Microsoft

Clifford Neural Layers for PDE Modeling

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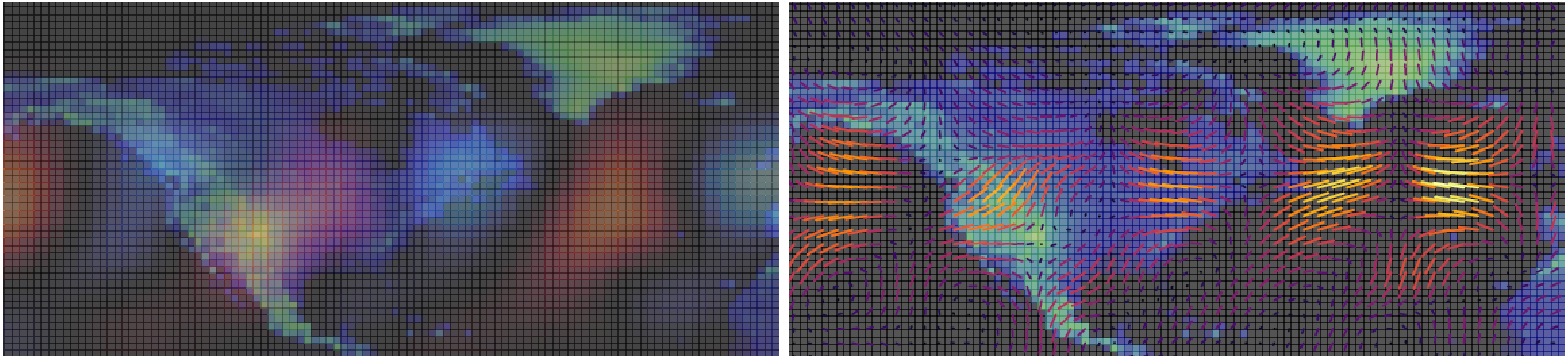
PDEs - the language of science / simulation



(a) Scalar pressure field **(b)** Vector wind velocity field

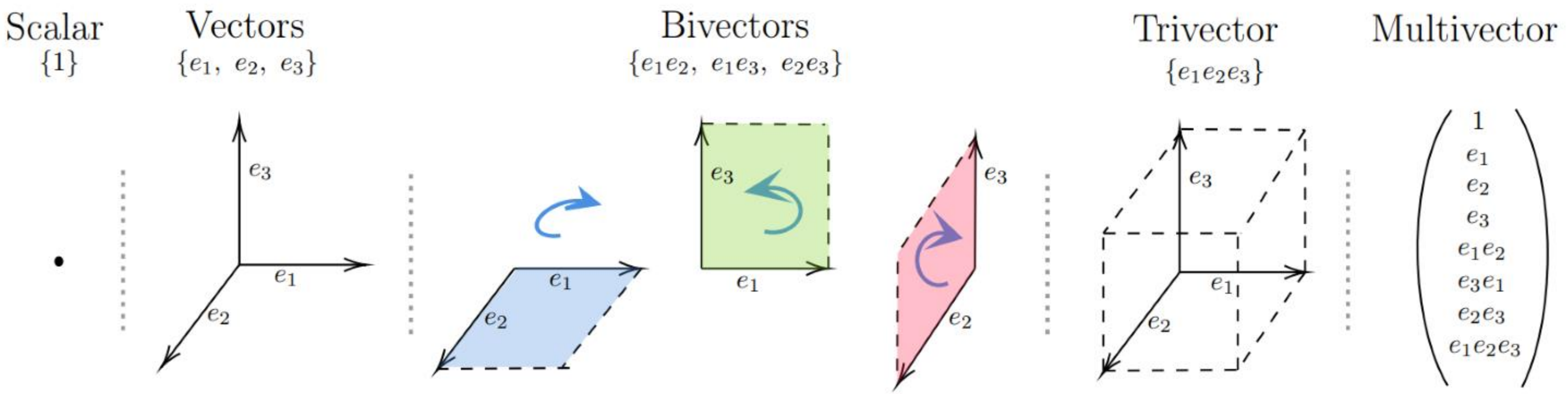
$$\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + g \frac{\partial \eta}{\partial x} = 0$$

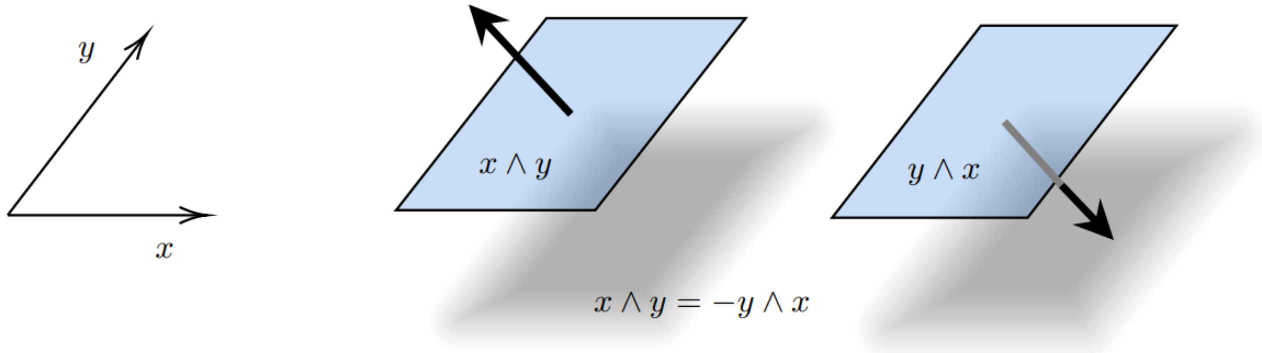
$$\frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + g \frac{\partial \eta}{\partial y} = 0$$

$$\frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x}\left[(\eta + h) v_x\right] + \frac{\partial}{\partial y}\left[(\eta + h) v_y\right] = 0$$

- Often, data shows relation between different fields and field components, which standard methods do not take into account.

Clifford algebras have multivector structure





Signature of Clifford algebra

- $Cl_{(p,q)}$ where (p,q) is the signature of the Clifford algebra:

$$
\begin{aligned}
e_i^2 &= +1 && \text{for } 1 \leq i \leq p\,, \\
e_j^2 &= -1 && \text{for } p < j \leq p+q\,, \\
e_i e_j &= -e_j e_i && \text{for } i \neq j\,.
\end{aligned}
$$

- $Cl_{(0,1)}$ with base vectors (1, e_1) is isomorph to the complex numbers with e_1= i.
- $Cl_{(0,2)}$ with base vectors (1, e_1, e_2, e_1e_2) is isomorph to the quaternions with e_1 = i, e_2 = j, e_1e_2 = k.

Geometric product

- Bilinear operation on multivectors:
- For example, geometric product for $Cl_{(2,0)}$:

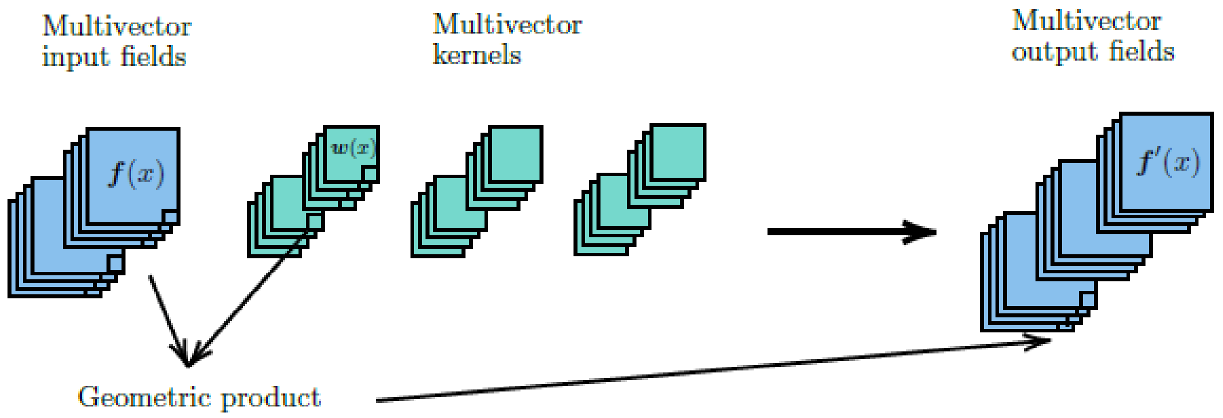
$$\begin{aligned}\boldsymbol{ab} &= a_0b_0 - a_1b_1 - a_2b_2 - a_{12}b_{12} \\ &+ (a_0b_1 + a_1b_0 + a_2b_{12} - a_{12}b_2)\ e_1 \\ &+ (a_0b_2 - a_1b_{12} + a_2b_0 + a_{12}b_1)\ e_2 \\ &+ (a_0b_{12} + a_1b_2 - a_2b_1 + a_{12}b_0)\ e_1e_2\end{aligned}$$

Clifford convolution

- Replace convolution with Clifford convolution:

$$[f \star w_i](x) = \sum_{y \in \mathbb{Z}^2} \langle f(y), w^i(y-x) \rangle = \sum_{y \in \mathbb{Z}^2} \sum_{j=1}^{c_{\text{in}}} f^j(y) w^{i,j}(y-x) \ .$$

$$\longrightarrow \quad [\boldsymbol{f} \star \boldsymbol{w}^i](x) = \sum_{y \in \mathbb{Z}^2} \sum_{j=1}^{c_{\text{in}}} \underbrace{\boldsymbol{f}^j(y) \boldsymbol{w}^{i,j}(y-x)}_{\boldsymbol{f}^j \boldsymbol{w}^{i,j} \ : \ G^2 \times G^2 \to G^2} \ .$$



Dual representation

Definition 2: Dual of a multivector

The dual $\boldsymbol{a}^*$ of a multivector $\boldsymbol{a}$ is defined as:

$$\boldsymbol{a}^* = \boldsymbol{a} i_{p+q} \; , \tag{22}$$

where i_{p+q} represents the respective pseudoscalar of the Clifford algebra.

$$\boldsymbol{a} = a_0 + a_1 e_1 + a_2 e_2 + a_{12} e_{12} \; ,$$

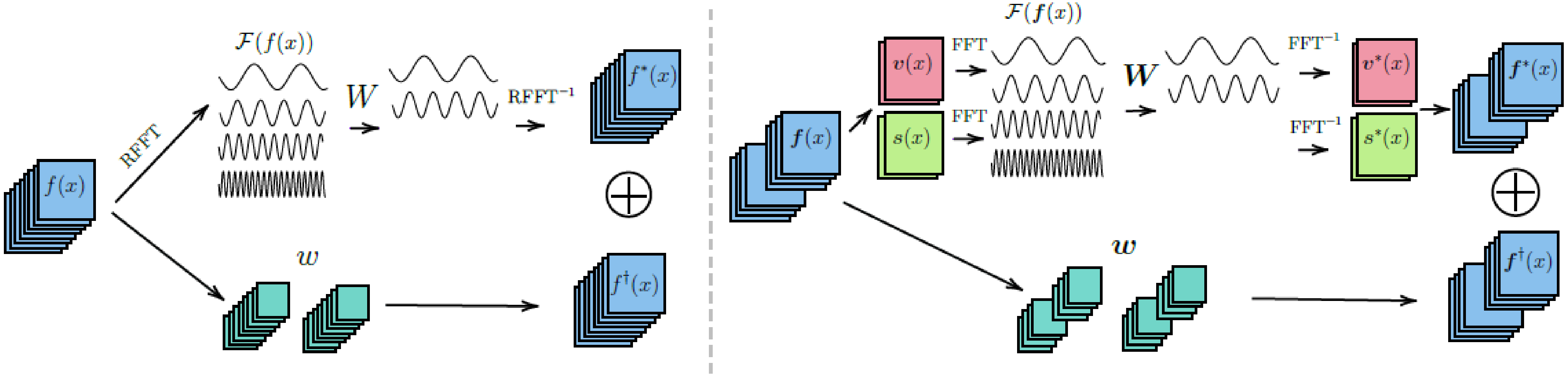
$$\boldsymbol{a} = 1 \underbrace{\left(a_0 + a_{12} i_2\right)}_{\text{spinor part}} + e_1 \underbrace{\left(a_1 + a_2 i_2\right)}_{\text{vector part}}$$

$$1 \leftrightarrow e_1 e_2 e_3 = i_3$$
$$e_1 \leftrightarrow e_2 e_3$$
$$e_2 \leftrightarrow e_3 e_1$$
$$e_3 \leftrightarrow e_1 e_2 \; .$$

$$\boldsymbol{F} = E + B i_3$$

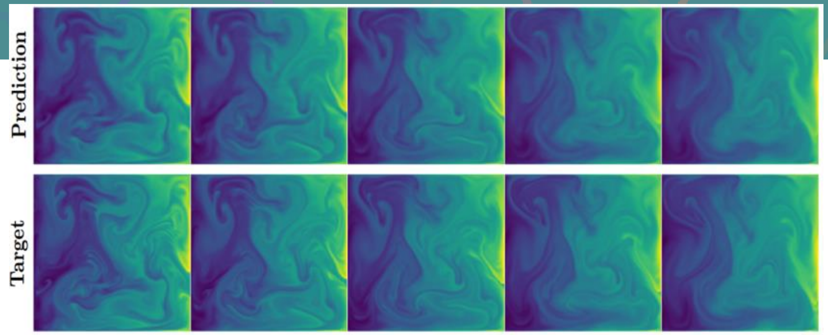
Clifford Fourier Transform

$$\hat{f}(\xi) = \mathcal{F}\{f\}(\xi) = \hat{f}_0(\xi) + \hat{f}_1(\xi)e_1 + \hat{f}_2(\xi)e_2 + \hat{f}_{12}(\xi)e_{12}$$

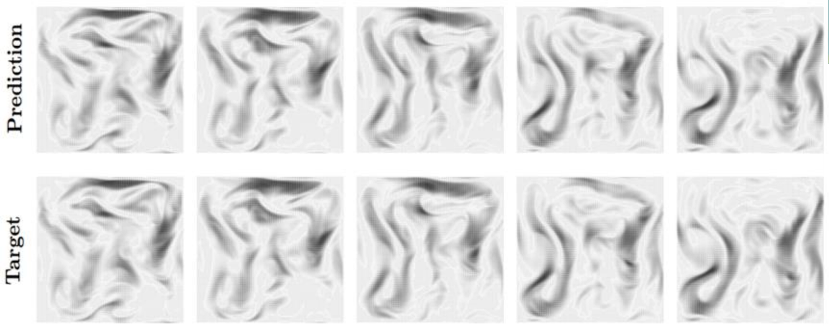


(a) FNO layer **(b)** Clifford FNO layer

Results

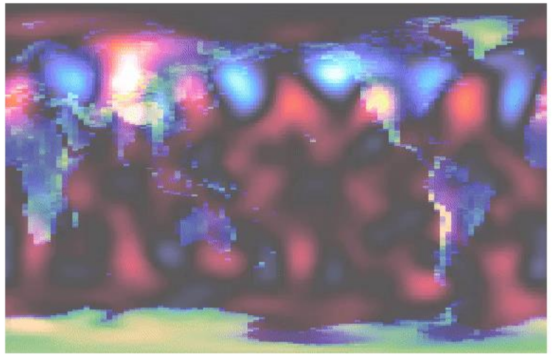


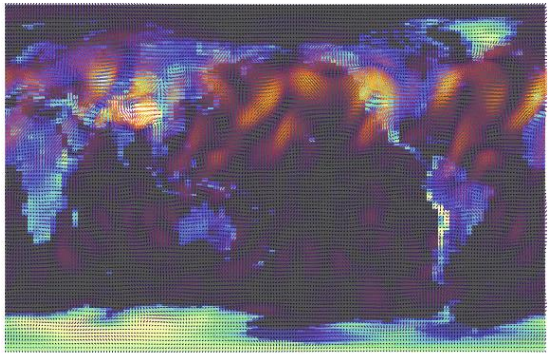
(a) Scalar field



(b) Vector field

$$\frac{\partial v}{\partial t} = -v \cdot \nabla v + \mu \nabla^2 v - \nabla p + f \ ,$$
$$\nabla \cdot v = 0 \ .$$





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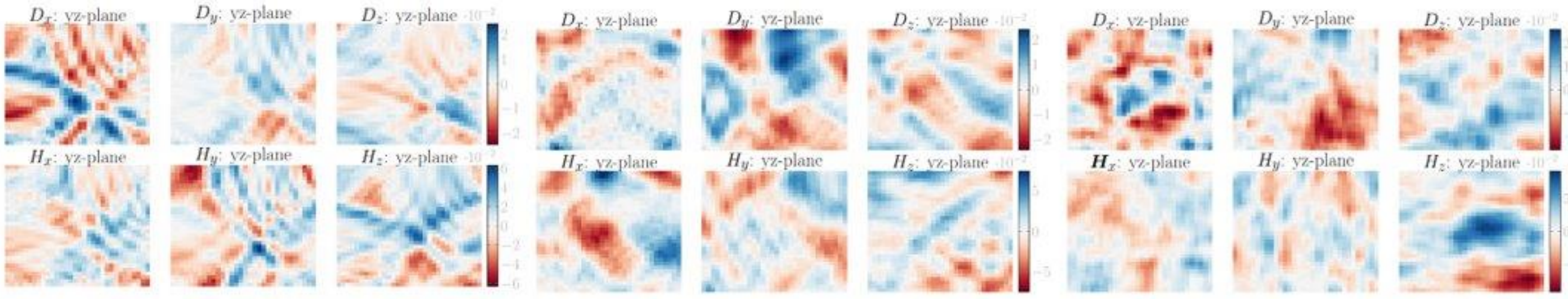

$$\boldsymbol{F} = E + Bi_3$$

ResNets vs CResNets / FNOs vs CFNOs

$$\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + g \frac{\partial \eta}{\partial x} = 0$$

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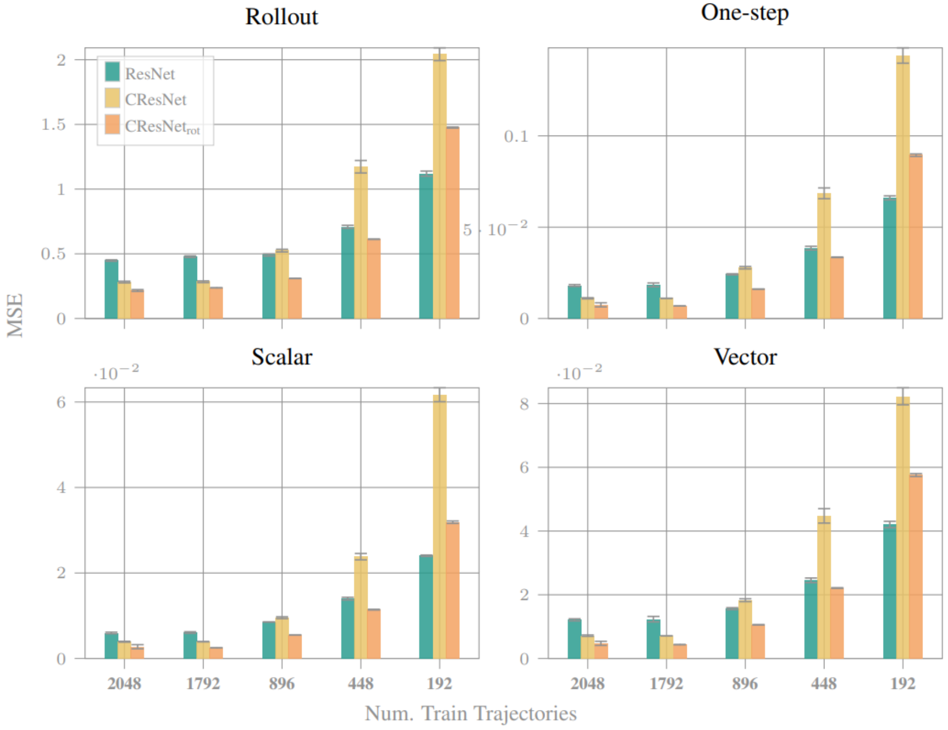

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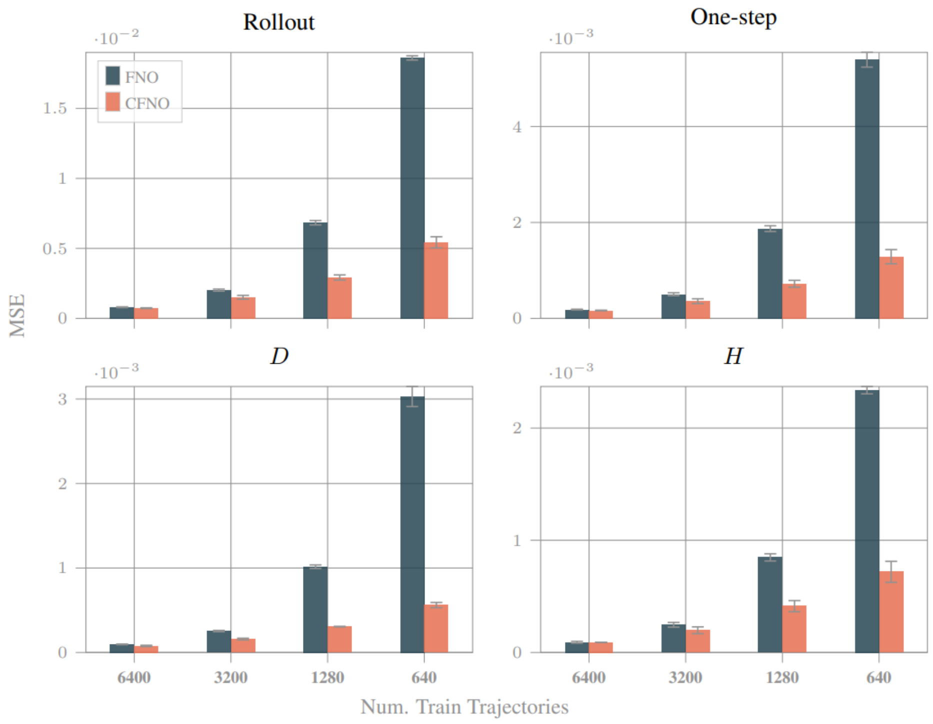
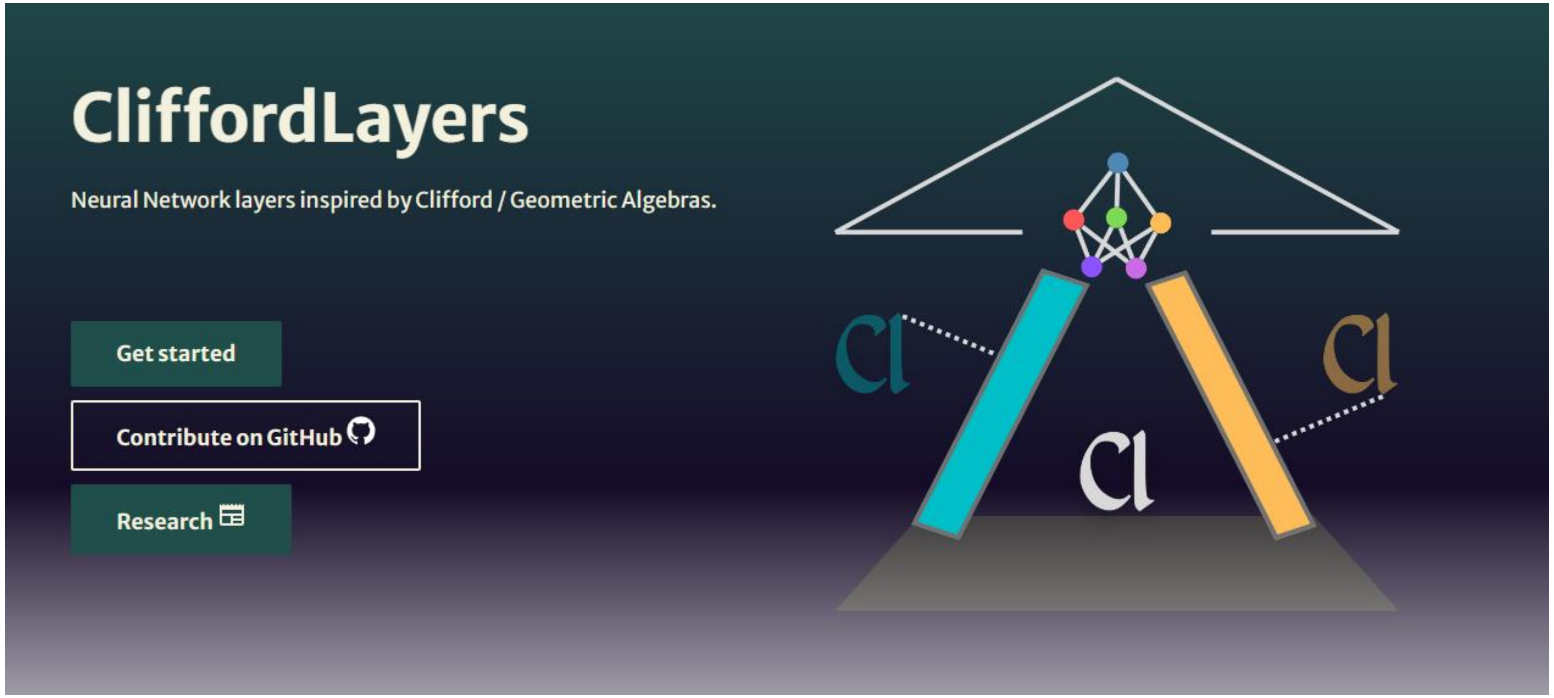
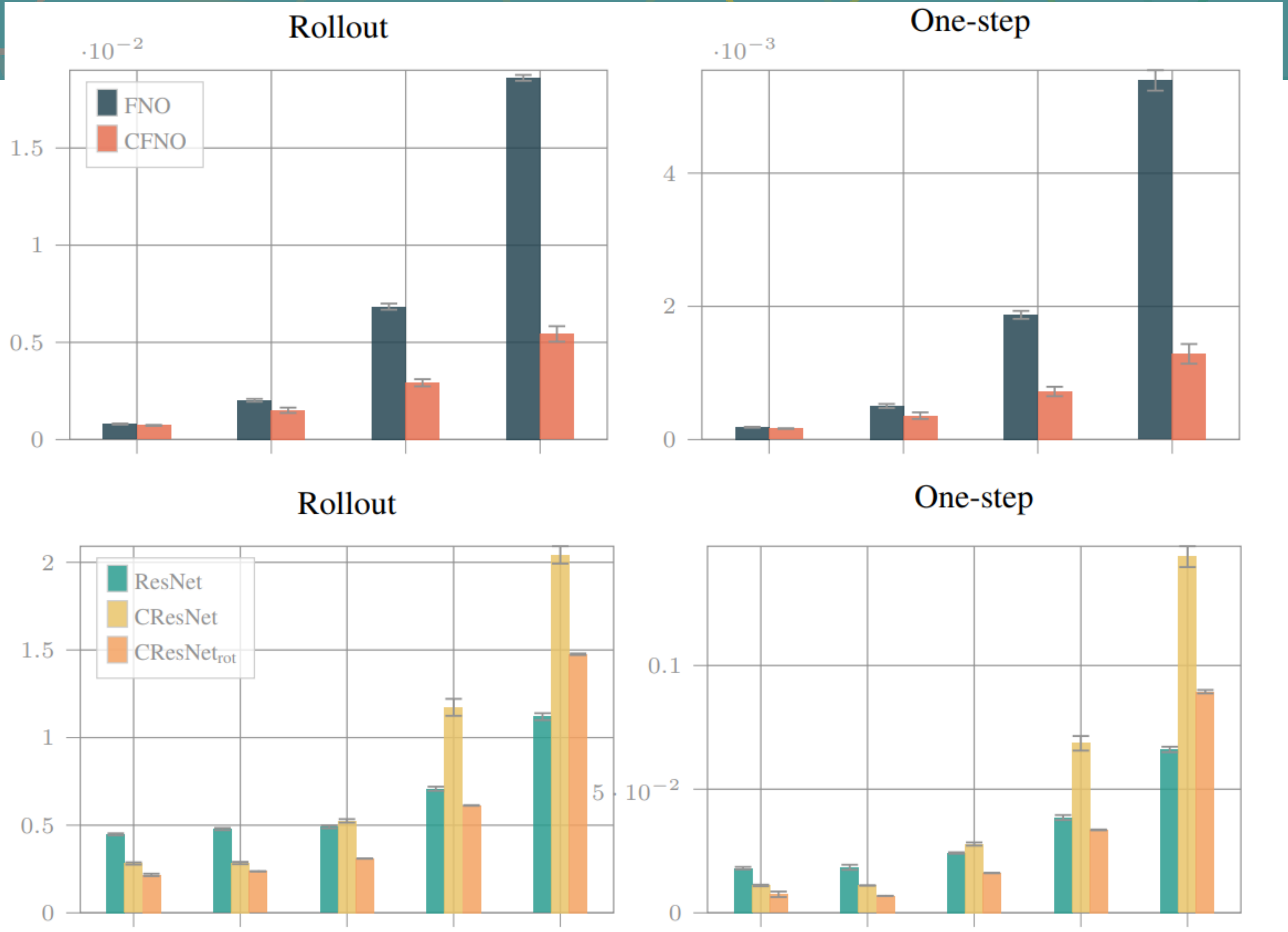


Material

- **Paper**: [2209.04934] Clifford Neural Layers for PDE Modeling (arxiv.org)
- **Codebase**: CliffordLayers - CliffordLayers (microsoft.github.io)




Rollout
One-step
$\cdot 10^{-2}$
$\cdot 10^{-3}$
FNO
CFNO
1.5
1
0.5
0
4
2
0
Rollout
One-step
ResNet
CResNet
$\text{CResNet}_{\text{rot}}$
2
1.5
1
0.5
0
0.1
$5 \cdot 10^{-2}$
0