A gentle introduction to neural operator

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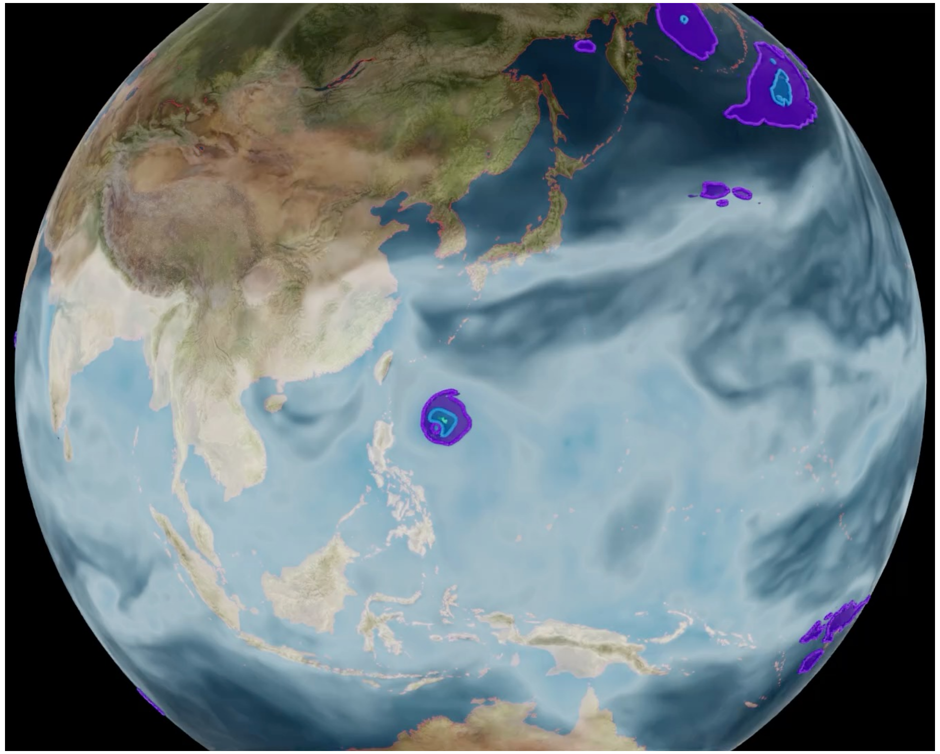
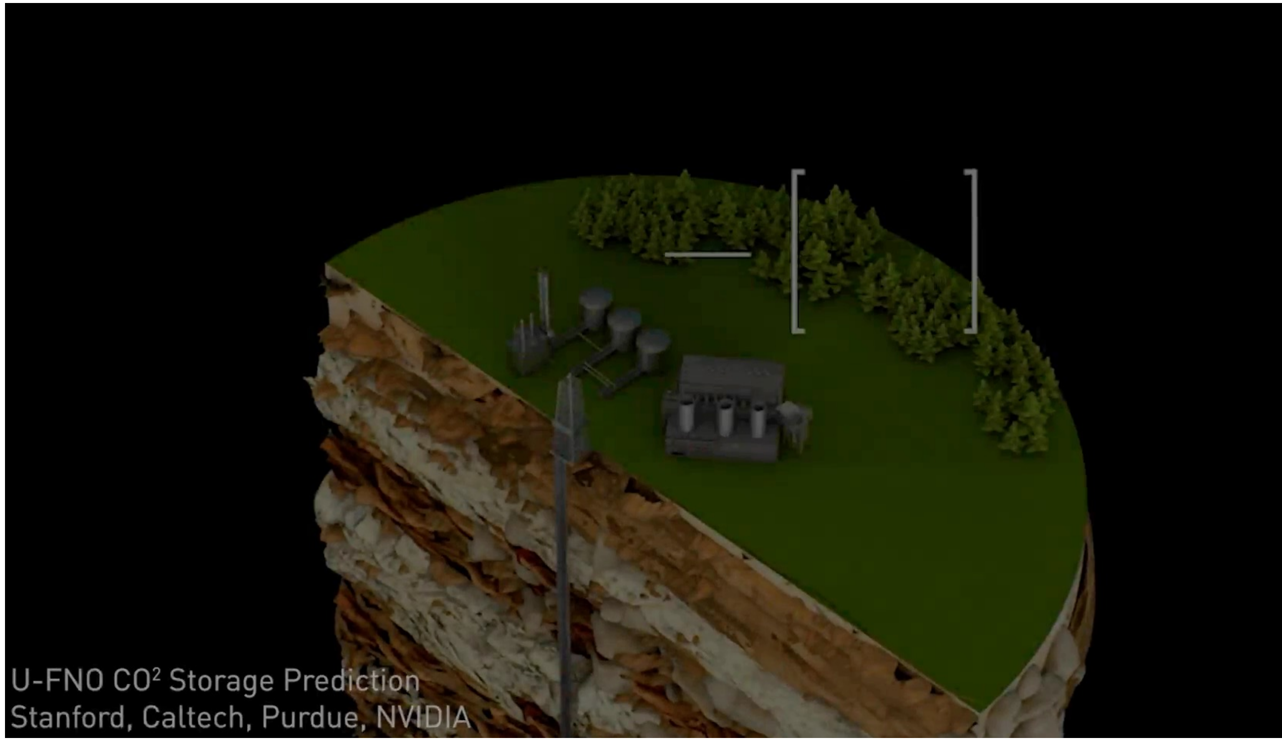
SZ4D Virtual Workshop



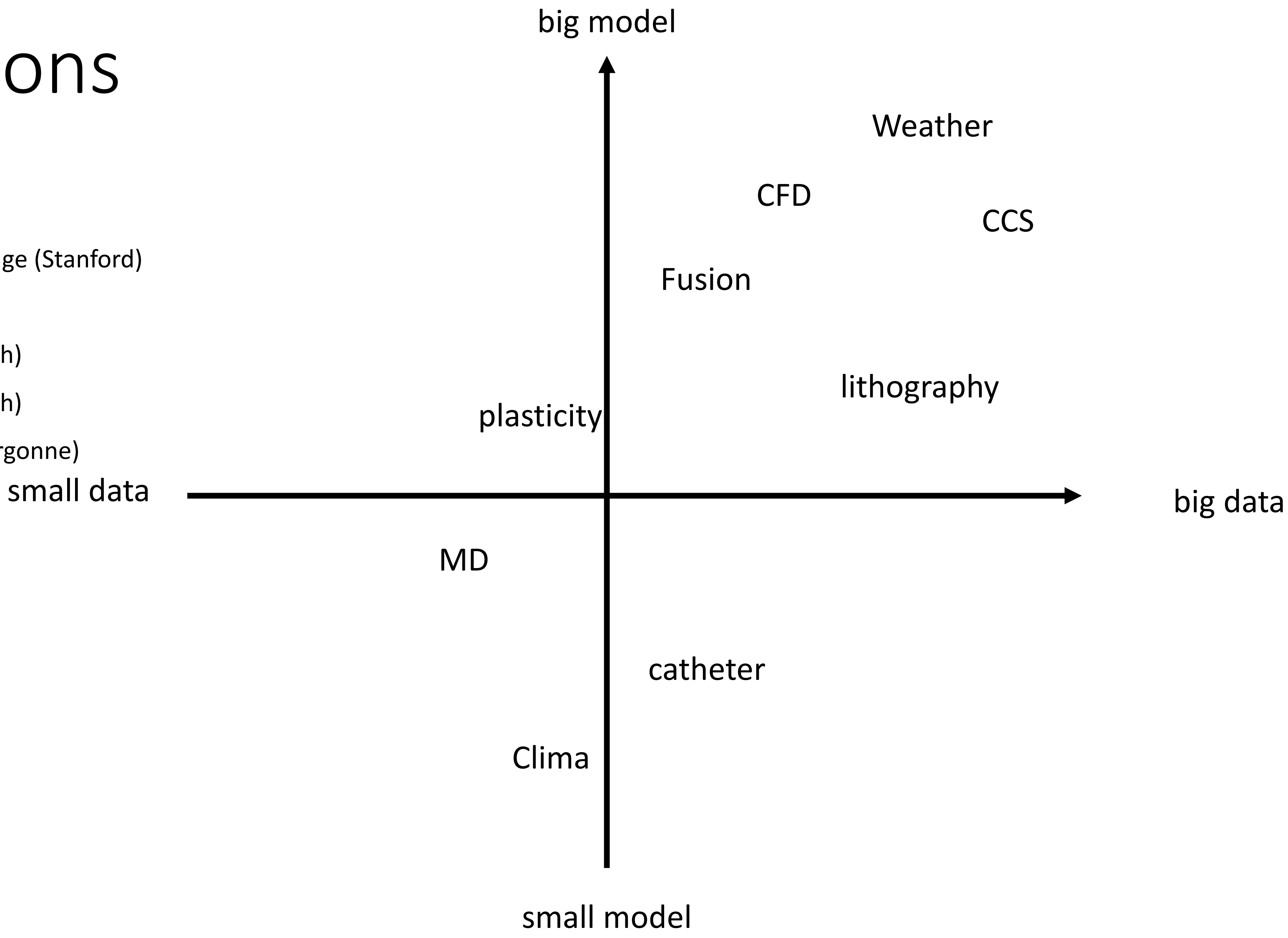
Weather prediction: Unprecedented Resolution for AI, “**100,000x**” faster than traditional methods
[1] PSHRCMKHLAHKA



CO2 storage: Multiphase flow for CO2-water interactions, “**60,000x**” faster (2d), **“700,000x”** faster (3d).
[2] WLLAAB

Applications

- Weather (Nvidia)
- Carbon Capture & Storage (Stanford)
- Lithography (Nvidia)
- Fluid Mechanics (Caltech)
- Solid Mechanics (Caltech)
- Molecular Dynamics (Argonne)
- Fusion (UK atomic)
- Catheter (Caltech)
- Clima Cloud (Caltech)



Operator learning

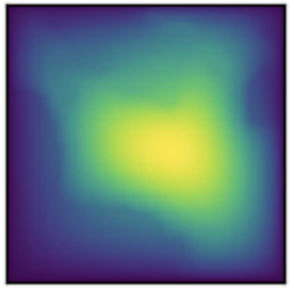
Operators are map between function space.

Given a dataset of input-output pairs, find the map (operator)

F: a->u

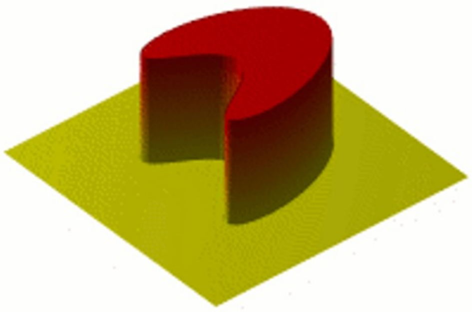
Input: coefficient

→



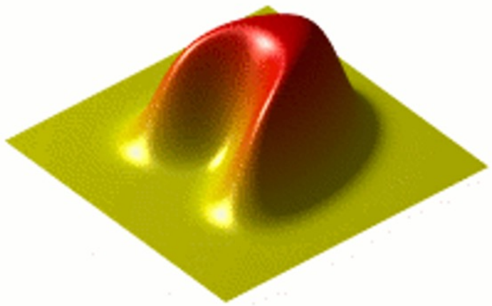
Output: solution

F: u0->u1



Input: initial

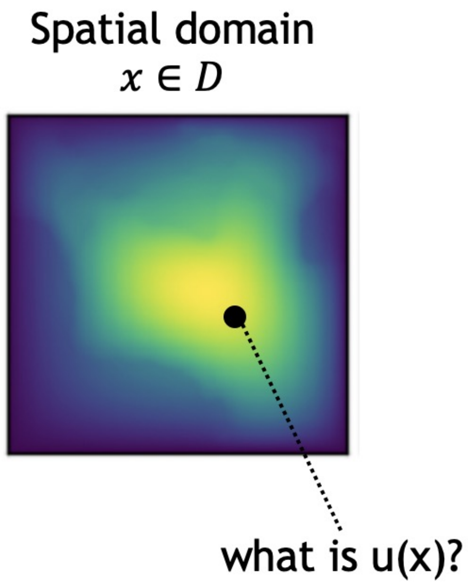
→



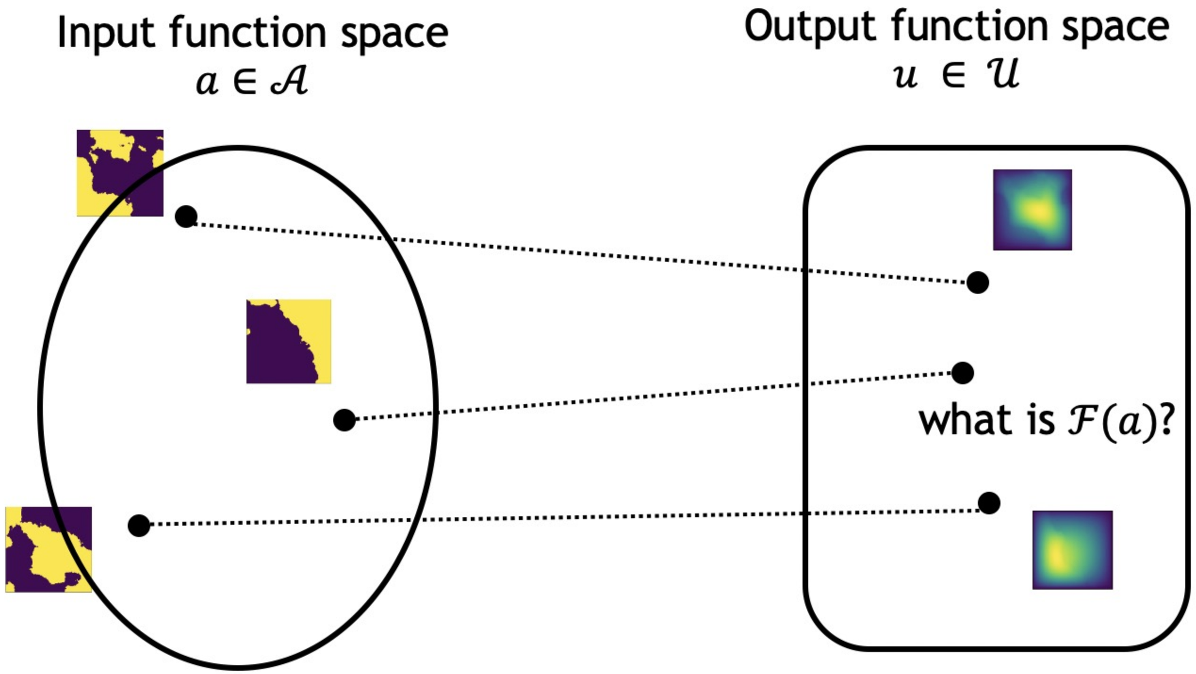
Output: solution

Solve vs learn

Solving for a PDE instance u
approximate $u(x)$ in the spatial space.



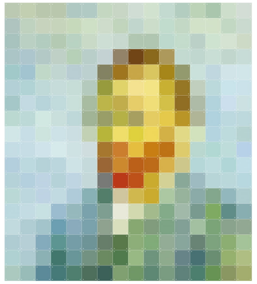
learn the solution operator $\mathcal{F}$
interpolate u in the function space.

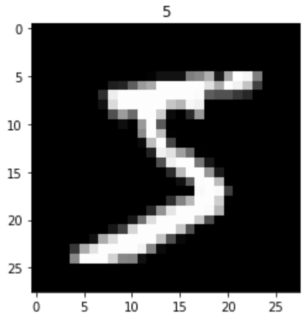


$$\mathcal{F}: \mathcal{A} \rightarrow \mathcal{U}$$

Neural networks vs Neural operators

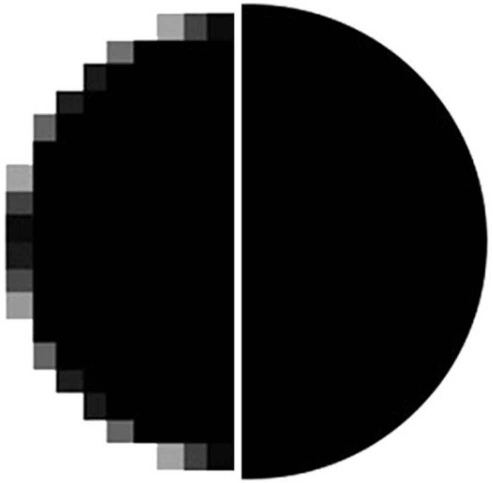
We want to define the model in the function spaces of the PDE.

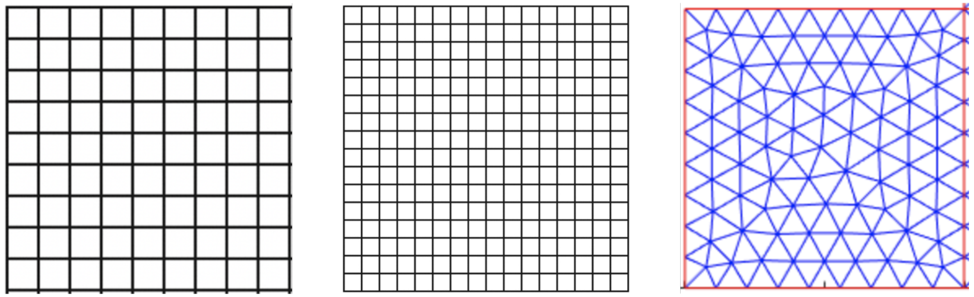


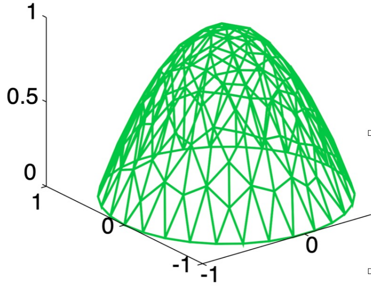


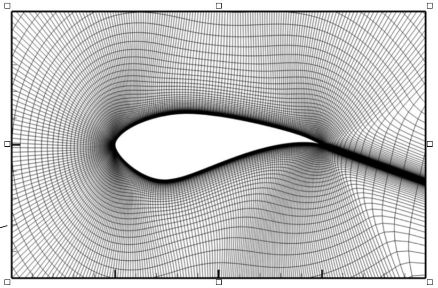
Vocabulary:
Man, woman, boy, girl, prince, princess, queen, king, monarch

	1	2	3	4	5	6	7	8	9
man	1	0	0	0	0	0	0	0	0
woman	0	1	0	0	0	0	0	0	0
boy	0	0	1	0	0	0	0	0	0
girl	0	0	0	1	0	0	0	0	0
prince	0	0	0	0	1	0	0	0	0
princess	0	0	0	0	0	1	0	0	0
queen	0	0	0	0	0	0	1	0	0
king	0	0	0	0	0	0	0	1	0
monarch	0	0	0	0	0	0	0	0	1







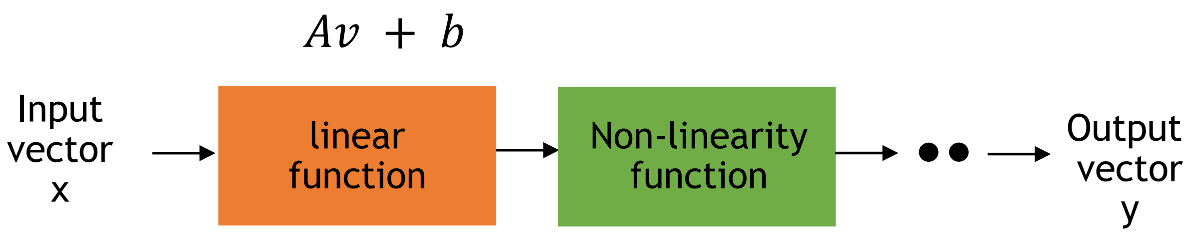


Discretized vector

Continuous function

Neural networks

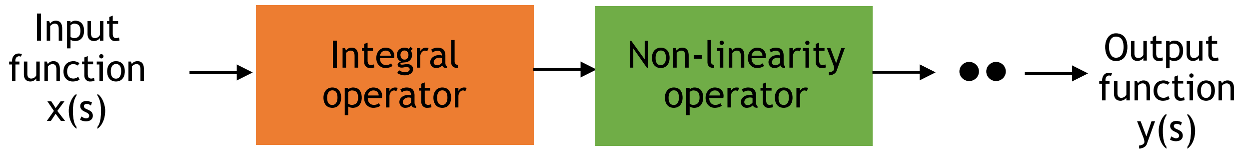
$$f: \ x \rightarrow y$$



Neural operators

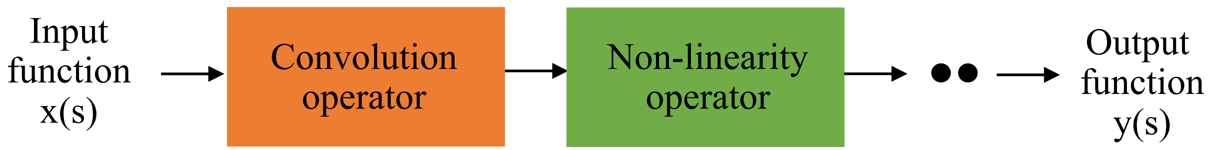
$$F: \; x(s) \rightarrow y(s)$$

$$\int \kappa(x, y)\, v(y)\, dy$$



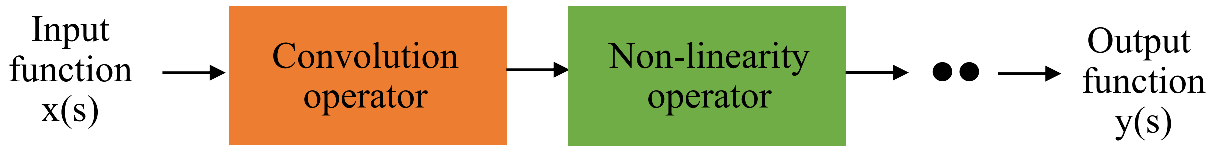
Fourier neural operators

$$F: \; x(s) \rightarrow y(s)$$



Fourier neural operators

F: x(s) → y(s)



Architecture

$$v_{l+1}(s) = \sigma\left(W_l v_l(s) + \int_D \kappa_l(s,z) v_l(z)\, dz + b_l(s) \right)$$

Fourier space

- Assume $\kappa_l(s,z) = \kappa_l(s-z)$ and parametrize its Fourier components θ_l.
  - Convolution theorem: $\int_D \kappa_l(s-z) v_l(z)\, dz = \mathcal{F}^{-1}(\theta_l \cdot \mathcal{F}(v_l))(s)$ $\quad \mathcal{O}(n \log n)$

[4] Fourier neural operator. LKALBSA (2021)

Approximation theory

- Neural operator can approximate any continuous operator.

[5] Nikola Kovachki et. al. 2021

- FNO can mimic pseudospectral solvers to get a bound on the number parameters.

[6] Nikola Kovachki et. al. 2021

- FNO (non-linear decoder) can be more efficient than DeepONet

[7] Samuel Lanthaler et. al. 2023

- FNO (non-linear decoder) can approximate any continuous operator with 1 Fourier mode (but higher channel dimensions).

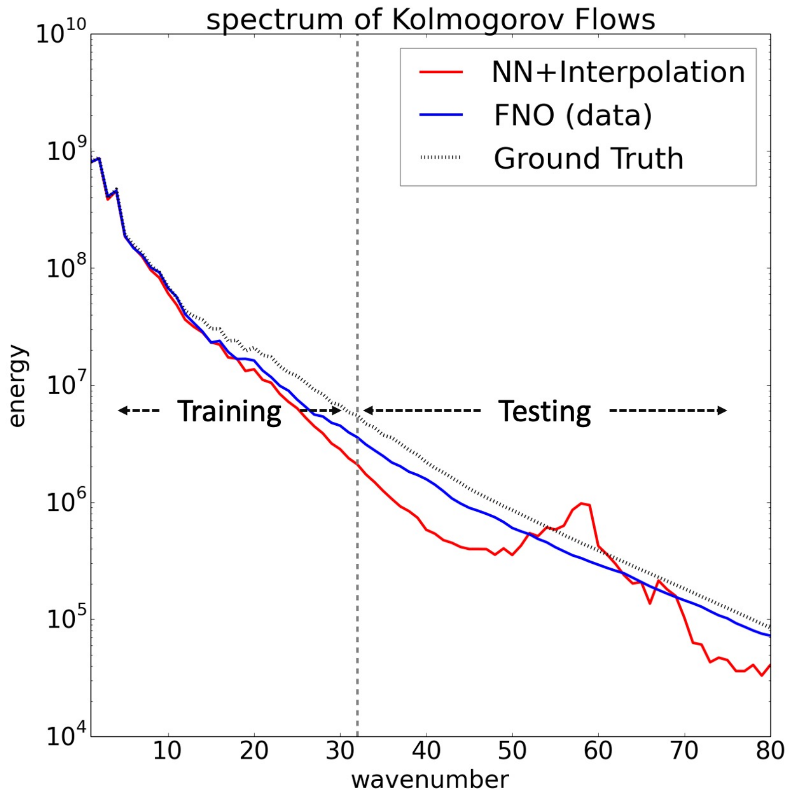
[8] Samuel Lanthaler et. al. 2023

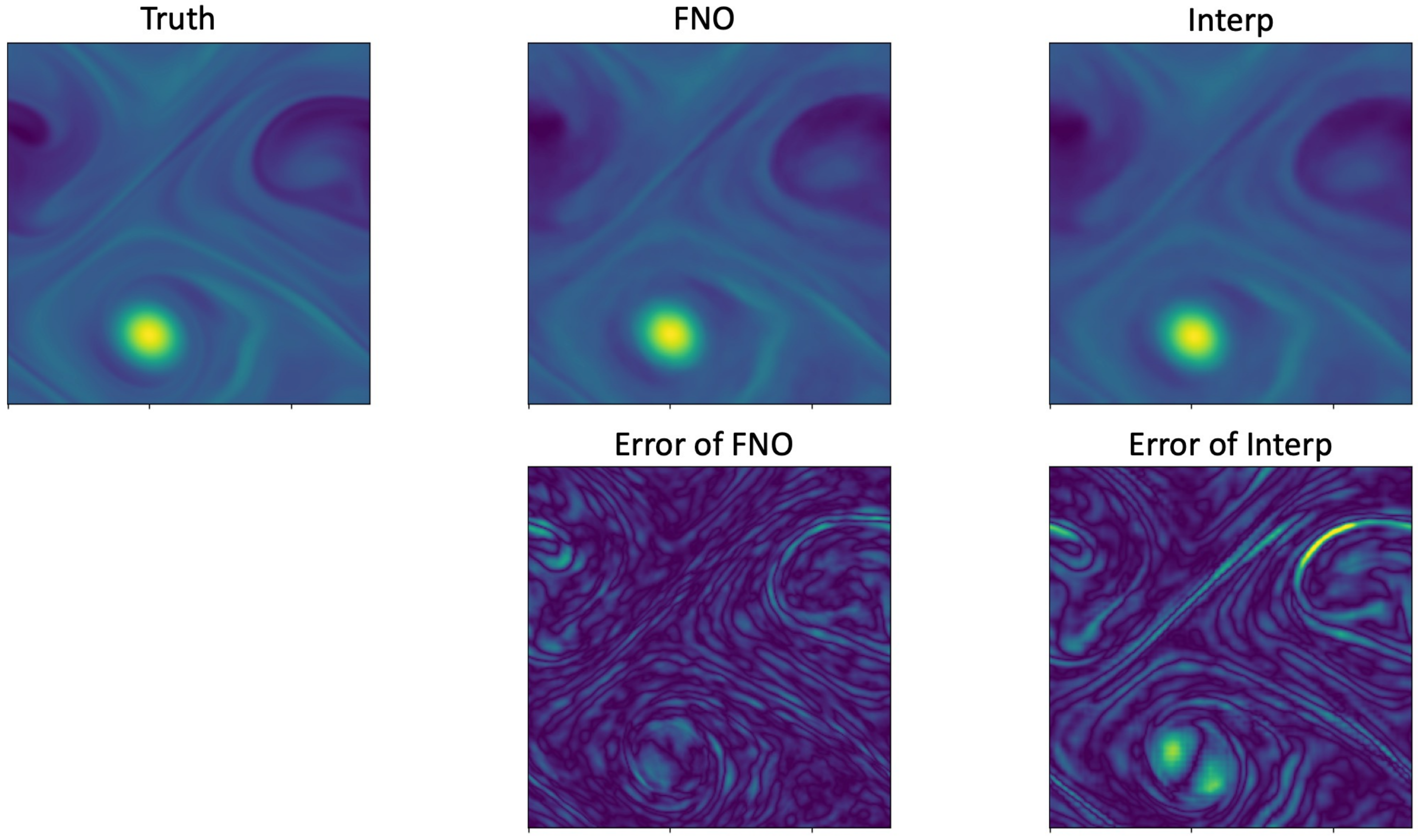
Discretization convergent (wrt refinement)

Property \ Model	CNNs	DeepONets	CNNs+Interpolation	Neural Operators
Discretization Invariance	✗	✗	✓	✓
Query at any point	✗	✓	✓	✓
Input at any point	✗	✗	✓	✓
Universal Approximation	✗	✓	✗	✓

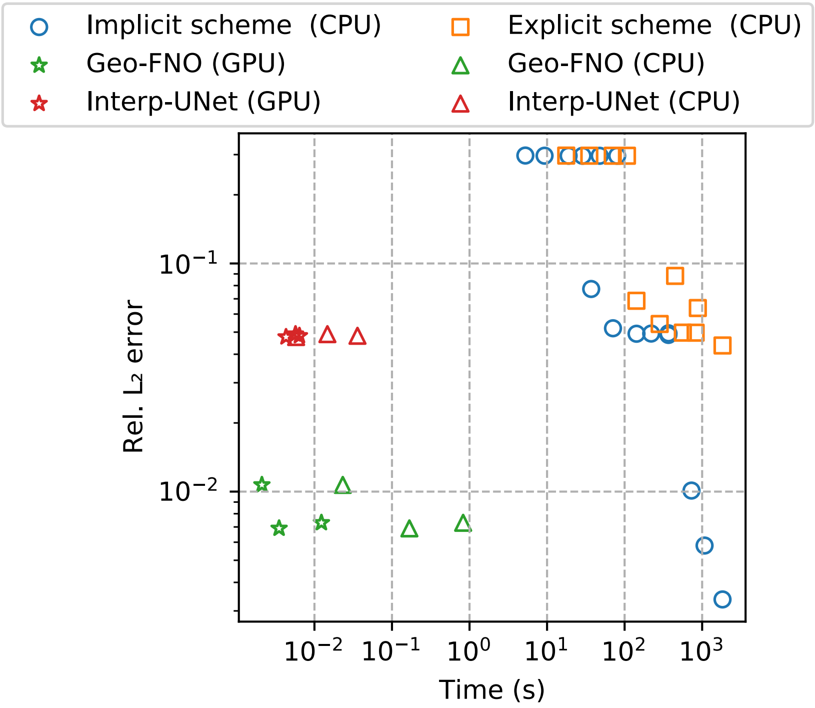
Discretization-invariance is a design philosophy. We define the problem in infinite space and then discretize the model.
In practice, many recently-developed NNs are indeed discretization-invariant (e.g. GraphCast, Transformer)

Extrapolation to unseen frequencies

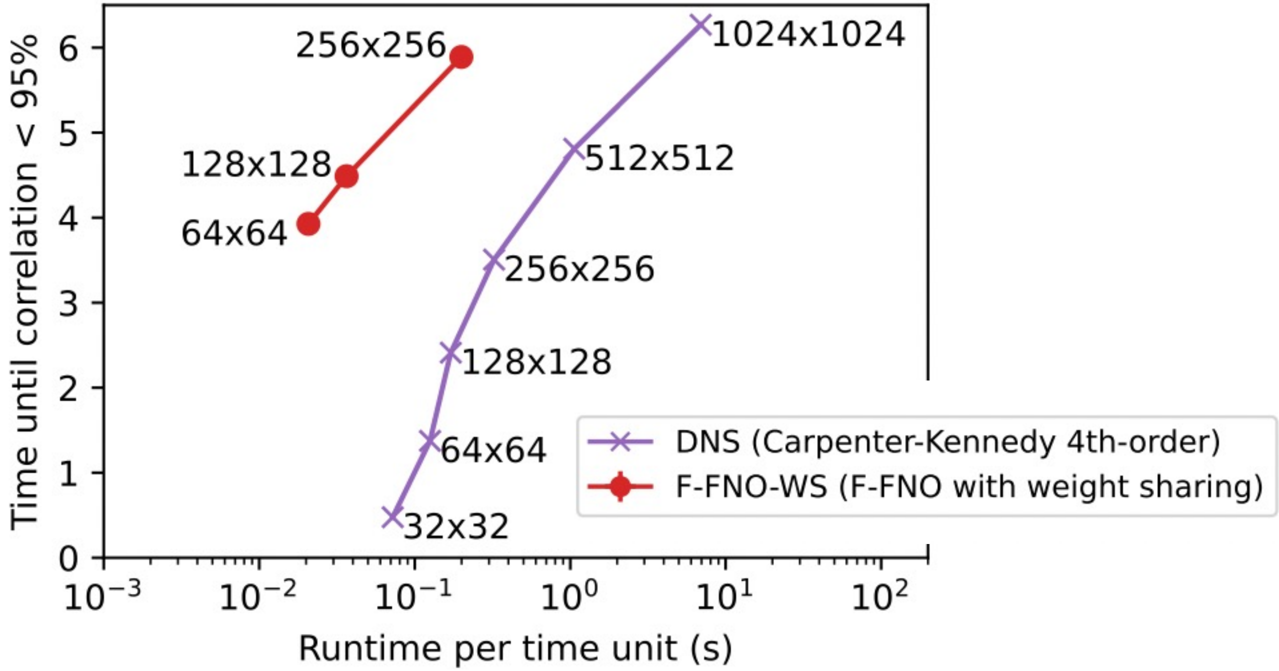




FNO compared to numerical solvers



2d Euler



2d NS

[13] F-FNO. Alasdair Tran et. al.

For larger scale, higher dimension, time-dependent problems, the neural operators seems to converge faster.

PINO: Physics-informed neural operator

Data loss: compare the prediction and ground-truth solution

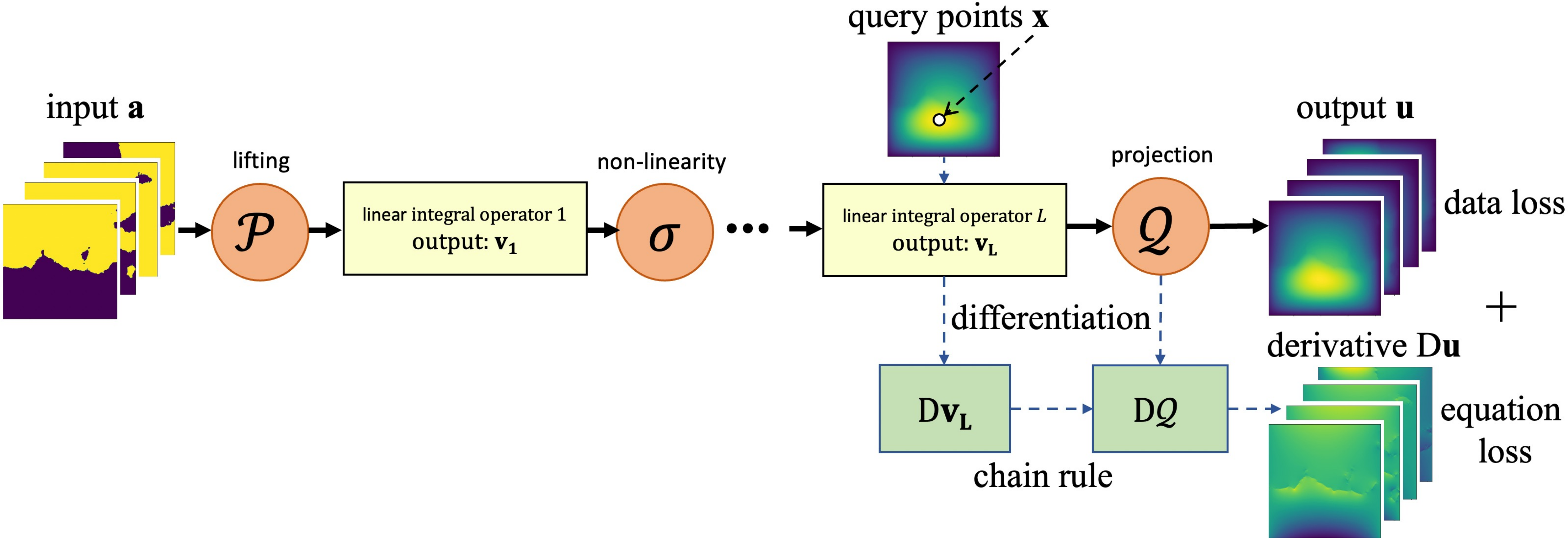
Equation loss: plug the prediction into PDE and compute the residual

$$\begin{aligned} -\nabla \cdot (a(x)\nabla u(x)) &= f(x), \quad && x \in D \\ u(x) &= 0, && x \in \partial D \end{aligned}$$

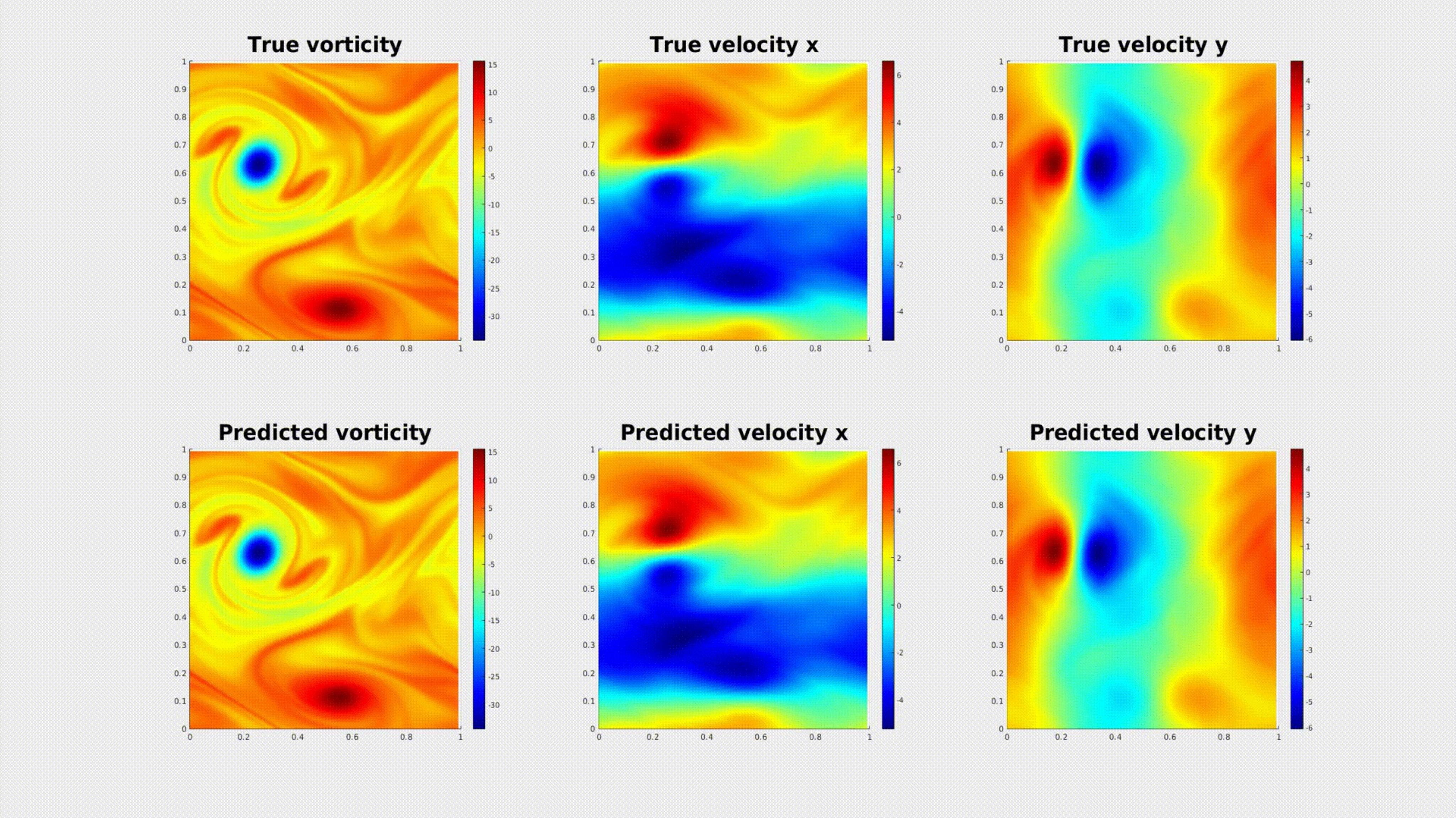
[14] PINO: LZKJCLAA

[15] Fourier-continuation PINO: MLWLBHA

PINO: Physics-informed neural operator

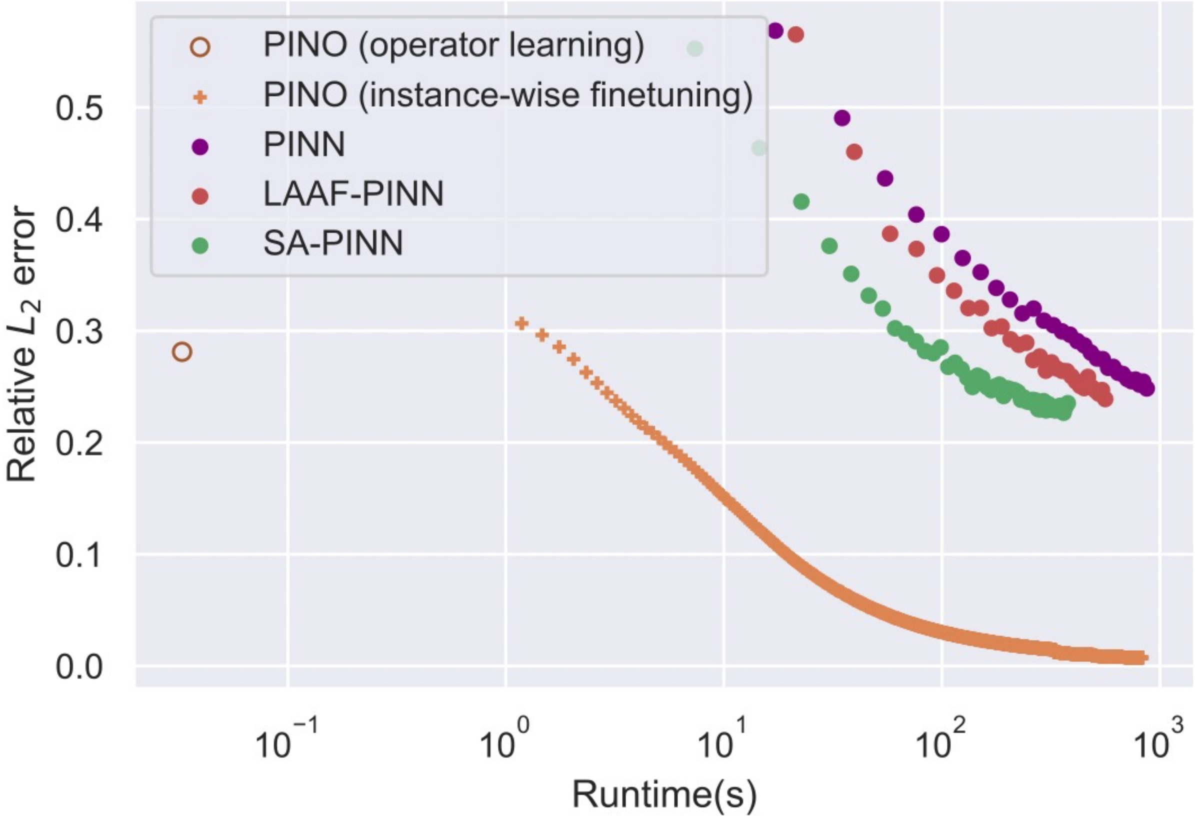


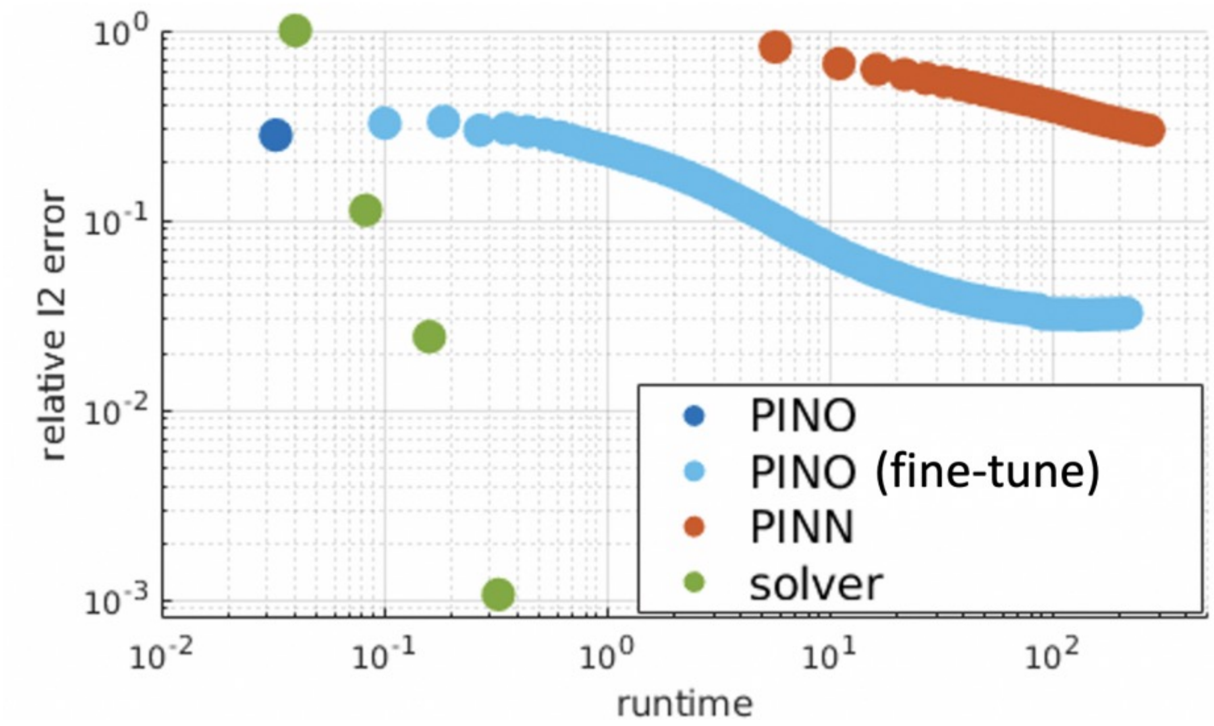
- PINO gets 2% error on Re500 [2π x 2π x 1s]
- Easily generalize from one Re to another



Relative error: PINO: 0.9%, PINN:18.7%

Convergence

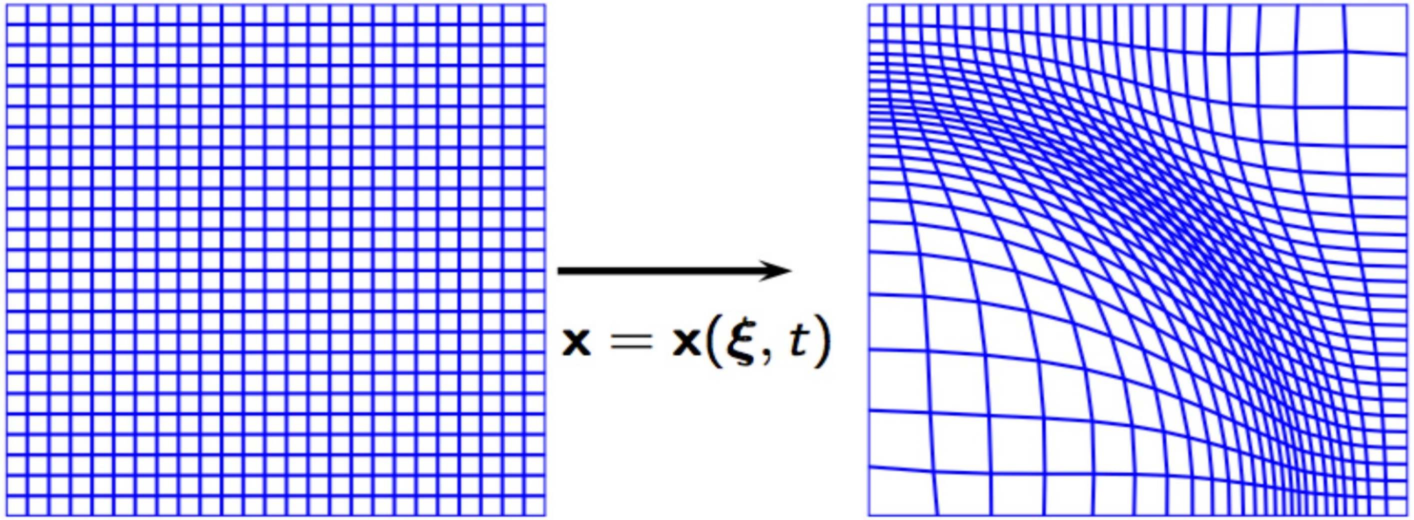




PINO converges faster than PINNs but slower than solvers

Geo-FNO: geometric-aware neural operator

Use deformation to construct adaptive meshes for complex geometries and multiscale structures.

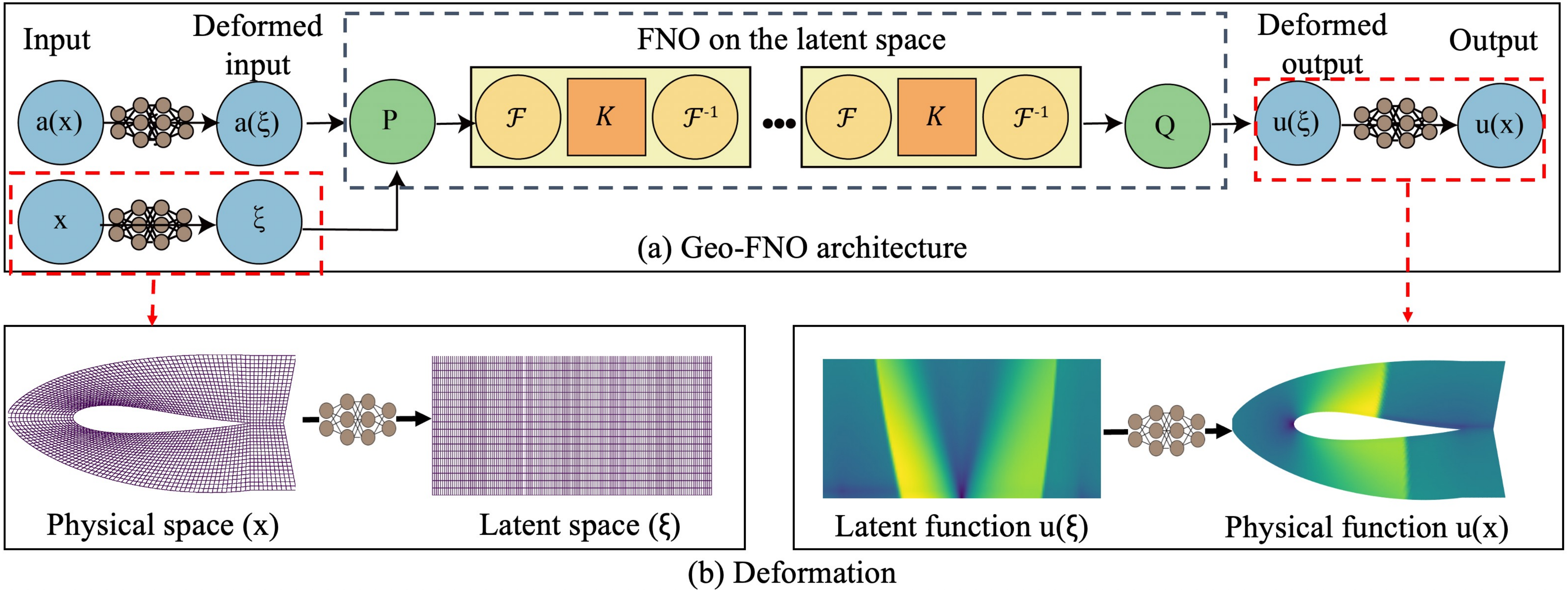


FFT computation mesh

Adaptive mesh

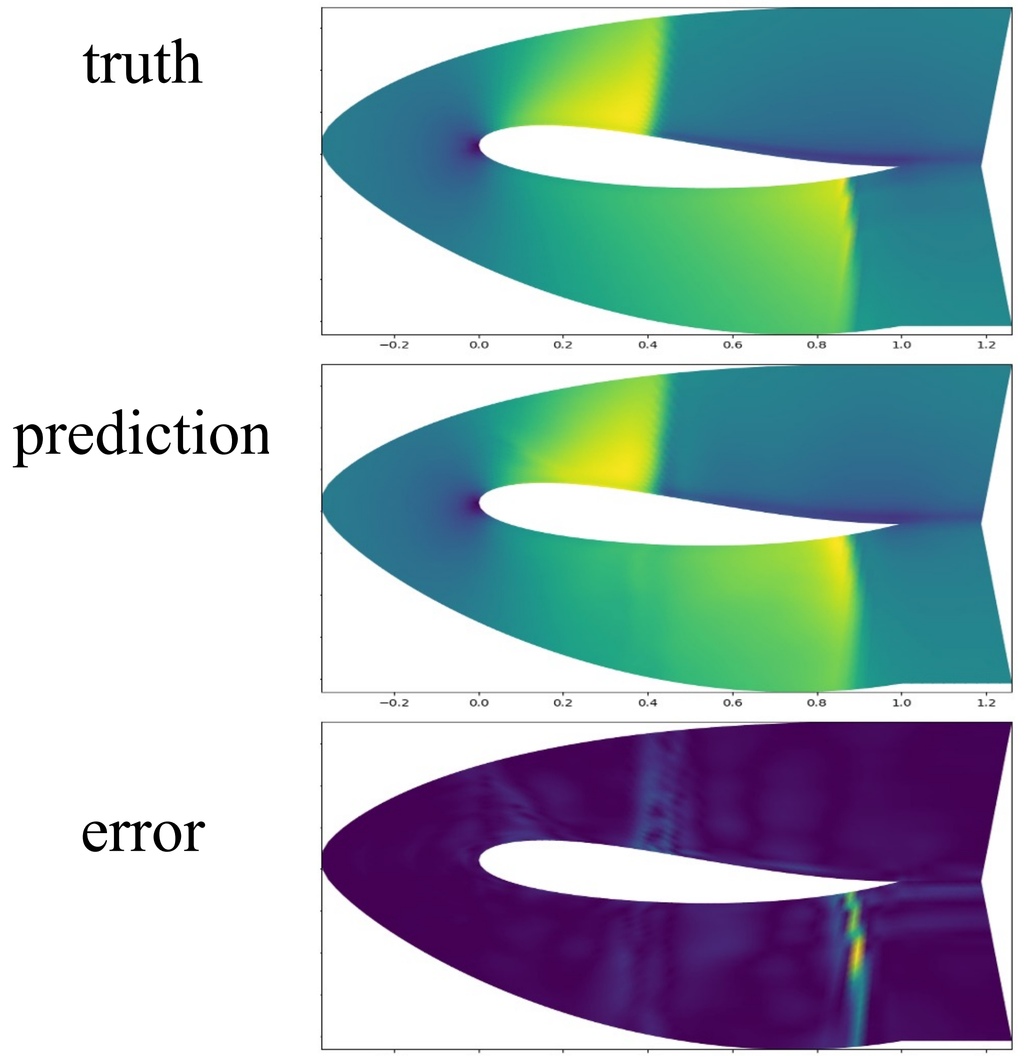
Geo-FNO

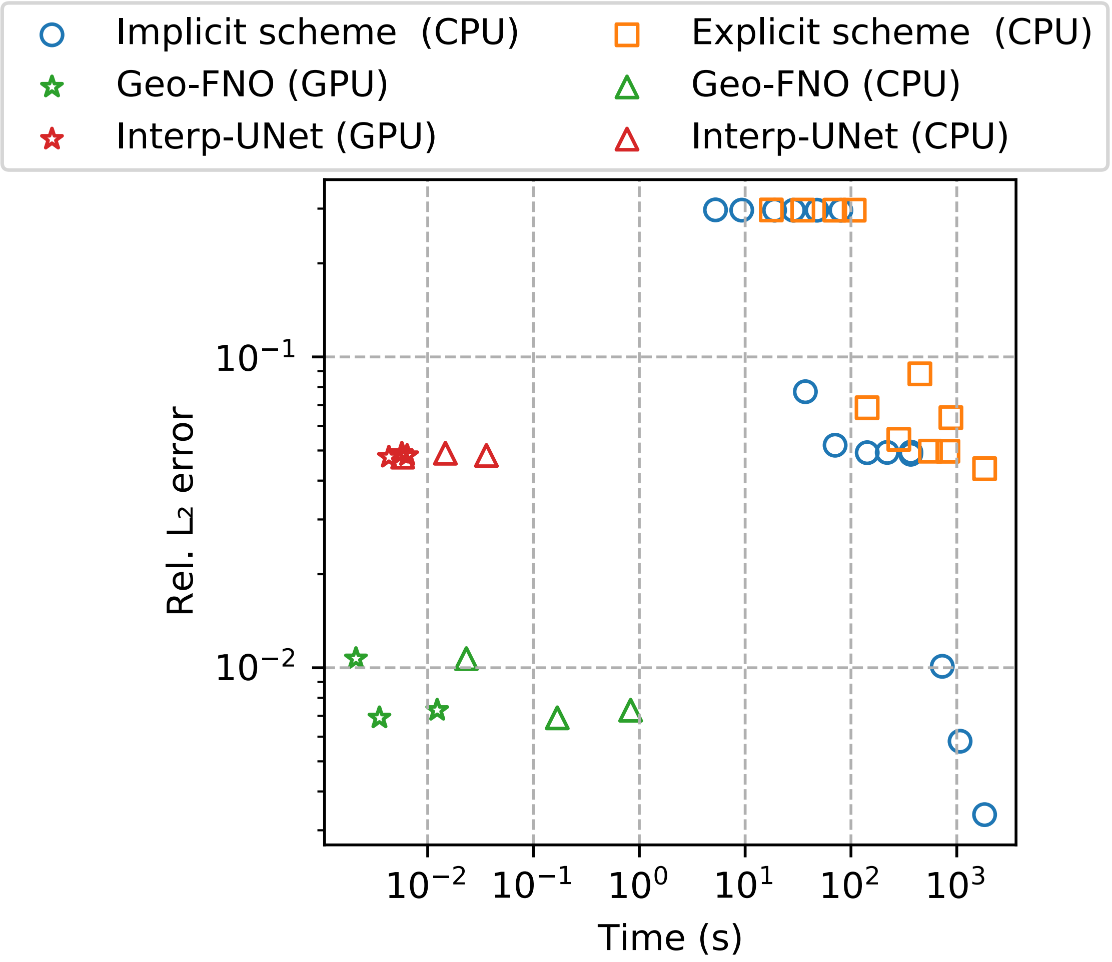
Idea: deform the irregular physical space to a uniform latent space, so the FFT can be applied in the latent space.



[19] Geo-FNO: LZLA

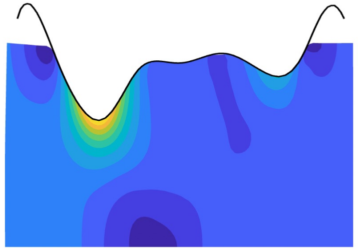
Examples: Airfoils

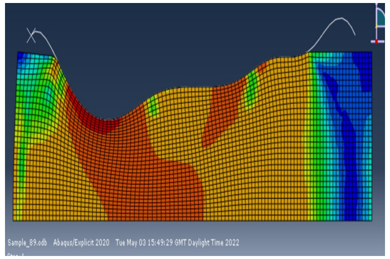




Error = 1.3%
10^5 speedup

Examples: Plastic equation

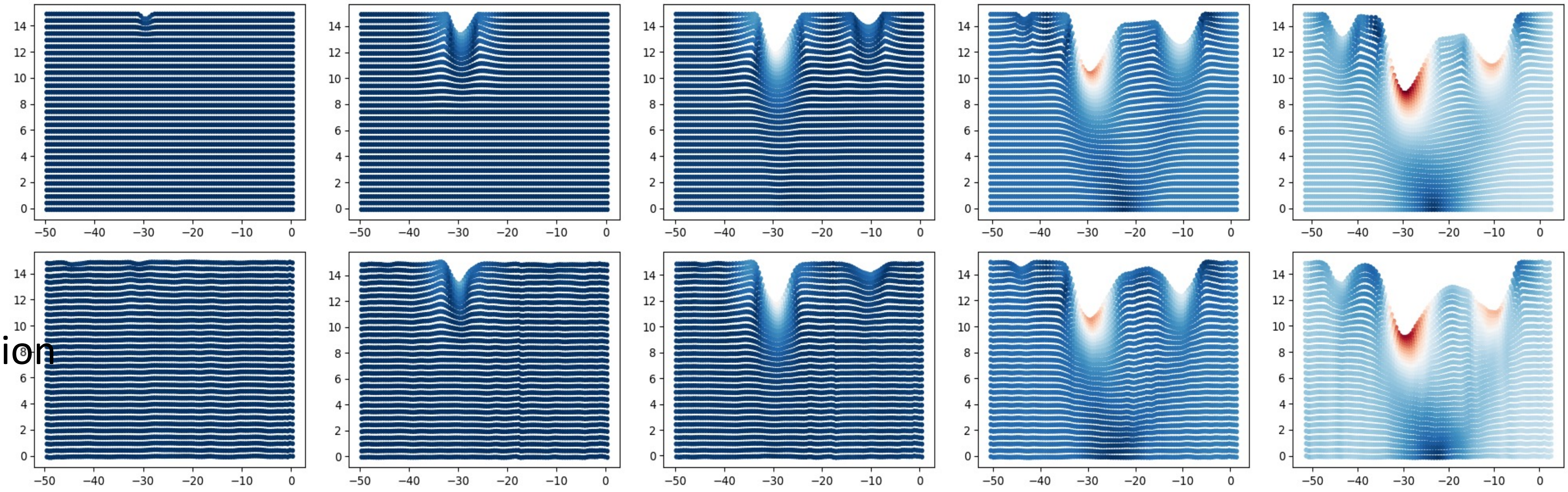




Plastic forging problem: a block of material is impacted by a frictionless, rigid die from top.

Truth

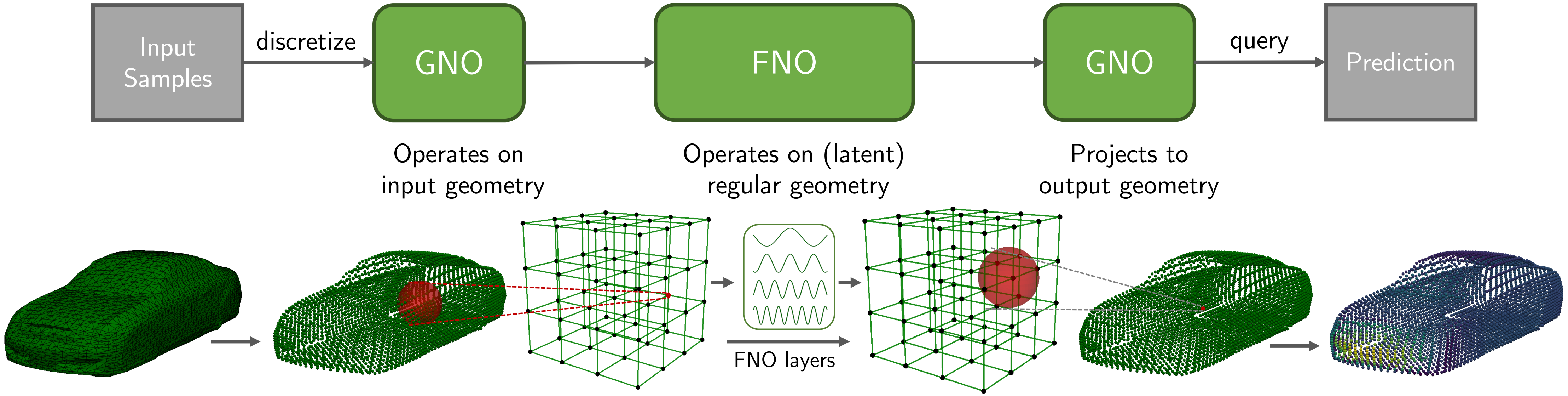
Prediction



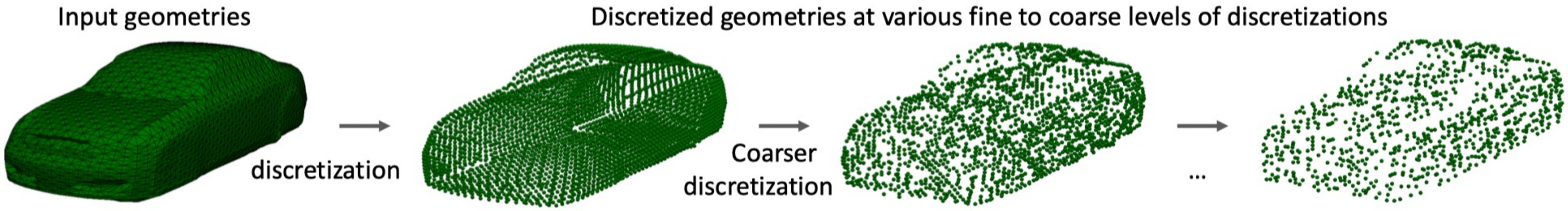
t=4 t=8 t=12 t=16 t=20

Error = 0.7%

Fourier + Graph representation

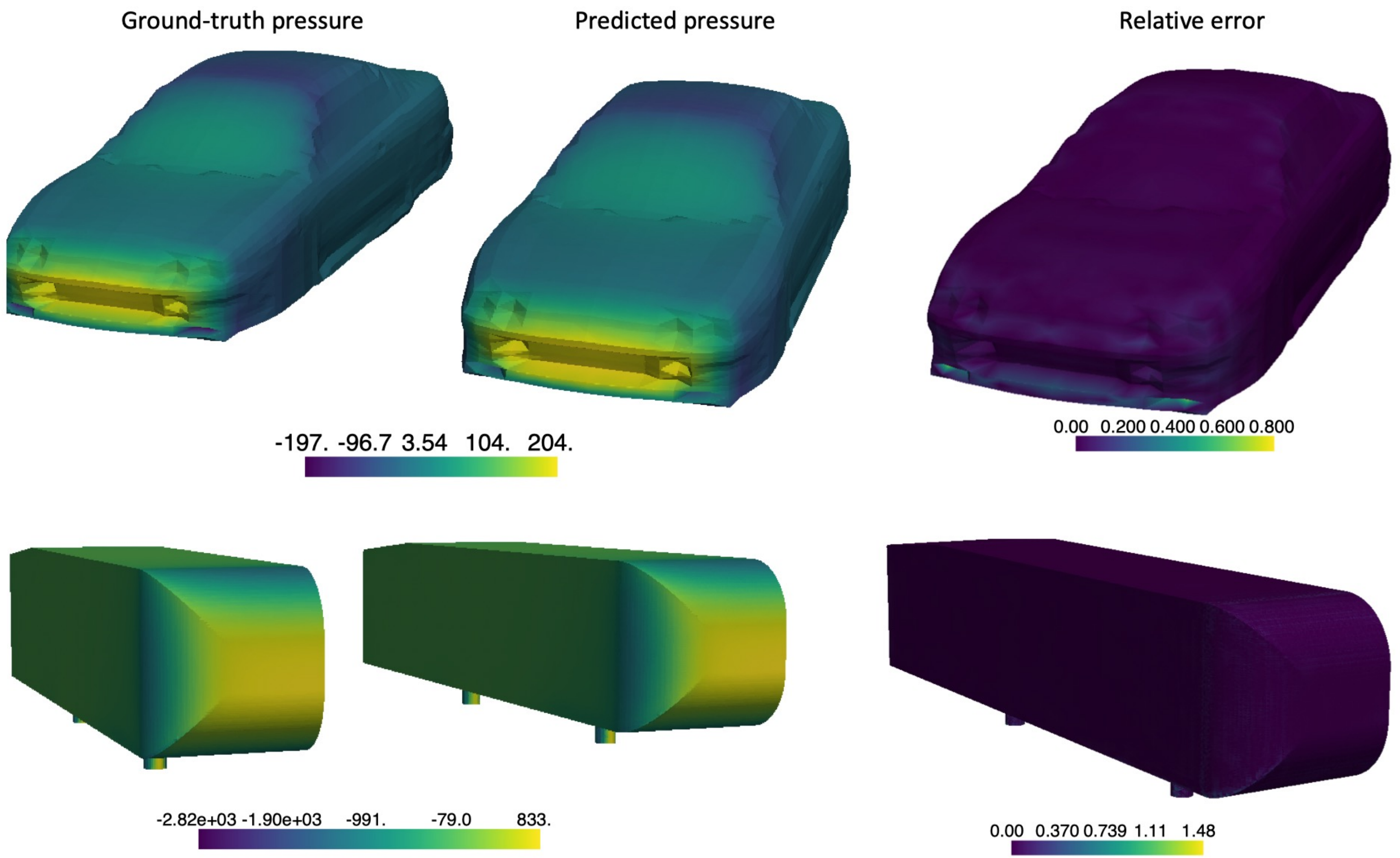


Irregular grid + Discretization consistent

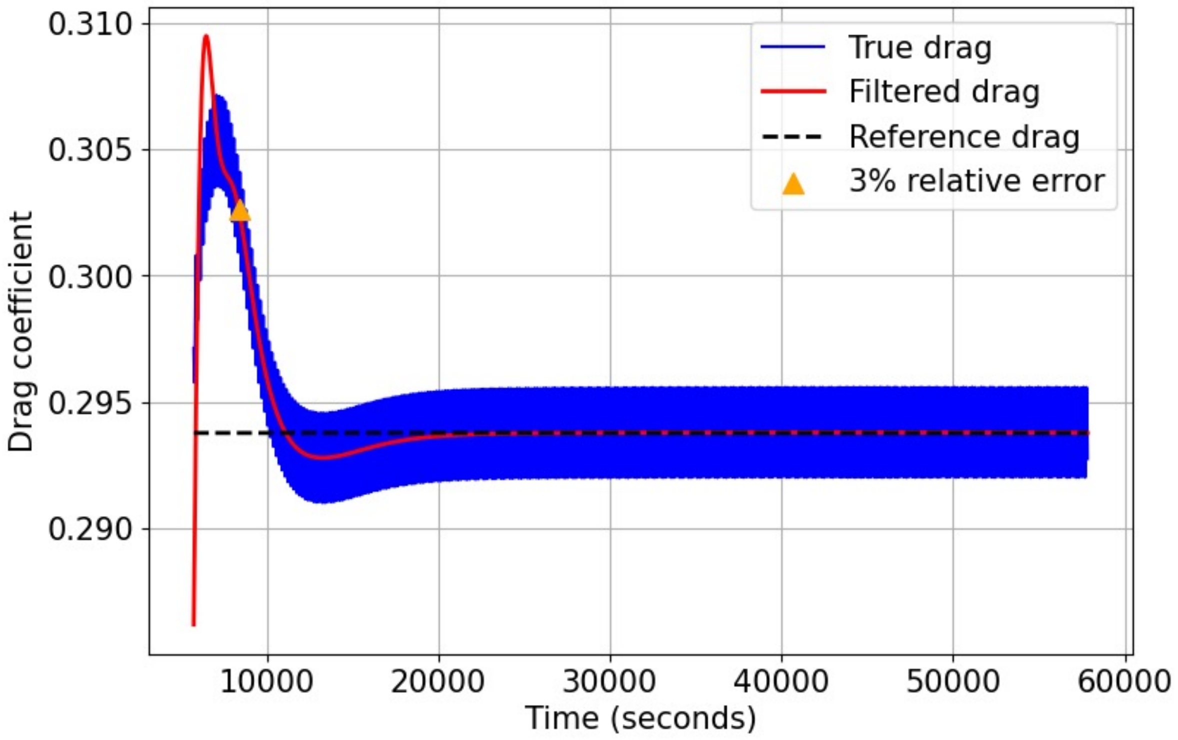


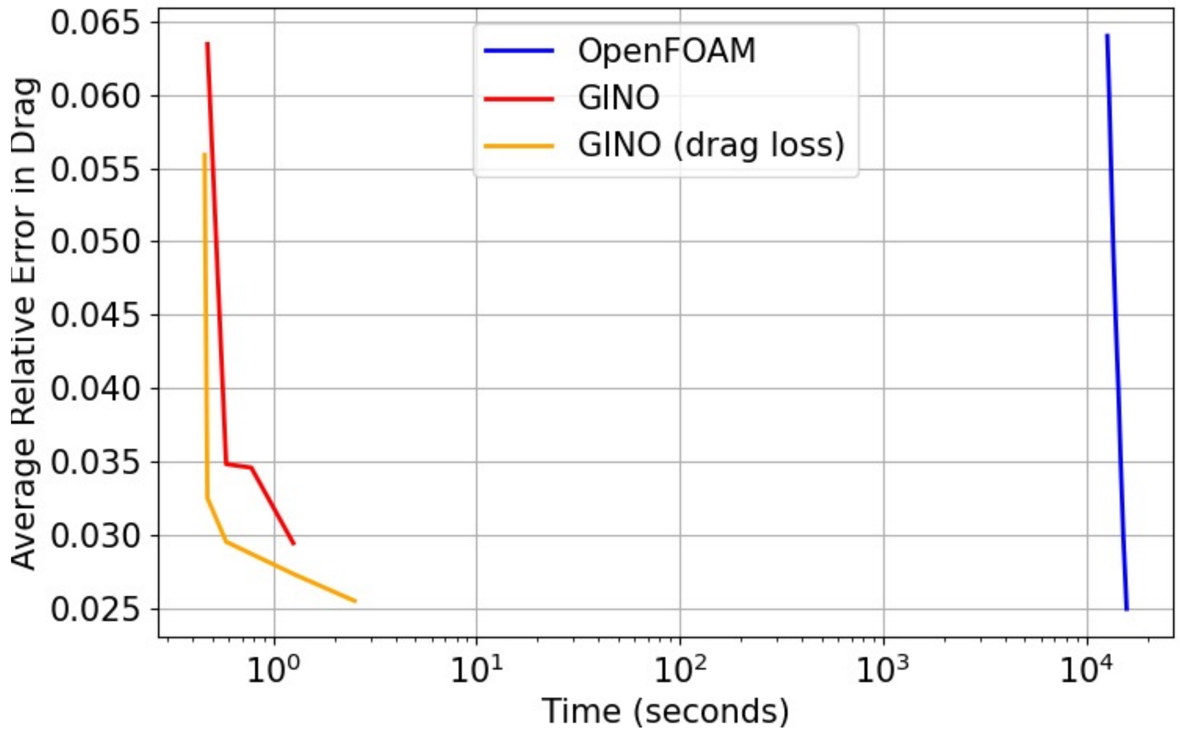
Model	Range	Complexity	Irregular grid	Discretization invariant
GNN	local	$O(N\text{degree})$	✔	✗
CNN	local	$O(N)$	✗	✗
UNet	global	$O(N)$	✗	✗
Transformer	global	$O(N^2)$	✔	✔
GNO (kernel)	radius r	$O(N\text{degree})$	✔	✔
FNO (FFT)	global	$O(N \log N)$	✗	✔
GINO [**Ours**]	global	$O(N \log N + N\text{degree})$	✔	✔

High accuracy



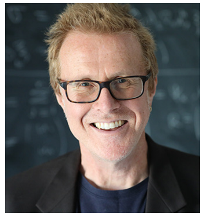
Drag coefficient





Caltech


Anima Anandkumar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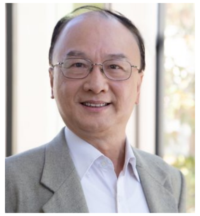
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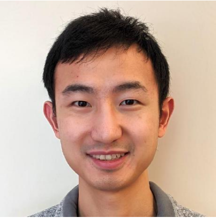
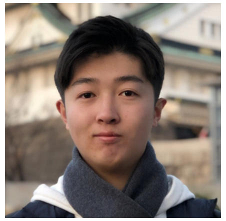

Daniel Zhengyu Huang


Jiawei Zhao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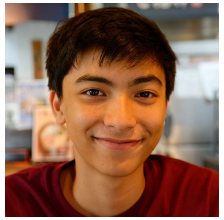
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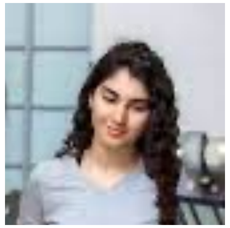
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Nikola B. Kovachki


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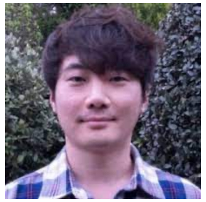
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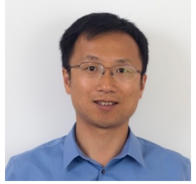
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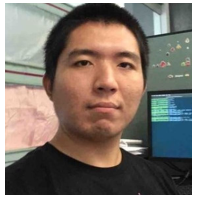
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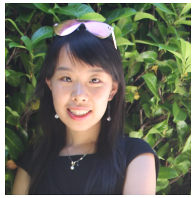
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Shashank Subramanian


Peter Harrington

References

1. Pathak, Jaideep, et al. "Fourcastnet: A global data-driven high-resolution weather model using adaptive fourier neural operators." *arXiv preprint arXiv:2202.11214* (2022).
2. Wen, Gege, et al. "Real-time high-resolution CO 2 geological storage prediction using nested Fourier neural operators." *Energy & Environmental Science* (2023).
3. Li, Zongyi, et al. "Neural operator: Graph kernel network for partial differential equations." *arXiv preprint arXiv:2003.03485* (2020).
4. Li, Zongyi, et al. "Fourier neural operator for parametric partial differential equations." *arXiv preprint arXiv:2010.08895* (2020).
5. Kovachki, Nikola, et al. "Neural operator: Learning maps between function spaces." *arXiv preprint arXiv:2108.08481* (2021).
6. Kovachki, Nikola, Samuel Lanthaler, and Siddhartha Mishra. "On universal approximation and error bounds for fourier neural operators." *The Journal of Machine Learning Research* 22.1 (2021): 13237-13312.
7. Lanthaler, Samuel, et al. "Nonlinear reconstruction for operator learning of pdes with discontinuities." *arXiv preprint arXiv:2210.01074* (2022).
8. De Hoop, Maarten, et al. "The cost-accuracy trade-off in operator learning with neural networks." *arXiv preprint arXiv:2203.13181* (2022).
9. Takamoto, Makoto, et al. "PDEBench: An extensive benchmark for scientific machine learning." *Advances in Neural Information Processing Systems* 35 (2022): 1596-1611.
10. Gupta, Jayesh K., and Johannes Brandstetter. "Towards Multi-spatiotemporal-scale Generalized PDE Modeling." *arXiv preprint arXiv:2209.15616* (2022).
11. Bi, Kaifeng, et al. "Pangu-Weather: A 3D High-Resolution Model for Fast and Accurate Global Weather Forecast." *arXiv preprint arXiv:2211.02556* (2022).
12. Lam, Remi, et al. "GraphCast: Learning skillful medium-range global weather forecasting." *arXiv preprint arXiv:2212.12794* (2022).
13. Tran, Alasdair, et al. "Factorized fourier neural operators." *arXiv preprint arXiv:2111.13802* (2021).
14. Li, Zongyi, et al. "Physics-informed neural operator for learning partial differential equations." *arXiv preprint arXiv:2111.03794* (2021).
15. Maust, Haydn, et al. "Fourier Continuation for Exact Derivative Computation in Physics-Informed Neural Operators." *arXiv preprint arXiv:2211.15960* (2022).
16. Liu, Burigede, et al. "A learning-based multiscale method and its application to inelastic impact problems." *Journal of the Mechanics and Physics of Solids* 158 (2022): 104668.
17. Williams, Francis, et al. "Neural fields as learnable kernels for 3d reconstruction." *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*. 2022.
18. Liu, Mingjie, et al. "An Adversarial Active Sampling-based Data Augmentation Framework for Manufacturable Chip Design." *arXiv preprint arXiv:2210.15765* (2022).
19. Li, Zongyi, et al. "Fourier neural operator with learned deformations for pdes on general geometries." *arXiv preprint arXiv:2207.05209* (2022).
20. Li, Zongyi, et al. "Multipole graph neural operator for parametric partial differential equations." *Advances in Neural Information Processing Systems* 33 (2020): 6755-6766.
21. Bruno, Oscar P., Jan S. Hesthaven, and Daniel V. Leibovici. "FC-based shock-dynamics solver with neural-network localized artificial-viscosity assignment." *Journal of Computational Physics: X* 15 (2022): 100110.