# AI in the Sciences and Engineering 2024

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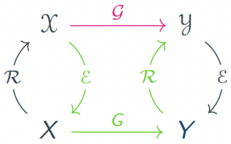
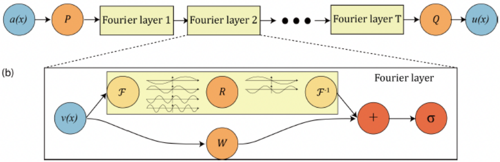
# What you learnt so far

- Operator learning: Given Abstract PDE: $\mathcal{D}_a(u) = f$
- Learn Solution Operator: $\mathcal{G} : \mathcal{X} \mapsto \mathcal{Y}$ with $\mathcal{G}(a, f) = u$
- Enforce Continuous-Discrete Equivalence via ReNO:

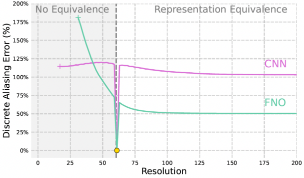



$$\mathcal{G} = \mathcal{R} \circ G \circ \mathcal{E}$$

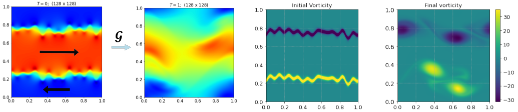
# FNO ?



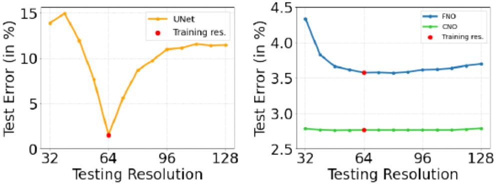

- Activations breaking Band limits $\Rightarrow$ FNO is not a ReNO !!



# A Practical Example

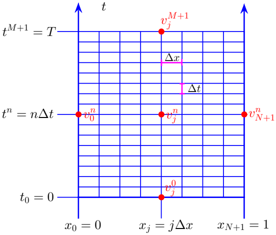



- FNO Results:

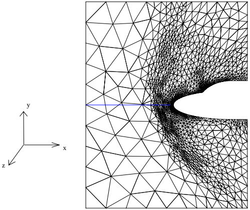



- Challenge: Design a ReNO

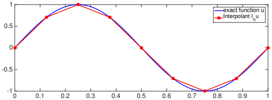
# Traditional Numerical Methods



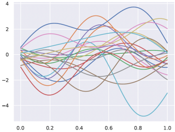

Finite Difference




Finite Volume



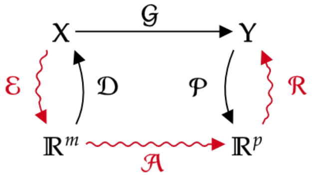

Finite Element



Spectral Method

# Revisiting Numerical Methods

- Can be reinterpreted in the following abstract Paradigm:




| Scheme | Encoder | Approximator | Reconstructor |
|---|---|---|---|
| Finite Difference | Point values | Scheme | Poly. Interpolant |
| Finite Element | Node Values | Scheme | Galerkin Basis |
| Finite Volume | Cell Averages | Scheme | Poly. Interpolant |
| Spectral | Fourier Coeffs. | Scheme | Fourier Interpolant |

# Spectral Neural Operators (SNO)

- A general structure

| Architecture | Encoder | Approximator | Reconstructor |
|---|---|---|---|
| SNO | Basis Coeffs | DNNs | Basis Functions |

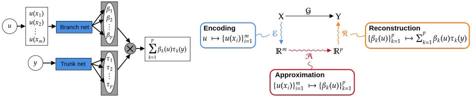
- A particular Instantiation: Fanaskov and Oseledets, 2022.
- $\mathcal{P}_K$: Periodic, bandlimited functions, Fourier basis $\Psi$.
- SNO: $T_{\Psi_{K'}} \circ \mathcal{N} \circ T_{\Psi_K} : \mathcal{P}_K \to \mathcal{P}_{K'}$, $\mathcal{N} : \mathbb{C}^{2K+1} \mapsto \mathbb{C}^{2K'+1}$
- SNO is a ReNO:

$$\begin{array}{ccccccc}
\mathcal{P}_K & \xrightarrow{T^*_{\Psi_K}} & \mathbb{C}^{2K+1} & \xrightarrow{\mathcal{N}} & \mathbb{C}^{2K'+1} & \xrightarrow{T_{\Psi_{K'}}} & \mathcal{P}_{K'} \\
T_{\Psi_K} \updownarrow T^*_{\Psi_K} & & \updownarrow \mathrm{Id} & & \updownarrow \mathrm{Id} & & T_{\Psi_{K'}} \updownarrow T^*_{\Psi_{K'}} \\
\mathbb{C}^{2K+1} & \xrightarrow{\mathrm{Id}} & \mathbb{C}^{2K+1} & \xrightarrow{\mathcal{N}} & \mathbb{C}^{2K'+1} & \xrightarrow{\mathrm{Id}} & \mathbb{C}^{2K'+1}
\end{array}$$

# A Variant

- DeepONets: Chen,Chen 1995, Lu et al, 2020:

$$\mathcal{N}(a)(y) = \sum_{k=1}^{p} \beta_k(a)\tau_k(y) \approx \mathcal{G}(a)(y)$$




| Architecture | Encoder | Approximator | Reconstructor |
| --- | --- | --- | --- |
| DeepOnet | Sensor Evals. | DNNs | DNNs |
| PCA-Net[1] | Input PCA | DNNs | Output PCA |

[1] Bhattacharya et al, 2020

# Are DeepONets ReNOs ?

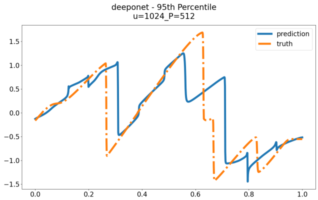
$$
\begin{array}{ccccccc}
\mathcal{P}_N & \xrightarrow{T^*_{\Psi_N}} & \mathbb{R}^{2N+1} & \xrightarrow{\mathcal{N}} & \mathbb{R}^K & \xrightarrow{T_{\mathcal{T}_K}} & \mathcal{Q}_K \\
T_{\Psi_N} \big\downarrow \big\uparrow T^*_{\Psi_N} & & \big\updownarrow \mathrm{Id} & & \big\updownarrow \mathrm{Id} & & T_{\mathcal{T}_K} \big\downarrow \big\uparrow T^*_{\mathcal{T}_K} \\
\mathbb{R}^{2N+1} & \xrightarrow{\mathrm{Id}} & \mathbb{R}^{2N+1} & \xrightarrow{\mathcal{N}} & \mathbb{R}^K & \xrightarrow{\mathrm{Id}} & \mathbb{R}^K
\end{array}
$$

- YES (if)
  - Bandlimited Functions $\mapsto$ span(TrunkNets)
  - Non-Uniform input sampling can lead to aliasing errors [2]
  - Trunk Nets need not be Basis for Function spaces.

[2] Observed in Lanthaler,SM,Karniadakis, 2022

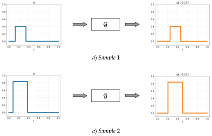
# Do DeepONets work in practice ?

- Yes, in some cases.
- However, Error of 30% for Burgers' equation with GRF initial data !!



# DeepONet vs. FNO

- Theory of (Lanthaler, Molinaro, Hadorn, SM, 2022):
- For Linear Advection Equation with Discontinuities:

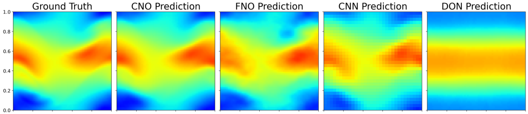



- Thm: To obtain $\epsilon$ error:
  - Size(DeepOnet) $\sim \mathcal{O}(\epsilon^{-2})$
  - Size(FNO) $\sim \mathcal{O}(\log(\epsilon^{-1}))$ !!
- Results:

| Architecture | ResNet | FCNN | DONet | FNO |
|---|---|---|---|---|
| Error | 14.8% | 23.3% | 7.9% | 0.7% |

- Analogous theorem for Burgers' equation.

# Poor performance of DeepONets




- Challenge: Design a ReNO that works