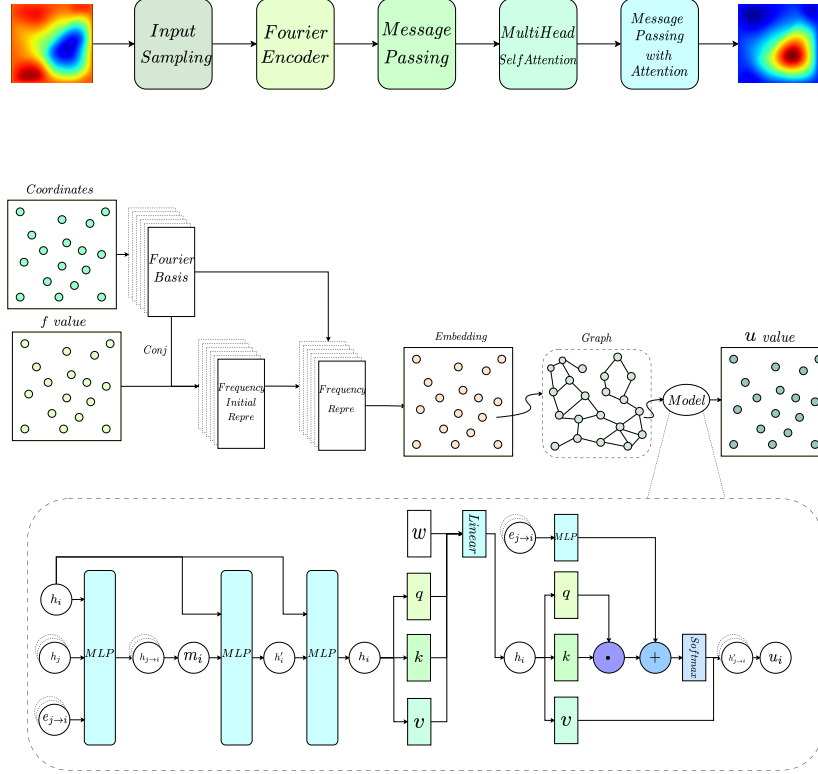


Figure 1: *GOLA: Graph-based Operator Learning with Attention*. The model first encodes input function values sampled on irregular spatial coordinates using a learnable Fourier encoder to obtain spectral node features. A graph is constructed based on spatial proximity, enabling message passing and multi-head self-attention to capture local and global dependencies. A final attention-based message passing layer refines the representation to predict the output solution values. GOLA effectively handles irregular domains and sparse samples, achieving strong generalization for PDE operator learning.

3.2 GRAPH CONSTRUCTION

To represent PDE solutions over irregular domains, we begin by randomly sampling a subset of points $\{x_i\}_{i=1}^N$ from a uniform grid in 2D space. We then construct a graph $G = (V, E)$ with nodes $V = \{x_i\}$ and edges E determined by a radius r . Edges are created based on spatial proximity. Two nodes are connected if the Euclidean distance between them is less than a threshold r such that $(i, j) \in E$ if and only if $\|x_i - x_j\|_2 \leq r$. Each edge (i, j) carries edge attributes e_{ij} that encode both geometric and feature-based information, such as the relative coordinates and function values at nodes i and j such that $e_{ij} = \|(x_i, x_j, f(x_i), f(x_j))\|$, where $\|$ is the concatenation operation. This graph-based representation allows us to model unstructured spatial domains and enables message passing among nonuniform samples.

3.3 FOURIER ENCODER

We define a set of learnable frequencies $\{\omega_m \in \mathbb{R}^2 \mid m = 1, \dots, M\}$.

For any coordinate $x \in \mathbb{R}^2$, the m -th basis function is given by the complex exponential

$$\varphi_m(x) = e^{2\pi i \langle \omega_m, x \rangle} \quad (2)$$

where $\langle \cdot, \cdot \rangle$ denotes the standard Euclidean inner product, and i is the imaginary unit.

At the discrete level, for a batch of B samples and N points per sample, the basis matrix is defined as

$$\Phi \in \mathbb{C}^{B \times N \times M}, \quad \Phi_{b,i,m} = e^{2\pi i \langle \omega_m, x_i^{(b)} \rangle} \quad (3)$$

where $x_i^{(b)}$ denotes the i -th coordinate point in the b -th batch sample.

Given the input $f \in \mathbb{R}^{B \times C_{\text{in}} \times N}$ sampled at points $\{x_i\}$, we first project onto the Fourier basis. We compute the Fourier coefficients by

$$\hat{u}_{b,c,m} = \frac{1}{N} \sum_{i=1}^N f_{b,c,i} \overline{\varphi_m(x_i^{(b)})} \quad (4)$$

where $\overline{(\cdot)}$ denotes complex conjugation.

We introduce a learnable set of complex Fourier coefficients $W \in \mathbb{C}^{C_{\text{in}} \times C_{\text{out}} \times M}$. The spectral filtering operation is

$$\hat{v}_{b,o,m} = \sum_{c=1}^{C_{\text{in}}} \hat{u}_{b,c,m} W_{c,o,m} \quad (5)$$

We reconstruct the output in the physical domain by applying the inverse transform

$$v_{b,o,i} = \sum_{m=1}^M \hat{v}_{b,o,m} \varphi_m(x_i^{(b)}) \quad (6)$$

Since v is complex-valued, we only take its real part for the output as $h = \text{Re}(v) \in \mathbb{R}^{B \times C_{\text{out}} \times N}$. The output h serves as the input node features for the downstream GNN model.

3.4 MESSAGE PASSING

Given a node $i \in V$ and its set of neighbors $\mathcal{N}(i)$, the pre-processed messages $\{m_{ij}\}_{j \in \mathcal{N}(i)}$ are first computed using a learnable neural network g_{Θ} as

$$m_{ij} = g_{\Theta}(h_i, h_j, e_{ij}) \quad (7)$$

where h_i and h_j are node features, and e_{ij} denotes edge attributes.

Then we aggregate message from neighbors such that

$$\hat{m} = \left\| \left(\frac{1}{|\mathcal{N}(i)|} \sum_{j \in \mathcal{N}(i)} m_{ij}, \max_{j \in \mathcal{N}(i)} m_{ij}, \min_{j \in \mathcal{N}(i)} m_{ij}, \sqrt{\frac{1}{|\mathcal{N}(i)|} \sum_{j \in \mathcal{N}(i)} \left(m_{ij} - \frac{1}{|\mathcal{N}(i)|} \sum_{j \in \mathcal{N}(i)} m_{ij} \right)^2} \right) \right\| \quad (8)$$

This concatenated feature vector is processed by a post-aggregation neural network γ_{Θ} to produce the updated node representation by

$$h'_i = \gamma_{\Theta}(h_i, \hat{m}) \quad (9)$$

The updated node representation is passed through additional MLP layers with residual connections to enhance expressiveness.

3.5 MULTI-HEAD SELF-ATTENTION

We employ H independent attention heads. For each head h , the query, key and value functions are computed as linear projections

$$q^{(h)}(x) = W_q h'(x), \quad k^{(h)}(y) = W_k h'(y), \quad v^{(h)}(y) = W_v h'(y) \quad (10)$$

where $W_q, W_k, W_v \in \mathbb{R}^{d_h \times C_{\text{out}}}$, $q^{(h)}(x), k^{(h)}(y), v^{(h)}(y) \in \mathbb{R}^{d_h}$ are learned head-specific features, and d_h is the dimension per attention head.

Before computing attention, the keys and values are normalized

$$\tilde{k}^{(h)}(y) = \text{Norm}(k^{(h)}(y)), \quad \tilde{v}^{(h)}(y) = \text{Norm}(v^{(h)}(y)) \quad (11)$$

where $\text{Norm}(\cdot)$ denotes instance normalization.

We compute

$$G_h = \sum_{j=1}^N \tilde{k}^{(h)}(y_j)^\top \tilde{v}^{(h)}(y_j) w(y_j), \quad (\mathcal{K}_h h')(x_i) = q^{(h)}(x_i) G_h \quad (12)$$

The outputs are concatenated and projected to the output space by

$$(\mathcal{K} h')(x_i) = \|((\mathcal{K}_1 h')(x_i), \dots, (\mathcal{K}_H h')(x_i)), \quad \hat{h}(x_i) = W_{\text{out}}(\mathcal{K} h')(x_i) \quad (13)$$

where where $G_h \in \mathbb{R}^{d_h \times d_h}$, w is calculated by the number of points, $W_{\text{out}} \in \mathbb{R}^{C_{\text{out}} \times (C_{\text{out}} \cdot H)}$.

The result is then passed through a linear projection layer to update the node features.

3.6 MESSAGE PASSING WITH ATTENTION

We update node features and add a skip connection by

$$\hat{h}'_i = W_1 \hat{h}_i + \sum_{j \in \mathcal{N}(i)} \alpha_{ij} (W_2 \hat{h}_j + W_3 e_{ij}), \quad \hat{h}'_i = \hat{h}'_i + W_s \hat{h}_i \quad (14)$$

The attention weights α_{ij} are computed using a scaled dot-product attention mechanism by

$$\alpha_{ij} = \text{softmax}_j \left(\frac{(W_4 \hat{h}_i)^\top (W_5 \hat{h}_j + W_3 e_{ij})}{\sqrt{d}} \right) \quad (15)$$

where d is the dimensionality of the head, and the softmax is applied over the set of neighbors $j \in \mathcal{N}(i)$. Then we add a linear projection to produce the predicted solution $\hat{u}$.

3.7 TRAINING

The model is trained to minimize the relative L_2 error between predicted and true solutions by

$$\mathcal{L}_2(\theta) = \frac{\|u - \mathcal{G}_\theta(f)\|_{L^2(\Omega)}}{\|u\|_{L^2(\Omega)}} \quad (16)$$

4 THEORETICAL ANALYSIS

Following the universal approximation theorem for operators (Lu et al., 2019), neural operator architectures can approximate any continuous operator $\mathcal{G}$ between Banach spaces when provided with sufficient capacity.

Proposition. Let $\mathcal{G} : \mathcal{F} \rightarrow \mathcal{U}$ be a continuous nonlinear operator between separable Banach spaces. Then, under sufficient model capacity, the GOLA architecture $\mathcal{G}_\theta$ can approximate $\mathcal{G}$ arbitrarily well in the $L^2(\Omega)$ norm over a compact domain Ω , i.e., $\sup_{f \in \mathcal{F}_\delta} \|\mathcal{G}(f) - \mathcal{G}_\theta(f)\|_{L^2(\Omega)} < \epsilon$, for any $\epsilon > 0$ and compact subset $\mathcal{F}_\delta \subset \mathcal{F}$.

Proof. Given a function $f \in \mathcal{F} \subset L^2(\Omega)$, we sample it at N spatial locations $\{x_i\}_{i=1}^N \subset \Omega$ to obtain a discrete representation $f_N = (f(x_1), \dots, f(x_N)) \in \mathbb{R}^N$. Since Ω is compact, by increasing N the point cloud $\{x_i\}$ becomes dense in Ω . Thus, f_N can approximate f arbitrarily well in $L^2(\Omega)$ norm via interpolation over the sampling set.

Define a set of complex Fourier basis functions $\{\phi_m(x) = e^{2\pi i \langle \omega_m, x \rangle}\}_{m=1}^M$. The Fourier basis is complete in $L^2(\Omega)$, so for any $f \in \mathcal{F}$ and $\delta > 0$, there exists M such that

$$\left\| f(x) - \sum_{m=1}^M \hat{f}_m \phi_m(x) \right\|_{L^2(\Omega)} < \delta.$$

This guarantees that the learnable Fourier encoder in GOLA can approximate the functional input f to arbitrary precision.

Construct a graph $G = (V, E)$ with node set $V = \{x_i\}_{i=1}^N$, where edges encode local spatial relationships. According to universal approximation results for GNNs (Xu et al., 2019), (Morris et al., 2019), for any continuous function defined on graphs, a GNN with sufficient depth and width can approximate it arbitrarily well. Thus, the GNN decoder can approximate the mapping from input features to solution values

$$(f(x_1), \dots, f(x_N)) \mapsto (\mathcal{G}(f)(x_1), \dots, \mathcal{G}(f)(x_N))$$

Let $\mathcal{T}_N$ denote the sampling operator, $\mathcal{F}_\theta$ the Fourier encoder, and $\mathcal{D}_\theta$ the GNN decoder. Then the GOLA operator can be written as

$$\mathcal{G}_\theta = \mathcal{D}_\theta \circ \mathcal{F}_\theta \circ \mathcal{T}_N$$

Each component is continuous and approximates its target arbitrarily well. Since composition of continuous approximations preserves continuity, and $\mathcal{F}_\delta$ is compact, the total approximation error can be made less than any $\epsilon > 0$ by choosing N , M , and model capacity large enough such that

$$\sup_{f \in \mathcal{F}_\delta} \|\mathcal{G}(f) - \mathcal{G}_\theta(f)\|_{L^2(\Omega)} < \epsilon$$

5 EXPERIMENTS

We evaluate the proposed model GOLA on four 2D PDE benchmarks including Darcy Flow, Nonlinear Diffusion, Eikonal, and Advection. For each dataset, we simulate training data with 5, 10, 20, 30, 40, 50, 80, 100 samples and use 100 examples for testing. To construct graphs, we randomly sample 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000 points from a uniform 128×128 grid over the domain $[0, 1] \times [0, 1]$. The sampled points define the nodes of the graph. Our model learns to approximate the solution operator from these irregularly sampled inputs. We aim to test generalization under both limited data and resolution changes. We compare against the following baselines including DeepONet (Lu et al., 2019), AFNO (Guibas et al., 2021) and Graph Kernel Network (GKN) (Li et al., 2020b).

Comparisons with baselines. Table 1 reports the averaged test errors over 5 runs with different seeds across four PDE benchmarks—Darcy Flow, Advection, Eikonal, and Nonlinear Diffusion—in the low-data regime of 100 training samples with sample density = 1000 randomly selected from a uniform 128×128 grid over the domain $[0, 1] \times [0, 1]$. The proposed GOLA method consistently achieves the lowest error across all datasets. For Darcy Flow, GOLA attains an error of 0.1088 ± 0.0027 , representing a 40.8% relative improvement over the best baseline, GKN (0.1840 ± 0.0040). In Advection, GOLA achieves 0.2227 ± 0.0185 , reducing the error by 26.7% compared to GKN and by over 77% relative to AFNO and DeepONet. For Eikonal, GOLA obtains 0.0657 ± 0.0011 , a 45.7% improvement over GKN, while Nonlinear Diffusion exhibits the largest relative gain— 0.0430 ± 0.0005 , which is 59.2% lower than GKN. Moreover, GOLA maintains standard deviations

on par with or below those of the best-performing baselines, indicating both superior accuracy and stable convergence.

Table 1: Test errors for different models in irregular sampling points trained on 100 training data samples with sample density=1000 across various PDE benchmarks. The results are averaged over 5 runs in this paper.

Dataset	AFNO	DeepONet	GKN	Ours(GOLA)
Darcy Flow	0.4310 ± 0.0040	0.5897 ± 0.0026	0.1840 ± 0.0040	0.1088 ± 0.0027
Advection	0.9845 ± 0.0007	0.9979 ± 0.0001	0.3043 ± 0.0041	0.2227 ± 0.0185
Eikonal	0.1828 ± 0.0017	0.1918 ± 0.0004	0.1210 ± 0.0043	0.0657 ± 0.0011
Nonlinear Diffusion	0.1686 ± 0.0016	0.2781 ± 0.0005	0.1052 ± 0.0038	0.0430 ± 0.0005

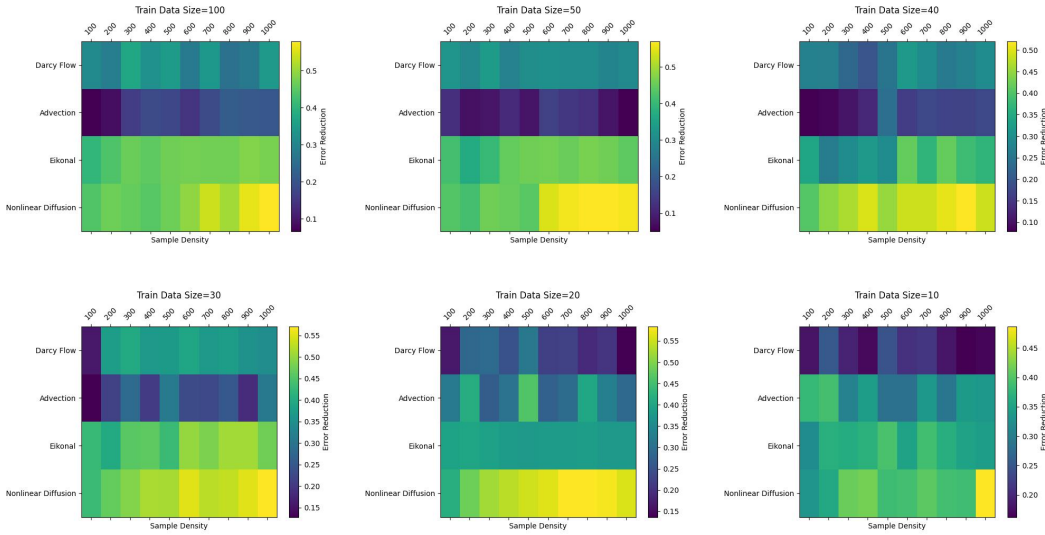


Figure 2: Error reduction heatmaps across training data sizes and sample densities for PDE Benchmarks. Nonlinear Diffusion consistently shows the highest error reduction across all training sizes and densities and it becomes more prominent at high sample densities even under very small training size 10.

Generalization across sample densities. From Table 2, we use 100 training data, and choose three types of sampling densities 20, 500, 1000 which represent small, medium and high sample densities. We observe a consistent trend that increasing sample density leads to significant performance improvements across all PDEs. The results highlight that higher sampling density substantially improves generalization, particularly for PDEs with more complex solution manifolds such as Darcy flow and nonlinear diffusion, and that even moderate densities 500 are sufficient to close much of the performance gap for Eikonal equations.

Table 2: Test errors for small, medium, and high sampling densities with training data size=100.

Sample Density	20	500	1000
Darcy flow	0.4422 ± 0.0213	0.1298 ± 0.0043	0.1088 ± 0.0027
Advection	0.4374 ± 0.0177	0.2654 ± 0.0163	0.2227 ± 0.0185
Eikonal	0.1267 ± 0.0019	0.0675 ± 0.0020	0.0657 ± 0.0011
Nonlinear diffusion	0.1901 ± 0.0060	0.0542 ± 0.0015	0.0430 ± 0.0005

Resolution generalization. From Table 3 and Figure 3, we use 100 training data and sample 1000 training sample points, then we test the relative L_2 error in different test sample densities 100, 500, 1000, 2000, 4000. We observe that higher test sample densities consistently reduce the error for all PDE families, reflecting improved approximation accuracy with denser test points.

Table 3: Test errors for different test sampling densities with training sample density=1000.

Test Sample Density	100	500	1000	2000	4000
Darcy flow	0.2475 ± 0.0041	0.1304 ± 0.0020	0.1088 ± 0.0027	0.0971 ± 0.0033	0.0895 ± 0.0035
Advection	0.3641 ± 0.0117	0.2505 ± 0.0149	0.2227 ± 0.0185	0.2218 ± 0.0202	0.2182 ± 0.0141
Eikonal	0.0790 ± 0.0031	0.0672 ± 0.0020	0.0657 ± 0.0011	0.0654 ± 0.0024	0.0654 ± 0.0019
Nonlinear diffusion	0.0893 ± 0.0020	0.0511 ± 0.0015	0.0430 ± 0.0005	0.0386 ± 0.0012	0.0368 ± 0.0015

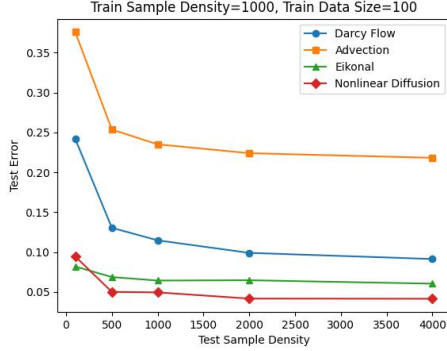


Figure 3: Test error trend with test sample density

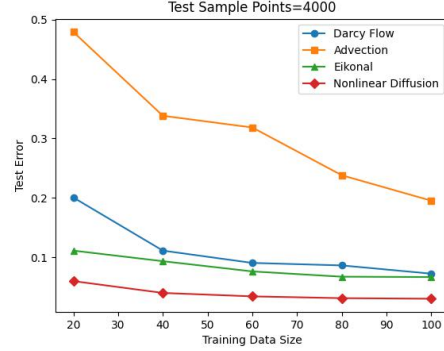


Figure 4: Test error trend with train data size

Data Efficiency. From Table 4, we use 2000 sample points and change different training data size to test the performance. From Figure 4, we report the results for 4000 sample points with different training data size. In Figure 5, we report the results for test error trend with respect to training data size in test sample points $\in \{200, 300, 400, 500, 600, 700, 800, 900\}$. Across all PDEs, we observe a clear trend of decreasing test error with increasing training data size, indicating effective data scaling behavior.

Table 4: Test errors under varying numbers of training data size with sample density=2000.

Training data size	20	40	60	80	100
Darcy flow	0.2027 ± 0.0161	0.1372 ± 0.0095	0.1071 ± 0.0073	0.0983 ± 0.0057	0.0913 ± 0.0029
Advection	0.5253 ± 0.0273	0.4026 ± 0.0182	0.3192 ± 0.0388	0.2709 ± 0.0243	0.2228 ± 0.0172
Eikonal	0.1029 ± 0.0047	0.0763 ± 0.0033	0.0678 ± 0.0028	0.0648 ± 0.0023	0.0647 ± 0.0021
Nonlinear diffusion	0.0815 ± 0.0139	0.0538 ± 0.0023	0.0429 ± 0.0036	0.0394 ± 0.0033	0.0360 ± 0.0013

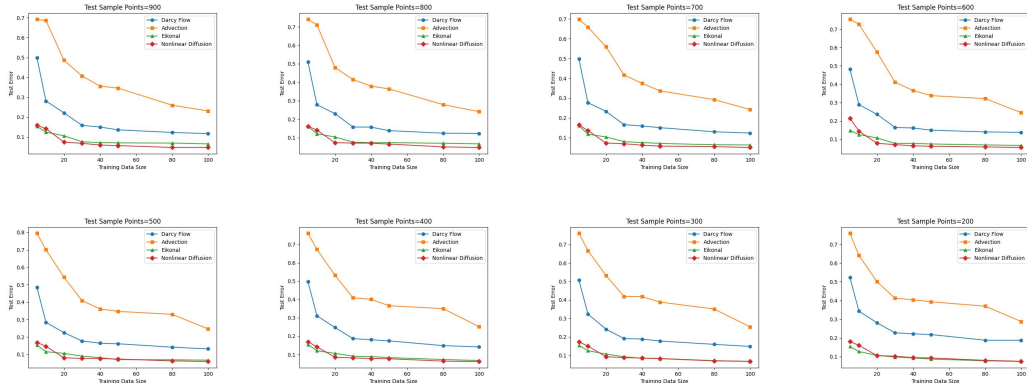


Figure 5: Test error trends across varying sample densities for PDE benchmarks.

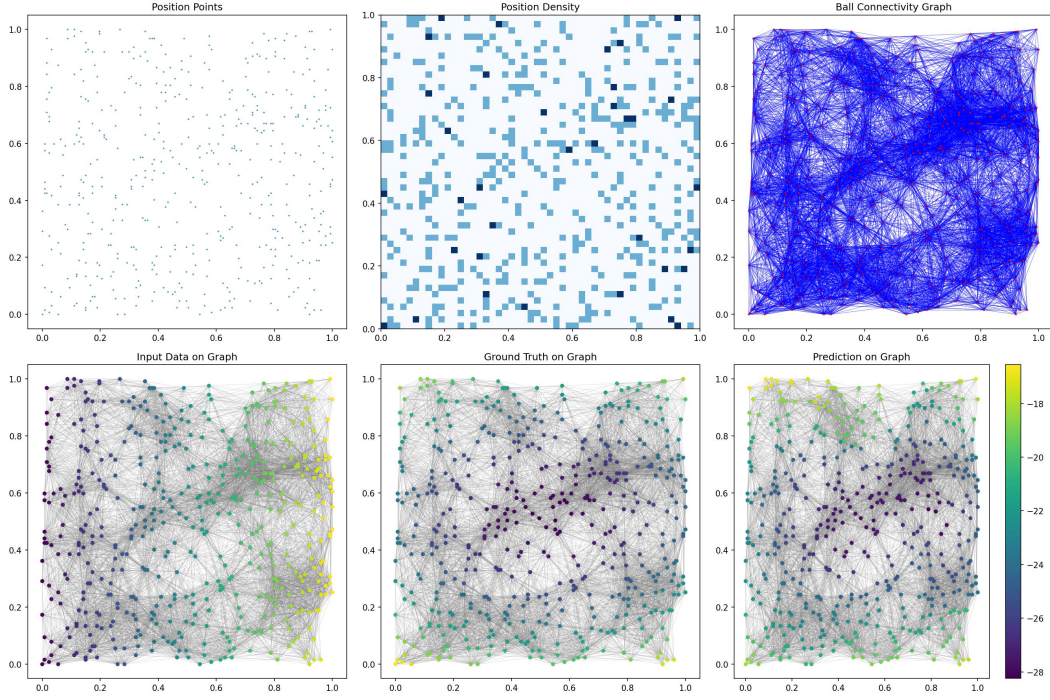


Figure 6: Visualizations for graph with 1000 sample points on Advection.

Graph Visualizations. We visualize graph construction in Figure 6. We randomly sample 1000 node positions in the unit square and use ball connectivity with a fixed radius 0.2 to construct graph. These results are shown on the top row. Then in this graph, we visualize input function values on the graph, ground-truth solution, and model prediction on the bottom row. Figure 6 demonstrates that (i) the graph construction preserves locality and global connectivity; (ii) the learned model generalizes well to unseen node configurations and accurately reconstructs the solution field; (iii) visual comparison between ground truth and predictions reveals minimal discrepancy, supporting the effectiveness of our proposed model GOLA.

Time Complexity and Memory Cost. We analyze the computational complexity of the GOLA architecture in terms of the number of spatial points N , Fourier modes M , feature channels C , and edges $E \sim \mathcal{O}(Nk)$, where k is the average number of neighbors in the sparse spatial graph. The time complexity for GOLA is $\mathcal{O}(MNC') + \mathcal{O}(NkC^2) + \mathcal{O}(NkC)$. The count of parameters for GOLA is 2,900,249.

6 CONCLUSION

In this work, We introduce **Graph-based Operator Learning with Attention (GOLA)** framework, which combines a learnable Fourier encoder with attention-enhanced message passing to solve PDEs over irregular domains. By representing the spatial domain as a proximity graph and embedding inputs into a learnable spectral basis, GOLA effectively captures both local and global dependencies, enabling accurate operator approximation even under sparse sampling and complex geometries. Through comprehensive experiments across diverse PDE benchmarks including Darcy Flow, Advection, Eikonal, and Nonlinear Diffusion, GOLA consistently outperforms baselines including AFNO, DeepONet, GKN particularly in data-scarce regimes. We demonstrate GOLA’s superior generalization, resolution scalability, and robustness to sparse sampling. These results highlight the potential of combining spectral encoding and localized message passing with attention to build continuous, data-efficient operator approximators that adapt naturally to non-Euclidean geometries. This study demonstrates that graph-based representations provide a powerful and flexible foundation for advancing operator learning in real-world physical systems with irregular data.

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A ADDITIONAL RESULTS

A.1 TEST ERROR TRENDS ACROSS VARYING SAMPLE DENSITIES(30-100) FOR PDE BENCHMARKS

In Figure 7, it shows the test error for four PDE benchmarks as a function of training data size, under different test point resolutions ranging from 30 to 100.

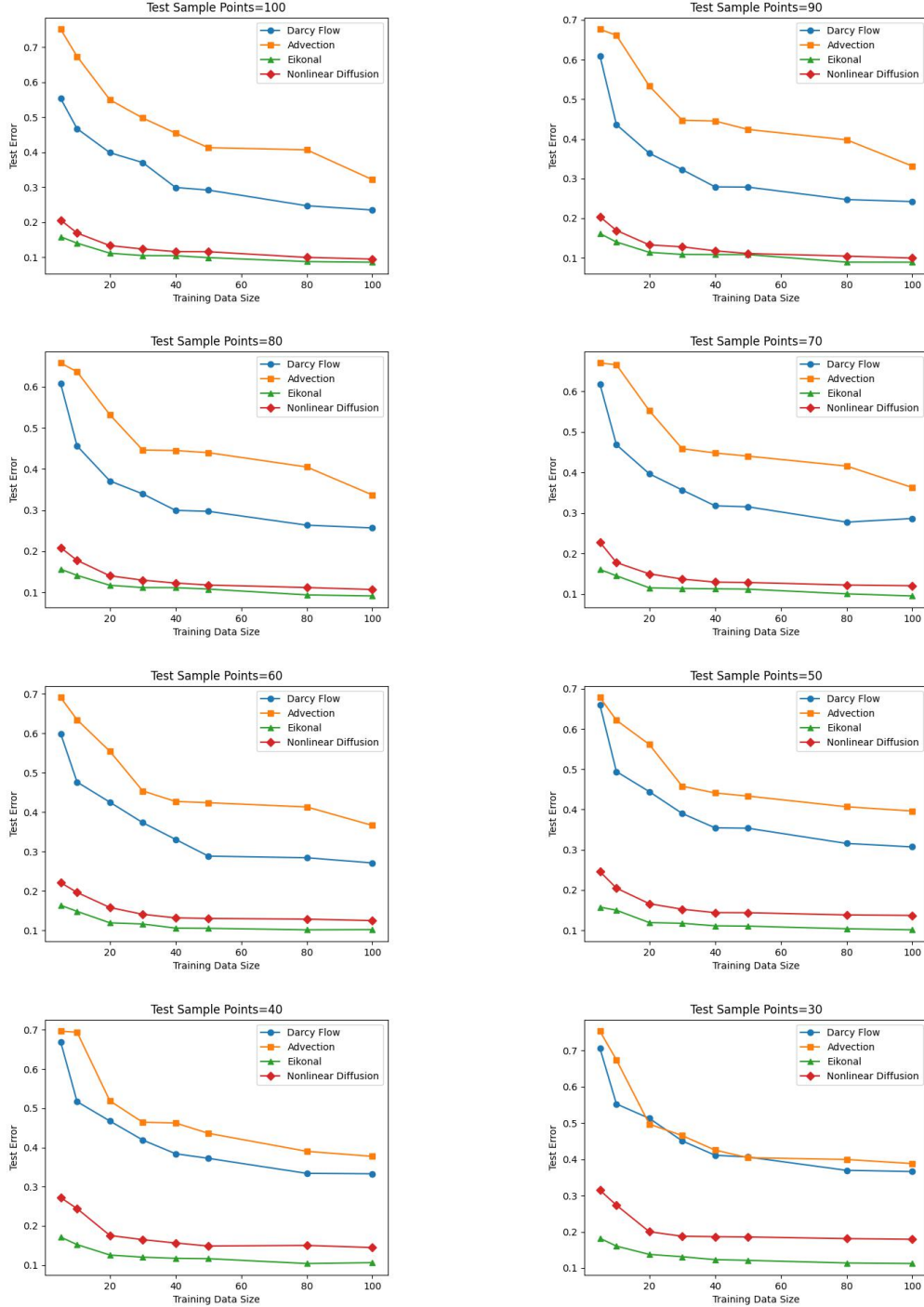


Figure 7: Test error trends across varying sample densities(30-100) for PDE benchmarks

A.2 ERROR REDUCTION ON 30, 50, 100 TRAINING DATA ACROSS VARIOUS SAMPLING DENSITY

From Table 5, 6, 7, with 100, 50, 30 training data size respectively, for each PDE benchmark, we choose sample density from 20 to 1000 to compare GKN and GOLLA, and calculate the error reduction. It shows that our method is better than GKN and error reduction is significant.

Table 5: Test errors trained on 100 training data size across various sampling density

(a) <i>Darcy Flow</i>				(b) <i>Eikonal</i>			
Density	GKN	Ours	Error Reduction	Density	GKN	Ours	Error Reduction
20	0.5027	0.4073	18.98%	20	0.1808	0.1236	31.64%
30	0.4746	0.3663	22.82%	30	0.1723	0.1125	34.71%
40	0.4572	0.3328	27.21%	40	0.1671	0.1066	39.80%
50	0.4283	0.3072	28.27%	50	0.1620	0.0981	39.44%
60	0.3995	0.2711	32.14%	60	0.1588	0.0962	39.42%
70	0.3885	0.2710	30.24%	70	0.1546	0.0953	38.36%
80	0.3760	0.2566	31.76%	80	0.1472	0.0911	38.11%
90	0.3646	0.2420	33.63%	90	0.1442	0.0871	39.47%
100	0.3402	0.2349	30.95%	100	0.1442	0.0857	40.57%
200	0.2633	0.1878	28.67%	200	0.1325	0.0745	43.77%
300	0.2355	0.1479	37.20%	300	0.1238	0.0664	46.37%
400	0.2097	0.1415	32.52%	400	0.1203	0.0658	45.30%
500	0.2020	0.1315	34.90%	500	0.1205	0.0640	46.89%
600	0.1911	0.1242	35.01%	600	0.1199	0.0632	47.29%
700	0.1874	0.1235	34.10%	700	0.1159	0.0614	47.02%
800	0.1788	0.1226	31.43%	800	0.1148	0.0607	47.13%
900	0.1777	0.1168	34.27%	900	0.1173	0.0606	48.34%
1000	0.1748	0.1147	34.38%	1000	0.1168	0.0611	47.69%
(c) <i>Nonlinear Diffusion</i>				(d) <i>Advection</i>			
Density	GKN	Ours	Error Reduction	Density	GKN	Ours	Error Reduction
20	0.2407	0.1958	18.65%	20	0.9035	0.3980	55.95%
30	0.2181	0.1795	17.70%	30	0.5409	0.3883	28.21%
40	0.2133	0.1446	32.21%	40	0.4563	0.3773	17.31%
50	0.2066	0.1369	33.74%	50	0.4208	0.3747	10.96%
60	0.1922	0.1248	35.07%	60	0.3823	0.3662	4.21%
70	0.1876	0.1206	35.71%	70	0.3736	0.3626	2.94%
80	0.1851	0.1067	42.36%	80	0.3468	0.3362	2.88%
90	0.1760	0.0995	43.47%	90	0.3422	0.3315	3.13%
100	0.1689	0.0947	43.93%	100	0.3446	0.3216	6.67%
200	0.1415	0.0755	46.64%	200	0.3150	0.2880	8.57%
300	0.1245	0.0674	45.86%	300	0.3017	0.2537	15.91%
400	0.1118	0.0618	44.72%	400	0.3084	0.2516	18.42%
500	0.1115	0.0594	46.73%	500	0.2997	0.2462	17.85%
600	0.1093	0.0553	49.41%	600	0.2886	0.2453	14.47%
700	0.1101	0.0507	53.95%	700	0.2972	0.2421	18.54%
800	0.1073	0.0469	56.29%	800	0.3038	0.2408	21.89%
900	0.1054	0.0463	56.07%	900	0.2926	0.2310	21.05%
1000	0.1044	0.0439	57.95%	1000	0.2886	0.2290	20.65%

Table 6: Test errors trained on 50 training data size across various sampling densities

(a) <i>Darcy Flow</i>				(b) <i>Eikonal</i>			
Density	GKN	Ours	Error Reduction	Density	GKN	Ours	Error Reduction
20	0.5690	0.4484	21.20%	20	0.1908	0.1361	28.67%
30	0.5192	0.4064	21.73%	30	0.1870	0.1213	35.13%
40	0.5085	0.3722	26.80%	40	0.1839	0.1162	36.81%
50	0.4783	0.3536	26.07%	50	0.1764	0.1103	37.47%
60	0.4467	0.2884	35.44%	60	0.1739	0.1052	39.51%
70	0.4328	0.3099	28.40%	70	0.1670	0.1024	38.68%
80	0.4310	0.2934	31.93%	80	0.1640	0.1000	39.02%
90	0.4099	0.2785	32.06%	90	0.1643	0.0943	42.60%
100	0.4068	0.2756	32.25%	100	0.1592	0.0927	41.77%
200	0.3092	0.2182	29.43%	200	0.1386	0.0873	37.01%
300	0.2673	0.1771	33.74%	300	0.1380	0.0824	40.29%
400	0.2421	0.1741	28.09%	400	0.1341	0.0741	44.74%
500	0.2326	0.1609	30.83%	500	0.1292	0.0702	45.67%
600	0.2173	0.1497	31.11%	600	0.1309	0.0705	46.14%
700	0.2114	0.1470	30.46%	700	0.1299	0.0713	45.11%
800	0.1990	0.1381	30.60%	800	0.1288	0.0688	46.58%
900	0.1901	0.1360	28.46%	900	0.1300	0.0704	45.85%
1000	0.1890	0.1328	29.74%	1000	0.1273	0.0710	44.23%
(c) <i>Nonlinear Diffusion</i>				(d) <i>Advection</i>			
Density	GKN	Ours	Error Reduction	Density	GKN	Ours	Error Reduction
20	0.2817	0.2202	21.83%	20	0.8899	0.4338	51.25%
30	0.2554	0.1858	27.25%	30	0.6991	0.4046	42.13%
40	0.2413	0.1485	38.46%	40	0.5983	0.3987	33.36%
50	0.2339	0.1437	38.56%	50	0.5569	0.4052	27.24%
60	0.2266	0.1303	42.50%	60	0.6016	0.4143	31.13%
70	0.2117	0.1285	39.30%	70	0.4733	0.4067	14.07%
80	0.2081	0.1177	43.44%	80	0.4585	0.3984	13.11%
90	0.1955	0.1110	43.22%	90	0.4559	0.3819	16.23%
100	0.1903	0.1083	43.09%	100	0.4467	0.3925	12.13%
200	0.1597	0.0932	41.64%	200	0.4156	0.3845	7.48%
300	0.1506	0.0818	45.68%	300	0.4132	0.3796	8.13%
400	0.1390	0.0766	44.89%	400	0.4126	0.3658	11.34%
500	0.1301	0.0733	43.66%	500	0.3767	0.3468	7.94%
600	0.1349	0.0618	54.19%	600	0.3981	0.3378	15.15%
700	0.1308	0.0575	56.04%	700	0.3893	0.3364	13.59%
800	0.1284	0.0552	57.01%	800	0.3778	0.3304	12.55%
900	0.1258	0.0542	56.92%	900	0.3619	0.3328	8.04%
1000	0.1218	0.0532	56.32%	1000	0.3717	0.3528	5.08%

Table 7: Test errors trained on 30 training data size across various sampling densities

(a) <i>Darcy Flow</i>				(b) <i>Eikonal</i>			
Density	GKN	Ours	Error Reduction	Density	GKN	Ours	Error Reduction
20	0.5574	0.4984	10.58%	20	0.1929	0.1402	27.32%
30	0.5203	0.4509	13.34%	30	0.1920	0.1313	31.61%
40	0.5028	0.4190	16.67%	40	0.1893	0.1200	36.61%
50	0.4881	0.3902	20.06%	50	0.1852	0.1174	36.61%
60	0.4667	0.3733	20.01%	60	0.1801	0.1162	35.48%
70	0.4576	0.3565	22.09%	70	0.1757	0.1138	35.23%
80	0.4568	0.3394	25.70%	80	0.1803	0.1115	38.16%
90	0.4513	0.3225	28.54%	90	0.1817	0.1088	40.12%
100	0.4404	0.3134	28.84%	100	0.1825	0.1047	42.63%
200	0.3651	0.2275	37.69%	200	0.1633	0.0981	39.93%
300	0.3168	0.1906	39.84%	300	0.1701	0.0921	45.86%
400	0.2938	0.1864	36.56%	400	0.1684	0.0908	46.08%
500	0.2810	0.1772	36.94%	500	0.1582	0.0901	43.05%
600	0.2702	0.1646	39.08%	600	0.1553	0.0776	50.03%
700	0.2618	0.1659	36.63%	700	0.1550	0.0764	50.71%
800	0.2524	0.1576	37.56%	800	0.1541	0.0756	50.94%
900	0.2454	0.1572	35.94%	900	0.1550	0.0736	52.52%
1000	0.2375	0.1554	34.57%	1000	0.1530	0.0762	50.20%
(c) <i>Nonlinear Diffusion</i>				(d) <i>Advection</i>			
Density	GKN	Ours	Error Reduction	Density	GKN	Ours	Error Reduction
20	0.2958	0.2365	20.05%	20	0.9881	0.4798	51.44%
30	0.2761	0.1878	31.98%	30	0.7924	0.4655	41.25%
40	0.2581	0.1647	36.19%	40	0.7468	0.4642	37.81%
50	0.2512	0.1523	39.37%	50	0.6657	0.4580	31.20%
60	0.2423	0.1408	41.89%	60	0.6622	0.4537	31.49%
70	0.2353	0.1369	41.82%	70	0.5756	0.4464	22.45%
80	0.2219	0.1295	41.64%	80	0.5646	0.4460	21.01%
90	0.2135	0.1279	40.09%	90	0.5889	0.4470	24.10%
100	0.2168	0.1234	43.08%	100	0.5708	0.4457	21.92%
200	0.1919	0.1024	46.64%	200	0.5242	0.4123	21.35%
300	0.1709	0.0873	48.92%	300	0.5841	0.4191	28.25%
400	0.1683	0.0815	51.57%	400	0.5157	0.4090	20.69%
500	0.1588	0.0773	51.32%	500	0.5915	0.4089	30.87%
600	0.1582	0.0709	55.18%	600	0.5344	0.4019	24.79%
700	0.1547	0.0685	55.72%	700	0.5387	0.4172	22.55%
800	0.1495	0.0703	52.98%	800	0.5527	0.4148	24.95%
900	0.1519	0.0683	55.04%	900	0.4994	0.4074	18.42%
1000	0.1520	0.0652	57.11%	1000	0.5353	0.3707	30.75%

A.3 TEST ERRORS ACROSS TRAINING DATA SIZE FOR DIFFERENT SAMPLE DENSITY

We choose sample density from 20 to 900, and for training data size from 5 to 100, we test on four PDE benchmarks as follows.

Table 8: Test sample density=900

Training data size	5	10	20	30	40	50	80	100
Darcy Flow	0.4996	0.2812	0.2215	0.1587	0.1503	0.1360	0.1230	0.1168
Advection	0.6921	0.6862	0.4866	0.4074	0.3560	0.3460	0.2601	0.2310
Eikonal	0.1540	0.1245	0.1059	0.0760	0.0718	0.0704	0.0694	0.0655
Nonlinear Diffusion	0.1589	0.1420	0.0740	0.0683	0.0595	0.0567	0.0474	0.0463

Table 9: *Test sample density=800*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.5102	0.2781	0.2303	0.1576	0.1572	0.1381	0.1243	0.1226
Advection	0.7407	0.7109	0.4799	0.4148	0.3789	0.3641	0.2791	0.2408
Eikonal	0.1606	0.1210	0.1038	0.0756	0.0731	0.0730	0.0697	0.0625
Nonlinear Diffusion	0.1623	0.1406	0.0728	0.0706	0.0701	0.0652	0.0501	0.0469

Table 10: *Test sample density=700*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.4985	0.2768	0.2332	0.1659	0.1592	0.1506	0.1301	0.1235
Advection	0.6978	0.6590	0.5594	0.4172	0.3747	0.3364	0.2926	0.2421
Eikonal	0.1605	0.1180	0.1038	0.0801	0.0755	0.0713	0.0643	0.0635
Nonlinear Diffusion	0.1642	0.1363	0.0731	0.0696	0.0623	0.0575	0.0548	0.0507

Table 11: *Test sample density=600*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.4817	0.2886	0.2362	0.1646	0.1616	0.1497	0.1401	0.1376
Advection	0.7537	0.7271	0.5754	0.4109	0.3661	0.3378	0.3216	0.2453
Eikonal	0.1483	0.1255	0.1073	0.0776	0.0772	0.0745	0.0691	0.0665
Nonlinear Diffusion	0.2149	0.1440	0.0781	0.0709	0.0644	0.0618	0.0583	0.0553

Table 12: *Test sample density=500*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.4855	0.2842	0.2247	0.1772	0.1643	0.1609	0.1414	0.1315
Advection	0.7947	0.7011	0.5431	0.4089	0.3609	0.3468	0.3299	0.2462
Eikonal	0.1537	0.1155	0.1060	0.0901	0.0811	0.0702	0.0689	0.0671
Nonlinear Diffusion	0.1686	0.1464	0.0801	0.0773	0.0760	0.0733	0.0626	0.0594

Table 13: *Test sample density=400*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.4970	0.3109	0.2471	0.1864	0.1804	0.1741	0.1481	0.1415
Advection	0.7604	0.6733	0.5317	0.4090	0.4005	0.3658	0.3499	0.2516
Eikonal	0.1547	0.1203	0.1058	0.0908	0.0883	0.0829	0.0725	0.0669
Nonlinear Diffusion	0.1695	0.1411	0.0847	0.0815	0.0776	0.0766	0.0637	0.0618

Table 14: *Test sample density=300*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.5075	0.3233	0.2416	0.1906	0.1880	0.1771	0.1592	0.1479
Advection	0.7606	0.6674	0.5323	0.4191	0.4178	0.3882	0.3505	0.2537
Eikonal	0.1533	0.1246	0.1066	0.0921	0.0835	0.0824	0.0709	0.0664
Nonlinear Diffusion	0.1722	0.1498	0.0920	0.0873	0.0849	0.0818	0.0694	0.0674

Table 15: *Test sample density=200*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.5227	0.3431	0.2812	0.2275	0.2222	0.2182	0.1880	0.1878
Advection	0.7586	0.6407	0.5004	0.4123	0.4040	0.3931	0.3697	0.2880
Eikonal	0.1538	0.1276	0.1069	0.0981	0.0934	0.0873	0.0780	0.0745
Nonlinear Diffusion	0.1807	0.1605	0.1060	0.1024	0.0951	0.0932	0.0804	0.0755

Table 16: *Test sample density=100*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.5534	0.4673	0.3986	0.3705	0.2994	0.2918	0.2471	0.2349
Advection	0.7513	0.6738	0.5498	0.4977	0.4547	0.4130	0.4069	0.3216
Eikonal	0.1583	0.1402	0.1115	0.1047	0.1044	0.0988	0.0876	0.0857
Nonlinear Diffusion	0.2062	0.1691	0.1332	0.1234	0.1161	0.1157	0.0995	0.0947

Table 17: *Test sample density=90*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.6094	0.4362	0.3638	0.3225	0.2791	0.2785	0.2471	0.2420
Advection	0.6764	0.6612	0.5334	0.4470	0.4452	0.4238	0.3977	0.3315
Eikonal	0.1612	0.1401	0.1140	0.1088	0.1084	0.1083	0.0893	0.0891
Nonlinear Diffusion	0.2036	0.1693	0.1329	0.1279	0.1179	0.1110	0.1046	0.0995

Table 18: *Test sample density=80*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.6076	0.4561	0.3709	0.3394	0.2994	0.2970	0.2633	0.2566
Advection	0.6579	0.6365	0.5318	0.4460	0.4450	0.4397	0.4049	0.3368
Eikonal	0.1561	0.1412	0.1170	0.1115	0.1113	0.1078	0.0937	0.0911
Nonlinear Diffusion	0.2086	0.1777	0.1401	0.1295	0.1225	0.1177	0.1116	0.1067

Table 19: *Test sample density=70*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.6176	0.4682	0.3965	0.3565	0.3176	0.3151	0.2773	0.2864
Advection	0.6697	0.6654	0.5524	0.4583	0.4479	0.4400	0.4156	0.3626
Eikonal	0.1606	0.1450	0.1154	0.1138	0.1128	0.1121	0.1005	0.0953
Nonlinear Diffusion	0.2279	0.1776	0.1498	0.1369	0.1294	0.1285	0.1223	0.1206

Table 20: *Test sample density=60*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.5989	0.4762	0.4251	0.3733	0.3308	0.2884	0.2842	0.2711
Advection	0.6906	0.6342	0.5541	0.4537	0.4270	0.4238	0.4131	0.3662
Eikonal	0.1637	0.1483	0.1192	0.1162	0.1058	0.1052	0.1015	0.1020
Nonlinear Diffusion	0.2211	0.1963	0.1580	0.1408	0.1318	0.1303	0.1286	0.1248

Table 21: *Test sample density=50*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.6595	0.4944	0.4445	0.3902	0.3546	0.3536	0.3158	0.3072
Advection	0.6784	0.6219	0.5618	0.4580	0.4412	0.4334	0.4069	0.3747
Eikonal	0.1576	0.1498	0.1191	0.1174	0.1111	0.1103	0.1038	0.0981
Nonlinear Diffusion	0.2458	0.2048	0.1661	0.1523	0.1439	0.1437	0.1382	0.1369

Table 22: *Test sample density=40*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.6693	0.5169	0.4674	0.4190	0.3840	0.3722	0.3339	0.3328
Advection	0.6966	0.6941	0.5189	0.4642	0.4625	0.4361	0.3901	0.3773
Eikonal	0.1712	0.1521	0.1255	0.1200	0.1172	0.1162	0.1038	0.1060
Nonlinear Diffusion	0.2720	0.2439	0.1755	0.1647	0.1563	0.1485	0.1500	0.1446

Table 23: *Test sample density=30*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.7064	0.5529	0.5131	0.4509	0.4114	0.4064	0.3697	0.3663
Advection	0.7536	0.6746	0.4973	0.4655	0.4256	0.4046	0.3996	0.3883
Eikonal	0.1822	0.1606	0.1377	0.1313	0.1232	0.1213	0.1140	0.1125
Nonlinear Diffusion	0.3148	0.2735	0.2003	0.1878	0.1867	0.1858	0.1812	0.1795

Table 24: *Test sample density=20*

<i>Training data size</i>	5	10	20	30	40	50	80	100
Darcy Flow	0.7416	0.5963	0.5363	0.4984	0.4567	0.4484	0.4176	0.4073
Advection	0.8587	0.7329	0.5114	0.4798	0.4661	0.4338	0.4186	0.3980
Eikonal	0.1875	0.1797	0.1543	0.1402	0.1392	0.1361	0.1292	0.1236
Nonlinear Diffusion	0.3202	0.3074	0.2403	0.2365	0.2297	0.2202	0.2000	0.1958

A.4 ERROR REDUCTIONS FOR TRAINING DATA SIZE=40

Table 25: *Sample density=100, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4122	0.2994	27.37%
Advection	0.4938	0.4547	7.92%
Eikonal	0.1668	0.1102	33.93%
Nonlinear Diffusion	0.1947	0.1161	40.37%
Poisson	0.3754	0.3707	1.25%

Table 26: *Sample density=200, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3281	0.2388	27.22%
Advection	0.4840	0.4420	8.68%
Eikonal	0.1429	0.1050	26.52%
Nonlinear Diffusion	0.1714	0.0951	44.52%

Table 27: *Sample density=300, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2746	0.2126	22.58%
Advection	0.4660	0.4178	10.34%
Eikonal	0.1390	0.0982	29.35%
Nonlinear Diffusion	0.1589	0.0849	46.57%

Table 28: *Sample density=400, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2446	0.1968	19.54%
Advection	0.4590	0.4005	12.75%
Eikonal	0.1396	0.0952	31.81%
Nonlinear Diffusion	0.1536	0.0776	49.48%

Table 29: *Sample density=500, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2505	0.1878	25.03%
Advection	0.4746	0.3609	23.96%
Eikonal	0.1355	0.0957	29.37%
Nonlinear Diffusion	0.1389	0.0760	45.28%

Table 30: *Sample density=600, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2416	0.1648	31.79%
Advection	0.4352	0.3661	15.88%
Eikonal	0.1323	0.0772	41.65%
Nonlinear Diffusion	0.1441	0.0739	48.72%

Table 31: *Sample density=700, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2257	0.1592	29.46%
Advection	0.4546	0.3747	17.58%
Eikonal	0.1294	0.0819	36.71%
Nonlinear Diffusion	0.1424	0.0731	48.67%

Table 32: *Sample density=800, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2120	0.1572	25.85%
Advection	0.4558	0.3789	16.87%
Eikonal	0.1304	0.0761	41.64%
Nonlinear Diffusion	0.1413	0.0701	50.39%

Table 33: *Sample density=900, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2068	0.1503	27.32%
Advection	0.4292	0.3560	17.05%
Eikonal	0.1306	0.0805	38.36%
Nonlinear Diffusion	0.1441	0.0691	52.05%

Table 34: *Sample density=1000, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2257	0.1592	29.46%
Advection	0.4546	0.3747	17.58%
Eikonal	0.1294	0.0819	36.71%
Nonlinear Diffusion	0.1424	0.0731	48.67%

Table 35: *Sample density=20, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5527	0.4567	17.37%
Advection	0.9735	0.5219	46.39%
Eikonal	0.1868	0.1451	22.32%
Nonlinear Diffusion	0.2892	0.2297	20.57%

Table 36: *Sample density=30, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5180	0.4114	20.58%
Advection	0.7502	0.4694	37.43%
Eikonal	0.1847	0.1354	26.69%
Nonlinear Diffusion	0.2638	0.1867	29.23%

Table 37: *Sample density=40, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5074	0.3840	24.32%
Advection	0.6341	0.4714	25.66%
Eikonal	0.1833	0.1234	32.68%
Nonlinear Diffusion	0.2464	0.1563	36.57%

Table 38: *Sample density=50, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4819	0.3546	26.42%
Advection	0.5321	0.4897	7.97%
Eikonal	0.1798	0.1194	33.59%
Nonlinear Diffusion	0.2417	0.1439	40.46%

Table 39: *Sample density=60, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4664	0.3308	29.07%
Advection	0.5688	0.4993	12.22%
Eikonal	0.1777	0.1181	33.54%
Nonlinear Diffusion	0.2349	0.1318	43.89%

Table 40: *Sample density=70, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4518	0.3176	29.70%
Advection	0.5410	0.4766	11.90%
Eikonal	0.1663	0.1147	31.03%
Nonlinear Diffusion	0.2195	0.1294	41.05%

Table 41: *Sample density=80, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4558	0.2994	34.31%
Advection	0.5175	0.4535	12.37%
Eikonal	0.1642	0.1132	31.06%
Nonlinear Diffusion	0.2127	0.1225	42.41%

Table 42: *Sample density=90, train data size=40*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4378	0.2791	36.25%
Advection	0.5039	0.4452	11.65%
Eikonal	0.1706	0.1122	34.23%
Nonlinear Diffusion	0.1996	0.1179	40.93%

A.5 ERROR REDUCTIONS FOR TRAINING DATA SIZE=20

Table 43: *Sample density=100, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4790	0.3986	16.78%
Advection	0.8125	0.5498	32.33%
Eikonal	0.1848	0.1115	39.66%
Nonlinear Diffusion	0.2284	0.1332	41.68%

Table 44: *Sample density=200, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3937	0.2812	28.58%
Advection	0.8552	0.5004	41.49%
Eikonal	0.1780	0.1069	39.94%
Nonlinear Diffusion	0.2056	0.1060	48.44%

Table 45: *Sample density=300, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3414	0.2416	29.23%
Advection	0.7282	0.5323	26.90%
Eikonal	0.1757	0.1066	39.33%
Nonlinear Diffusion	0.1923	0.0920	52.16%

Table 46: *Sample density=400, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3291	0.2471	24.92%
Advection	0.7667	0.5317	30.65%
Eikonal	0.1716	0.1058	38.34%
Nonlinear Diffusion	0.1831	0.0847	53.74%

Table 47: *Sample density=500, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3285	0.2247	31.60%
Advection	1.0101	0.5431	46.23%
Eikonal	0.1703	0.1060	37.76%
Nonlinear Diffusion	0.1783	0.0801	55.08%

Table 48: *Sample density=600, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3030	0.2362	22.05%
Advection	0.7948	0.5754	27.60%
Eikonal	0.1739	0.1073	38.30%
Nonlinear Diffusion	0.1780	0.0781	56.12%

Table 49: *Sample density=700, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3001	0.2332	22.29%
Advection	0.7928	0.5594	29.44%
Eikonal	0.1682	0.1038	38.29%
Nonlinear Diffusion	0.1755	0.0731	58.35%

Table 50: *Sample density=800, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2841	0.2303	18.94%
Advection	0.8037	0.4799	40.29%
Eikonal	0.1696	0.1038	38.80%
Nonlinear Diffusion	0.1749	0.0728	58.38%

Table 51: *Sample density=900, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2787	0.2215	20.52%
Advection	0.7267	0.4866	33.04%
Eikonal	0.1705	0.1059	37.89%
Nonlinear Diffusion	0.1755	0.0740	57.83%

Table 52: *Sample density=1000, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.2660	0.2297	13.65%
Advection	0.7421	0.5268	29.01%
Eikonal	0.1697	0.1059	37.60%
Nonlinear Diffusion	0.1716	0.0757	55.89%

Table 53: *Sample density=20, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5909	0.5363	9.24%
Advection	1.0704	0.5114	52.22%
Eikonal	0.1985	0.1543	22.27%
Nonlinear Diffusion	0.3053	0.2403	21.29%

Table 54: *Sample density=30, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5712	0.5131	10.17%
Advection	1.0391	0.4973	52.14%
Eikonal	0.1941	0.1377	29.06%
Nonlinear Diffusion	0.2804	0.2003	28.57%

Table 55: *Sample density=40, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5493	0.4674	14.91%
Advection	0.9612	0.5189	46.02%
Eikonal	0.1916	0.1255	34.50%
Nonlinear Diffusion	0.2655	0.1755	33.90%

Table 56: *Sample density=50, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5221	0.4445	14.86%
Advection	0.9652	0.5618	41.79%
Eikonal	0.1880	0.1191	36.65%
Nonlinear Diffusion	0.2525	0.1661	34.22%

Table 57: *Sample density=60, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5013	0.4251	15.20%
Advection	0.8556	0.5541	35.24%
Eikonal	0.1864	0.1192	36.05%
Nonlinear Diffusion	0.2459	0.1580	35.75%

Table 58: *Sample density=70, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4975	0.3965	20.30%
Advection	0.8128	0.5524	32.04%
Eikonal	0.1838	0.1154	37.21%
Nonlinear Diffusion	0.2420	0.1498	38.10%

Table 59: *Sample density=80, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4937	0.3709	24.87%
Advection	0.7770	0.5318	31.56%
Eikonal	0.1835	0.1170	36.24%
Nonlinear Diffusion	0.2387	0.1401	41.31%

Table 60: *Sample density=90, train data size=20*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4920	0.3638	26.06%
Advection	0.8157	0.5334	34.61%
Eikonal	0.1847	0.1140	38.28%
Nonlinear Diffusion	0.2313	0.1329	42.54%

A.6 ERROR REDUCTIONS FOR TRAINING DATA SIZE=10

Table 61: *Sample density=100, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5692	0.4673	17.90%
Advection	1.0858	0.6738	37.94%
Eikonal	0.2061	0.1402	31.98%
Nonlinear Diffusion	0.2531	0.1691	33.19%

Table 62: *Sample density=200, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4593	0.3431	25.30%
Advection	1.0516	0.6407	39.07%
Eikonal	0.2018	0.1276	36.77%
Nonlinear Diffusion	0.2500	0.1605	35.80%

Table 63: *Sample density=300, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.4014	0.3233	19.46%
Advection	0.9618	0.6674	30.61%
Eikonal	0.1955	0.1246	36.27%
Nonlinear Diffusion	0.2548	0.1498	41.21%

Table 64: *Sample density=400, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3750	0.3109	17.09%
Advection	1.0257	0.6733	34.36%
Eikonal	0.1913	0.1203	37.11%
Nonlinear Diffusion	0.2430	0.1411	41.93%

Table 65: *Sample density=500, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3764	0.2842	24.50%
Advection	0.9785	0.7011	28.35%
Eikonal	0.1905	0.1155	39.37%
Nonlinear Diffusion	0.2383	0.1464	38.56%

Table 66: *Sample density=600, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3645	0.2886	20.82%
Advection	1.0162	0.7271	28.45%
Eikonal	0.1929	0.1255	34.94%
Nonlinear Diffusion	0.2360	0.1440	38.98%

Table 67: *Sample density=700, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3522	0.2768	21.41%
Advection	0.9918	0.6590	33.56%
Eikonal	0.1929	0.1180	38.83%
Nonlinear Diffusion	0.2289	0.1363	40.45%

Table 68: *Sample density=800, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3400	0.2781	18.21%
Advection	1.0006	0.7109	28.95%
Eikonal	0.1909	0.1210	36.62%
Nonlinear Diffusion	0.2304	0.1406	38.98%

Table 69: *Sample density=900, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3356	0.2812	16.21%
Advection	1.0374	0.6862	33.85%
Eikonal	0.1913	0.1245	34.92%
Nonlinear Diffusion	0.2319	0.1420	38.77%

Table 70: *Sample density=1000, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.3345	0.2787	16.68%
Advection	1.0026	0.6668	33.49%
Eikonal	0.1956	0.1286	34.25%
Nonlinear Diffusion	0.2346	0.1204	48.68%

Table 71: *Sample density=20, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.6578	0.5963	9.35%
Advection	1.1149	0.7329	34.26%
Eikonal	0.2144	0.1797	16.18%
Nonlinear Diffusion	0.3280	0.3074	6.28%

Table 72: *Sample density=30, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.6580	0.5529	15.97%
Advection	1.1036	0.6746	38.87%
Eikonal	0.2073	0.1606	22.53%
Nonlinear Diffusion	0.3017	0.2735	9.35%

Table 73: *Sample density=40, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.6207	0.5169	16.72%
Advection	1.1147	0.6941	37.73%
Eikonal	0.2090	0.1521	27.22%
Nonlinear Diffusion	0.2920	0.2439	16.47%

Table 74: *Sample density=50, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5909	0.4944	16.33%
Advection	1.0714	0.6219	41.95%
Eikonal	0.2063	0.1498	27.39%
Nonlinear Diffusion	0.2788	0.2048	26.54%

Table 75: *Sample density=60, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5624	0.4762	15.33%
Advection	1.1333	0.6342	44.04%
Eikonal	0.2051	0.1483	27.69%
Nonlinear Diffusion	0.2751	0.1963	28.64%

Table 76: *Sample density=70, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5629	0.4682	16.82%
Advection	1.1024	0.6654	39.64%
Eikonal	0.2039	0.1450	28.89%
Nonlinear Diffusion	0.2609	0.1776	31.93%

Table 77: *Sample density=80, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5795	0.4561	21.29%
Advection	1.0573	0.6365	39.80%
Eikonal	0.2041	0.1412	30.82%
Nonlinear Diffusion	0.2600	0.1777	31.65%

Table 78: *Sample density=90, train data size=10*

<i>Dataset</i>	GKN	Ours	Error Reduction
Darcy Flow	0.5824	0.4362	25.10%
Advection	1.1247	0.6612	41.21%
Eikonal	0.2047	0.1401	31.56%
Nonlinear Diffusion	0.2597	0.1693	34.81%

A.7 GRAPH VISULIZATIONS

Some examples about graph visualizations for Advection and Darcy.

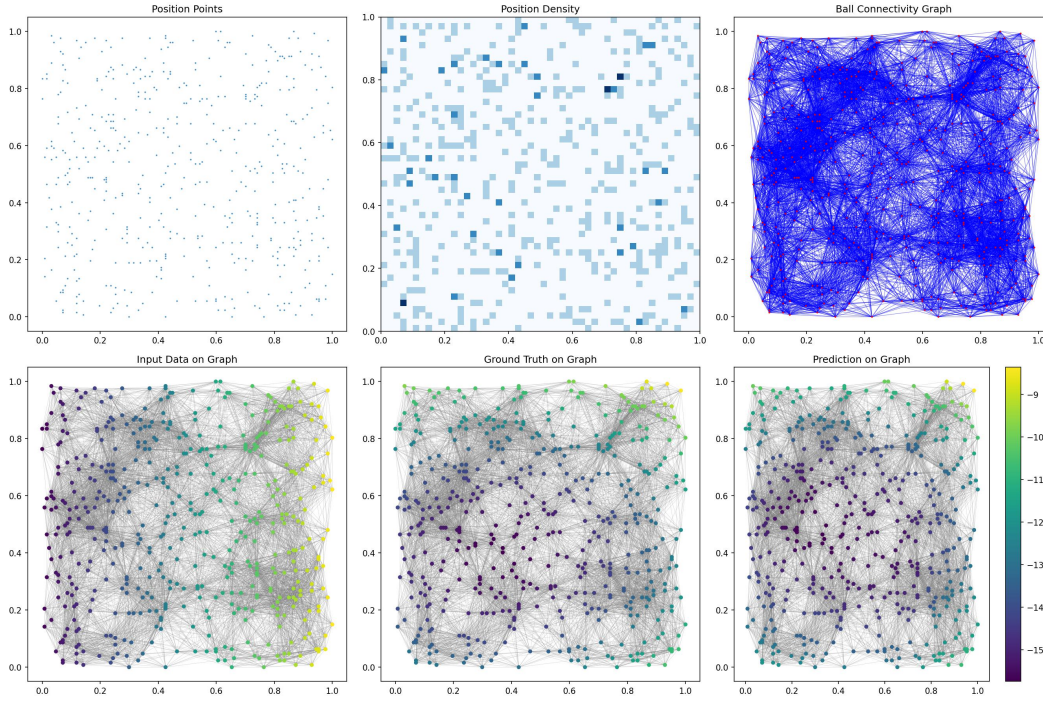


Figure 8: Graph Visualizations for Advection.

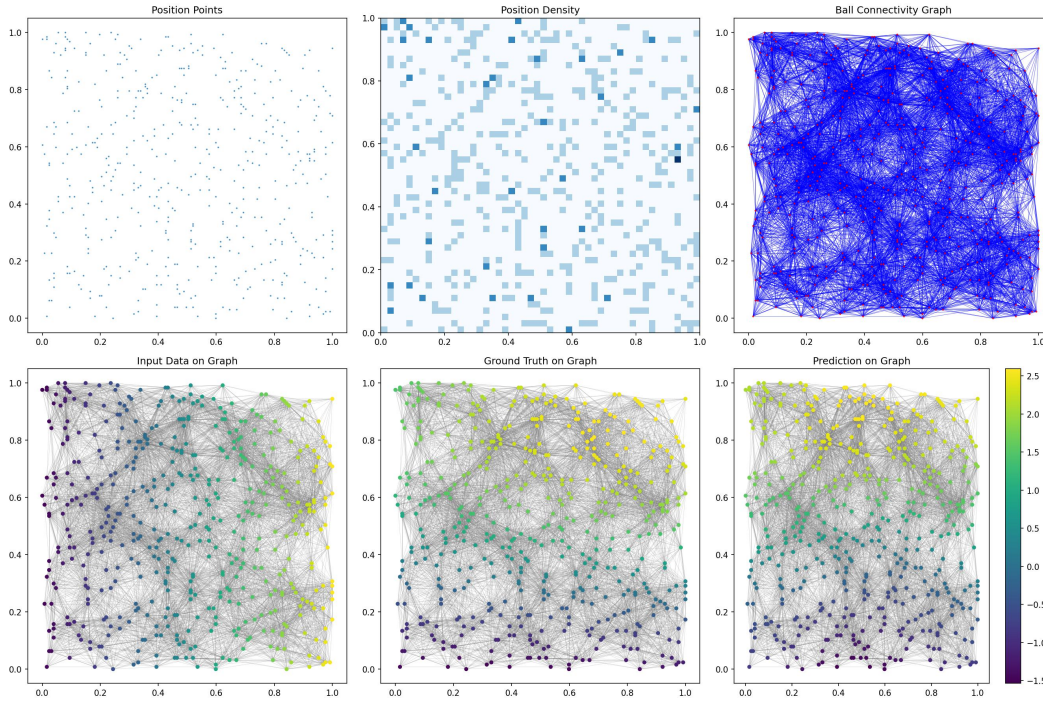


Figure 9: Graph Visualizations for Advection.

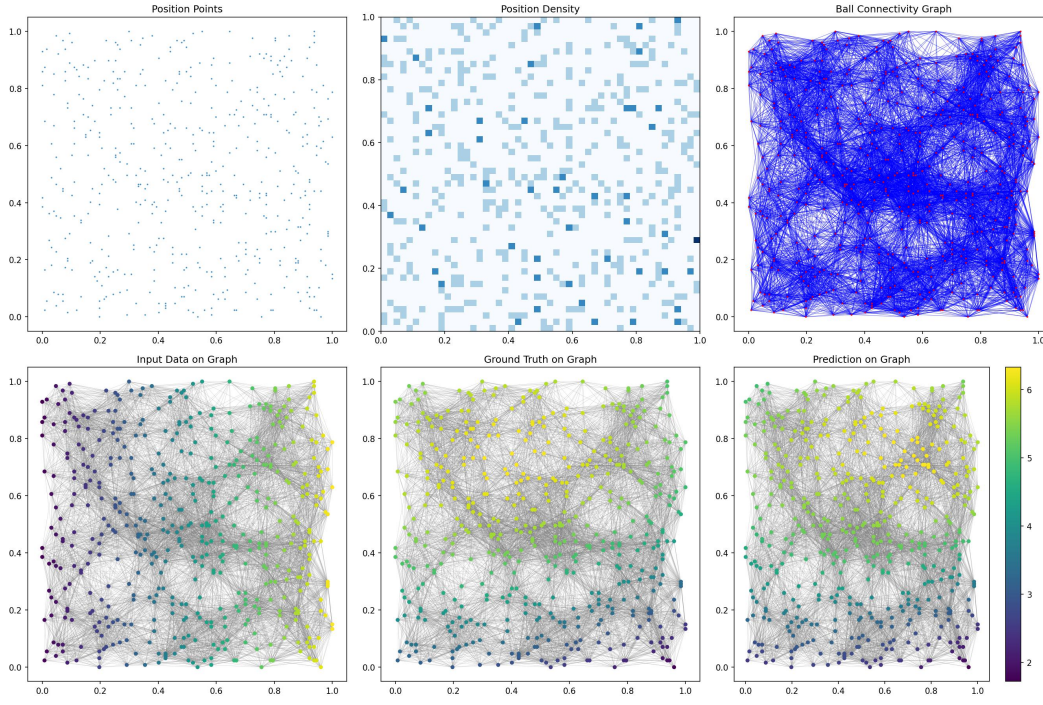


Figure 10: Graph Visualizations for Advection.

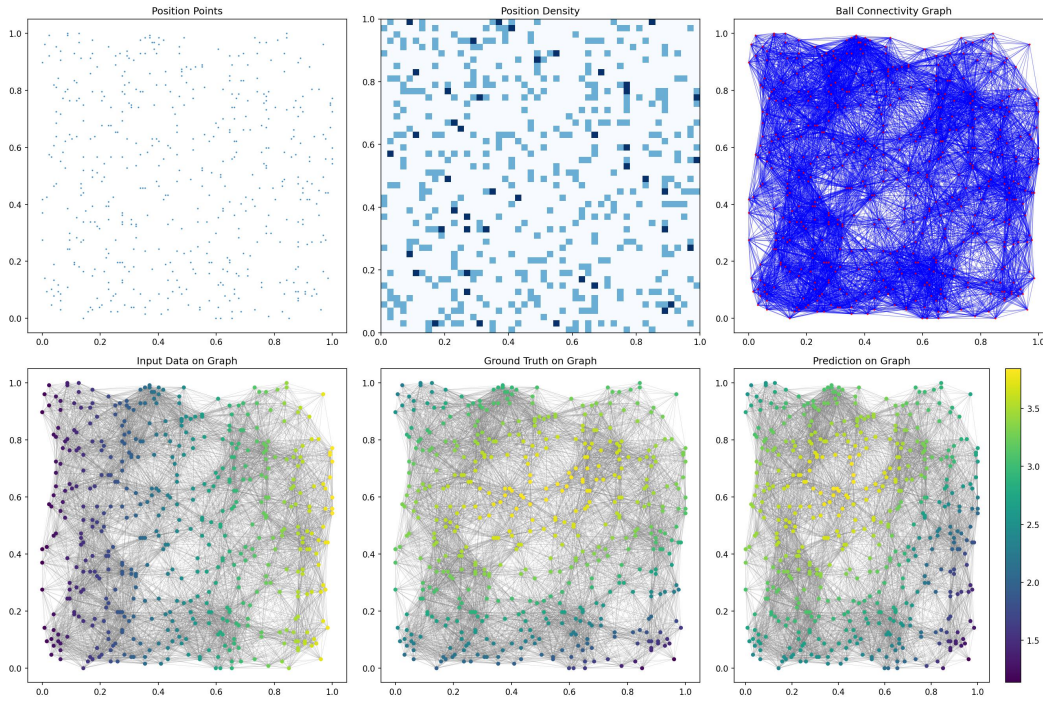


Figure 11: Graph Visualizations for Advection.

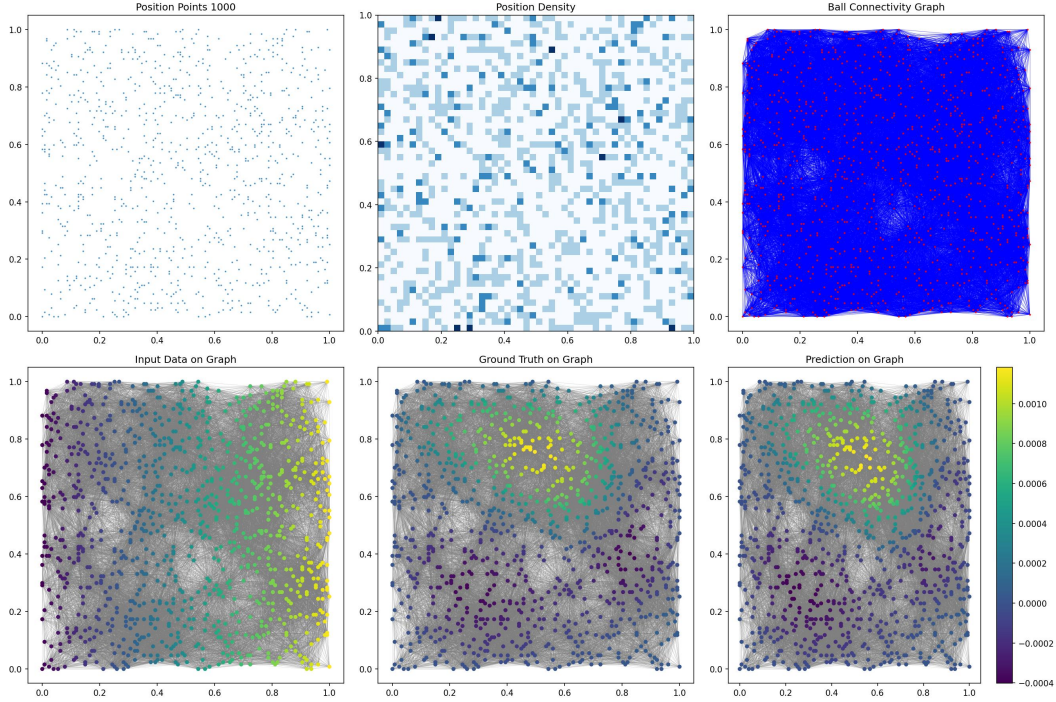


Figure 12: Graph Visualizations for Darcy.

B DATASETS DESCRIPTIONS

B.1 DARCY FLOW

We considered a steady-state 2D Darcy Flow equation (Li et al., 2020a),

$$\begin{aligned} -\nabla \cdot (a(x) \nabla u(x)) &= f(x) \quad x \in (0, 1)^2, \\ u(x) &= 0 \quad x \in \partial(0, 1)^2, \end{aligned} \quad (17)$$

where $u(x)$ is the velocity of the flow, $a(x)$ characterizes the conductivity of the media, and $f(x)$ is the source function that can represent flow sources or sinks within the domain. In the experiment, our goal is to predict the solution u given the external source f . To this end, we fixed the conductivity a , which is generated by first sampling a Gauss random field α in the domain and then applying a thresholding rule: $a(x) = 4$ if $\alpha(x) < 0$, otherwise $a(x) = 12$. We then used another Gauss random field to generate samples of f . We followed (Li et al., 2020a) to solve the PDE using a second-order finite difference solver and collected the source and solution at a 128×128 grid.

B.2 NONLINEAR DIFFUSION PDE

We next considered a nonlinear diffusion PDE,

$$\begin{aligned} \partial_t u(x, t) &= 10^{-2} \partial_{xx} u(x, t) + 10^{-2} u^2(x, t) + f(x, t), \\ u(-1, t) &= u(1, t) = 0, \quad u(x, 0) = 0, \end{aligned} \quad (18)$$

where $(x, t) \in [-1, 1] \times [0, 1]$. Our objective is to predict the solution function u given the source function f . We used the solver provided in (Lu et al., 2022), and discretized both the input and output functions at a 128×128 grid. The source f was sampled from a Gaussian process with an isotropic square exponential (SE) kernel for which the length scale was set to 0.2.

B.3 EIKONAL EQUATION

Third, we employed the Eikonal equation, widely used in geometric optics and wave modeling. It describes given a wave source, the propagation of wavefront across the given media where the wave

speed can vary at different locations. The equation is as follows,

$$|\nabla u(\mathbf{x})| = \frac{1}{f(\mathbf{x})}, \quad \mathbf{x} \in [0, 256] \times [0, 256], \quad (19)$$

where $u(\mathbf{x})$ is the travel time of the wavefront from the source to location $\mathbf{x}$, $|\cdot|$ denotes the Euclidean norm, and $f(\mathbf{x}) > 0$ is the speed of the wave at $\mathbf{x}$.

In the experiment, we set the wave source at $(0, 10)$. The goal is to predict the travel time u given the heterogeneous wave speed f . We sampled an instance of f using the expression:

$$f(\mathbf{x}) = \max(g(\mathbf{x}), 0) + 1.0,$$

where $g(\cdot)$ is sampled from a Gaussian process using the isotropic SE kernel with length-scale 0.1. We employed the `eikonal_fm` library (https://github.com/kevinganster/eikonal_fm/tree/master) that implements the Fast Marching method Sethian (1999) to compute the solution u .

B.4 POISSON EQUATION

Fourth, we considered a 2D Poisson Equation,

$$-\Delta u = f, \quad \text{in } \Omega = [0, 1]^2, \quad u|_{\partial D} = 0. \quad (20)$$

where Δ is the Laplace operator. The solution is designed to take the form, $u(x_1, x_2) = \frac{1}{\pi K^2} \sum_{i=1}^K \sum_{j=1}^K a_{ij} (i^2 + j^2)^r \sin(i\pi x_1) \cos(j\pi x_2)$, and $f(x_1, x_2)$ is correspondingly computed via the equation. To generate the dataset, we set $K = 5$ and $r = 0.5$, and independently sampled each element a_{ij} from a uniform distribution on $[0, 1]$.

B.5 ADVECTION EQUATION

Fifth, we considered a wave advection equation,

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = f, \quad x \in [0, 1], \quad t \in [0, 1]. \quad (21)$$

The solution is represented by a kernel regressor, $u(\mathbf{x}) = \sum_{j=1}^M w_j k(\mathbf{x}, \mathbf{z}_j)$, and the source f is computed via the equation. To collect instances of (f, u) , we used the square exponential (SE) kernel with length-scale 0.25. We randomly sampled the locations $\mathbf{z}_j$ from the domain and the weights w_j from a standard normal distribution.

C LLM USAGE

LLMs were used for grammar refinement and LaTeX formatting.