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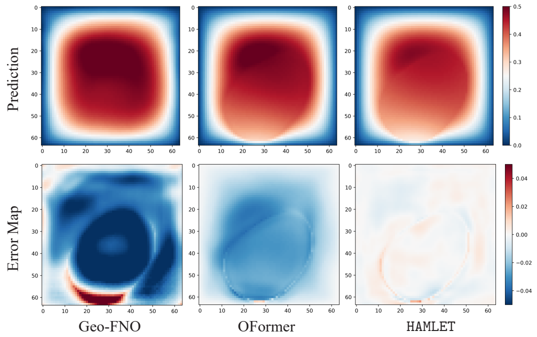

HAMLET

GrapH TrAnsforMer NeuraL OpEraTor for Partial Differential Equations

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Outline

- Section 1: Understanding the Significance of Partial Differential Equations
- Section 2: Limitations of Current Numerical Techniques
- Section 3: Introducing HAMLET: Graph Transformer Neural Operator for PDEs
- Section 4: Methodology and Experimental Results
- Section 5: Implications and Future Directions

Importance of Partial Differential Equations

Problems in science and engineering reduce to PDEs

Two main cases: Initial condition problems

Heat equation:

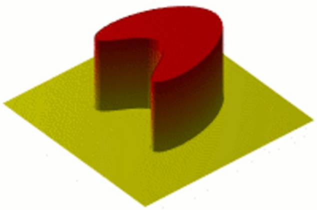
Spatial domain: $D = [0,1] \times [0,1]$

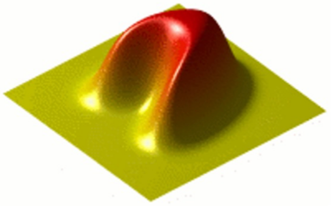
Time domain: $T = [0,1]$

Points: $\vec{x} = (x, y) = (x_1, x_2)$

Solution function (Temperature): $u: T \times D \rightarrow \mathbb{R}$

Equation: $u_t = \Delta u$





Initial value problem: given the temperature at time $t = 0$, What is the temperature a time $t = 1$?

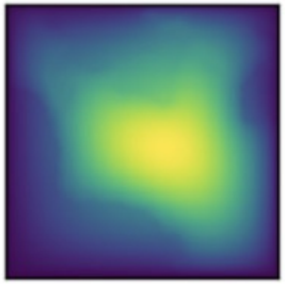
Given $u(0, x)$what is $u(1, x)$?

Two main cases: Boundary condition problems

For example a two dimensional elliptic PDE:

$$-\nabla \cdot \big(a(x)\nabla u(x)\big) = f(x), \qquad x \in D$$

Input: a(x)



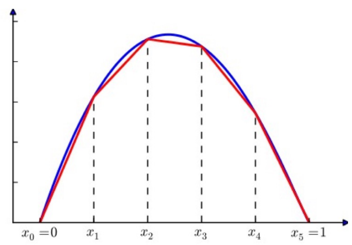
Output: u(x)

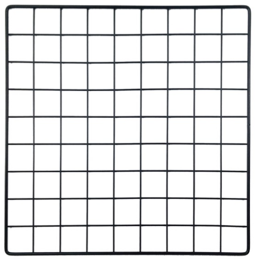
Given $a(x)$, what is $u(x)$?

Numerical Solver

Pipeline

1. Discretize the space
2. Write out a system
3. Solve the system





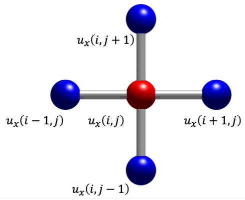
Commong numerical methods:

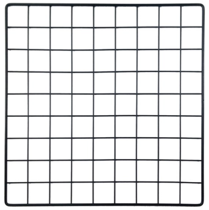
- Finite difference methods
- Finite element methods
- Spectral methods
- Iterative methods

$$u_x(x) = \lim_{dx \to 0} \frac{[u(x+dx) - u(x)]}{dx}$$

$$u_x(x) \sim \frac{[u(x+dx) - u(x)]}{dx}$$

$$u_x(i,j) \sim \frac{[u(i+1,j) - u(i,j)]}{dx}$$





Trade-off: finer grids are more accurate, but also more expensive

Role of Deep Learning in PDEs

- Physics informed neural networks (PINN)
  - Underlying differential equation as a loss-function
- Operator Learning
  - Fourier Neural Operator (FNO)
  - Physics Informed Neural Operator (PINO)
  - Graph Neural Operator (GNO)
  - FNO Transformer
- Encoder-Decoder Networks
- Graph Neural Networks

The Need for Innovative Solutions

Adapting to Varied Geometries:

- The demand for PDE solutions that can adapt to arbitrary geometries and diverse input formats has driven the search for innovative neural network architectures.

Addressing Computational Challenges:

- There is a growing need for models that can handle increasing data complexity and noise while maintaining computational efficiency.

Challenges in Current Numerical Approaches

Limited Generalizability:

- Existing techniques may struggle to generalize across multiple PDE instances and lack discretization invariance, impacting their adaptability to diverse scenarios.

Inability to Generalize Beyond Specific Resolutions:

- Current methods may face limitations in generalizing beyond specific resolutions and geometries observed during training, hindering their applicability to varied scenarios.

Formulation of the Problem

$$P : \mathcal{P} \times \mathcal{D} \times \mathcal{V} \times \mathbb{R}^m \times \ldots \times \mathbb{R}^m \to \mathbb{R}^\ell, \quad \mathcal{D} \subset \mathbb{R}^n, \mathcal{V} \subset \mathbb{R}^m, \mathcal{P} \subset \mathbb{R}^p$$

$$P\left(\theta, x, u, \partial_{x_1} u, \ldots \partial_{x_n} u, \ldots, \partial_{x_1}^{\alpha_1} \cdots \partial_{x_n}^{\alpha_n} u\right) = 0.$$

For most of the problems at least one of the conditions is fulfilled:

$$u(x) = u_0(x), \quad x \in \mathcal{D}_\theta \times \{T_0\}, \quad \mathcal{D}_\theta \subset \mathbb{R}^{n-1}$$

$$u(x) = u_b(x), \quad x \in \partial\mathcal{D}_\theta \times \mathcal{T}, \quad \mathcal{T} \subset \mathbb{R}_{\geq 0}$$

Formulation as operator learning:

$$\mathcal{S} : \mathcal{P} \times \mathcal{D} \times \mathbb{R}^m \times \ldots \times \mathbb{R}^m \times \mathbb{R}^\ell \times \mathbb{R}^\ell \to \mathcal{V}$$

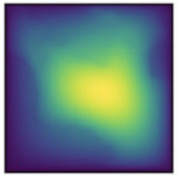
$$(\theta, x, \partial_{x_1} u, \ldots \partial_{x_n} u, \ldots, \partial_{x_1}^{\alpha_1} \cdots \partial_{x_n}^{\alpha_n} u, u_b, u_0) \mapsto u$$

Two examples from before

- Darcy flow PDE:

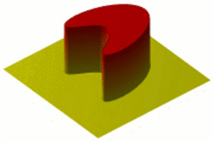
$$-\nabla \cdot \big(a(x)\nabla u(x)\big) = f(x) \qquad S : a \longmapsto u$$

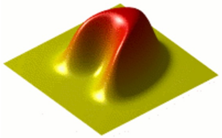

Input: a(x)


Output: u(x)

- Heat equation:

$$u_t = \Delta u \qquad S : u_0 \longmapsto u(t)$$





A discretization is needed

Addressing Limitations with Neural Operators

- Idea: We want to learn the solution operator directly from data
- Approximate the solution operator with a neural network -> Neural Operator
- The two main examples are the FNO (Fourier Neural Operator) and the GNO (Graph Neural Operator)

$\mathcal{S} : \mathcal{D} \to \mathcal{V}$

$\mathcal{D}_L$ be an L-point discretisation of $\mathcal{D}$.

$\tilde{\mathcal{S}}_\mu$ the approximate solution operator.

$$R_K\left(\mathcal{S}, \tilde{\mathcal{S}}_\mu, \mathcal{D}_L\right) = \sup_{\theta \in K} \left\| \hat{\mathcal{S}}\left(\mathcal{D}_L, \theta|_{\mathcal{D}}\right) - \mathcal{S}(\theta) \right\|_{\mathcal{V}}$$

$$\lim_{N \to \infty} R_K\left(\mathcal{S}(\cdot, \theta), \tilde{\mathcal{S}}^{(N)}(\cdot, \cdot, \theta), \mathcal{D}^{(N)}\right) = 0$$

Discretization invariance

Fourier Neural Operator

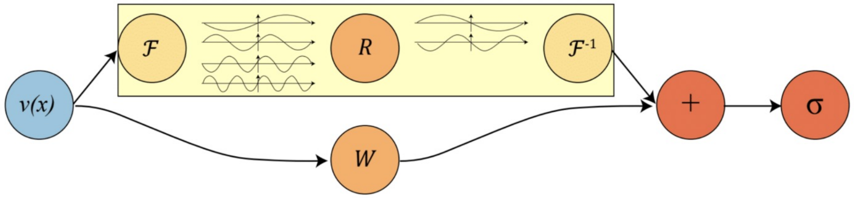


Figure 1 – layer of the Fourier neural operator

$$\tilde{\mathcal{S}}_\mu := \mathcal{Q} \circ (W_L + \mathcal{K}_L + b_L) \circ \cdots \circ \sigma (W_1 + \mathcal{K}_1 + b_1) \circ \mathcal{P}$$

Integral Kernel Operators

$$\mathcal{K}_l : \{\mathcal{D} \to \mathbb{R}^{d_l}\} \to \{\mathcal{U} \to \mathbb{R}^{d_{l+1}}\} \;:\; \mathcal{F}^{-1}\Big(R_\phi \cdot (\mathcal{F} v_t)\Big)(x) \qquad \forall x \in D$$

Depending on discretization and uniform grids

Graph Neural Operator [1]

$$v_{t+1}(x) = \sigma\left(W v_t(x) + \int_D \kappa_\phi(x, y, a(x), a(y)) v_t(y)\, \nu_x(dy)\right)$$

$$v_{t+1}(x) = W v_t(x) + \sum_{y \in N(x)} \kappa_\phi\big(e(x,y)\big) v_t(y)$$

[1] Li et al. [2020] https://arxiv.org/abs/2003.03485

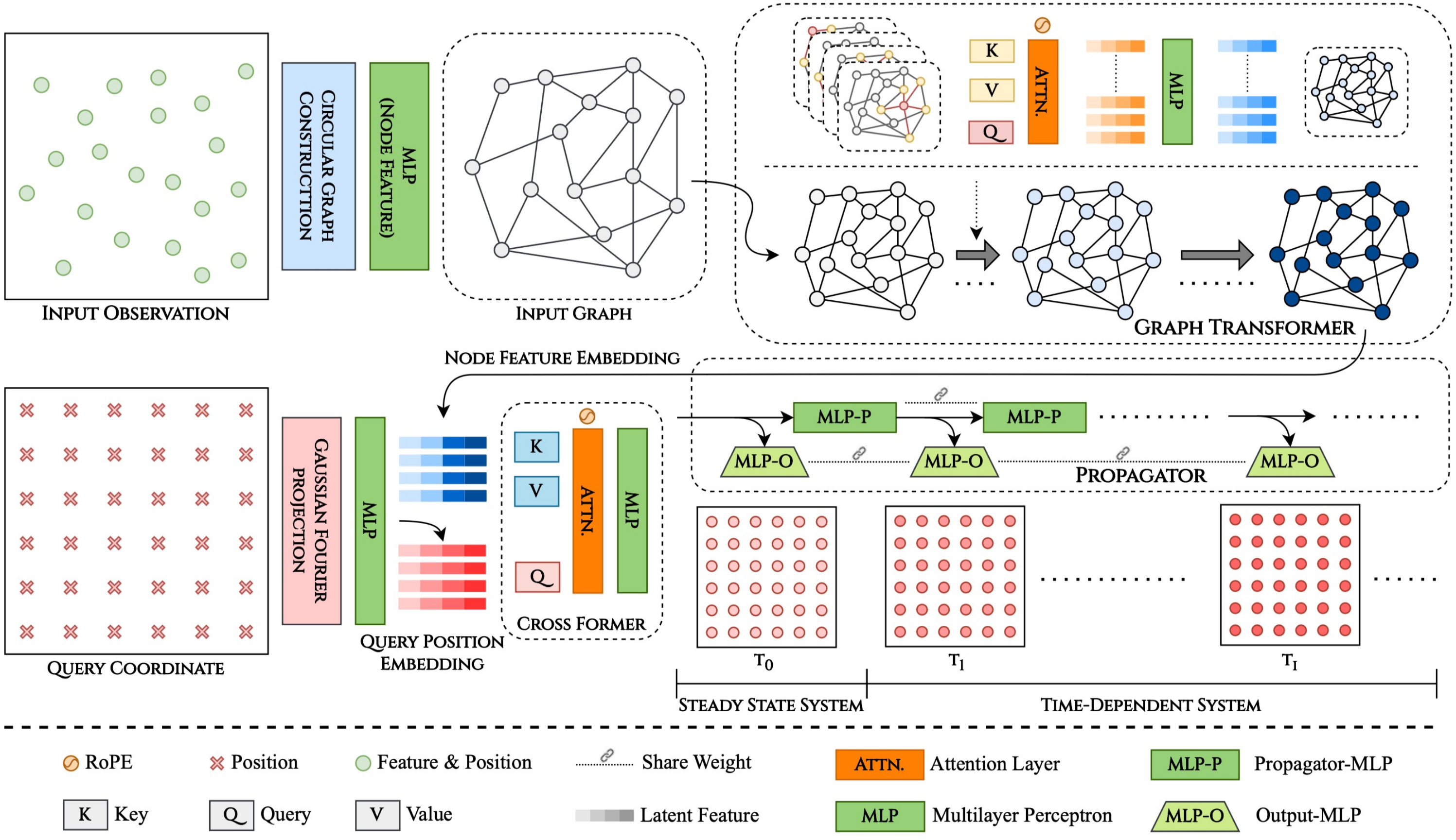
The Role of Graph Transformer Architectures

- Can we make a neural operator, which is adaptable to any grid realizations and can work with a multi-modality framework?
- Can we break down the efficiency of the neural operator and enhance the information in the data (data limitation)?
- Can we create a flexible approach with easy extendibility?
- A Graph Transformer indeed represents a neural operator

Outlook for the new architecture

- Include information for properties of the PDE directly in the architecture using multihead attention (with two output channels)
  - boundary conditions
  - Initial value conditions
- Use the flexibility and efficiency of graph transformer in the architecture
- Different graph structures are used to increase details resolutions
- Propagate the solution in the latent space and transform it afterwards into a graph structure

Introducing HAMLET



Results

Table 1. Numerical comparison of our approaches vs. existing techniques. The values reflect the nRMSE. The best-performing results are highlighted in green.

Dataset Setting		Normalised RMSE (nRMSE)							
Dataset	Param.	GNOT	U-Net	FNO	DeepONet	OFormer	GeoFNO	MAgNet	HAMLET
Darcy Flow	$\beta = 0.01$	–	1.10E+00	2.50E+00	3.25E-01	3.04E-01	1.03E+00	7.71E-02	**3.11E-01**
Darcy Flow	$\beta = 0.1$	–	1.80E-01	2.20E-01	1.67E-01	1.15E-01	3.13E-01	8.10E-02	**7.65E-02**
Darcy Flow	$\beta = 1.0$	–	3.30E-02	6.40E-02	5.12E-02	2.05E-02	6.34E-02	1.03E-01	**1.40E-02**
Darcy Flow	$\beta = 10.0$	–	8.20E-03	1.20E-02	3.97E-02	6.34E-03	2.51E-02	1.62E-01	**4.77E-03**
Darcy Flow	$\beta = 100.0$	–	4.40E-03	6.40E-03	3.64E-02	4.19E-03	2.04E-02	1.95E-01	**3.46E-03**
Shallow Water	–	4.16E-03	8.30E-02	4.40E-03	2.35E-03	2.90E-03	6.70E-03	–	**2.04E-03**
Diffusion Reaction	–	8.22E-01	8.40E-01	1.20E-01	8.42E-01	3.28E+00	7.72E+00	–	**9.02E-02**

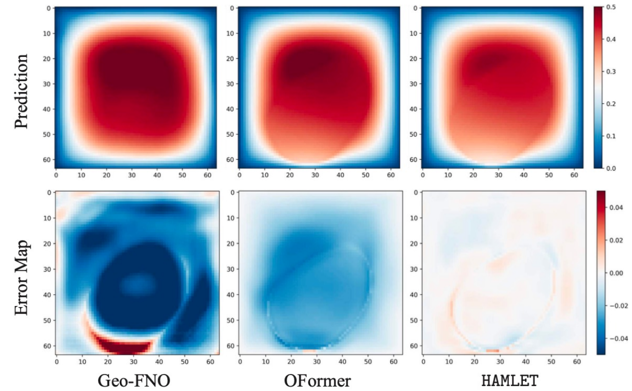
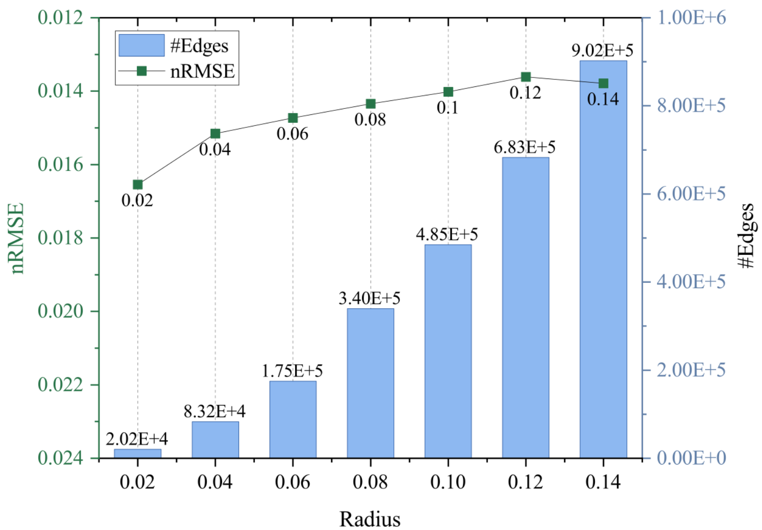


Figure 4. Predictions and corresponding error maps for Geo-FNO, OFormer, and HAMLET models using Darcy Flow ($\beta = 1.0$).

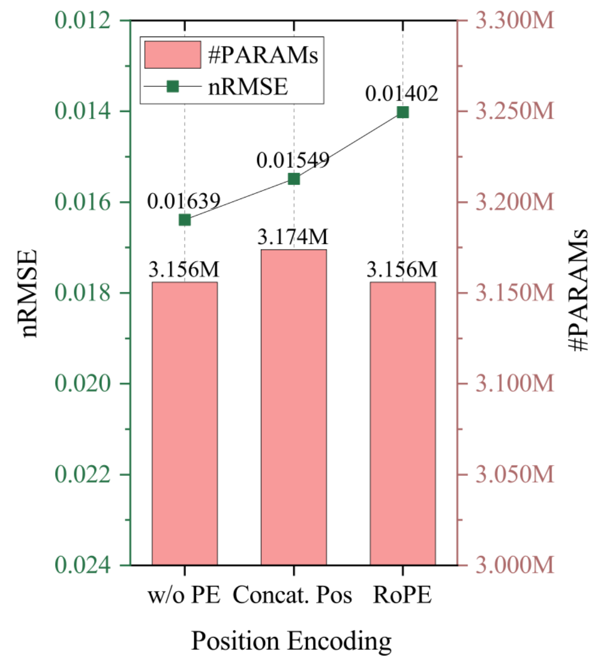
Scalability and Robustness



(A) Ablation Study
Radius for Circular Graph Construction

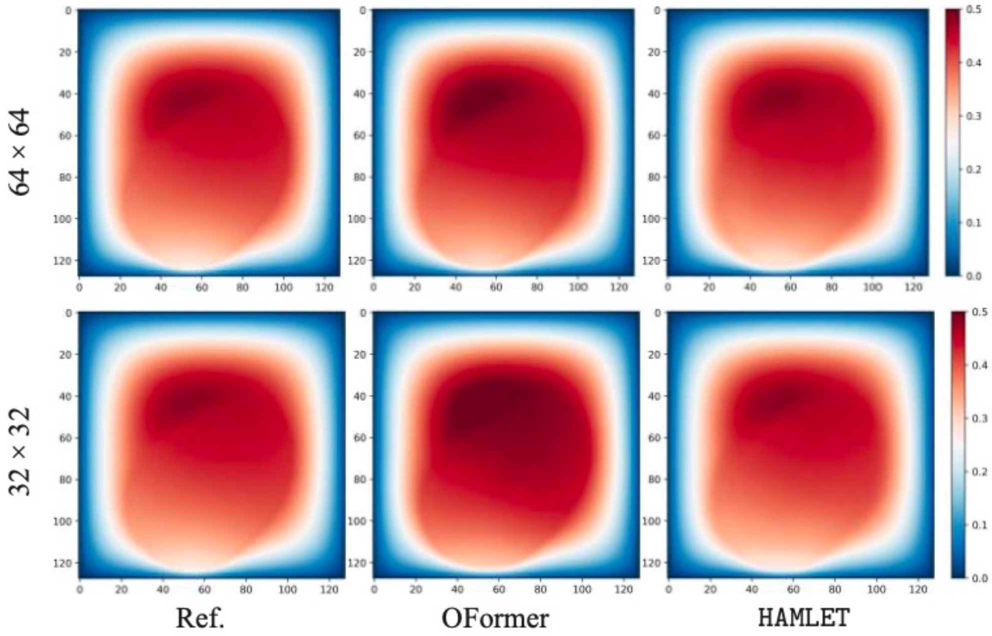
Table 2. Ablation studies for graph constructions on Darcy Flow 2D ($\beta = 1.0$) in 64×64 grid.

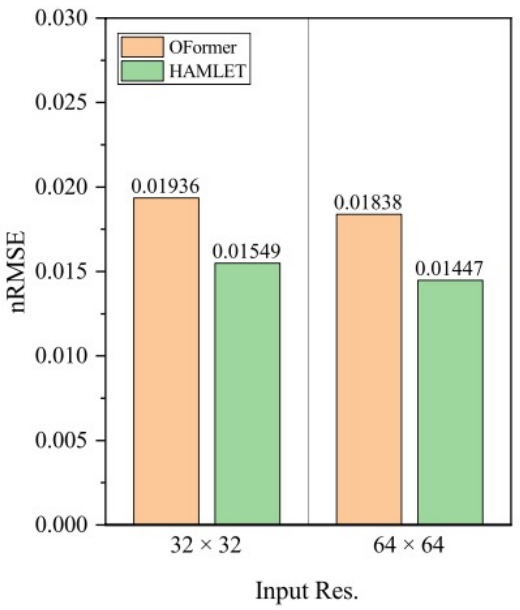
	KNN				Circular
	$k = 21$	$k = 51$	$k = 101$	$k = 151$	
nRMSE	0.02018	0.01996	0.02054	0.02094	**0.01402**



(B) Ablation Study
Position Encoding

Impact of Data Size on Model Performance





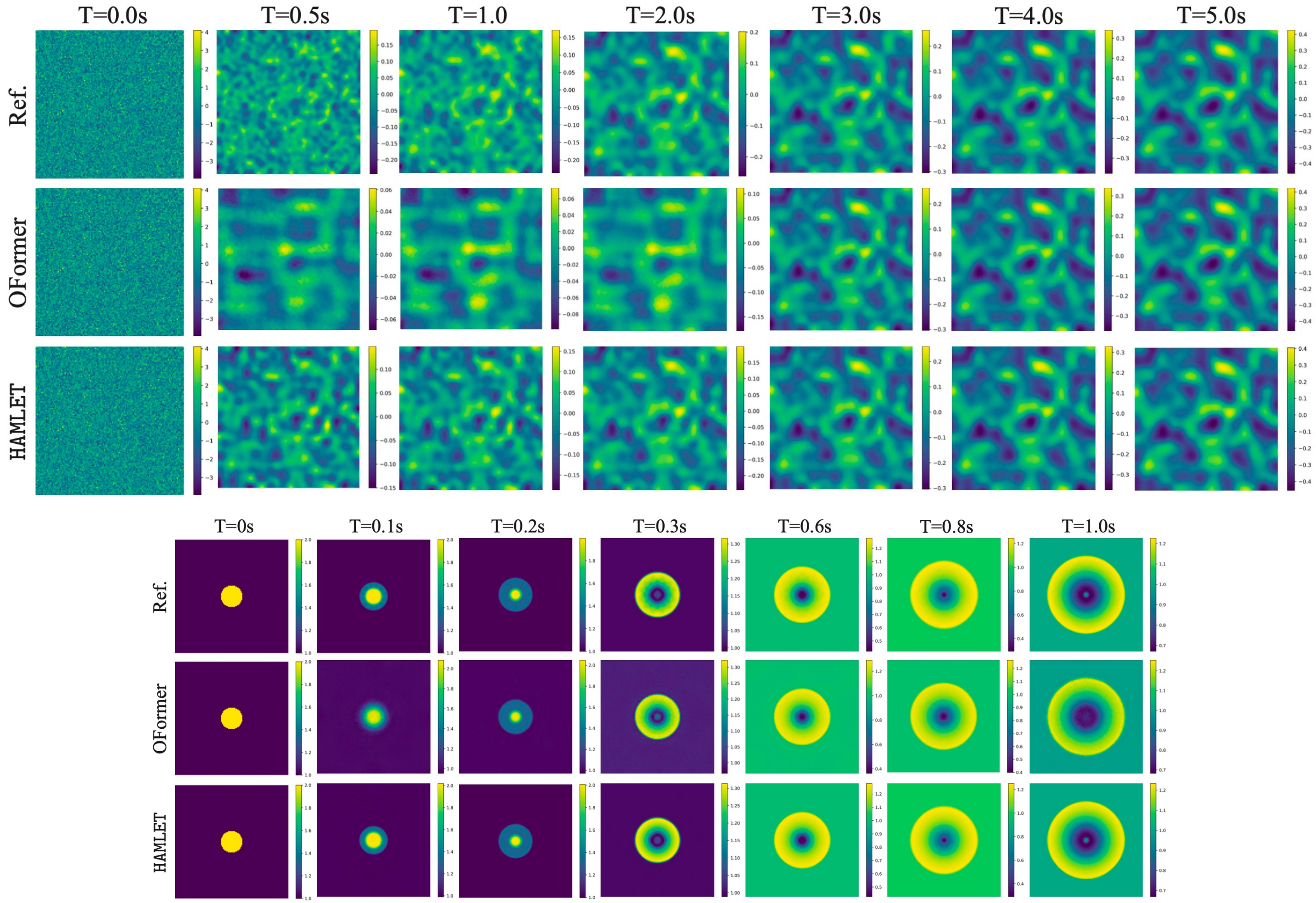
Darcy Flow (β = 1.0), nRMSE

#Training Data	9K	5K	2K	1K
OFormer	2.048E-02	2.093E-02	2.674E-02	3.321E-02
HAMLET	1.402E-02	1.642E-02	2.211E-02	2.779E-02

Shallow Water, nRMSE

#Training Data	900	500	200	100
OFormer	2.900E-03	1.190E-02	2.310E-02	2.910E-02
HAMLET	2.044E-03	2.320E-03	3.255E-03	4.746E-03

Evaluation Protocol in time dependent problems



Conclusion and Future Directions

- Offers a flexible and robust solution adaptable to various geometries and conditions. employs modular input encoders and establishes new benchmarks in scenarios with limited data availability.

Limitation:

- Graph construction time is a limitation, common in graph-based approaches. An increased number of parameters and lack of interpretability
- Not adaptable to every problem

Future Work:

- Integration of Lie-symmetry preservation and augmentation.
- Extension to handle higher-dimensional PDEs, including 3D problems.
- Dedicated exploration to refine the model architecture.
- Multiple parameter meshes and estimations

Call to Action

- Establish and promote the use of standardized benchmarks for evaluating neural operators of PDEs. Provide a common ground for comparison, ensuring consistent evaluation metrics.

- Rethink current evaluation methods to include a broader range of problem settings and conditions. Standardize the reporting of results to include crucial error analysis. Compare to existing methods like FEM, FDM, spectral methods…

- Encourage the publication and discussion of frameworks and approaches that did not succeed.

- Investigate the integration of physical laws and symmetries into neural operator frameworks. Explore hybrid models that combine traditional numerical methods with neural operators.

- Aim for the development of general-purpose neural operators capable of solving a wide variety of PDEs. Less parameter tuning and adaptability for datasets.

Thank you very much for your attention

References

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Li, Z., Meidani, K., and Farimani, A. B. Transformer for partial differential equations' operator learning. *Transactions on Machine Learning Research*, 2023.