Nuclear Fusion



Chip Design/Lithography



Weather and Climate



ensemble

Neural Operators: Machine Learning in Function Spaces

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Rise of Deep Learning

• Neural Networks such as CNN, AlexNet, LSTM, ResNet, UNet, EfficientNet, MobileNet, Transformer, ViT, Diffusion Models.

(shifted right

Compute + Domain Specific metrics

Hidder

laver '

Input

laver



Progress in CV + Language

Real world domain (Function) -> Data (Function)



Weather forecasting

However, we should view them as functions and not just time-series or pictures.

Fusion

Numerical Solvers

- Traditionally we model these phenomena using differential and algebraic equations. Examples include Darcy, Navier-Stokes, Helmotz etc.)
- Create numerical solvers to solve these equations at a certain discretization (resolution). For example: Finite difference, elements etc.

Finer discretization ➡ Converge to ground truth operator (more accurate solution)

$$\partial_t u(x,t) + u(x,t) \cdot
abla u(x,t) +
abla p(x,t) =
u(x,t) =
u(x,t) = 0, \ u(x,0) = u_0(x), \ i\hbarrac{\partial}{\partial t}\Psi(x,t) = \left[-rac{\hbar^2}{2m}rac{\partial^2}{\partial x^2} + V(x,t)
ight]\Psi(x,t)$$

Darcy Flow:
$$-\nabla (a(x)\nabla u(x)) = f(x)$$

Input: diffusion coefficients, a's



Limitations

Input function space

 $a \in \mathcal{A}$

0.....

Infinite dimension

- Generating good data is hard.
- Solvers are not differentiable; Not good for inverse problems
- Hard to incorporate domain knowledge into the solver
- Massive computation
- Discretization dependent

How about we learn the solution operator?

Given a, predict u

......

Output function space

 $u \in U$

what is $\mathcal{G}(a)$?

·····0

0

.....0



Moving on to learning Functions

- The classical development of neural networks has been primarily for mappings between a finitedimensional Euclidean space.
- However, many problems in physics and math involve learning the mapping between *function spaces*, which poses a limitation on the classical neural network-based methods.
- For a bold example, images should be considered as functions of light defined on a continuous region instead of as 32 x 32-pixel vectors.



One ML model for any discretization

Neural Network

Neural Operator

Input and output at fixed resolution

Input and output at any resolution



Discretization Agnostic Learning

Neural Operator (What are they?)

In mathematics, operators are usually referring to the mappings between function spaces. Consider a general differential equation represented as

Lu = f

where u and f are functions defined on the physical domain. Effectively, the task is akin to learning an operator, often seen as the inverse of L, capable of mapping the given function f back to the desired function u.

To deal with this problem, we propose operator learning. By encoding specific structures, we let the neural network learn the mapping of functions and generalize among different resolutions. As a result, we can first use a numerical method to generate some less-accurate, low-resolution data, but the learned solver can still give reasonable, high-resolution predictions. In some sense, both training and evaluation can be pain-free.





Discretization -Convergent

One ML model for any discretization

Mesh refinement

Definition: a trained AI model is discretization-convergent if

- We can query at any point.
- Converges upon mesh refinement to a limit.



Converging solution

Model	NNs	DeepONets	Interpolation	Neural Operators
Discretization Invariance	X	×	1	1
Is the output a function?	X	1	1	1
Can query the output at any point?	X	1	1	1
Can take the input at any point?	X	×	1	1
Universal Approximation	×	1	×	1





From Neural networks to Neural Operators

- Integral operator outputs functions (not just finite-dimensional vectors).
- Integral operator is discretization agnostic and discretization convergent.
- Neural Operators are universal approximator of operators.

Architectures



Graph Neural Operator (GNO)



Suppose we parameterize the kernel as a Neural Network.





Generalization of GNNs to neural operators

Fourier Neural Operator (FNO)

Again note that map $K: v_t \rightarrow v_{t+1}$ is parameterized as $v'(x) = \int k(x, y)v(y)dy + Wv(x)$ Where k is a kernel function and W is the bias term. Now if we restrict k(x, y) = k(x - y) then we get that our integral is indeed a convolution operator, which is a natural choice from the perspective of fundamental solutions. We can exploit the Fast Fourier Transform to do a convolution in Fourier space in quasilinear time.

The Fourier layer consists of three steps:

- 1. Fourier transform F
- 2. Linear transform on the lower Fourier modes $R K_{max}$
- 3. Inverse Fourier transform F^{-1}

FNO – Block + All Layers Filters in CNN Fourier Filters Filters in convolution neural networks are usually local. They are good to capture local patterns such as edges and shapes. Fourier filters are global sinusoidal functions. They are better for representing continuous functions.

Projection

Fourier laver

Target Dimension

Fourier lave

Note: When the input function is given on a regular grid

Other Architectures



Lots of variants of Neural Operators depending on how you parameterize the kernel.

PINO FNO-Transforme CoDA-NO UNO Differential FNO NO MNO IFNO SFNO UQO GNO-FNO GNO GINO Multipole GNO Diffusion NO Neural Operators Low Ranked NO Convolution NO DeepONets Multiwavele NO Generative Adversial NO Spectral NO Hyena Neura Operators PCANN

Zero shot super resolution

Train using coarse resolution data



Directly evaluate on higher resolution (no re-training)



Note: The data contains the effect of high-resolution components of the physics because the data is assumed from real world (very high resolution solver).

Universal Approximators of Operators





$$\|\hat{\mathcal{G}}_{\theta}(D_L, a|_{D_L}) - \mathcal{G}^{\dagger}(a)\|_{\mathcal{U}} \leq \underbrace{\|\hat{\mathcal{G}}_{\theta}(D_L, a|_{D_L}) - \mathcal{G}_{\theta}(a)\|_{\mathcal{U}}}_{\text{discretization error}} + \underbrace{\|\mathcal{G}_{\theta}(a) - \mathcal{G}^{\dagger}(a)\|_{\mathcal{U}}}_{\text{approximation error}}$$

Theorem (Universal approximation theorem of neural operators) :

Under a mild regularity condition, for any given arbitrary operator between general function spaces G^{\dagger} , and any $\epsilon > 0$, there exist a neural operator \mathcal{G}_{θ} , such that,

$$\sup_{a} \|\mathcal{G}^{\dagger}(a) - \mathcal{G}(a)\|_{\mathcal{U}} \le \epsilon.$$



Learning happens on discretized data

Big Impact Applications



Optimization difficulties in FNO

At the core of FNO is a spectral layer that leverages a discretization-convergent representation in the Fourier domain, which learns weights over a fixed set of frequencies. However, there are optimization difficulties in the training of FNO. However, training FNO presents two significant challenges, particularly in large-scale, high-resolution applications

- 1. Computing Fourier transform on *high-resolution inputs* is computationally intensive but necessary since fine-scale details are needed for solving many PDEs, such as fluid flows.
- 2. Selecting the *relevant set of frequencies* in the spectral layers is challenging, and too many modes can lead to overfitting, while too few can lead to underfitting.



Incremental FNO

Instead of fixing the frequency modes and data resolution, we propose iFNO that *progressively augments both frequency modes and training resolution.*

- Start from **minimal** frequency modes and **lowest** training resolution.
- When the optimization quality is **not improved**, increase both frequency modes and training resolution.
- Repeat the process multiple times until the network **converges**.

Why does it work?

- **iFNO follows spectral bias in deep neural networks** Spectral bias suggests that neural networks prioritize the learning of low-frequency components of the target function.
- iFNO adds explicit constraints over frequency modes and training resolution

Additional constraints further regularize the training of FNO.



Advantages:

- 1. **iFNO improves generalization performance** by regularizing frequency evolution and training resolution in particular a 10% lower testing and using 20% fewer frequency modes compared to the existing FNO.
- 2. **iFNO reduces training cost** as few frequency modes require less parameters, and low training resolution requires less dimensionality achieving a 30% faster performance, enabling larger scale simulations.



Figure 6: Number of frequency modes K in the converged FNO and iFNO models across datasets. We report K in the first Fourier convolution operator. NS denotes Navier-Stokes equations.

Moving towards a foundational model

Existing neural operator architectures face challenges when solving Multiphysics problems with coupled PDEs, due to complex geometries, interactions between physical variables, and the lack of large amounts of high-resolution training data.

- The architecture *should not be restricted to a fixed number of physical variables,* allowing it to handle PDEs with varying numbers of variables.
- It should be able to learn and predict different PDE systems, even when the number of physical variables differs between the training and target systems.
- When the training and target PDE systems have *overlapping physical variables*, the architecture should allow for transfer of learned knowledge between the systems.



Few Shot Supervised Finetuning

Codomain Attention Neural Operator -Architecture

- **1.** Permutation Equivariant Neural Operator: This allows CoDA-NO to process vector-valued input functions $a = [a_1, a_2, ..., a_d]$, where each a_i represents a different physical variable like velocity, pressure etc. It applies the same integral or pointwise operator to each component a_i sharing weights across variables.
- 2. CoDA-NO Layer: This is the core innovation. It extends the self-attention mechanism from standard transformers to operate on functions instead of finite-dimensional vectors. Specifically, for an input vector-valued function $w = [w_1, w_2, ..., w_d]$:
 - 1. It tokenizes w along the codomain/channel dimension into separate **token functions** w_i treating each physical variable w_i as a token.
 - 2. For each w_i , it computes query q_i , key k_i , and value v_i functions using learnable operators Q, K, V.
 - 3. It computes weighted sums of the value functions v_i , using weights from dot products between q_i and k_i in function space.
 - 4. This gives output token functions o_i for each variable.
 - 5. Finally, it concatenates these o_i back into the output vector-valued function o.

CoDA-NO Architecture (Cont'd)

- **1.** Variable Specific Positional Encoding (VSPE): It learns positional encodings e_j for each input variable a_j , concatenating e_j with a_j to obtain extended input functions. Then we just applied a shared point wise lifting operator to all of these extended input functions.
- 2. Function Space Normalization: It extends normalization layers like BatchNorm to operate on functions instead of vectors.

Lastly, to effectively handle non-uniform complex geometries, we follow the GINO architecture where a GNO is used as an encoding and decoding module. We note that all of the integral operators are FNO. Finally, by tokenizing along the codomain and applying self-attention there, CoDA-NO can explicitly model interactions between different physical variables of multiphysics PDEs within a single model.



Figure 3: Visualization of horizontal velocity u_x at t and $t + \delta t$ time step.

CoDA-NO – Diagram



Figure 2. On the left, we illustrate the architecture of the Codomain Attention Neural Operator. Each physical variable (or co-domain) of the input function is concatenated with variable specific positional encoding (VSPE). Each variable, along with the VSPE, is passed through a GNO layer, which maps from the given non-uniform geometry to a latent regular grid. Then, the output on a uniform grid is passed through a series of CoDA-NO layers. Lastly, the output of the stacked CoDA-NO layers is mapped onto the domain of the output geometry for each query point using another GNO layer. On the **right**, we illustrate the mechanism of codomain attention. At each CoDA-NO layer, the input function is tokenized codomain-wise, and each token function is passed through the \mathcal{K} , \mathcal{Q} , and \mathcal{V} operators to get key, query, and value functions $\{k^1, k^2\}, \{q^1, q^2\}, \text{ and } \{v^1, v^2\}$ respectively. The output function is calculated via an extension of the self-attention mechanism to the function space.

Codomain Attention Neural Operator (Training)

Self-supervised Pretraining:

- The objective is to train the model to reconstruct the original input function from its masked version.
- The input function is masked by setting values of a percentage of mesh points to zero for some variables, or by completely masking certain variables.
- The model's encoding component acts as the Encoder, while the decoding component is the Reconstructor during this phase

Supervised Fine-tuning:

- The Reconstructor from the pretraining phase is replaced by a randomly initialized Predictor module in the decoding component.
- The parameters of the Encoder and variable-specific positional encodings (VSPEs) are initialized from the pretrained weights.
- If the fine-tuning (target) PDE introduces new variables not present during pretraining, additional VSPEs are trained for these new variables to adapt to the expanded set of variables.



Figure 3. Test time adaptation to new physical variables. The model is pre-trained on the Navier-Stokes equation dataset, which comprises physical variables such as velocities u_x , u_y , and pressure p. To adapt this pre-trained model on a fluid-solid interaction dataset containing an additional Elastic wave equation with new displacement variables d_x and d_y , it is only necessary to add two additional VSPEs to the whole pipeline.

Datasets

- PDEBench features a much wider range of PDEs than existing benchmarks. Datasets employed in our study encompass diverse PDE types and parameters like Navier-Stokes equations, diffusion-reaction equations, and shallow-water equations.
- 2. Fluid Dynamics Problem (NS): Governed by the Navier-Stokes equation
 - Involves a Newtonian, incompressible fluid impinging on a rigid cylinder with an attached rigid strap. The physical variables are the fluid velocity (u) and pressure (p)
- **3.** Fluid-Structure Interaction Problem (NS+EW): Coupled system governed by both the Navier-Stokes equation for fluid and the Elastic wave equation for the solid
 - 1. Involves a Newtonian, incompressible fluid interacting with an elastic, compressible solid object (cylinder with an attached deformable elastic strap). The physical variables are the fluid velocity (u), pressure (p), and the solid displacement field (d).



•Model: CoDA-NO outperforms all baselines •Pre-training:

•NS+EW pre-training performs best overall
•NS pre-training also effective, especially for fluid dynamics (NS) tasks

•Few-shot learning:

CoDA-NO shows significant improvement with dimited data (5-25 samples)
Performance gap narrows but remains as

sample size increases to 100

•Viscosity/Reynolds number:

•Consistent performance across Re = 400 and Re = 4000

•Adapts well to more turbulent flows (Re = 4000)

Task generalization:

•Effectively transfers from fluid dynamics (NS) to fluid-structure interaction (NS+EW)

Table 1: Test L_2 loss for fluid dynamics (NS) and fluid-solid interaction (NS+EW) datasets with viscosity Re = 400 and Re = 4000 for different numbers of few-shot training samples.

		Re = 400					Re = 4000			
Model	Pretrain		# Few Shot Training Sample					les		
	Dataset		5		25		100		25	100
			Evaluation Dataset							
		NS	NS+EW	NS	NS+EW	NS	NS+EW	NS+EW	NS+EW	NS+EW
GINO	-	0.200	0.122	0.047	0.053	0.022	0.043	0.717	0.292	0.136
DeepO	-	0.686	0.482	0.259	0.198	0.107	0.107	0.889	0.545	0.259
GNN	-	0.038	0.045	0.008	0.009	0.008	0.009	0.374	0.310	0.132
ViT	-	0.271	0.211	0.061	0.113	0.017	0.021	0.878	0.409	0.164
U-Net	-	13.33	3.579	0.565	0.842	0.141	0.203	3.256	0.563	0.292
	-	0.182	0.051	0.008	0.084	0.006	0.004	0.326	0.264	0.070
Ours	NS	0.025	0.071	0.007	0.008	0.004	0.005	0.366	0.161	0.079
	NS+EW	0.024	0.040	0.006	0.005	<u>0.005</u>	0.003	0.308	0.143	0.069

•Full CoDA-NO:

Best performance across all scenarios
Especially effective with few-shot learning (5-25 samples)

•Impact of Components:

•CoDA-NO without VSPE & Norm: Significant performance drop

•Adding CoDA-NO alone: Major improvement, especially for NS+EW

•VSPE: Critical for model convergence with limited data -

•Normalization: Essential for effective training

•Pre-training Effects:

•NS+EW pre-training: Best overall performance

•NS pre-training: Effective, especially for NS tasks

•Generalization:

•Full CoDA-NO shows best adaptation from NS to NS+EW tasks

•Key Takeaway: All components (CoDA-NO, VSPE, Normalization) are crucial for optimal performance and generalization

CoDA-NO VSPE		PE Norm	Pretrain Dataset	# Few Shot Training Samples					
					5		25		100
			Dutaset	NS	NS+EW	NS	NS+EW	NS	NS+EW
×	×	×	×	0.271	0.211	0.061	0.113	0.017	0.020
\checkmark	×	×	×	0.182	0.051	0.008	0.084	0.006	0.004
\checkmark	×	\checkmark	NS	0.049	0.079	0.009	0.0132	0.004	0.009
\checkmark	×	\checkmark	NS EW	0.045	0.057	0.010	0.011	0.008	0.004
\checkmark	\checkmark	×	NS	*	*	0.023	*	0.008	0.006
\checkmark	\checkmark	×	NS EW	0.057	0.232	0.012	0.052	0.006	0.006
\checkmark	\checkmark	\checkmark	NS	0.025	0.071	0.007	0.008	0.004	0.005
\checkmark	\checkmark	\checkmark	NS EW	0.024	0.040	0.006	0.005	0.005	0.003

Zero-Shot Super Resolution Performance

•Task: Fluid-Solid (NS-EW) Interaction Problem

•Setting: Trained on 1317 mesh points, tested on 2193 points Key Findings:

1.CoDA-NO outperforms all baselines significantly

2.Pre-training improves performance:

1. NS pre-training slightly better than NS-ES pre-training 3.Performance across viscosities (μ):

1. Best: $\mu = 5$

- 2. Good: $\mu = 10$
- 3. Challenging: $\mu = 1$

4.Baseline comparisons:

- 1. ViT performs best among baselines
- 2. U-Net and DeepO struggle most with this task

Conclusion: CoDA-NO demonstrates superior generalization to higher resolution meshes without specific training.

Model	Pretrain	Fluid Viscocities			
model	Dataset	$\mu = 5$	$\mu = 1$	$\mu = 10$	
U-Net	-	0.144	0.267	0.216	
Vit	-	0.052	0.175	0.046	
GINO	-	0.069	0.103	0.0711	
DeepO	-	0.113	0.107	0.357	
GNN	-	0.223	0.211	0.247	
CoDA-NO	NS-ES	0.041	0.063	0.048	
CoDA-NO	NS	0.032	0.049	0.035	

•Single-Physics PDEs:

•Shallow Water Equations (SWE):

•CoDA-NO: 0.04072 (12% improvement over FNO) •Diffusion Equation (DIFF):

•CoDA-NO: 0.00810 (43% improvement over FNO)

•Multi-Physics Dataset (NS+DIFF+SWE): •CoDA-NO: 0.00302 (slightly higher than FNO's 0.00118)

•Reconstruction Error:

•CoDA-NO consistently lower than FNO across all datasets

•Model Size Comparison:

•CoDA-NO: 11 million parameters

•FNO: 1.9 billion parameters (98% larger)

•Performance vs. DPOT:

•Comparable performance to DPOT on DIFF dataset

•CoDA-NO: 0.0081 vs. DPOT-L-500: 0.0073

•Achieved with significantly fewer parameters and training epochs

Model	Dataset	Test Error				
Model	Dutuber	Prediction Error	Reconstruction Error			
CoDA-NO FNO	SWE	0.04072 0.04631	0.00460 0.03262			
CoDA-NO FNO	DIFF	0.00810 0.01415	0.00041 0.01894			
CoDA-NO FNO	NS+DIFF+SWE	0.00302 0.00118	0.00006 0.00287			

Model	Model Parameters
CoDA-NO	11M
FNO	1.9B
DPOT-FT-T	7M
DPOT-FT-S	30M
DPOT-FT-M	100M
DPOT-FT-L	500M

Overall picture

- 1. Superior Performance: Outperforms baselines in few-shot learning and zeroshot super-resolution tasks
- **2.** Adaptability: Seamlessly handles varying numbers of physical variables and complex geometries
- **3. Generalization:** Effectively transfers knowledge between single and multiphysics problems
- **4. Robustness:** Maintains performance across various Reynolds numbers, including turbulent flows

CoDA-NO demonstrates potential as a versatile foundation model for solving diverse multiphysics PDEs, opening new avenues for efficient scientific computing.

Some open problems in Neural Operator

- Scaling up is a big challenge
- The resolution in the intermediate layers is designer choice, how it should be done?
- Neural Operator architectures are still primitive.
- What can these architectures bring to CV?
- Uncertainty Quantification is essential, but how can it be done in function spaces?
- Reinforcement learning and control + Neural Operators = How can it be done?
- Unsupervised learning representation learning in function spaces?
- What about meta learning, adversarial robustness, transfer learning etc?

Takeaway: Lots to discover in this field.

Collaboration

Be aware of challenges:

- Often domain experts are pessimistic about ML
- Initial ML methods are often not as good as the existing paradigms
- Domain experts don't know much ML as MLists don't know much about other fields.
- Needs joint development and language bridge.
- The data is not generated having ML in mind





Codebase



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Neural Operator is an open-source library with a permissive license for scientific ML. It provides a unified API for different neural architectures for operator learning. Our mission is to democratize state-of-the-art algorithms like yours through a unified codebase.



In particular, we have added a Physics-based Informed Neural Operator (PINO) as an extension of PINNs that overcomes the critical limitations by incorporating both data and physics losses at varying resolutions. This allows for better generalization and extrapolation to resolutions beyond the training data and is much more suitable for multi-scale dynamic PDE systems.



The New codebase for all Neural Operators are present here: <u>neuraloperator/neuraloperator: Learning in infinite</u> <u>dimension with neural operators</u>

Must watch Resources

- <u>https://youtu.be/_j7bceE9AyA</u> ICML 2024 Tutorial"Machine Learning on Function spaces By Kamyar Azizzadensheli
- <u>https://youtu.be/6bl5XZ8kOzl</u> AI That Connects the Digital and Physical Worlds | Anima Anandkumar | TED
- <u>https://youtu.be/PpTkY8lgV3c</u> **Tutorial on Neural Operators by Zongyi Li**
- <u>https://youtu.be/y5EJr4ofGOc</u> ML for Solving PDEs: Neural Operators on Function Spaces by Anima Anandkumar
- <u>ETH Zürich DLSC: Course Introduction YouTube</u> Playlist by ETH on scientific computing
- <u>https://youtu.be/W8PybqAk6lk</u> Fourier Neural Operator (FNO) [Physics Informed Machine Learning] by Steve Brunton

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Conclusion

Al for science Ai of Science Ai + Science

Two Nobel Prizes this year:)

Any Questions?

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