REPRESENTATION EQUIVALENT NEURAL OPERATORS

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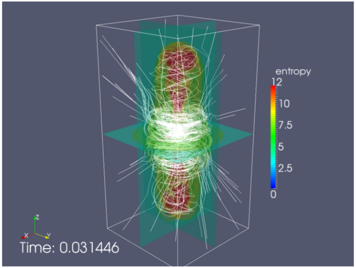
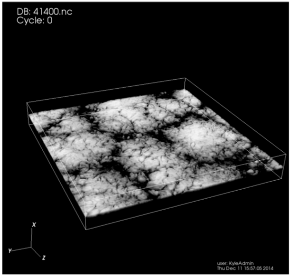
Outline of the presentation

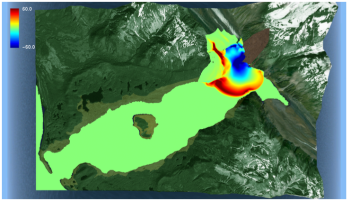
- What are neural operators for solving PDEs ?
- Are neural operators really operators ?
- How can we correctly define neural operators ?
- Can construct practical ones ?



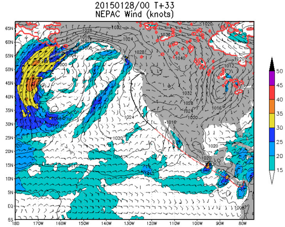
Supernovas



Clouds



Tsunamis



Weather

Solving PDEs as approximating solution operators

Theory

- We want to solve the PDE :

$$\mathcal{F}(u, p) = 0,\ x \in \Omega$$
$$B(u, p) = 0,\ x \in \partial\Omega$$

- p input, e.g. initial condition

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- Only finite number of computations,
- need to discretize u, p e.g. on a regular grid Δ
- consider discrete spaces X, Y
- consider approximation G

$$G : X \to Y,$$
$$p_\Delta \to u_\Delta$$

Link between discrete and continuous

$$\begin{tikzcd}
\mathcal{X} \arrow[r, "\mathcal{G}"] \arrow[d, dashed, bend right, "?"'] & \mathcal{Y} \arrow[d, dashed, bend right, "?"'] \\
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\end{tikzcd}$$

Having an **operator** perspective is very important :

- the solution lies in this function space,
- quantifying discrepancy between discrete and continuous solutions is at the basis of numerical analysis.
- Essential for structure preserving methods, as symmetries are at the operator level, etc...

For this reason,

- solution operator $\mathcal{G}$ approximated with **neural operator** $\mathcal{G}_\theta$,
- $\mathcal{G}_\theta$ mapping from functions to functions :

$$\begin{aligned} \mathcal{G}_\theta : \mathcal{X} &\to \mathcal{Y}, \\ p &\to u \end{aligned}$$

- potential for deep learning to drastically *accelerate* simulations,
- can be applied even when pde is unknown (e.g. climate)

Discretization invariance

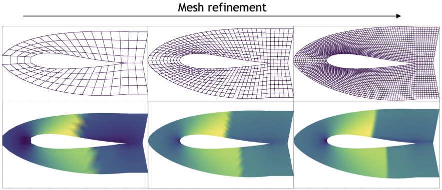
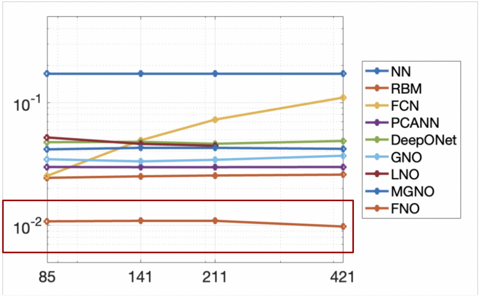


Figure 1: Discretization Invariance
An discretization-invariant operator has convergent predictions on a mesh refinement.



a prototypical example : the Fourier neural operator (fno)

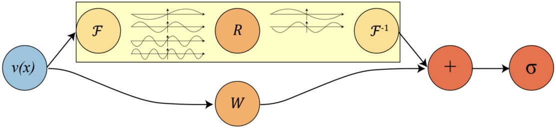
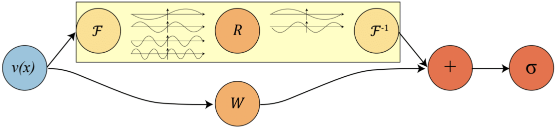


Figure 2 – layer of the Fourier neural operator **?**

- sequence of layers, as in classical nns

$$\mathcal{G} = \mathcal{N}_L \circ \mathcal{N}_{L-1} \circ \ldots \circ \mathcal{N}_1$$
$$(\mathcal{N}_\ell v)(x) = \sigma\left(A_\ell v(x) + B_\ell(x) + \mathcal{K}_\ell v(x)\right)$$



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- **novelty** : layers defined as mappings from functions to functions

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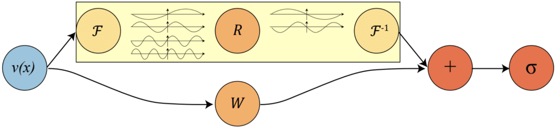

Figure 3 – layer of the Fourier neural operator

- for example, continuous convolution with Fourier layer :

$$\mathcal{K}_\ell v(x) = \int_D k_\ell(x-y)v(y)dy = \mathfrak{F}^{-1}(\mathcal{R}_\theta \odot \mathfrak{F}(v))(x)$$

claim : gives ability to handle different resolutions

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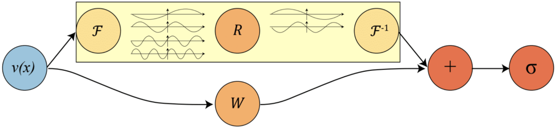

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- state of the art for many PDEs, claims to handle functions
- claim to be discretization invariant,
- how are these computed on a computer ?

FNO in practice

$$
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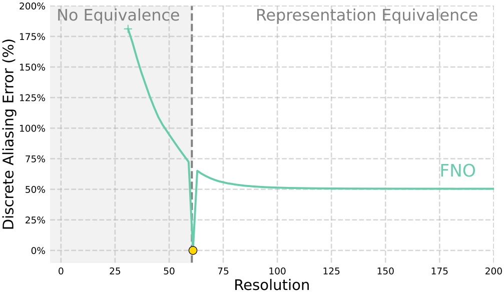
\mathcal{X} \arrow[r, "\mathcal{G}"] \arrow[d, bend right, "?"'] & \mathcal{Y} \arrow[d, bend right, dashed, "?"'] \\
X \arrow[r, red, "G"] \arrow[u, bend right, dashed, "?"'] & Y \arrow[u, bend right, dashed, "?"']
\end{tikzcd}
$$

- in practice, all computations done discretely using G, not $\mathcal{G}$
  - input and output function sampled on a grid
  - DFT is used instead of Fourier transform
  - activations computed on the grid (not the function)

- link between operator $\mathcal{G}$ and discrete map G ?

Discrete representations not equivalent



- random input $u \in \mathbb{R}^{61}$ and target data $v \in \mathbb{R}^{61}$, $u_i, v_i \sim \mathcal{G}(0, 1)$
- train mapping G to regress $u \to v$
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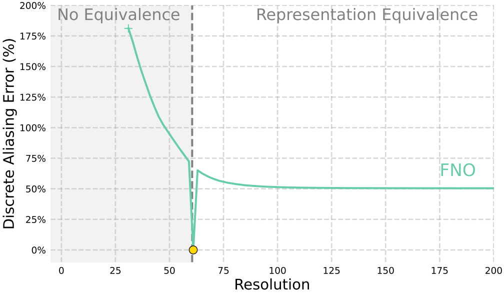

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- hints at discrepancy between continuous and discrete
- a bit of an extreme case, but shows that
- discretization invariance is only a property at the limit, does not say anything for practical resolutions

Representation equivalent neural operators (ReNO)

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Couple $(G, \mathcal{G})$, such that the diagram commutes :

$$\begin{tikzcd}
\mathcal{X} \arrow[r, "\mathcal{G}"] \arrow[d, bend right, "\mathcal{E}"'] & \mathcal{Y} \arrow[d, bend right, "\mathcal{E}"'] \\
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- i.e. discrepancy between continuous and discrete, aka *aliasing*

$$\varepsilon(G, \mathcal{G}) = \mathcal{G} - \mathcal{R} \circ G \circ \mathcal{E} = 0,$$

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$$\varepsilon(G, \mathcal{G}) = \mathcal{G} - \mathcal{R} \circ G \circ \mathcal{E} = 0,$$

- $\mathcal{X}, \mathcal{Y}$ separable Hilbert spaces, e.g. bandlimited functions, spanned by wavelets, fourier series coefficients, etc...

layer-wise Instantiation

- Design each layer $(\mathcal{G}_\ell, G_\ell)$ such that diagram **commutes** :

$$\mathcal{G}_\ell = \mathcal{R} \circ N_\ell \circ \mathcal{E}$$

- composition of layers is also a ReNO

Equivalence between discrete representations

Consider two discretizations G and G' of $\mathcal{G}$ (e.g. on different grids).

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

If both diagrams commute, **discrete representations are equivalent** :

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

- If **not** $\varepsilon(G, \mathcal{G}) \neq 0$, potential **discrepancy** at different resolutions.

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Instantiation : Bandlimited spaces

- input, output spaces : $\mathcal{X}, \mathcal{Y}$ *bandlimited* functions,

$$\mathcal{E}(v) = \{f(x_i)\}_{1,\dots,n}, \qquad \mathcal{R}(v)(x) = \sum_{i=1}^{n} v(x_i)\mathrm{sinc}(x - x_i)$$

- Natural spaces for point-wise evaluations on cartesian grid,

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- Natural spaces for point-wise evaluations on cartesian grid,
- Nyquist-Shannon : if grid dense enough, bijection between $\mathcal{X}$ and X
- $\varepsilon(G, \mathcal{G}) = \mathcal{G} - \mathcal{R} \circ G \circ \mathcal{E}$ reduces to classical aliasing.

per layer analysis

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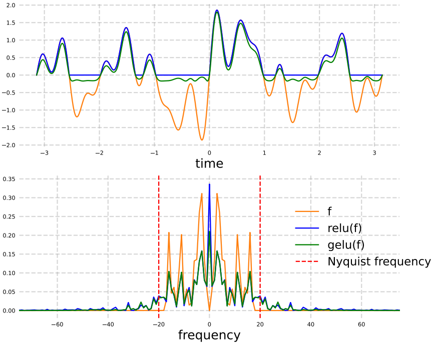
per layer analysis

- Continuous and discrete convolutions **equivalent**,
- Activation function is not : $\varepsilon(G, \mathcal{G}) \neq 0$, i.e. diagram does not commute



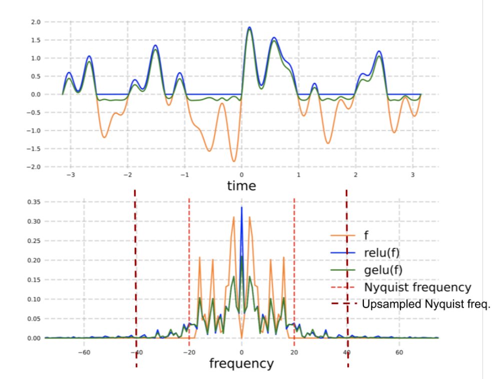
New convolutional based architecture

We propose to

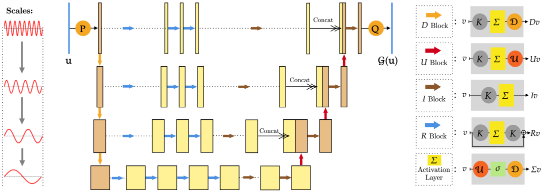
- *Fix* the activation function,
- Go back to standard convolutions (Fourier not essential),

Just as in StyleGAN3, new activation :

- upsample
- activation
- downsample



a convolutional based neural operator (CNO)



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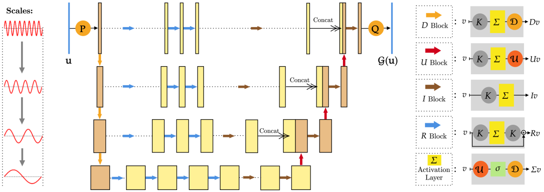
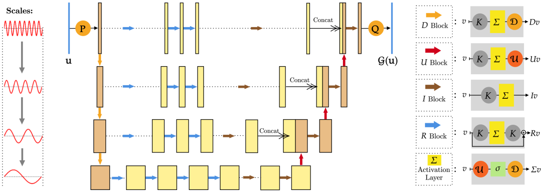


- convolution operation, implemented with simple convs :

$$K_\ell = \sum_{i,j=1}^{k} k_{ij} \cdot \delta_{z_{ij}}, \qquad \mathcal{K}_\ell v(x) = \int_D K_\ell(x-y)v(y)dy$$



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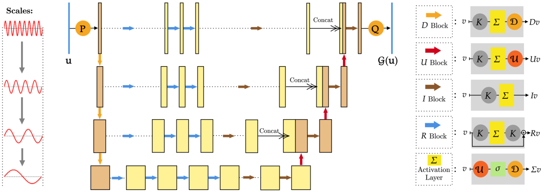

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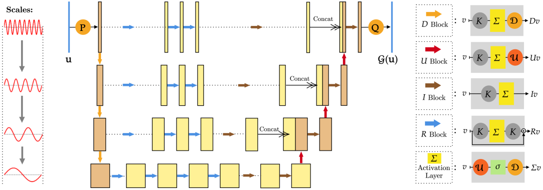

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$$\Sigma(f)(x) = \mathcal{D} \circ \sigma \circ \mathcal{U}$$

- upsampling $\mathcal{U}$ and downsampling $\mathcal{D}$: interpolation with sinc filter
- these operations all have a (unique) discrete N_ℓ (approximately)

$$\mathcal{G}_\ell(v) = \mathcal{R} \circ N_\ell \circ \mathcal{E}(v) \quad \text{for all} \quad v \in \mathcal{X}$$

- preservation of continuous structures, translation equivariance (better generalization ?)
- cno able to process at different grids, not restricted to fno layer
- *representation equivalence*

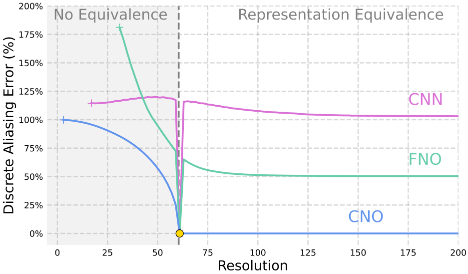

Table 1 – Relative median L^1 test errors.

	In/Out	FFNN	GT	UNet	ResNet	DON	FNO	CNO
Poisson Equation	In	5.74%	2.77%	0.71%	0.43%	12.92%	4.98%	**0.21%**
	Out	5.35%	2.84%	1.27%	1.10%	9.15%	7.05%	**0.27%**
Wave Equation	In	2.51%	1.44%	1.51%	0.79%	2.26%	1.02%	**0.63%**
	Out	3.01%	1.79%	2.03%	1.36%	2.83%	1.77%	**1.17%**
Smooth Transport	In	7.09%	0.98%	0.49%	0.39%	1.14%	0.28%	**0.24%**
	Out	650.6%	875.4%	1.28%	0.96%	157.2%	3.90%	**0.46%**
Discontinuous Transport	In	13.0%	1.55%	1.31%	**1.01%**	5.78%	1.15%	**1.01%**
	Out	257.3%	22691.1%	1.35%	1.16%	117.1%	2.89%	**1.09%**
Allen-Cahn Equation	In	18.27%	0.77%	0.82%	1.40%	13.63%	**0.28%**	0.54%
	Out	46.93%	2.90%	2.18%	3.74%	19.86%	**1.10%**	2.23%
Navier-Stokes Equations	In	8.05%	4.14%	3.54%	3.69%	11.64%	3.57%	**2.76%**
	Out	16.12%	11.09%	10.93%	9.68%	15.05%	9.58%	**7.04%**
Darcy Flow	In	2.14%	0.86%	0.54%	0.42%	1.13%	0.80%	**0.38%**
	Out	2.23%	1.17%	0.64%	0.60%	1.61%	1.11%	**0.50%**
Compressible Euler	In	0.78%	2.09%	0.38%	1.70%	1.93%	0.44%	**0.35%**
	Out	1.34%	2.94%	0.76%	2.06%	2.88%	0.69%	**0.59%**

Table 1 – Relative median L^1 test errors.

	In/Out	FFNN	GT	UNet	ResNet	DON	FNO	CNO
Poisson Equation	In	5.74%	2.77%	0.71%	0.43%	12.92%	4.98%	**0.21%**
	Out	5.35%	2.84%	1.27%	1.10%	9.15%	7.05%	**0.27%**
Wave Equation	In	2.51%	1.44%	1.51%	0.79%	2.26%	1.02%	**0.63%**
	Out	3.01%	1.79%	2.03%	1.36%	2.83%	1.77%	**1.17%**
Smooth Transport	In	7.09%	0.98%	0.49%	0.39%	1.14%	0.28%	**0.24%**
	Out	650.6%	875.4%	1.28%	0.96%	157.2%	3.90%	**0.46%**
Discontinuous Transport	In	13.0%	1.55%	1.31%	**1.01%**	5.78%	1.15%	**1.01%**
	Out	257.3%	22691.1%	1.35%	1.16%	117.1%	2.89%	**1.09%**
Allen-Cahn Equation	In	18.27%	0.77%	0.82%	1.40%	13.63%	**0.28%**	0.54%
	Out	46.93%	2.90%	2.18%	3.74%	19.86%	**1.10%**	2.23%
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quantitative results

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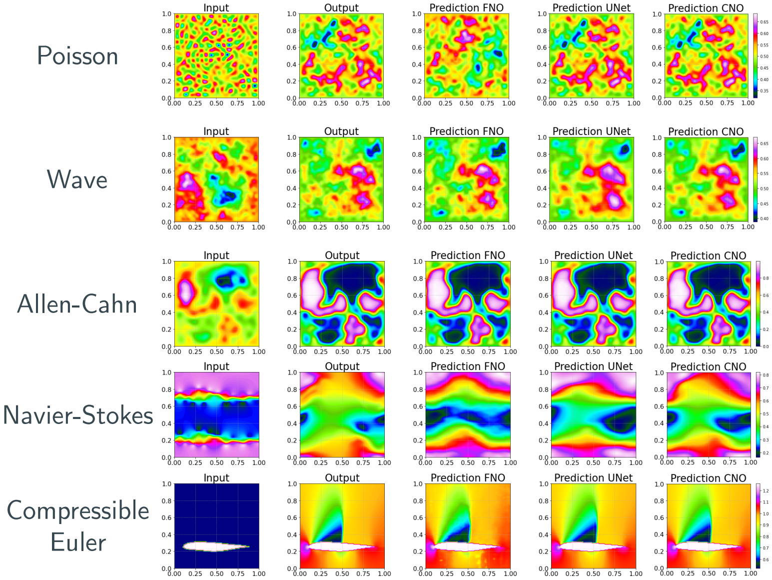
- e.g. for Navier Stokes, 10^{3-4} speedups wrt sota GPU codes


Poisson
Wave
Allen-Cahn
Navier-Stokes
Compressible Euler
Input
Output
Prediction FNO
Prediction UNet
Prediction CNO

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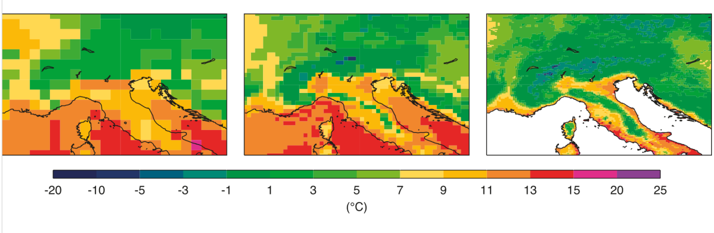

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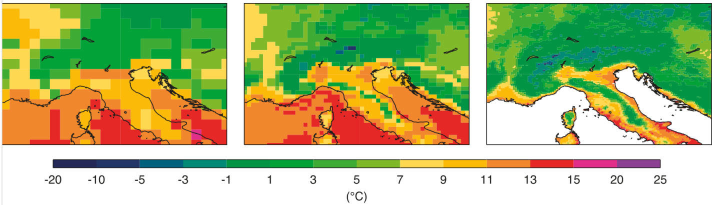

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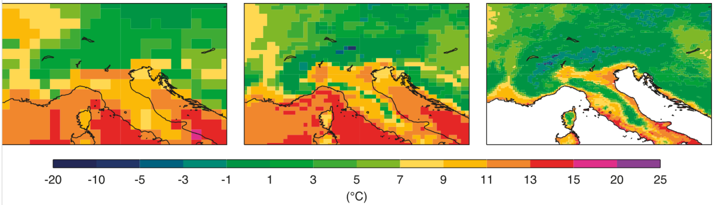
  - often different resolutions
  - there may be structures to preserve, e.g. conservation laws, etc,
  - can we learn one neural network for datasets at different resolutions ?
  - potentially useful to trade accuracy for compute and memory

limitations and future work



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- thanks for your time!

Appendix

Representation equivalent neural operators (ReNO)

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Couple $(G, \mathcal{G})$, such that the diagram commutes :

$$
\begin{tikzcd}
\mathcal{X} \arrow[r, "\mathcal{G}"] \arrow[d, bend right, "\mathcal{E}"'] & \mathcal{Y} \arrow[d, bend right, "\mathcal{E}"'] \\
X \arrow[r, "G"] \arrow[u, bend right, "\mathcal{R}"'] & Y \arrow[u, bend right, "\mathcal{R}"']
\end{tikzcd}
$$

- $f = \sum_{i \in I} c_i \Phi_i(x)$. discretize : $f \xrightarrow{\mathcal{E}} c$, reconstruct : $c \xrightarrow{\mathcal{R}} f$
- $\{\Phi_i\}_{i \in I}$ basis or frame spanning $\mathcal{X}, \mathcal{Y}$,
- i.e. discrepancy between continuous and discrete, aka *aliasing*

$$\varepsilon(G, \mathcal{G}) = \mathcal{G} - \mathcal{R} \circ G \circ \mathcal{E} = 0,$$

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$$\varepsilon(G, \mathcal{G}) = \mathcal{G} - \mathcal{R} \circ G \circ \mathcal{E} = 0,$$

- $\mathcal{X}, \mathcal{Y}$ separable Hilbert spaces, e.g. bandlimited functions, spanned by wavelets, fourier series coefficients, etc...

frame theory

synthesis and analysis operators

- $\mathcal{E}\colon \mathcal{X} \to \ell^2(I), \quad \mathcal{E}(\{f_i\}_{i\in I}) = \{\langle f, S^{-1} f_i\rangle\}_{i\in I}$
- $\mathcal{R}\colon \ell^2(I) \to \mathcal{X}, \quad \mathcal{R}(\{c_i\}_{i\in I}) = \sum_{i\in I} c_i f_i,$
- $S(f) = \sum_{i\in I} \langle f, f_i\rangle f_i$

definition : a frame

A countable sequence of vectors $\{f_i\}_{i\in I}$ in $\mathcal{X}$ is a frame for $\mathcal{X}$ if there exists constants $A, B > 0$ such that for all $f \in \mathcal{X}$

$$A\|f\|^2 \leq \sum_{i\in I} |< f, f_i >|^2 \leq B\|f\|^2$$

- e.g. orthogonal basis :$A = B = 1$,

frame decomposition theorem

Every element in $\mathcal{X}$ can be *uniquely and stably* reconstructed from its frame coefficients by means of the reconstruction formula

$$f = \mathcal{R}\mathcal{E}f = \sum_{i \in I} \langle f, S^{-1} f_i \rangle f_i = \sum_{i \in I} \langle f, f_i \rangle S^{-1} f_i, \tag{1}$$

where the series converge unconditionally.

Ablation Study

Table 13: Relative median L^1 test errors, for both in- and out-of-distribution testing, for the CNO models and two ablation models.

	In/Out	CNO	CNO w/o Filters	CNO w/o ResNets
Poisson Equation	In	**0.21%**	0.93%	0.85%
	Out	**0.27%**	1.65%	0.82%
Wave Equation	In	0.63%	**0.59%**	1.64%
	Out	1.17%	**1.12%**	1.64%
Smooth Transport	In	**0.24%**	0.31%	0.31%
	Out	**0.46%**	**0.46%**	0.76%
Discontinuous Transport	In	**1.03%**	1.21%	1.17%
	Out	**1.18%**	1.32%	1.60%
Allen-Cahn	In	**0.54%**	0.69%	0.71%
	Out	2.23%	**2.16%**	2.21%
Navier-Stokes	In	**2.76%**	3.20%	3.00%
	Out	7.04%	9.60%	**5.85%**
Darcy	In	**0.38%**	0.47%	0.41%
	Out	**0.50%**	0.65%	0.58%
Compressible Euler	In	**0.35%**	0.38%	0.37%
	Out	**0.59%**	0.62%	**0.59%**

Proposition 3.8. *Let (U, u) be an $\epsilon-$ReNO. For any two frame sequence pairs (Ψ, Φ) and (Ψ', Φ') satisfying conditions in Definition 3.4 and such that $\mathcal{M}_{\Phi'} \subseteq \mathcal{M}_{\Phi}$, we have*

$$\|\tau(u, u')\| \leq \frac{2\epsilon\sqrt{B_\Psi}}{\sqrt{A_\Phi}},$$