FOURIER NEURAL OPERATORS FOR FAST WEATHER MODELING

ANIMA ANANDKUMAR

CHALLENGE: DRAMATIC RISE IN EXTREME WEATHER ACROSS THE GLOBE

CLIMATE SCIENCE REQUIRES MILLION-X SPEEDUPS

Computational constraints limit model resolution

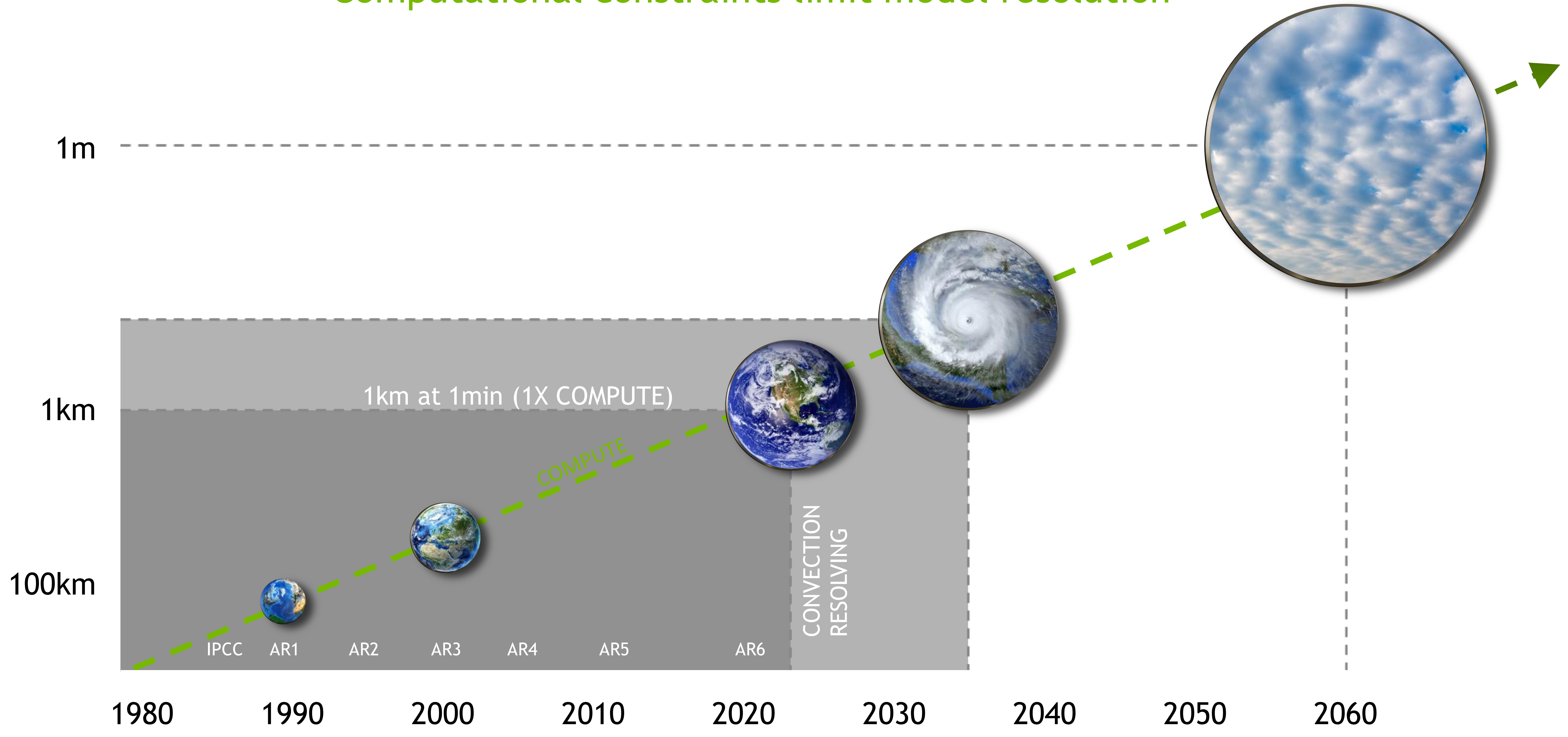
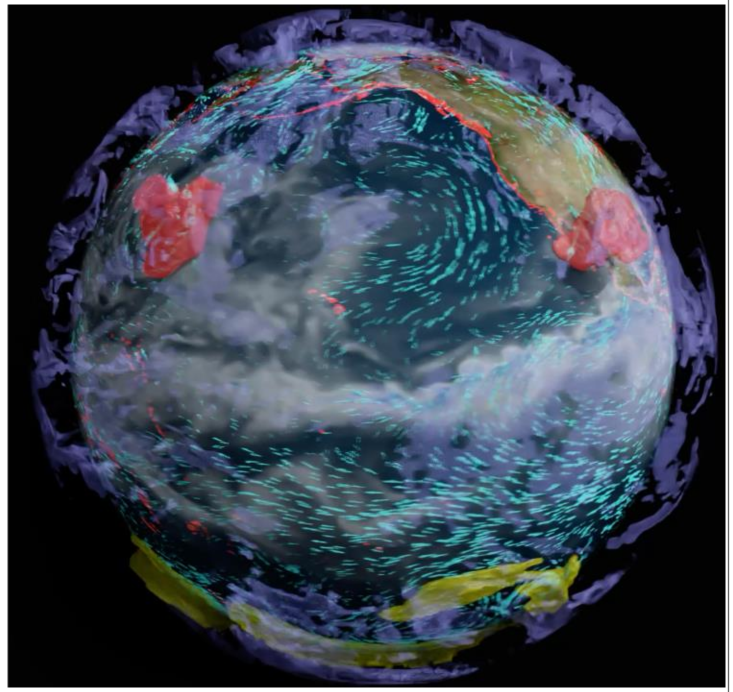
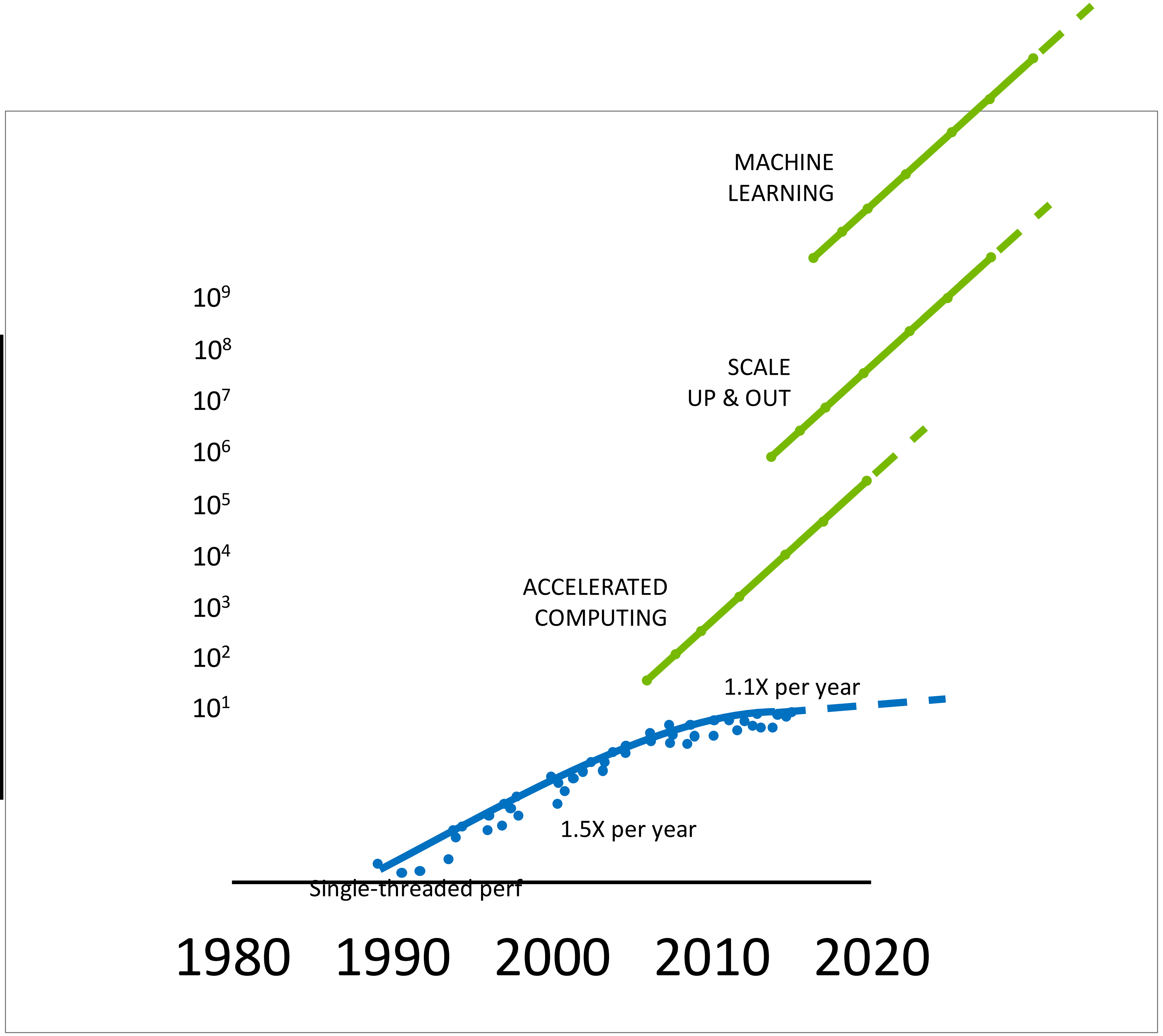


Figure adapted from: Schneider, T., Teixeira, J., Bretherton, C. *et al.* Climate goals and computing the future of clouds. *Nature Climate Change* **7,** 3–5 (2017). https://doi.org/10.1038/nclimate3190

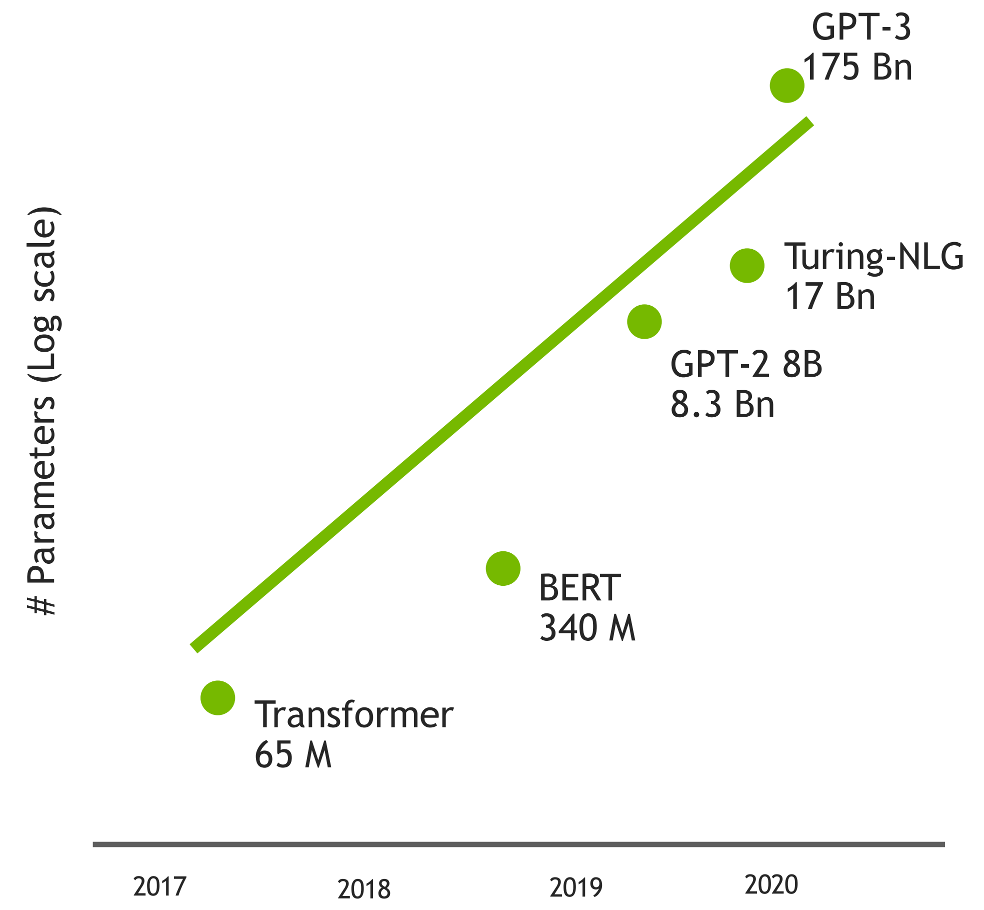
MILLION-X LEAP IN SCIENTIFIC COMPUTING





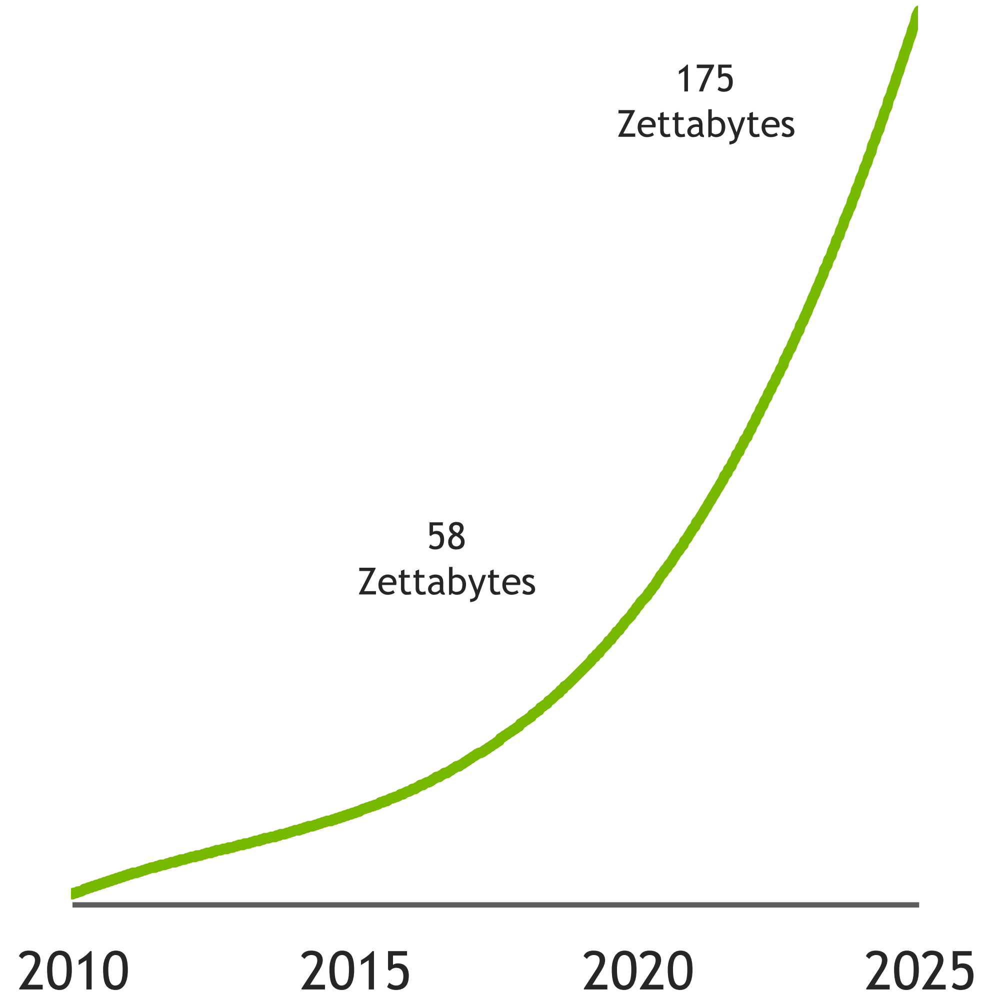
EXPLODING DATA AND MODEL SIZE

EXPLODING MODEL SIZE
Driving Superhuman Capabilities



BIG DATA GROWTH
90% of the World's Data in last 2 Years

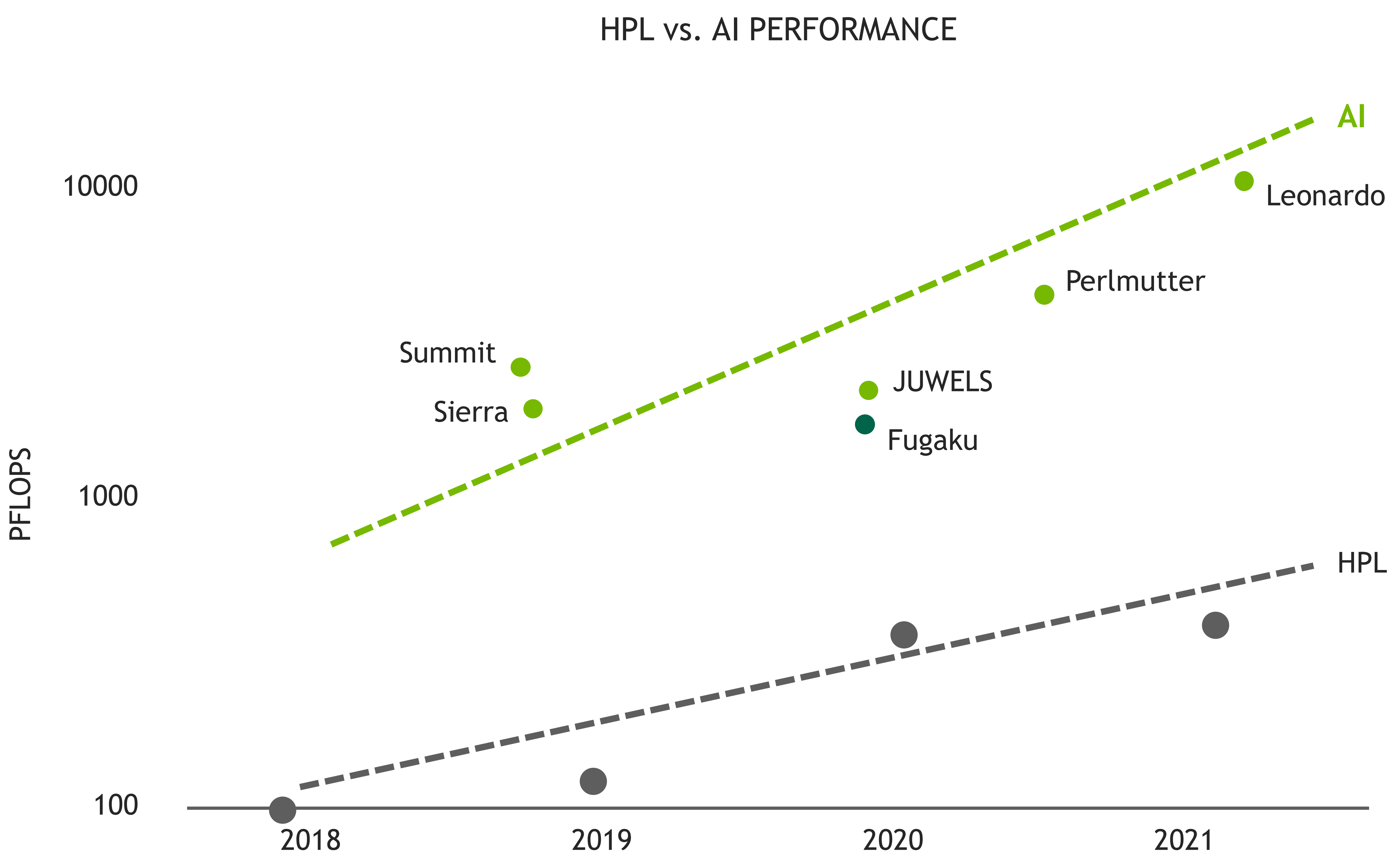
GROWTH IN SCIENTIFIC DATA
Fueled by Accurate Sensors & Simulations



Source for Big Data Growth chart: IDC — The Digitization of the World (May, 2020)

THE ERA OF EXASCALE AI SUPERCOMPUTING

AI is the New Growth Driver for Modern HPC

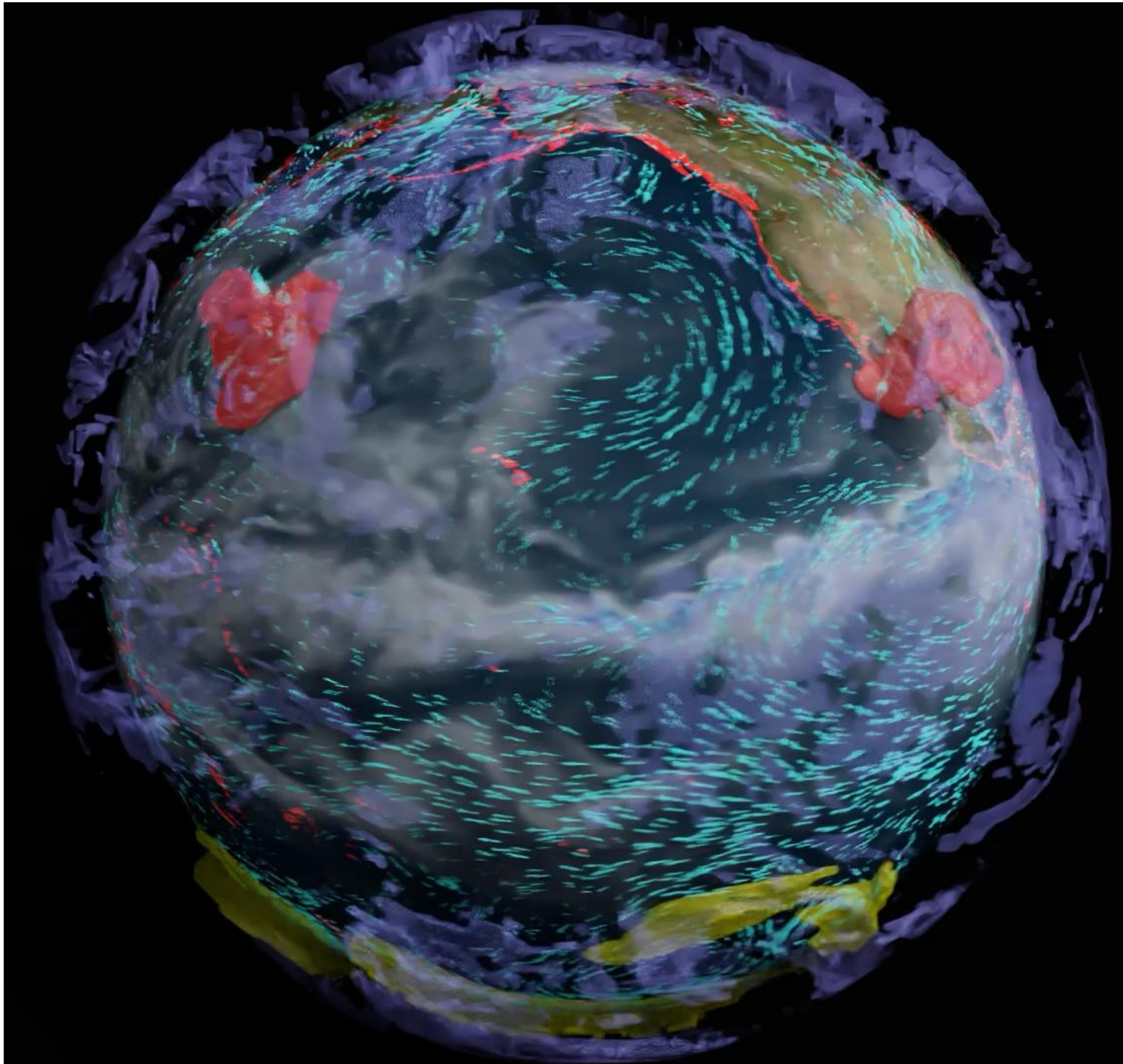


HPL: Based on #1 system in June Top500
AI: Peak system FP16 FLOPS

ANNOUNCING EARTH-2 SUPERCOMPUTER

Enabling Million-X Development
in Climate Modeling

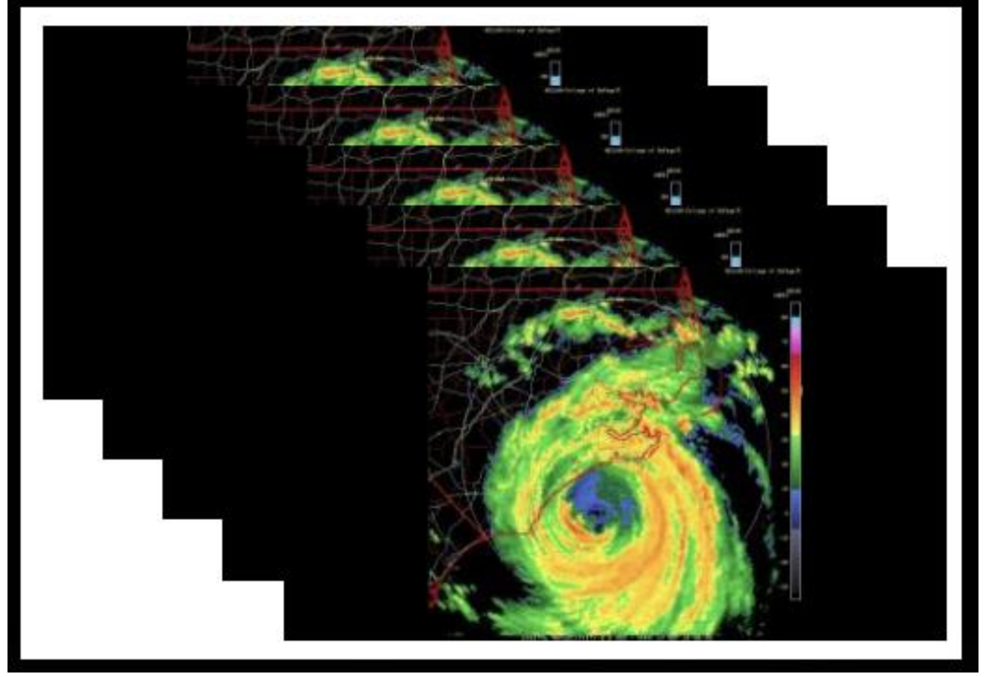
- Pledge to dedicate engineering and AI resources at NVIDIA
- Fine-scale weather and climate modeling
- Uncertainty calibration for extreme weather risks
- Simulation is the answer

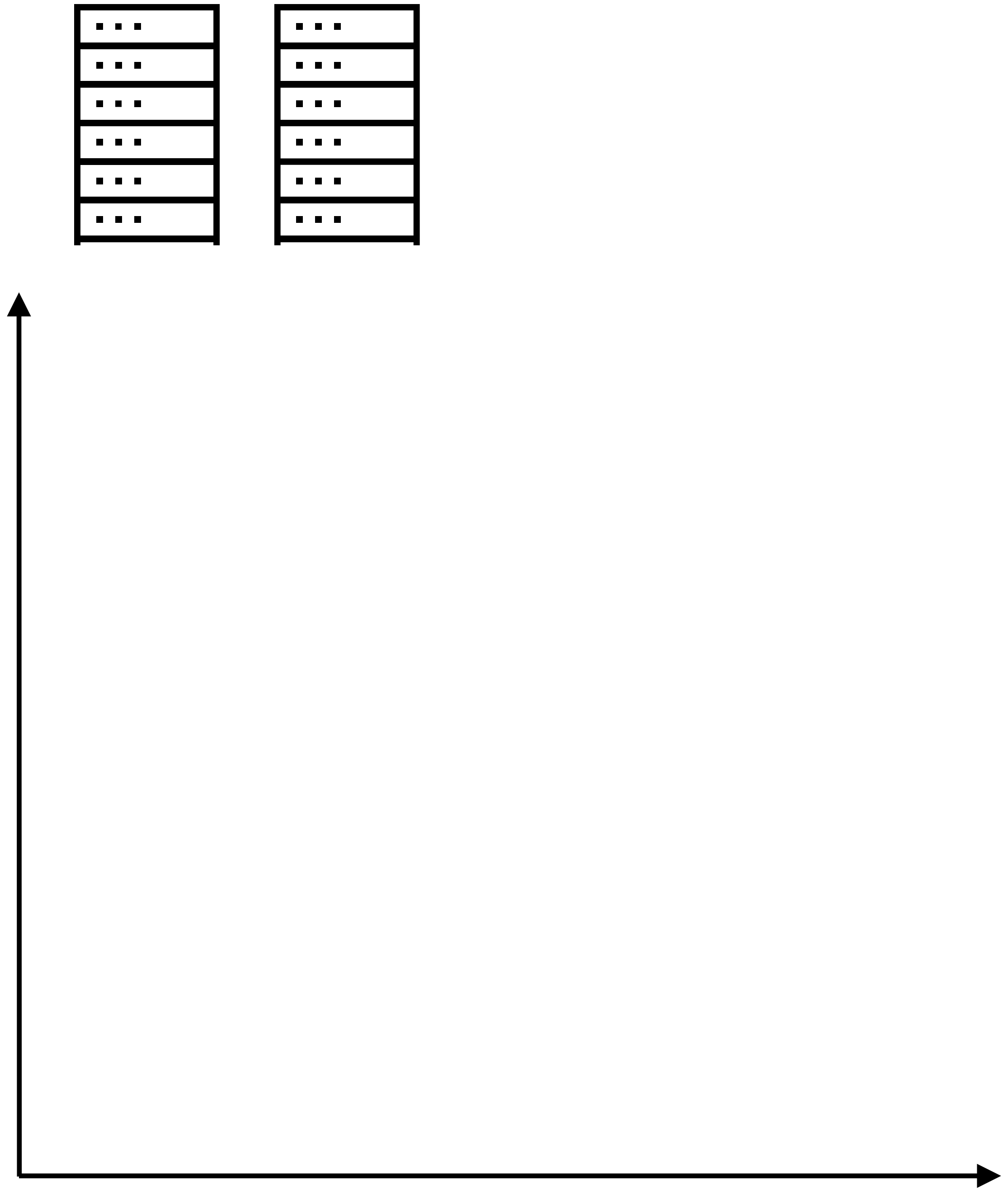


CLIMATE SCIENCE REQUIRES MILLION-X SPEEDUPS

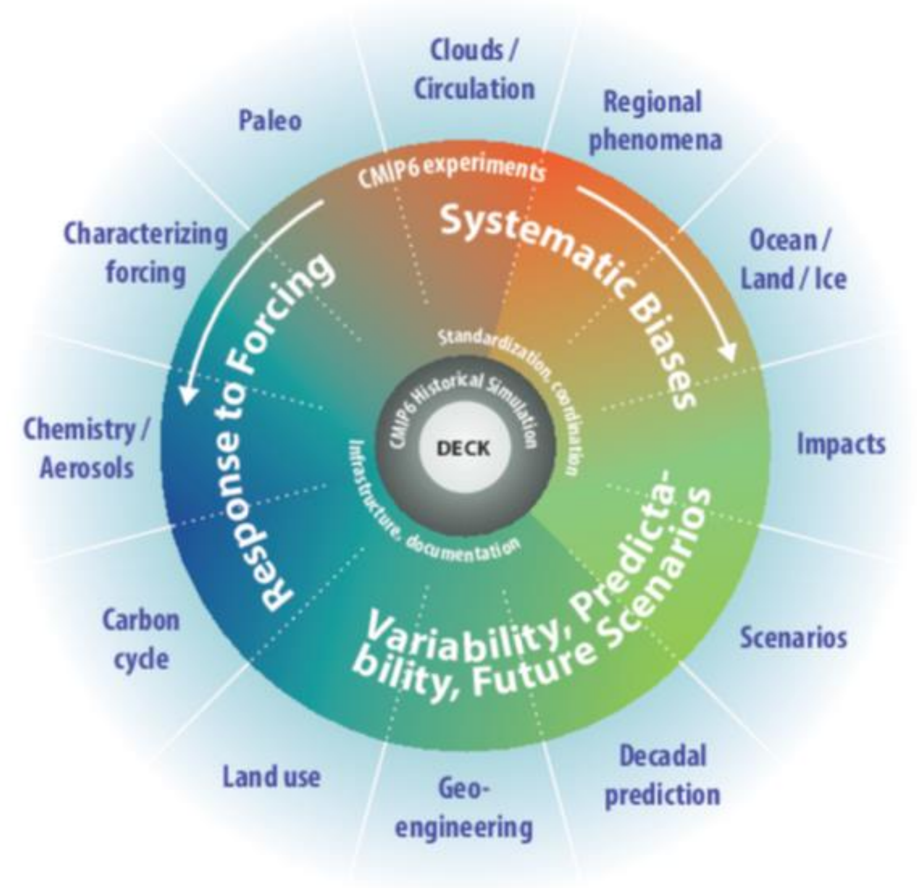
Computational constraints limit the size of ensembles and how many scenarios can be explored

10s —> 1000s OF MEMBERS

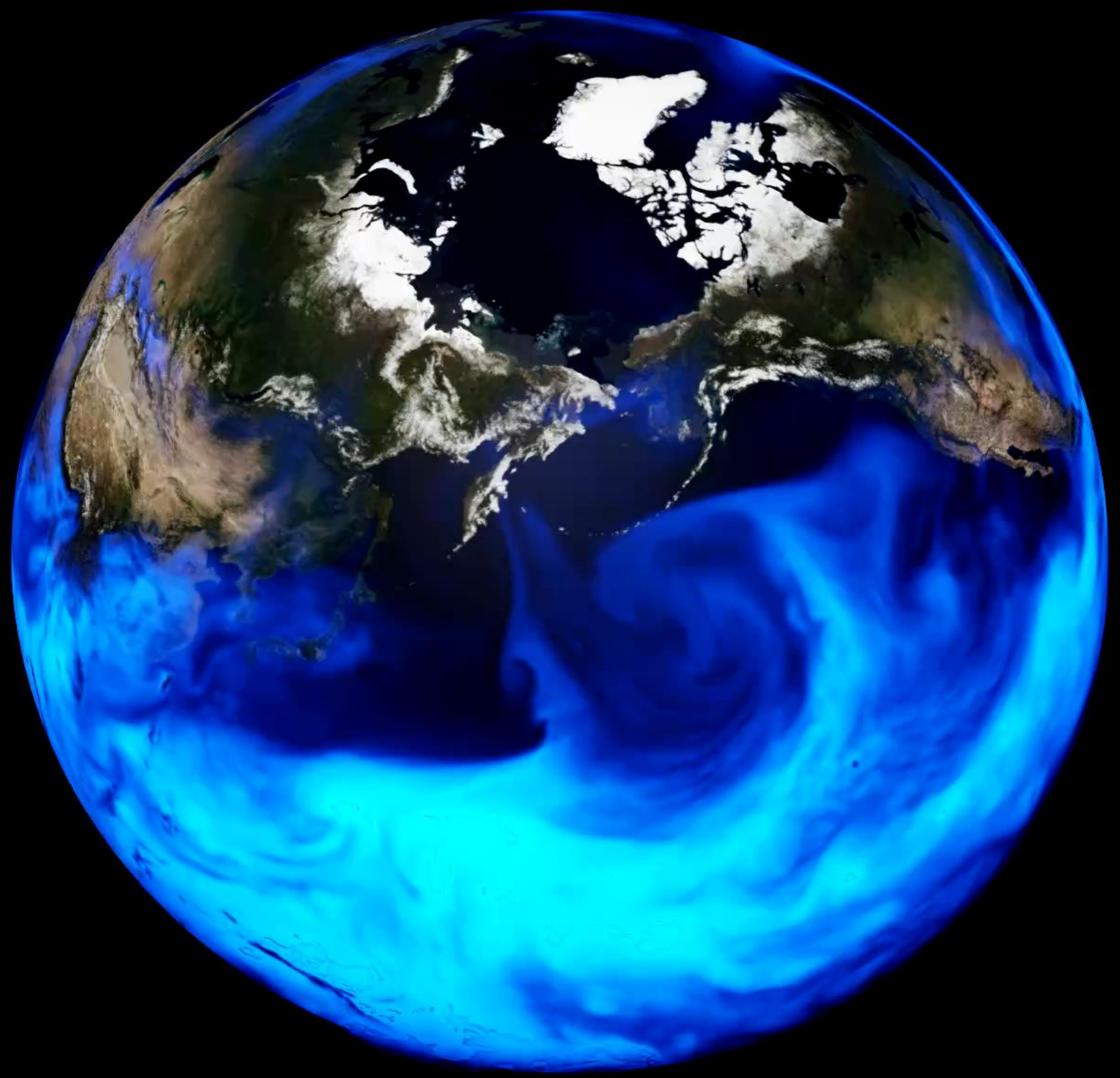




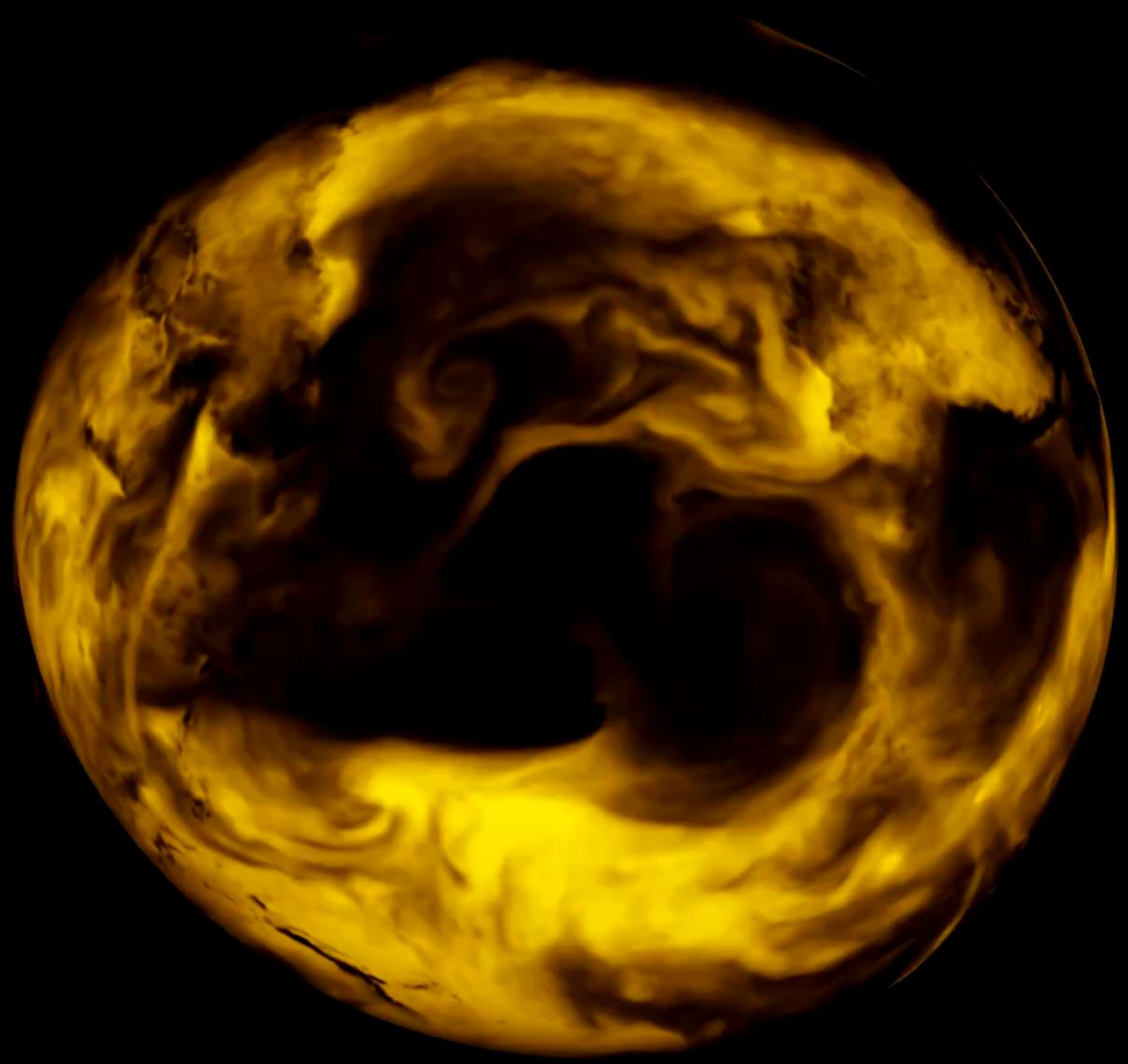
10s —> 1000s OF SCENARIOS



Ground Truth



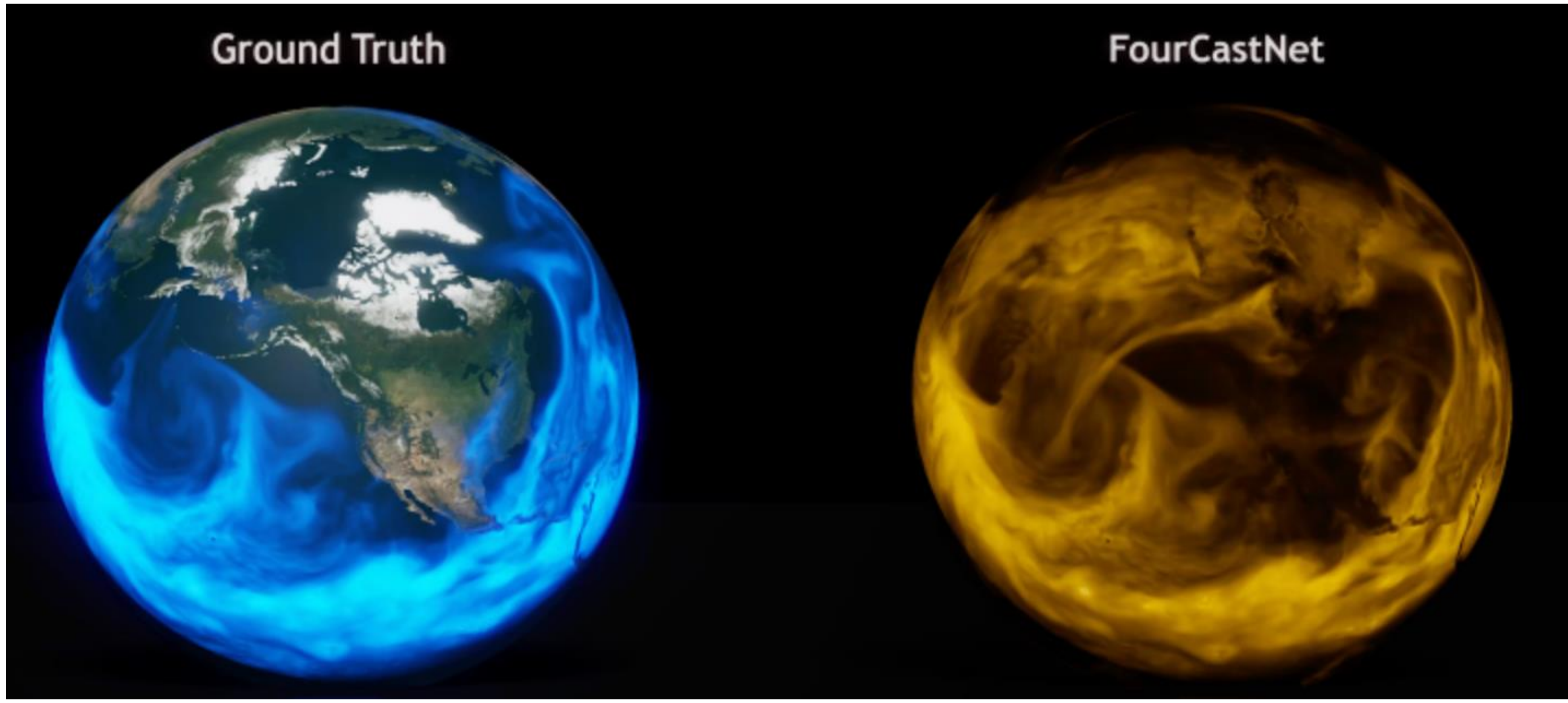
FourCastNet



FINE-SCALE WEATHER PREDICTION

FourCastNet uses FNO to obtain unprecedented speed and accuracy

- FourCastNet is a data-driven model trained on 10 TB of weather data
- Uses FNO with transformer backbone
- Unparalleled accuracy of surface winds and precipitation up to one week.
- 8x higher resolution than any other AI model for weather forecasting.
- 1000-member ensemble in a fraction of a second.
- 4 to 5 orders of magnitude speedup over NWP.
- 25000X smaller energy footprint.



GRID-FREE LEARNING FOR CONTINUOUS PHENOMENA

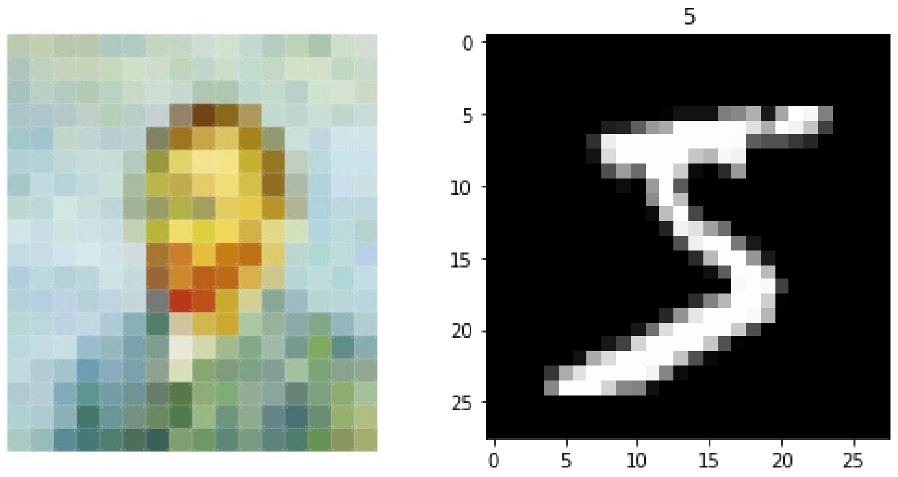
Learning operators between continuous inputs and outputs

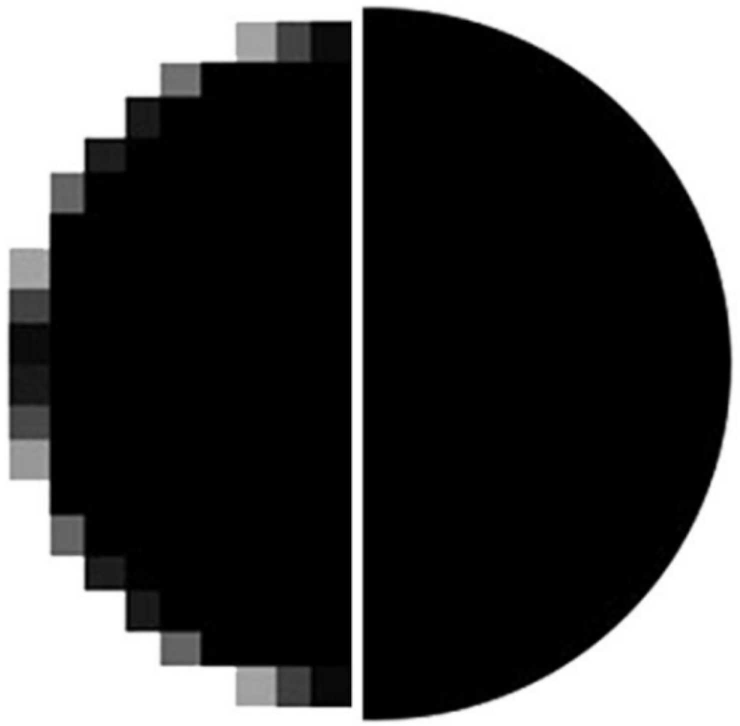
Neural Network

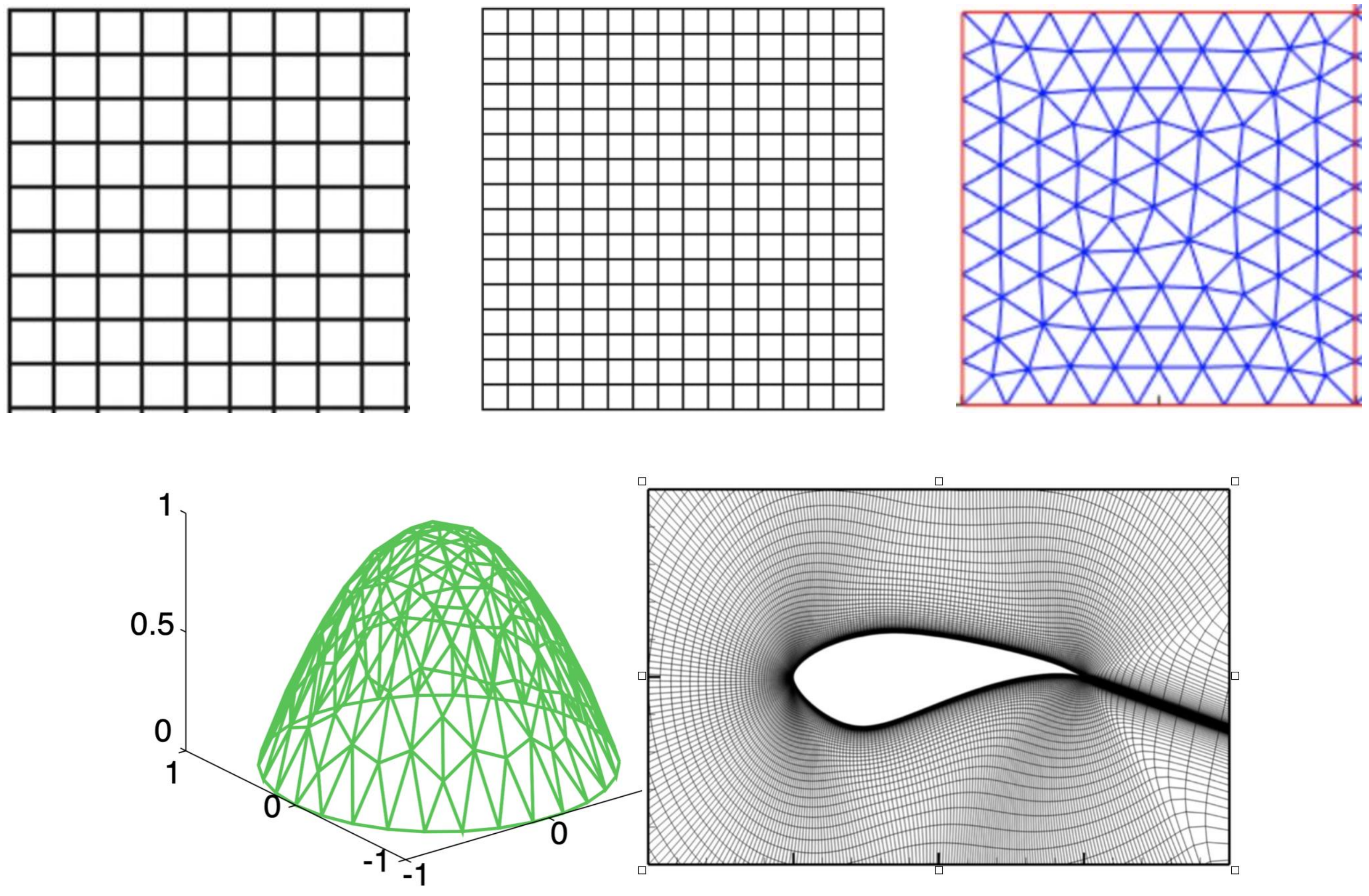
Function: Mapping in finite dimensions.

Neural Operator

Operator: Mapping in infinite dimensions (function space).







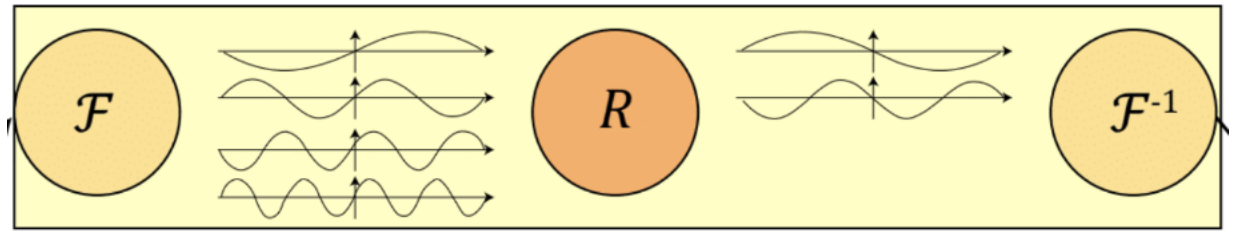
Discretized input

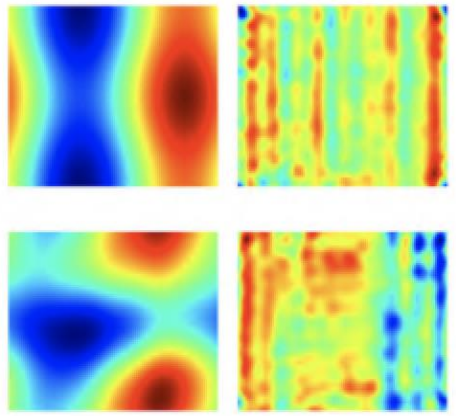
Continuous function

FNO: FOURIER NEURAL OPERATOR

New Framework for Learning PDEs

- Use Fourier Transform to implement kernel integration
- Reduce to learning weights in frequency domain





Input: coefficient function → Layer 1: Convolution operator → Non-linearity → • • → Output: solution function

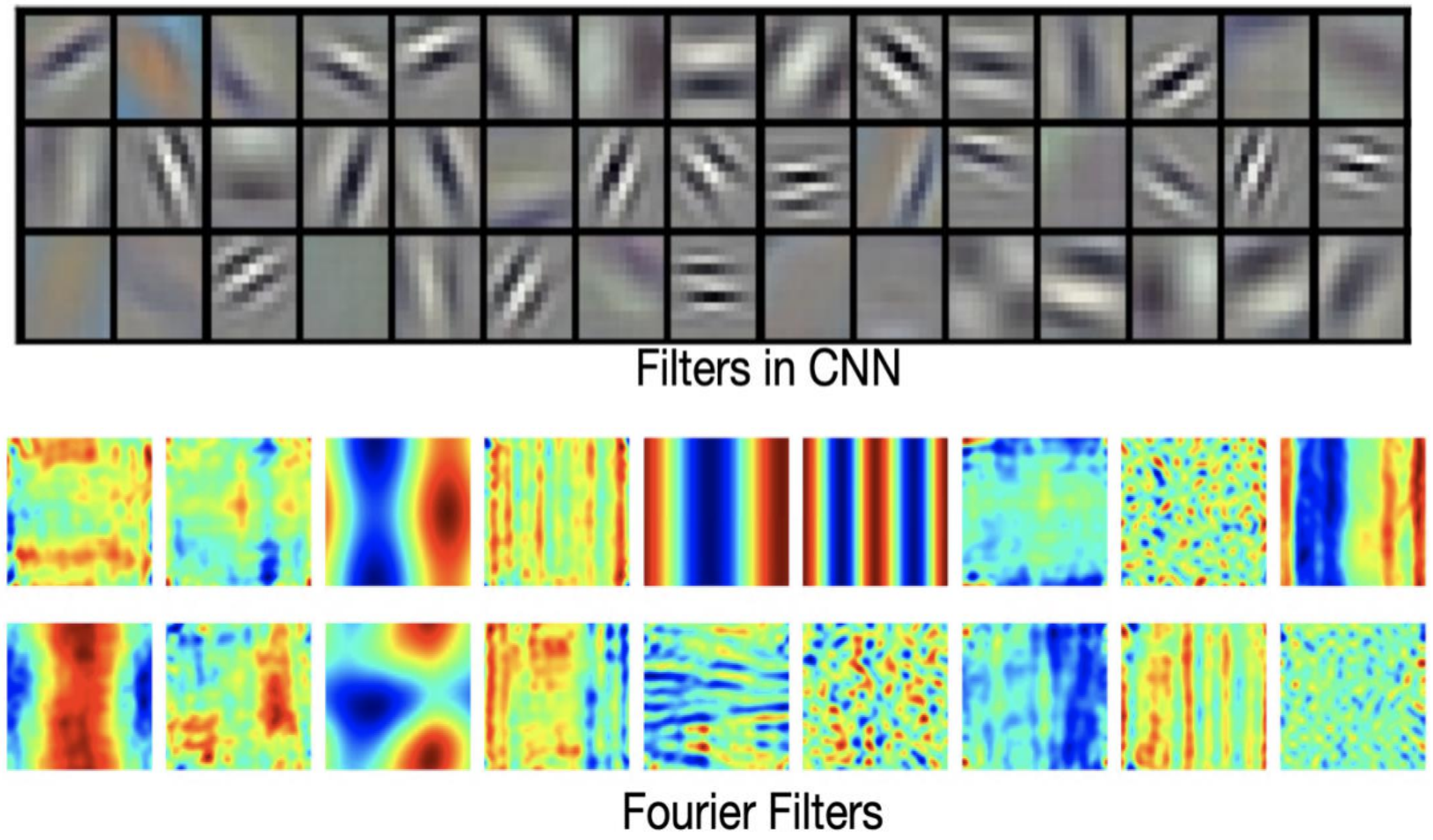
Fourier Neural Operator can approximate any operator: solutions of non-linear PDEs

Z. Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, A. Anandkumar "Fourier Neural Operator for Parametric Partial Differential Equations" ICLR 2021

FOURIER TRANSFORM FOR GLOBAL CONVOLUTION

$$
\begin{aligned}
Kv_l &= \int_D \kappa\big(x, y, a(x), a(y)\big) v_l(y) \mathrm{d}y \\
&\approx \int_D \kappa(x - y) v_l(y) \mathrm{d}y \\
&= \mathcal{F}^{-1}\big((\mathcal{F}\kappa) \cdot (\mathcal{F}v_l)\big) \\
&:= \mathcal{F}^{-1}\big(R \cdot (\mathcal{F}v_l)\big)
\end{aligned}
$$

Learn *R* in Fourier Domain



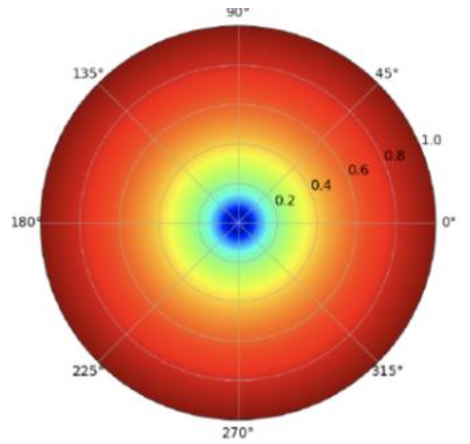
NEURAL OPERATOR

Learning in infinite dimensions

Composing linear integral operator with non-linearity.

Integral Operator

$$\int K(x, y)v(y)\mathrm{d}y$$



$K(x, y)$

Kernel of integral operator

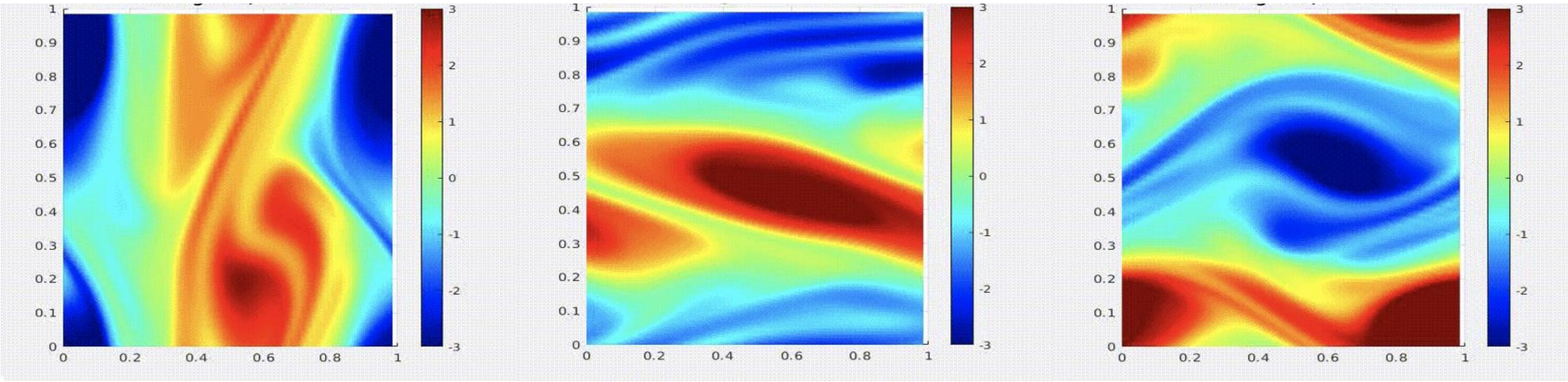
Input: Initial and boundary conditions → Linear operator → Non-linearity → • • → Output: Solution function

Neural Operator can approximate any continuous operator

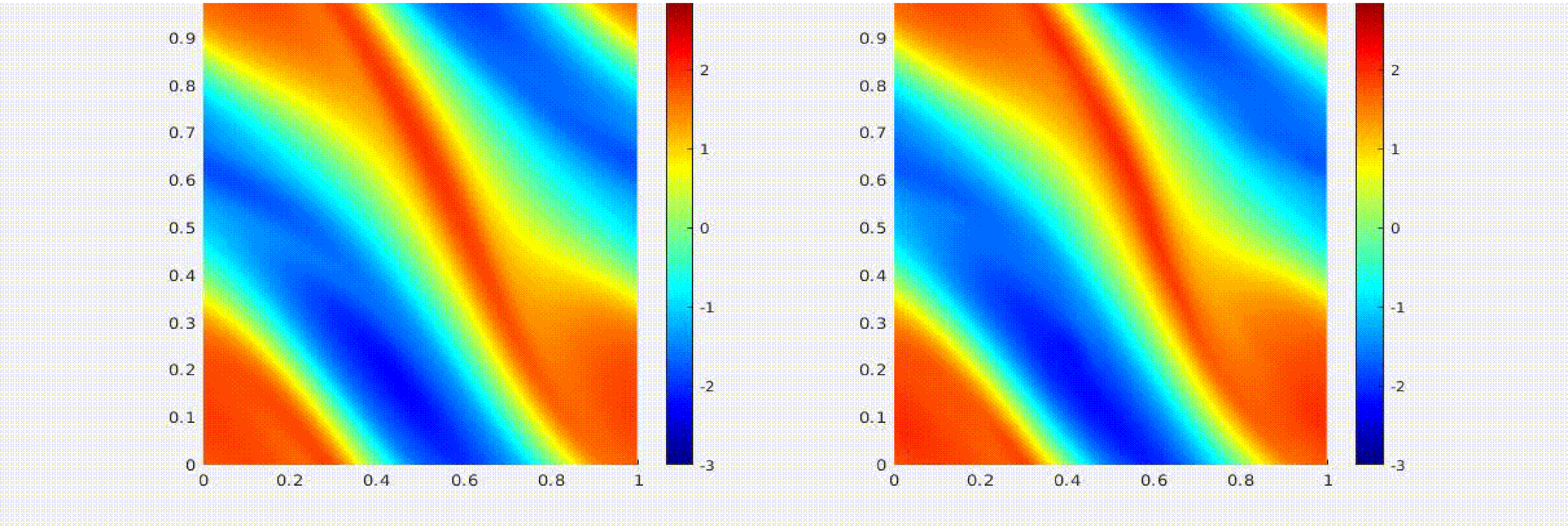
FIRST ML METHOD TO SOLVE FLUID FLOW

Solution in turbulent regime. 1000x faster than traditional solvers

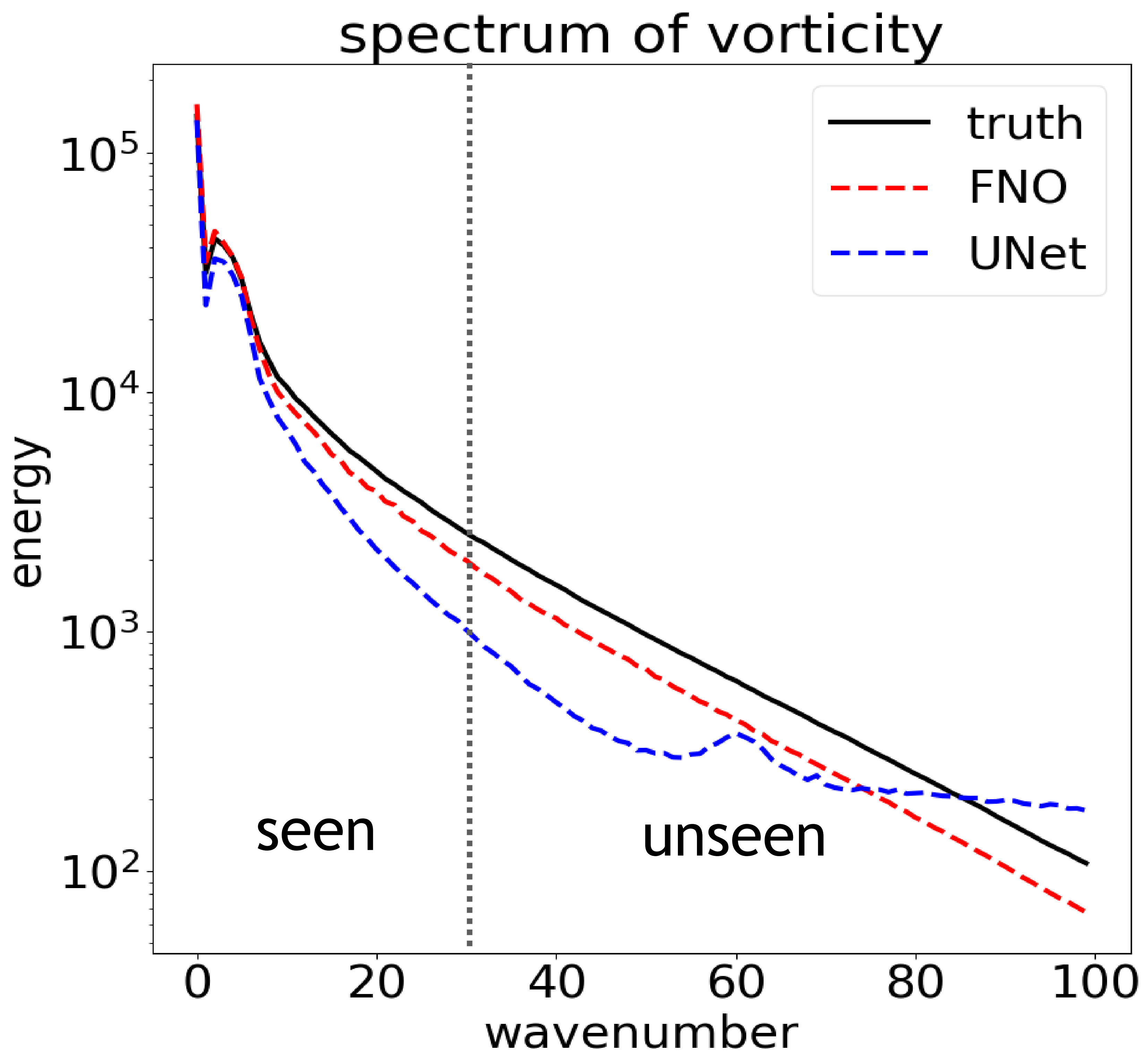
Train using 64*64*20 data (coarse)



Directly evaluate on 256*256*80 (zero-shot super resolution)



FNO CAPTURES THE ENERGY SPECTRUM



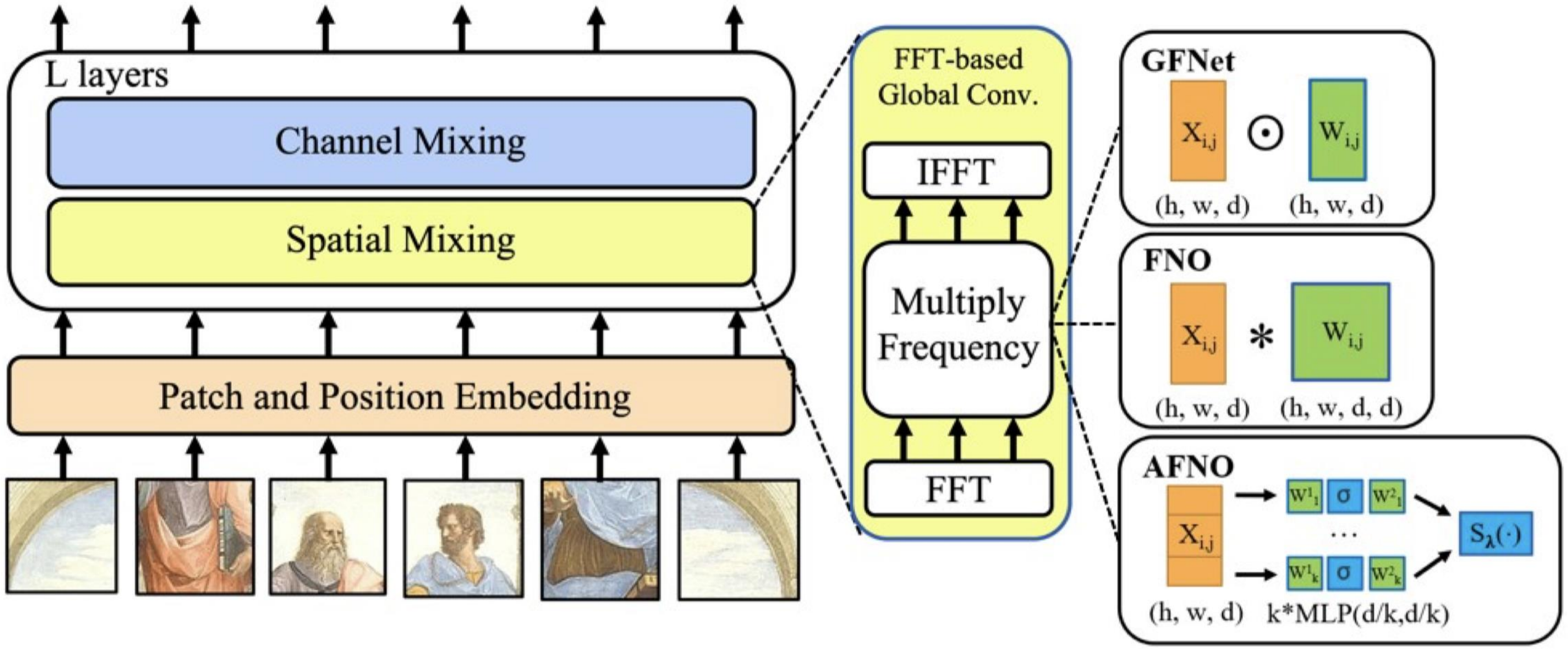
Zero shot super-resolution: train on 64x64, test on 256x256.
Extrapolate to unseen wavenumbers (32->128).

TRANSFORMERS ARE SPECIAL CASES OF NEURAL OPERATOR

Adaptive Fourier neural operator for efficiency

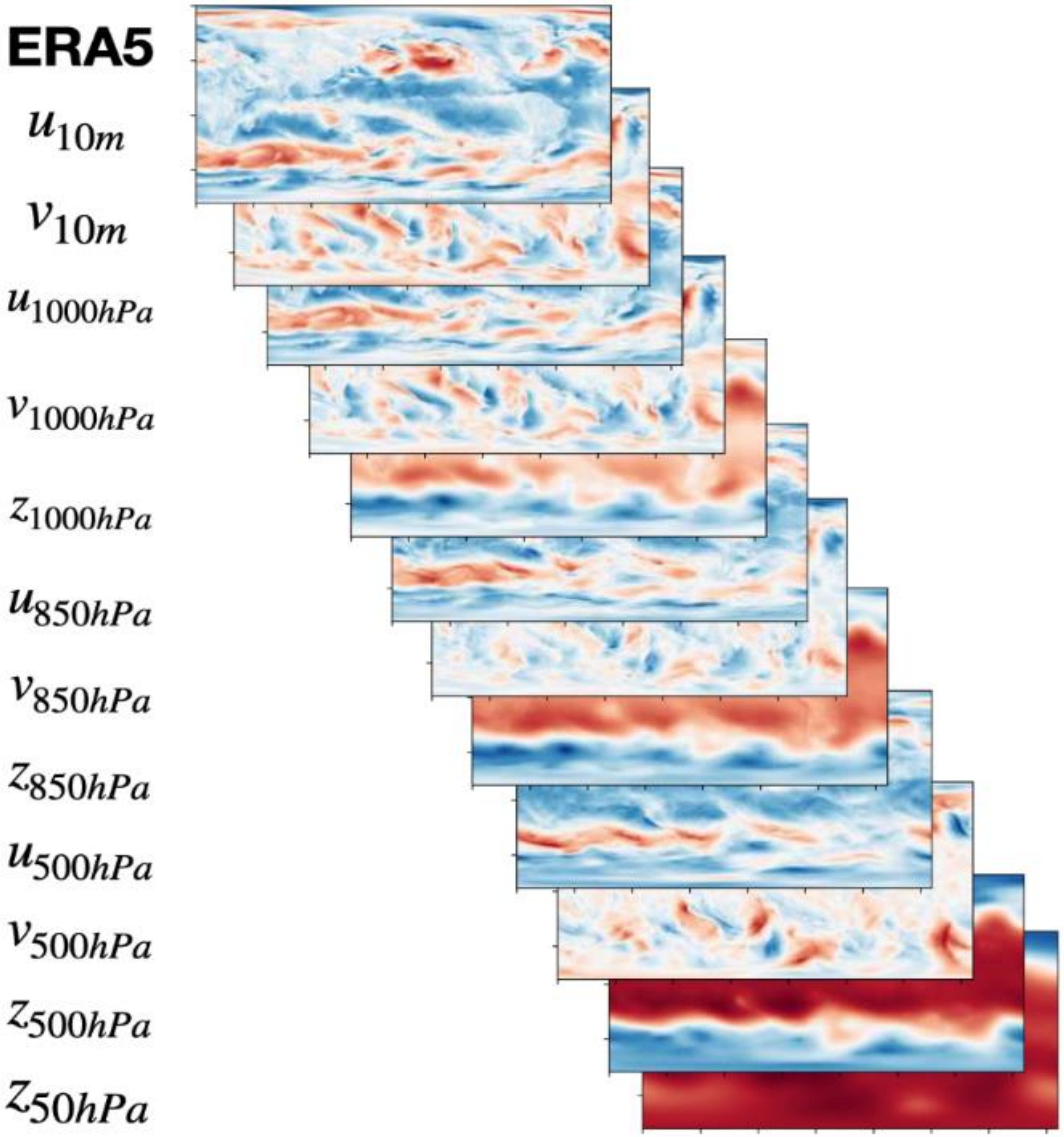
Neural operator is a continuous generalization of Transformers.

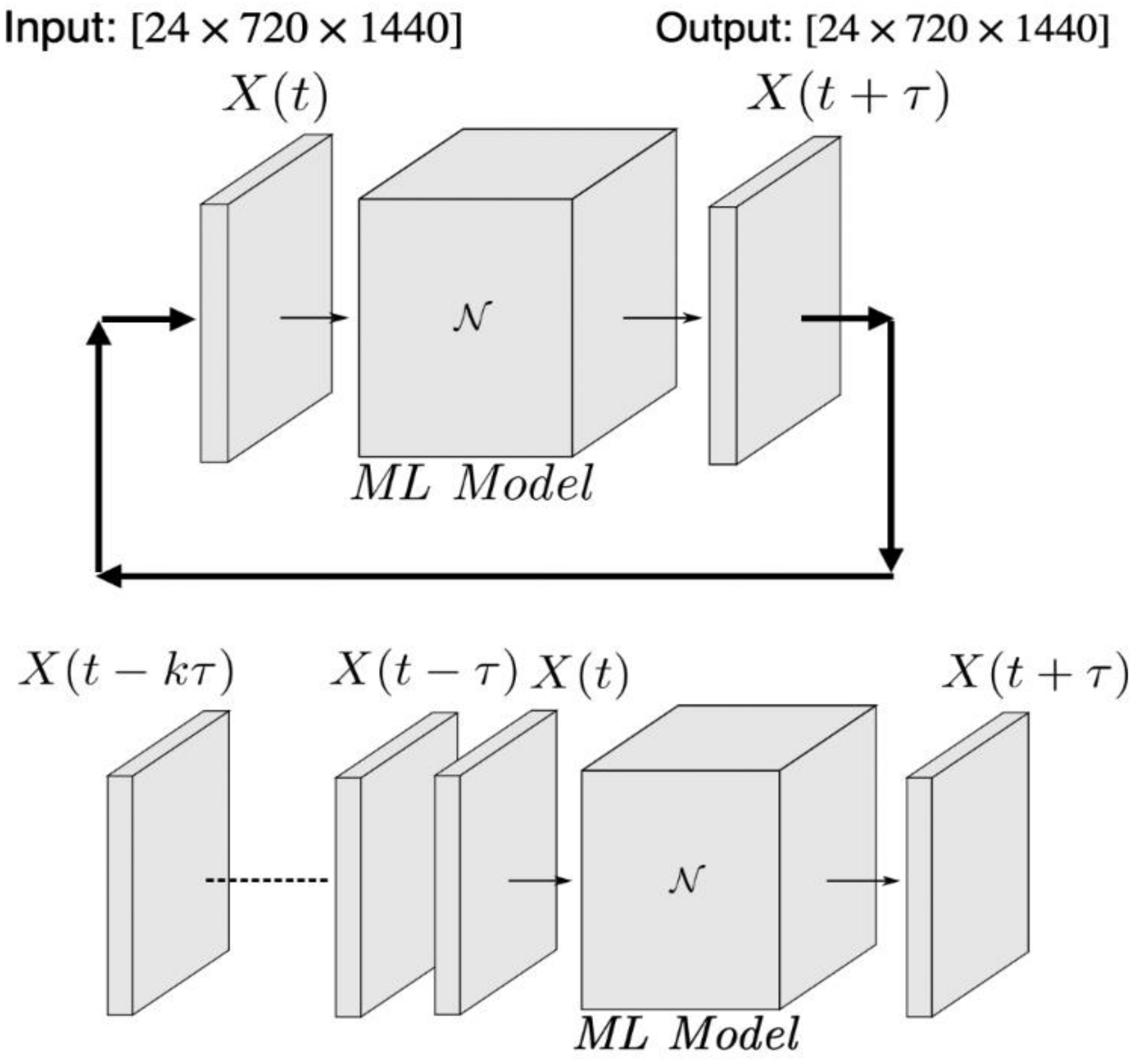
- Attention: kernel-integration.
- Query-key: low-rank kernel
- Use Fourier transform in kernel for efficiency.



John Guibas, Morteza Mardani, Zongyi Li, Andrew Tao, Anima Anandkumar, Bryan Catanzaro, Adaptive Fourier Neural Operators: Efficient Token Mixers for Transformers", *ICLR 2022*

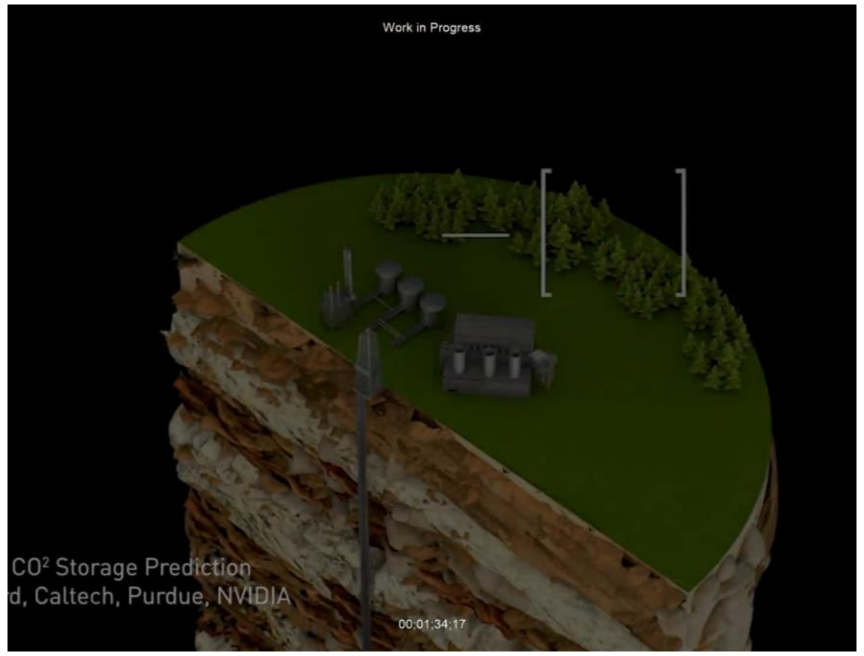
FOURCASTNET (FOURIER FORECASTING NETWORK)





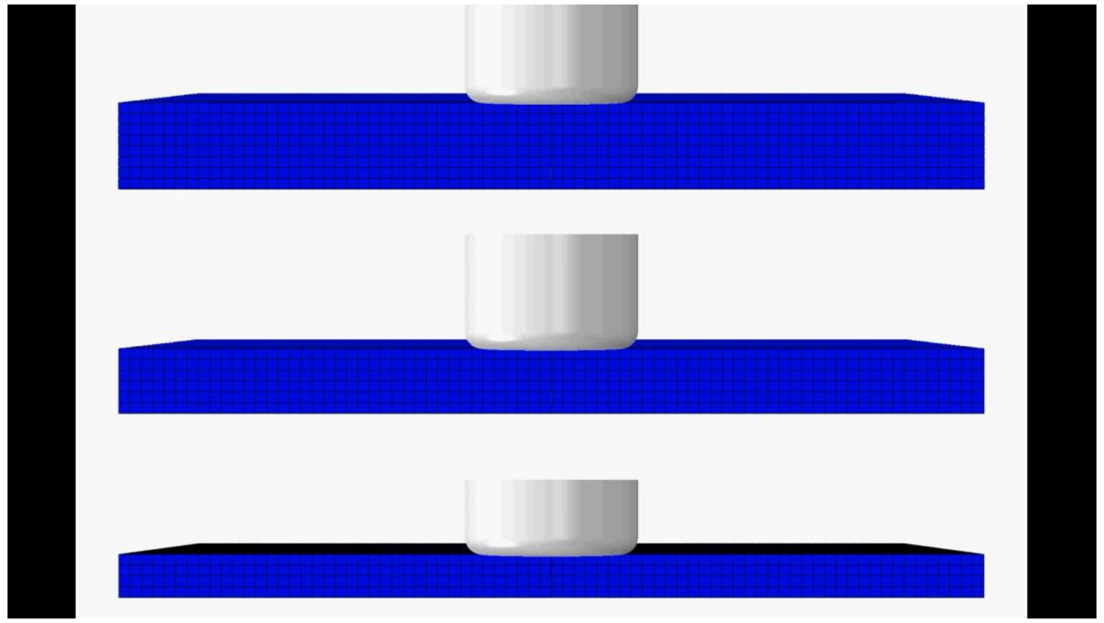
MANY OTHER APPLICATIONS FOR FNO

CO2 Sequestration



FNO is 10^4x faster

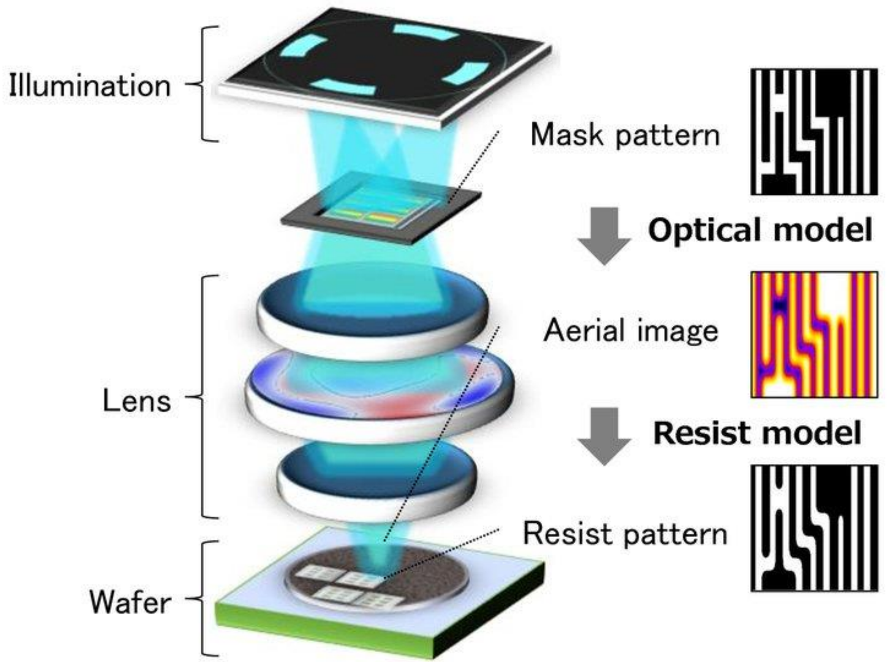
Stress Prediction in Materials



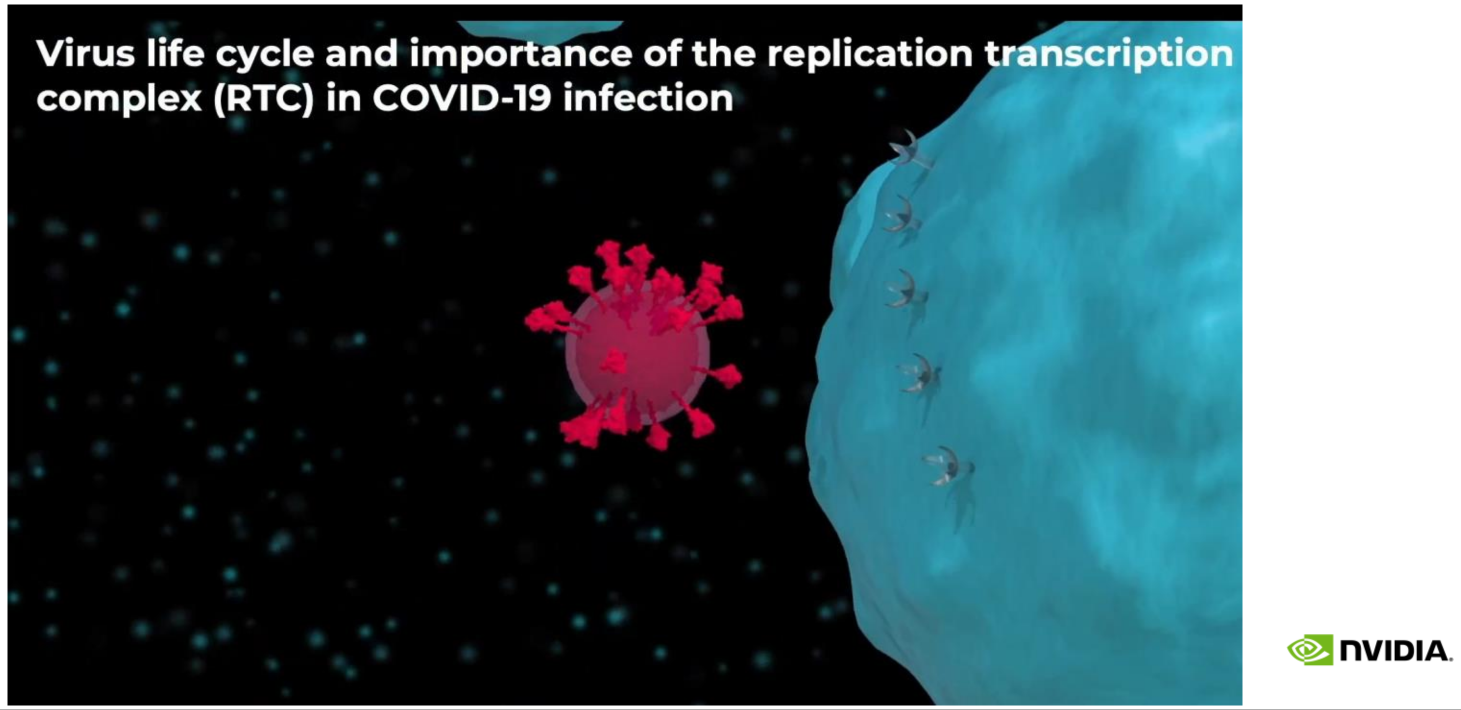
PCA-neural operator is 10^5x faster

Computational Lithography

For first time, metal layer contour simulation at 1nm^2 /pixel resolution with any tile size.



Molecular dynamics



PINO: PHYSICS-INFORMED NEURAL OPERATOR

Data loss: compare prediction and ground-truth solution

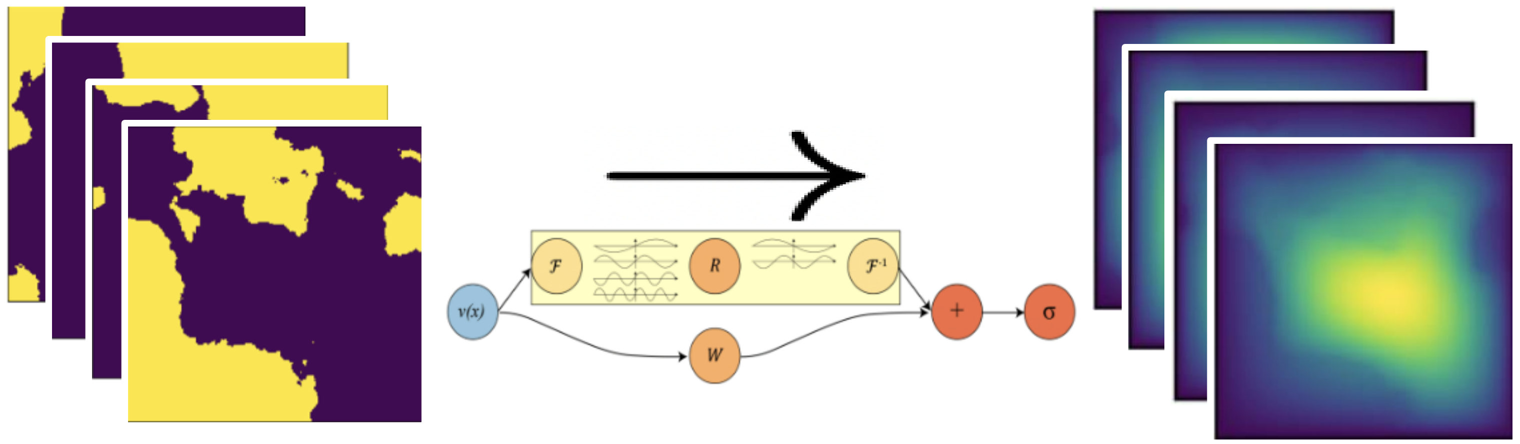
Equation loss: plug prediction in PDE and compute residual

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

PINO: PHYSICS-INFORMED NEURAL OPERATOR

1. Pre-train:

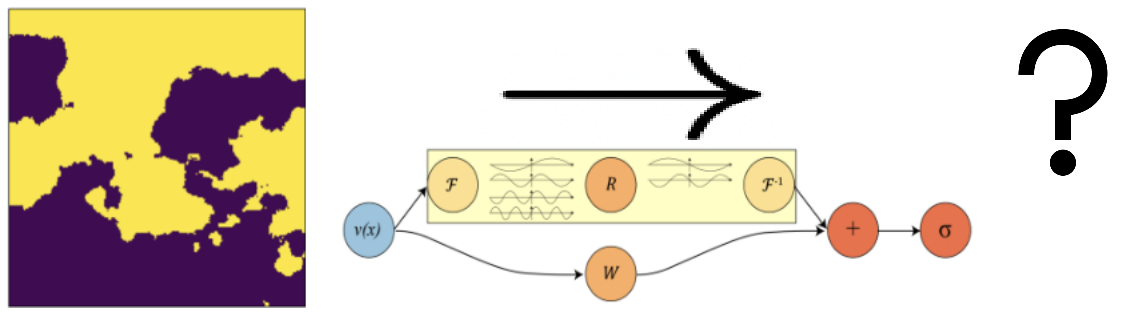
Learn a solution operator



Equation loss
Data loss (if available)

2. Test-time optimize:

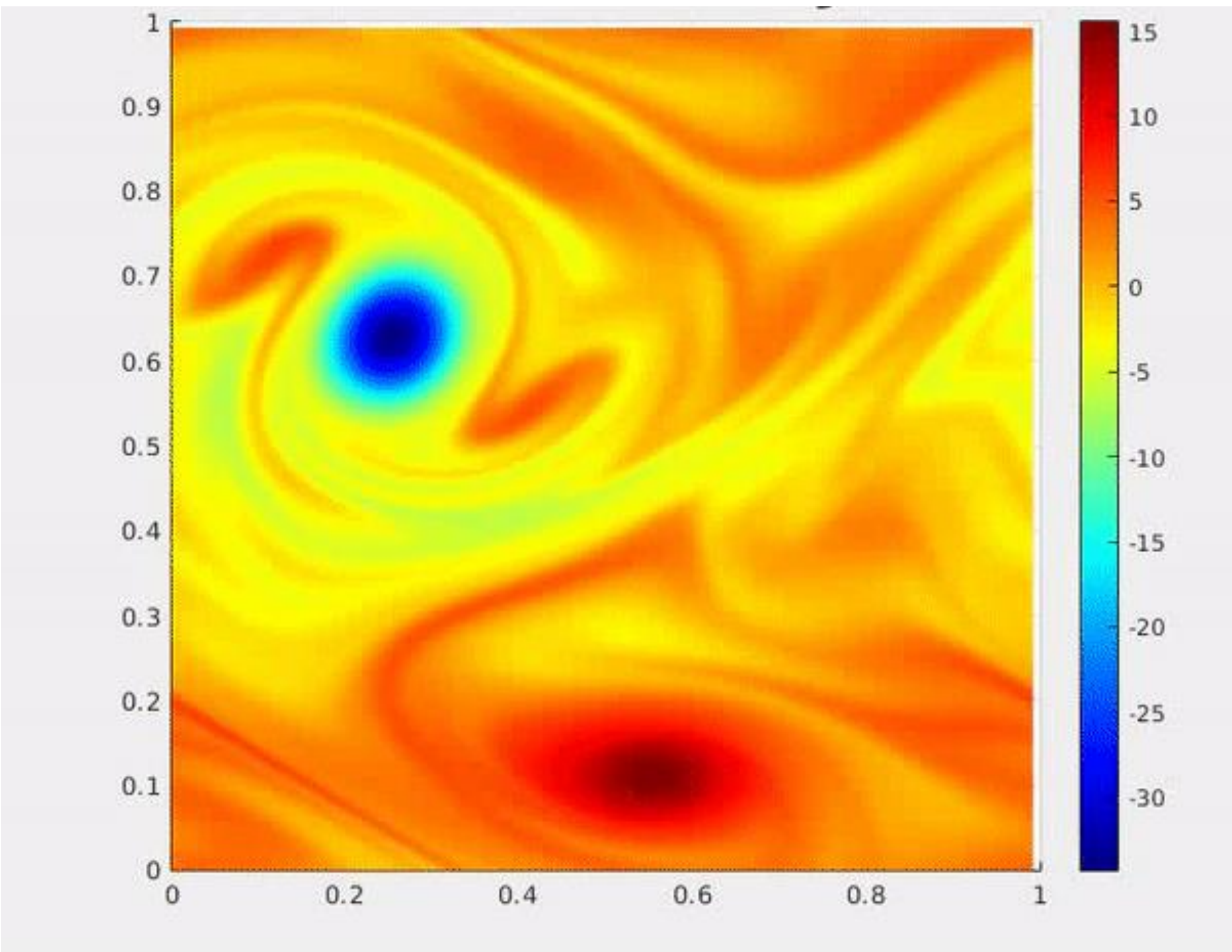
Fine-tune learned operator to solve for a specific instance



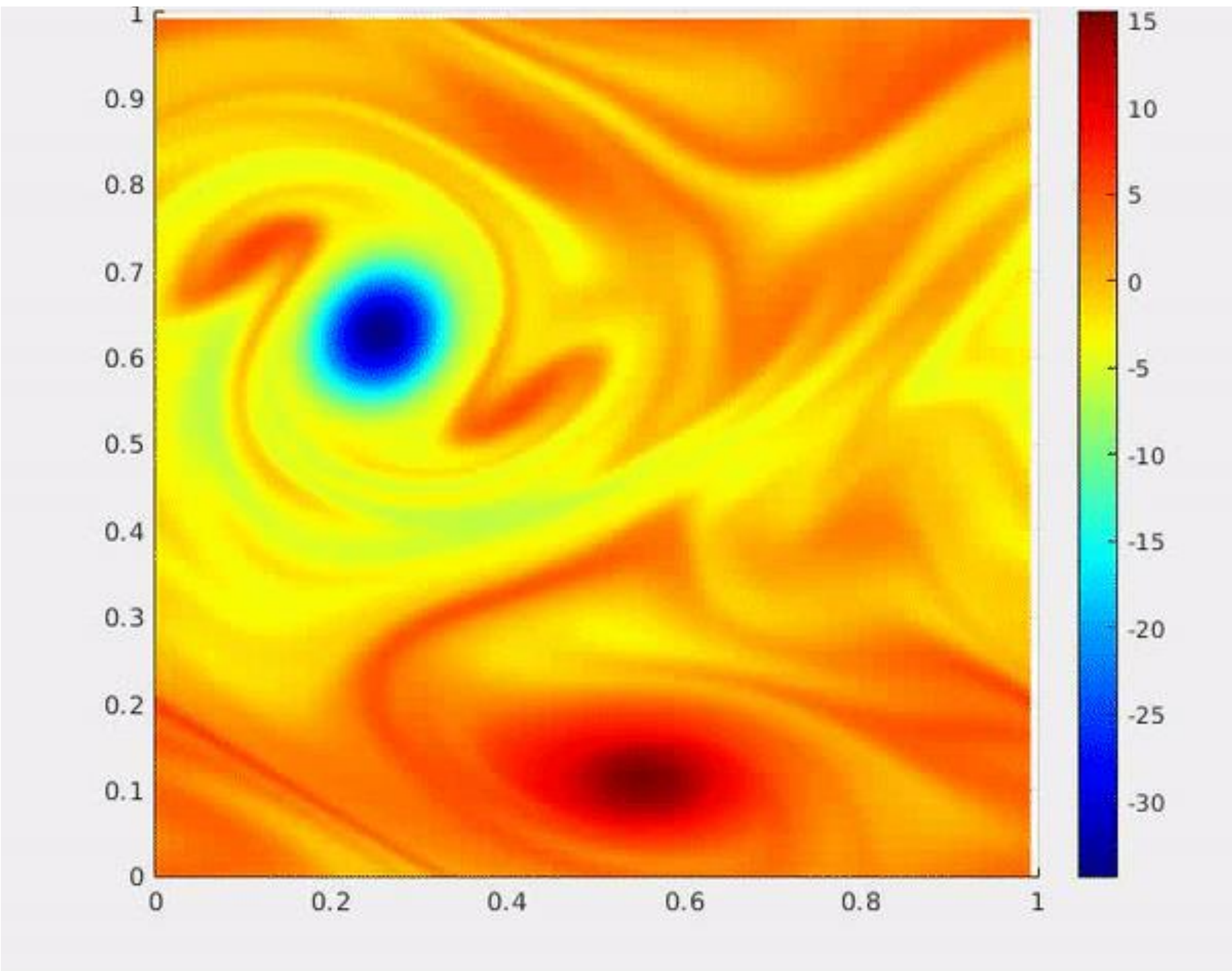
Equation loss
Operator loss (to prevent forgetting)

PINO: PHYSICS-INFORMED NEURAL OPERATOR

True vorticity

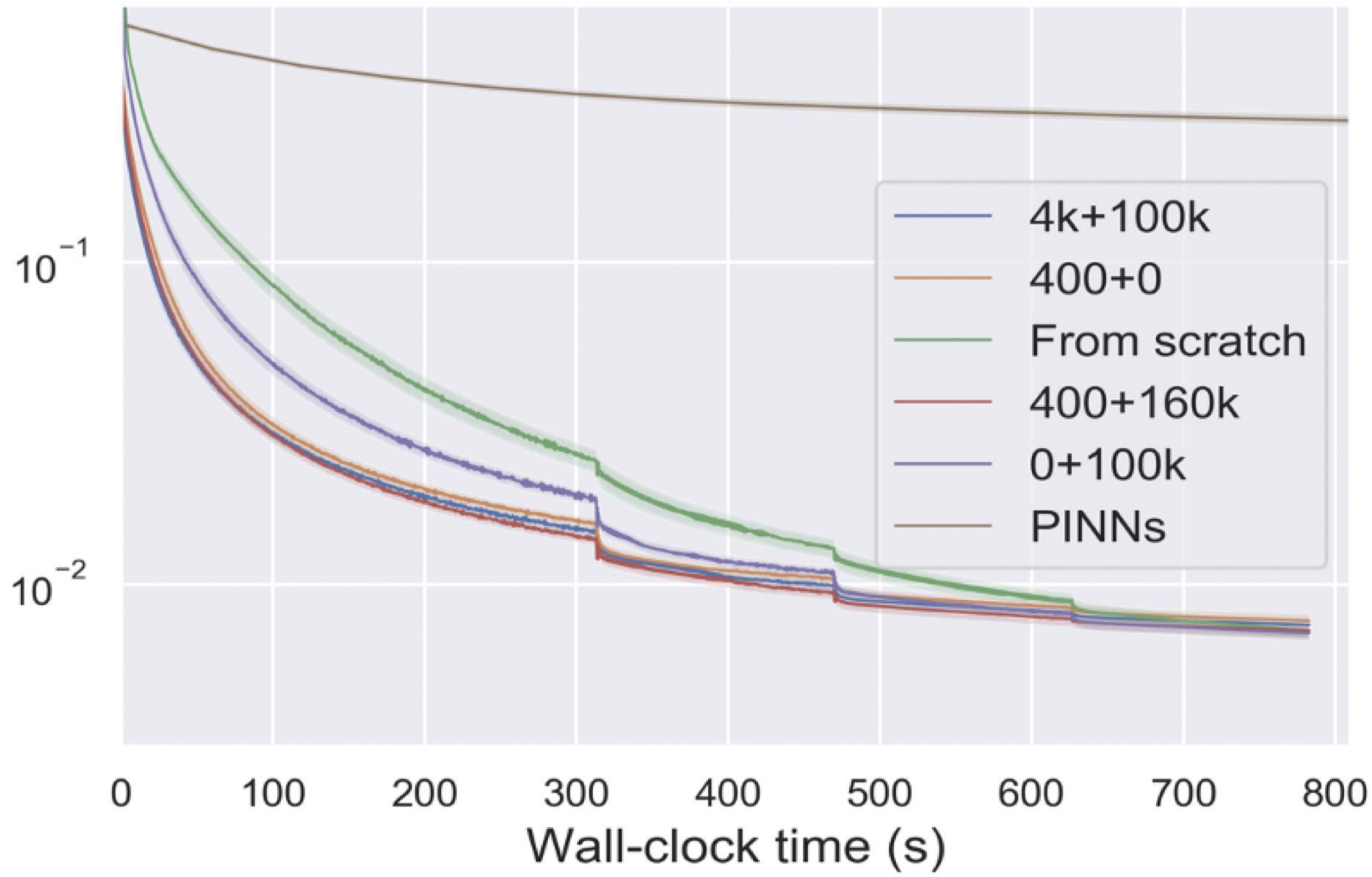


Predicted vorticity



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

PINO: PHYSICS-INFORMED NEURAL OPERATOR



No. of data samples + additional PDE instances

PINO vs PINN

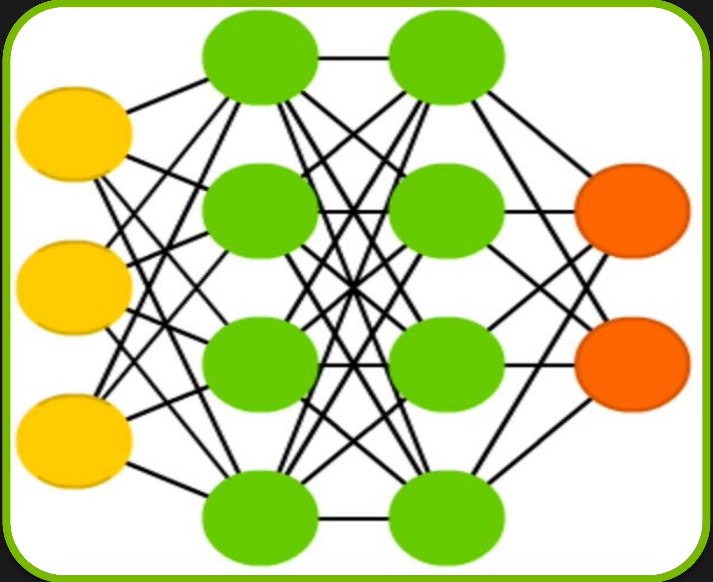
- Learned operator ansatz has better optimization landscape
- Optimize function-wise vs optimize pointwise

Physics-informed neural networks -- M.Raissi, P.Perdikaris, G.E.Karniadakis

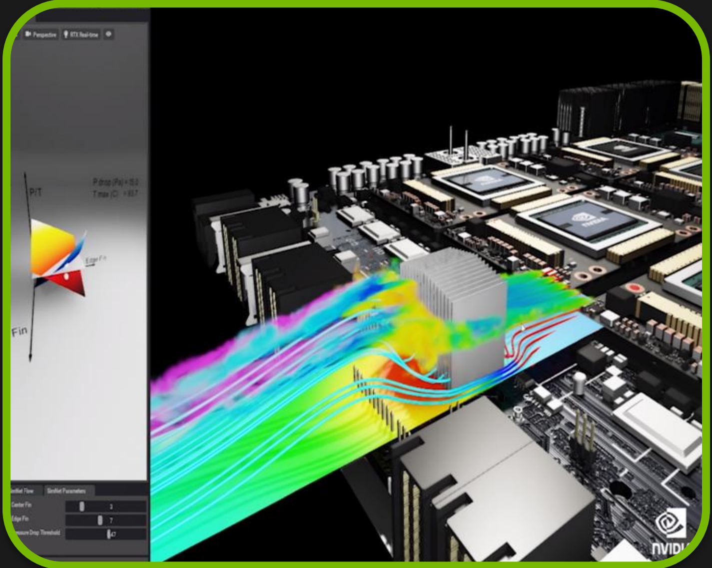
NVIDIA MODULUS

AI-accelerated Physics Simulation Platform

Solve larger problems faster *with* XLA, AMP and TF32 support, and Multi-GPU, Multi-Node implementation



Several advanced networks model Multiple Physics in ***Forward, Inverse and Data Assimilation simulations*** with accuracy & convergence



Parameterized system representation to solve ***multiple scenarios simultaneously***

APIs for implementing new Physics, Geometry, and Domains and detailed ***User Guide examples***

CONCLUSION

- AI4science is the future of science
- Principled algorithms for zero-shot generalization
- Operator learning extends neural networks to learning in infinite dimensional spaces
- Orders of magnitude speedup while maintaining accuracy