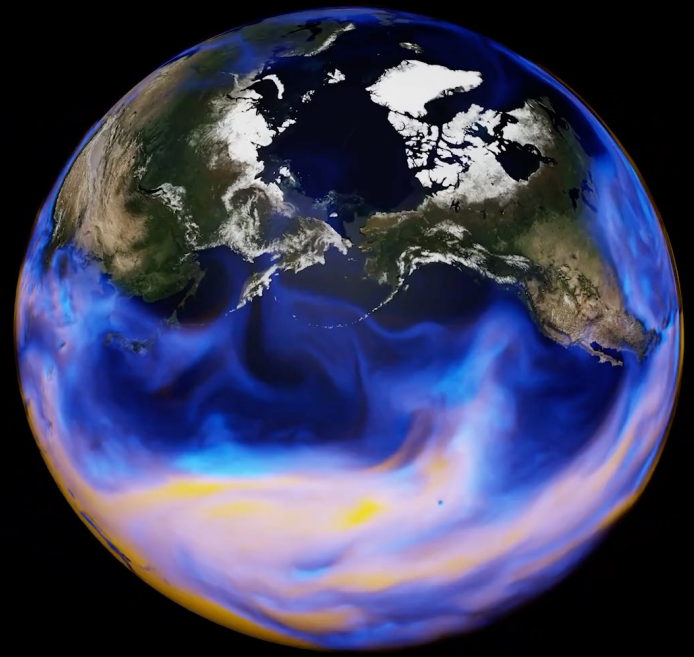
AI + SCIENCE
NEURAL OPERATORS

Anima Anandkumar

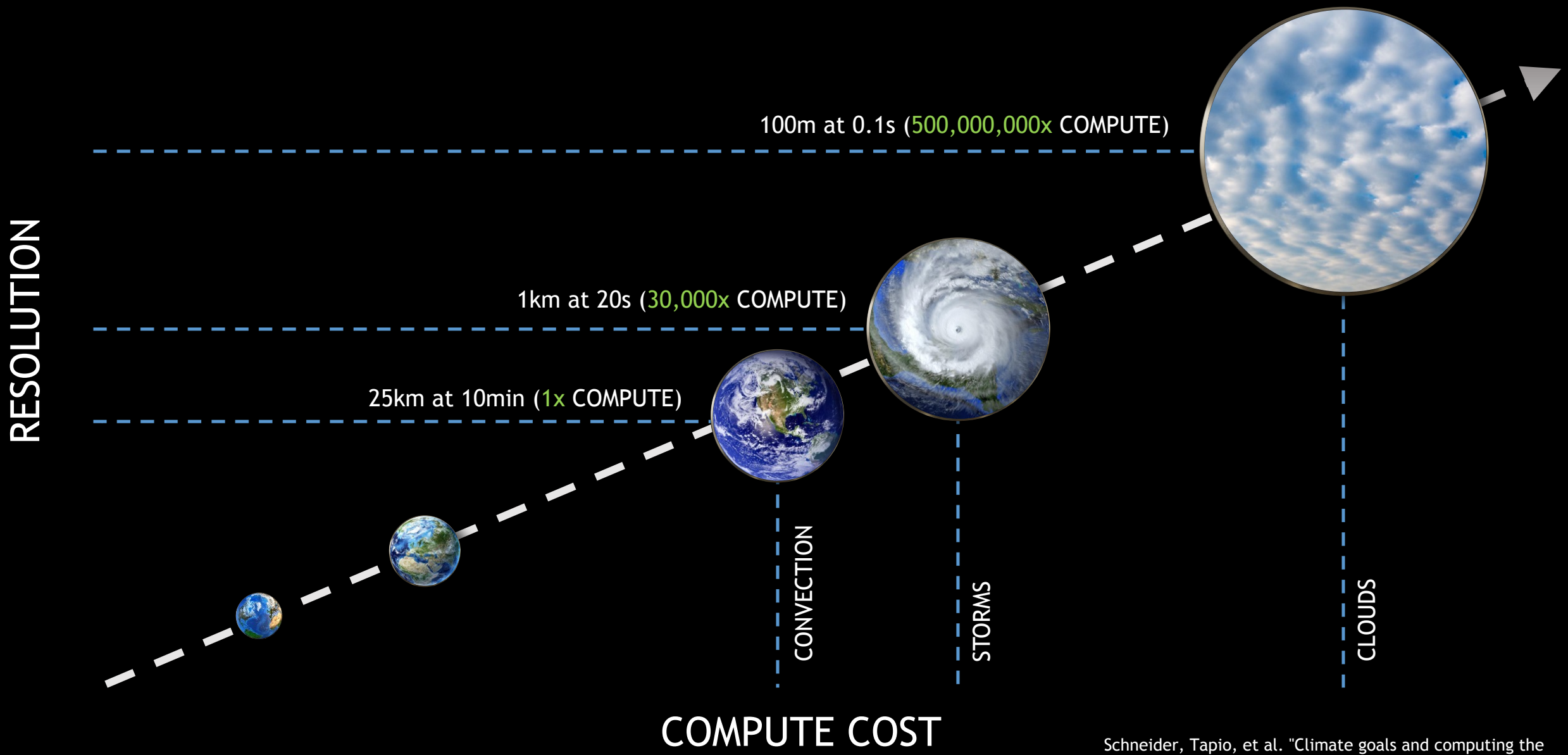
MULTI-SCALE PROCESSES IN NATURE





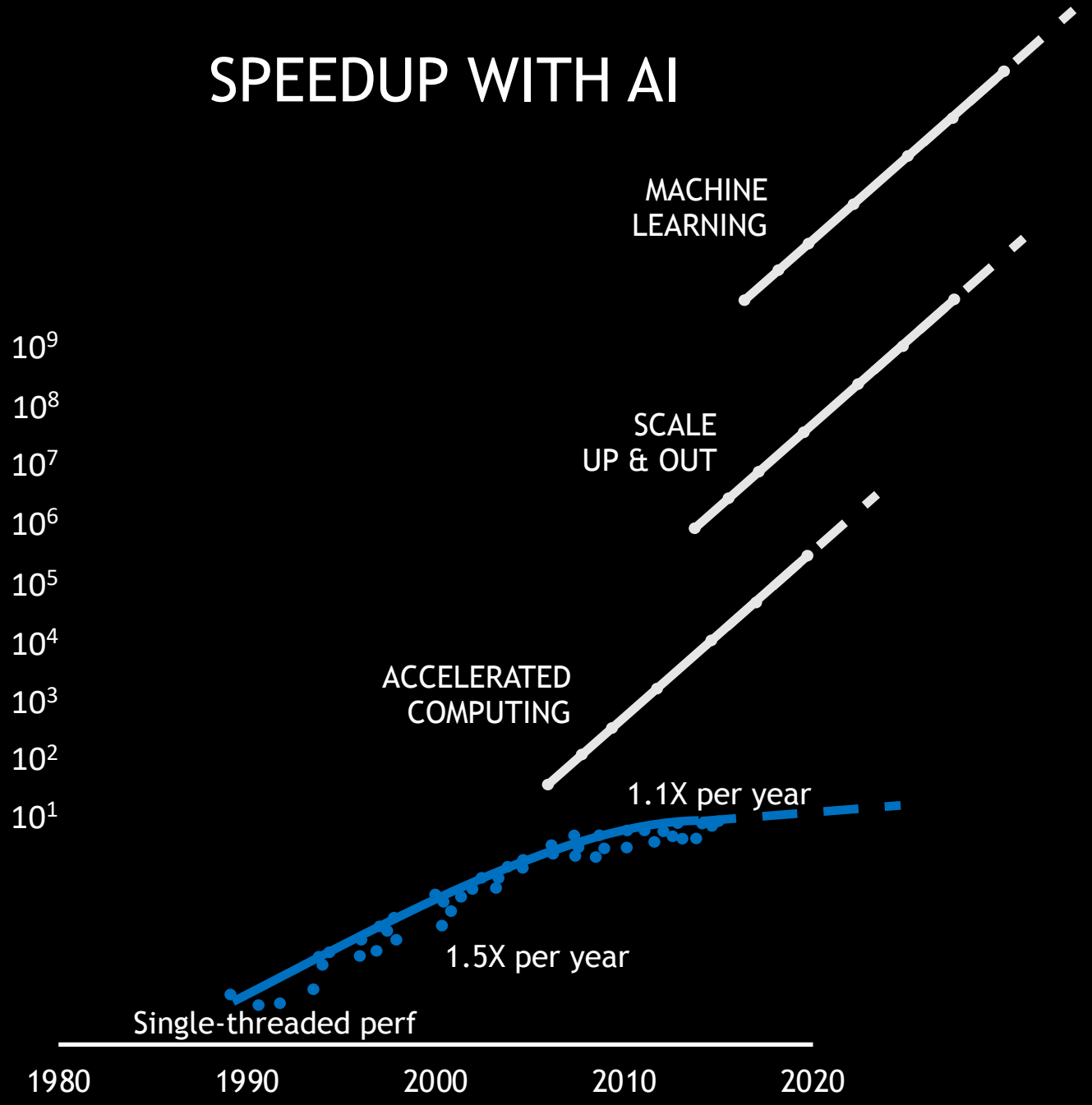
Mathematical equations govern the world at all scales

CAPTURING FINE-SCALES TOO EXPENSIVE CURRENTLY



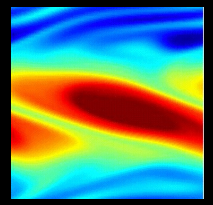
Schneider, Tapio, et al. "Climate goals and computing the future of clouds." *Nature Climate Change* (2017).

SPEEDUP WITH AI

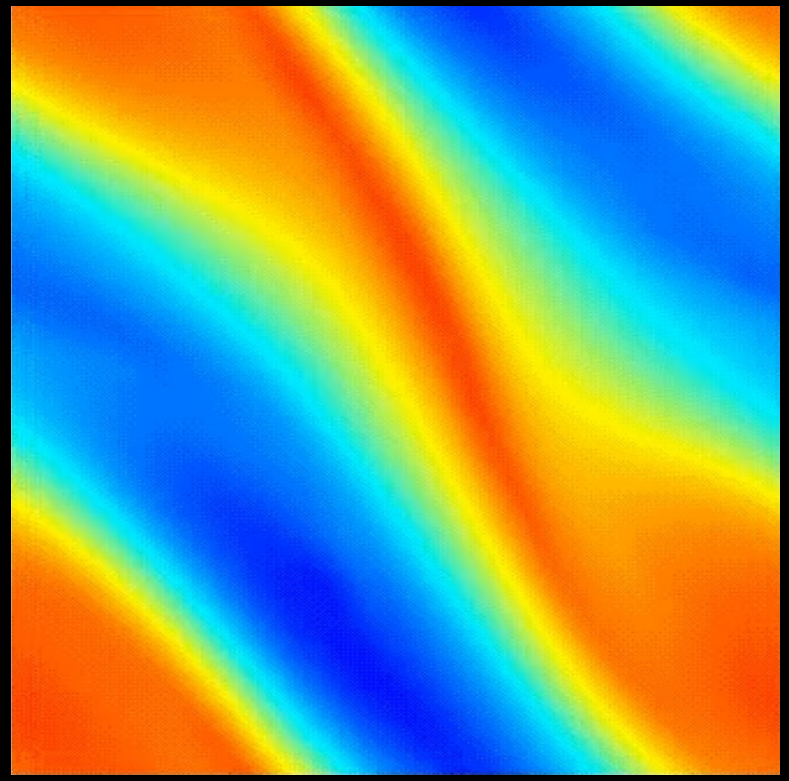


LEARNING ACROSS RESOLUTIONS WITH NEURAL OPERATORS

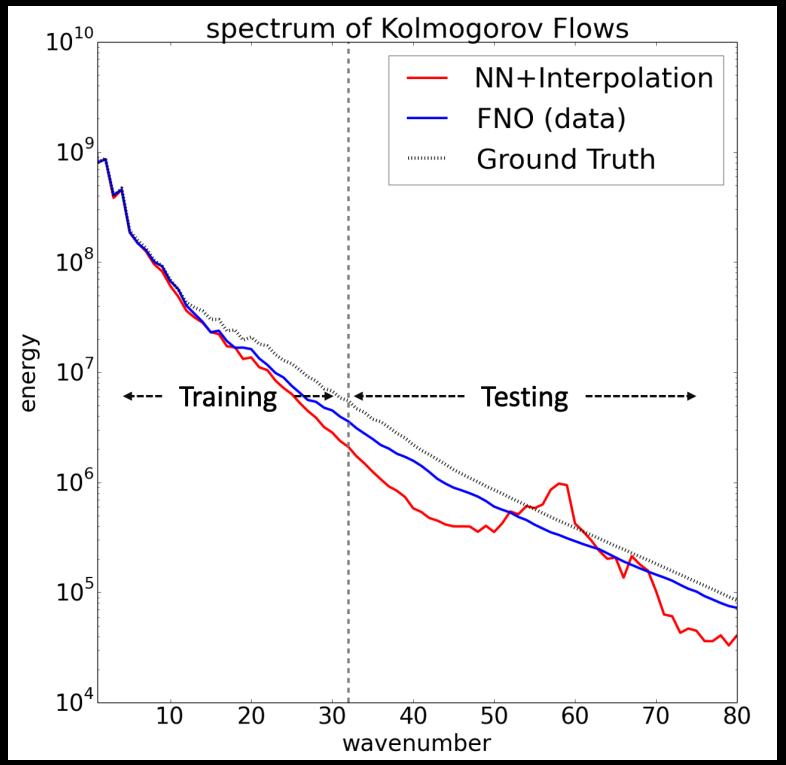
training data
(64x64)



prediction
(256x256)



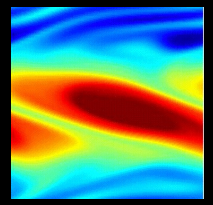
https://github.com/neuraloperator



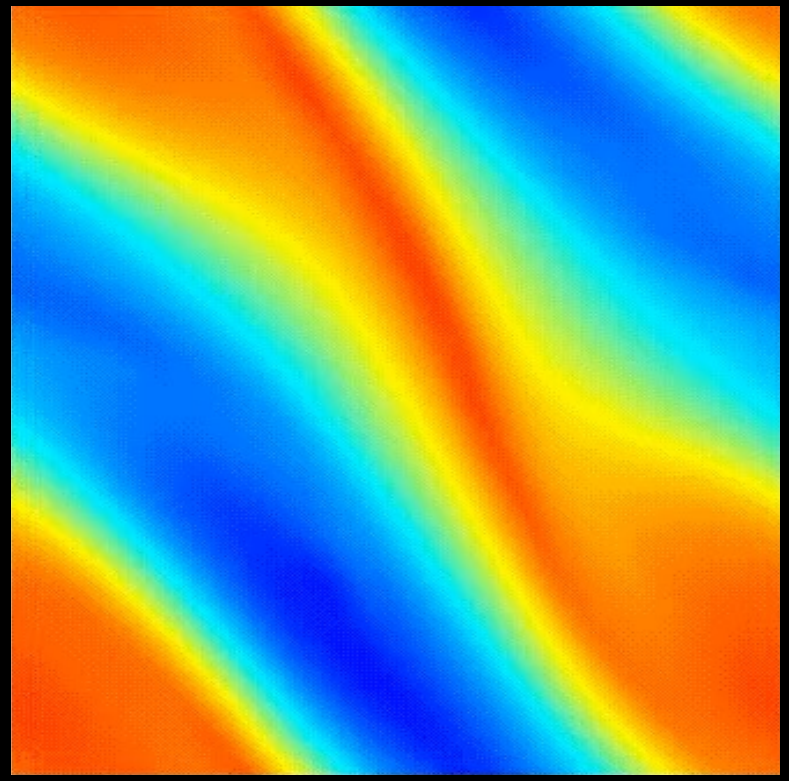
Our AI model (FNO) captures physical effects at all scales

PHYSICS INFORMED NEURAL OPERATORS

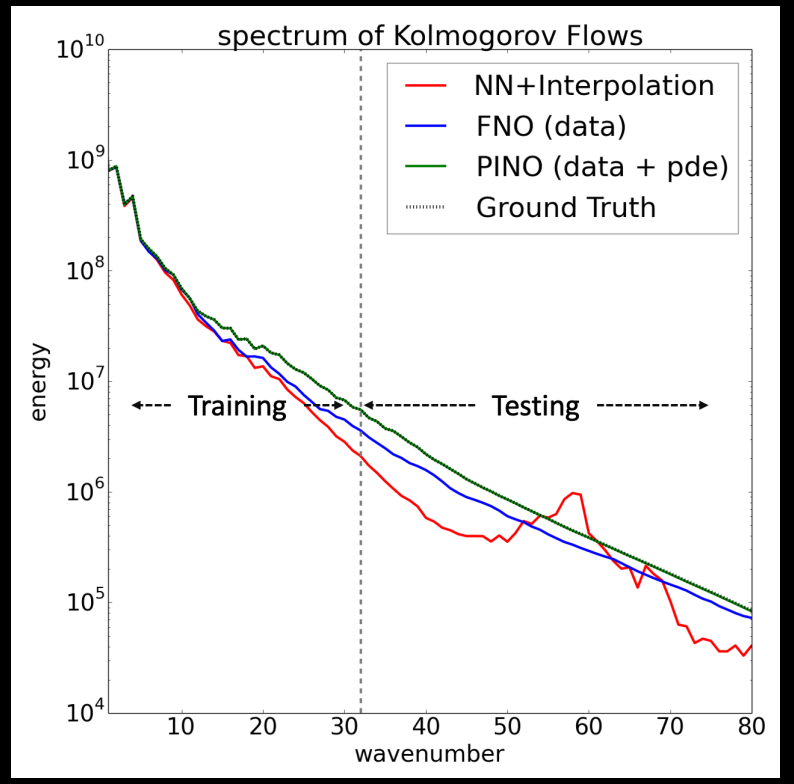
training data
(64x64)



prediction
(256x256)



https://github.com/neuraloperator

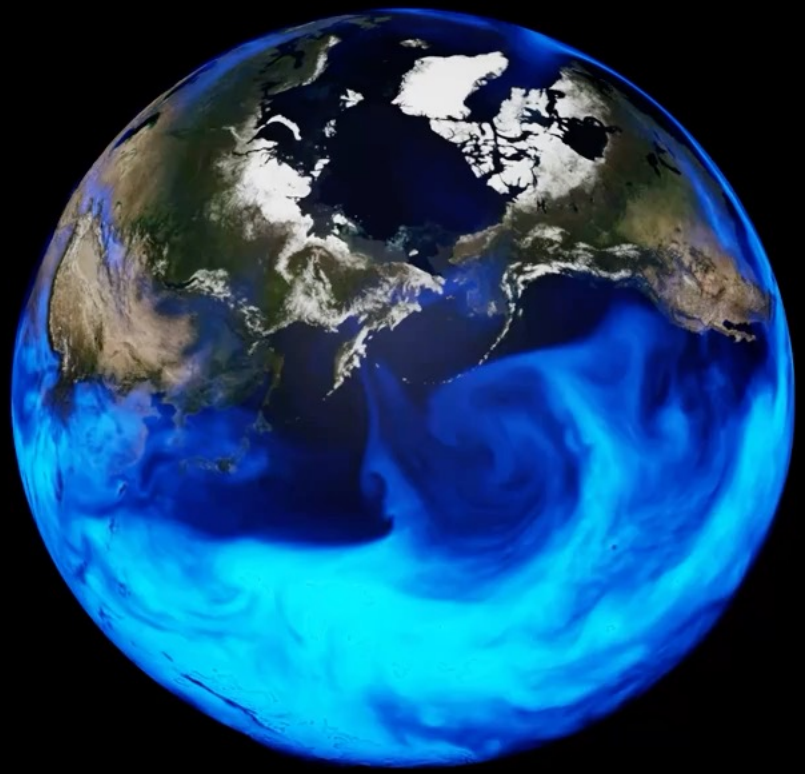


Our AI model (PINO) perfectly learns physical effects at all scales

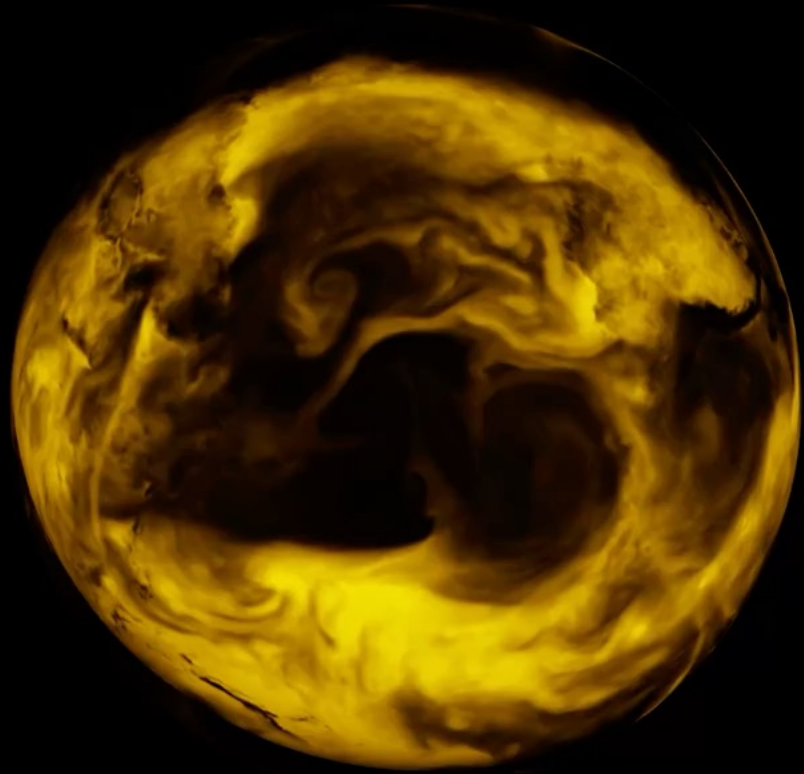
APPLICATIONS

AI ACCELERATES WEATHER FORECASTING

Ground Truth



FourCastNet



Our AI (FNO) is **45,000 times** faster than current weather models

AI ACCELERATES WEATHER FORECASTING

ECMWF | Charts

Help Log in

Home / Charts catalogue

FourCastNet

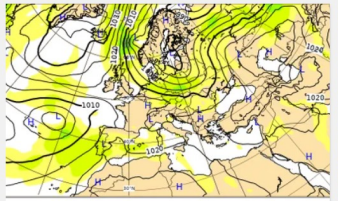
Range
- Medium (15 days)
- Extended (42 days)
- Long (Months)

Type
- Forecasts
- Verification

Component
- Surface
- Atmosphere

Product type
- High resolution forecast (HRES)
- Ensemble forecast (ENS)
- Combined (ENS + HRES)
- Extreme forecast index
- Point-based products
- Experimental: AIFS
- Experimental: Machine learning models
- Atmospheric composition

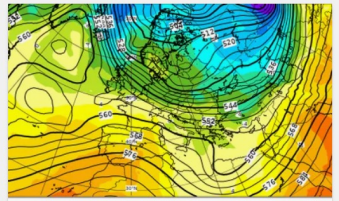
Parameters
- Wind



Latest forecast

Experimental: FourCastNet ML model: Mean sea level pressure and 850 hPa wind speed

FourCastNet v2-small:a deep learning-based system developed by NVIDIA in collaboration with researchers at several US universities.It is initialised with ECMWF HRES analysis. FourCastNet operates at 0.25° resolution.

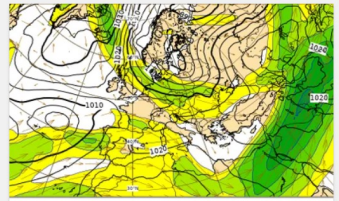


Latest forecast

Experimental: FourCastNet ML model: 500 hPa geopotential height and 850 hPa temperature

Experimental: FourCastNet ML model: 500 hPa geopotential height and 850 hPa temperature

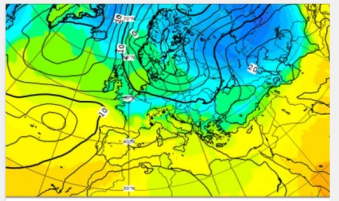
system developed by NVIDIA in collaboration with researchers at several US universities.It is initialised with ECMWF HRES analysis. FourCastNet operates at 0.25° resolution.



Latest forecast

Experimental: FourCastNet ML model: Mean sea level pressure and 200 hPa wind

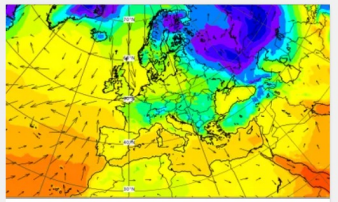
FourCastNet v2-small:a deep learning-based system developed by NVIDIA in collaboration with researchers at several US universities.It is initialised with ECMWF HRES analysis. FourCastNet operates at 0.25° resolution.



Latest forecast

Experimental: FourCastNet ML model: Temperature and geopotential at various pressure levels

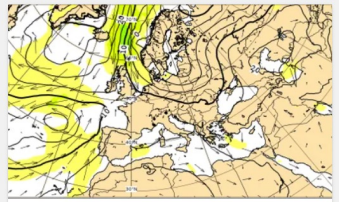
FourCastNet v2-small:a deep learning-based system developed by NVIDIA in collaboration with researchers at several US universities.It is initialised with ECMWF HRES analysis. FourCastNet operates at 0.25° resolution.



Latest forecast

Experimental: FourCastNet ML model: 2 m temperature and 10 m wind

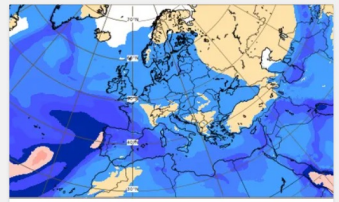
FourCastNet v2-small:a deep learning-based system developed by NVIDIA in collaboration with researchers at several US universities.It is initialised with ECMWF HRES analysis. FourCastNet operates at 0.25° resolution.



Latest forecast

Experimental: FourCastNet ML model: Wind and geopotential heights at various pressure levels

FourCastNet v2-small:a deep learning-based system developed by NVIDIA in collaboration with researchers at several US universities.It is initialised with ECMWF HRES analysis. FourCastNet operates at 0.25° resolution.



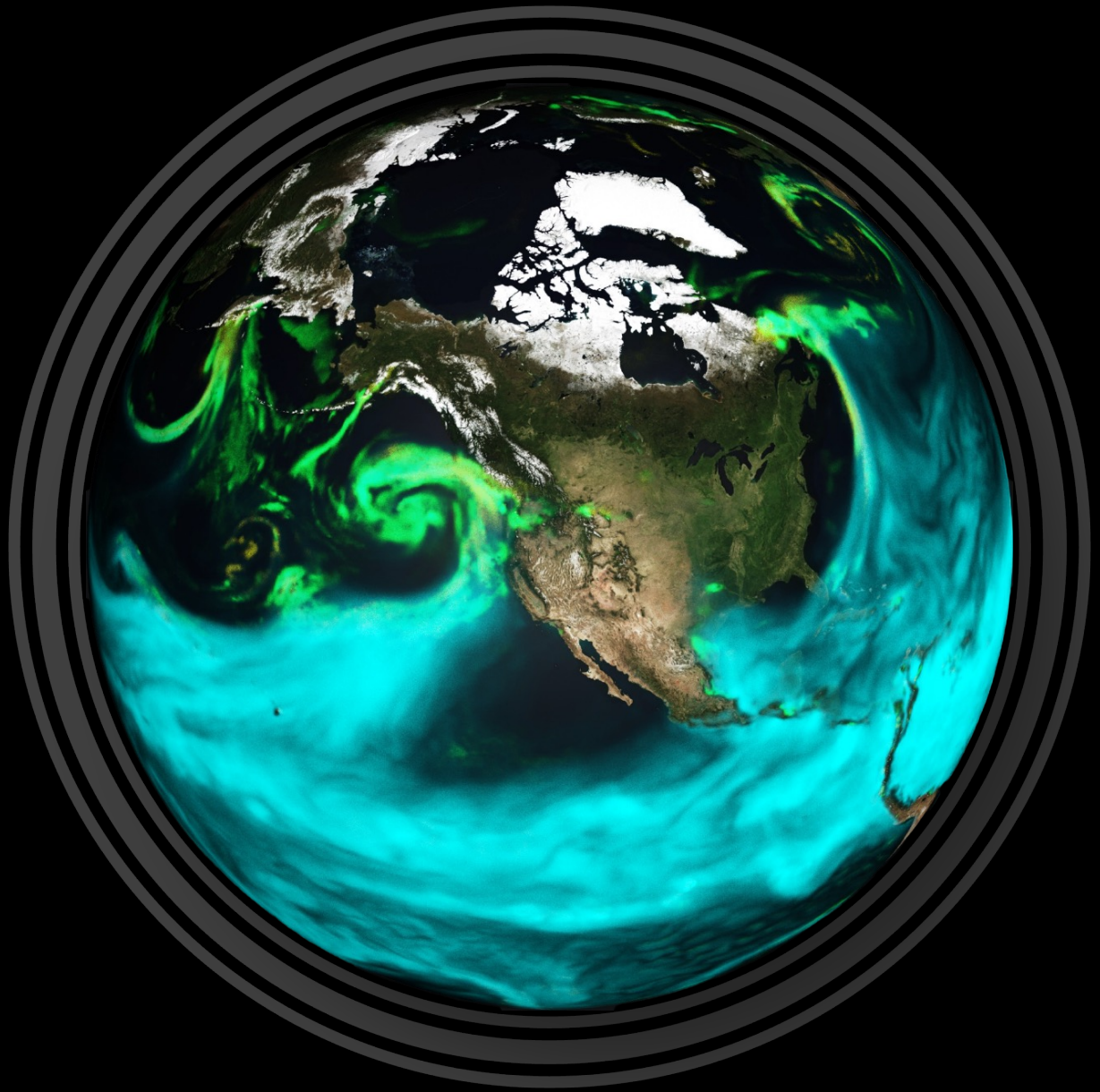
Latest forecast

Experimental: FourCastNet ML model: Total column water

FourCastNet v2-small:a deep learning-based system developed by NVIDIA in collaboration with researchers at several US universities.It is initialised with ECMWF HRES analysis. FourCastNet operates at 0.25° resolution.

https://charts.ecmwf.int/products/fourcast_medium-z500-t850

Our AI weather model is deployed at ECMWF, giving real-time forecasts



Full model emulation of ERA5

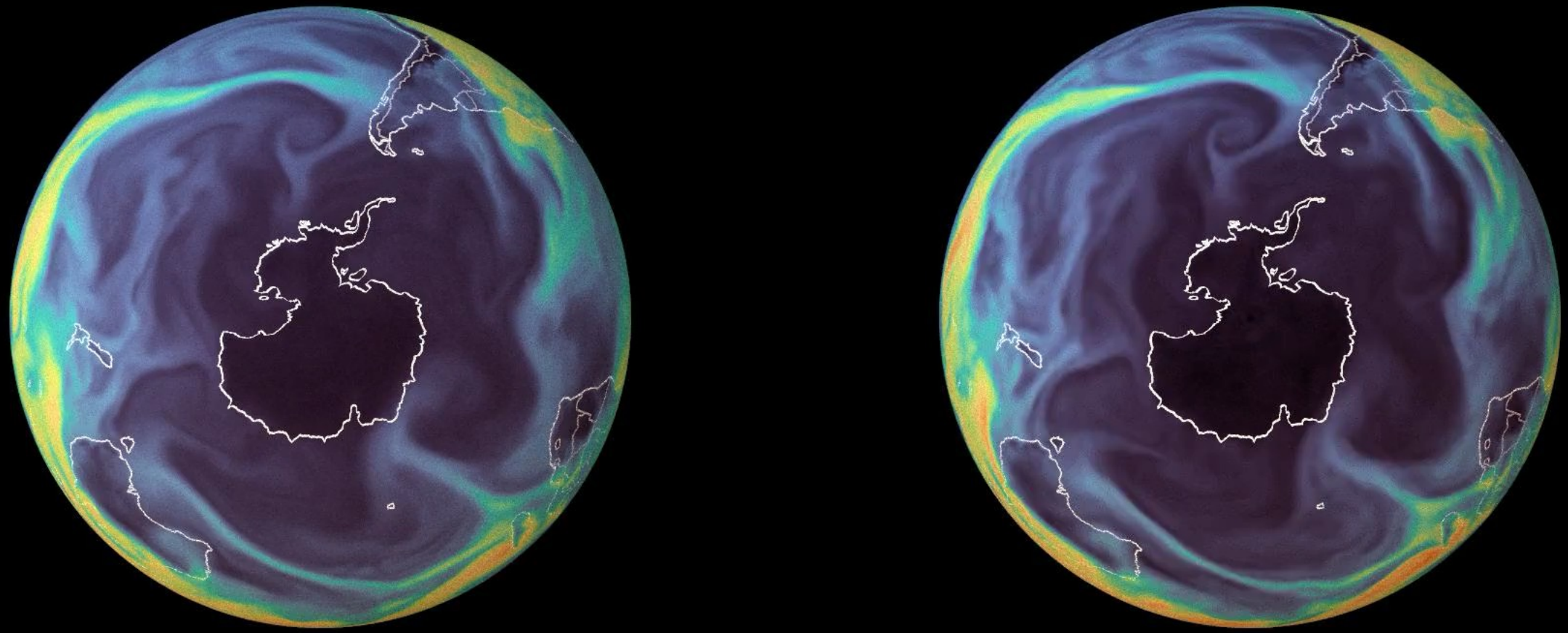
Scope	Global, Medium-Range Weather
Resolution	**25km**
Architecture	Spherical Fourier Neural Operator
Training Data	**ERA5 Reanalysis** (1979 – Present)
Speedup vs NWP	O(10,000 – 100,000)
Max Stable Rollout	250+ days
Project Type	Open-source Code

https://github.com/ecmwf-lab/ai-models-fourcastnetv2

https://www.ecmwf.int/en/about/media-centre/news/2023/how-ai-models-are-transforming-weather-forecasting-showcase-data

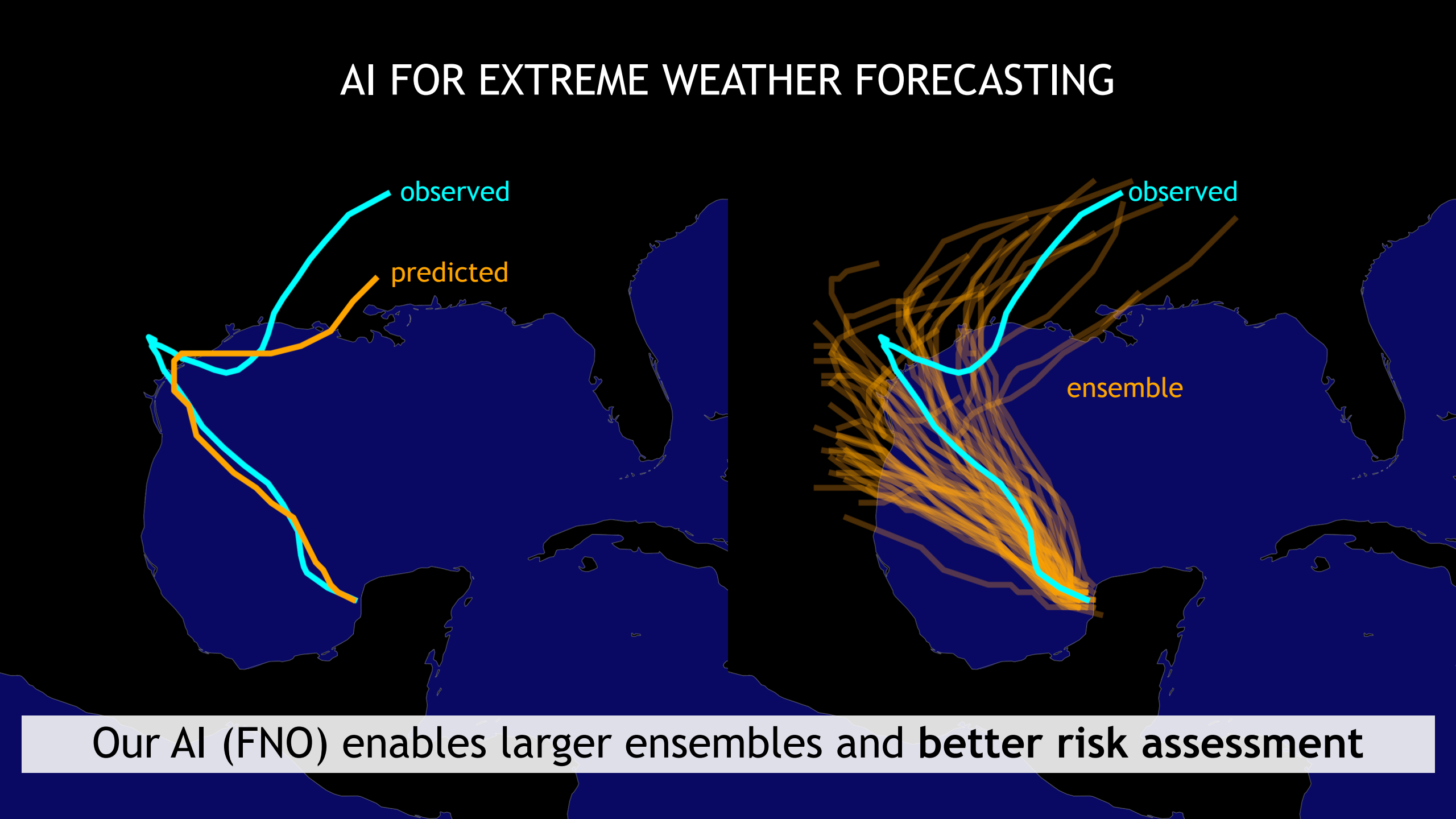
Bonev, Boris, et al. "Spherical Fourier Neural Operators: Learning Stable Dynamics on the Sphere." *ICML* (2023).

DATA + DOMAIN KNOWLEDGE



Adding spherical geometry to AI allows stable long roll-outs

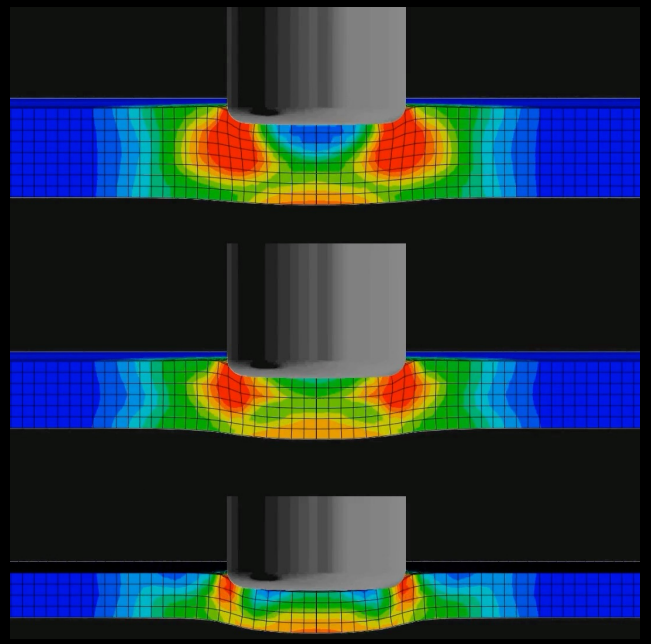
AI FOR EXTREME WEATHER FORECASTING



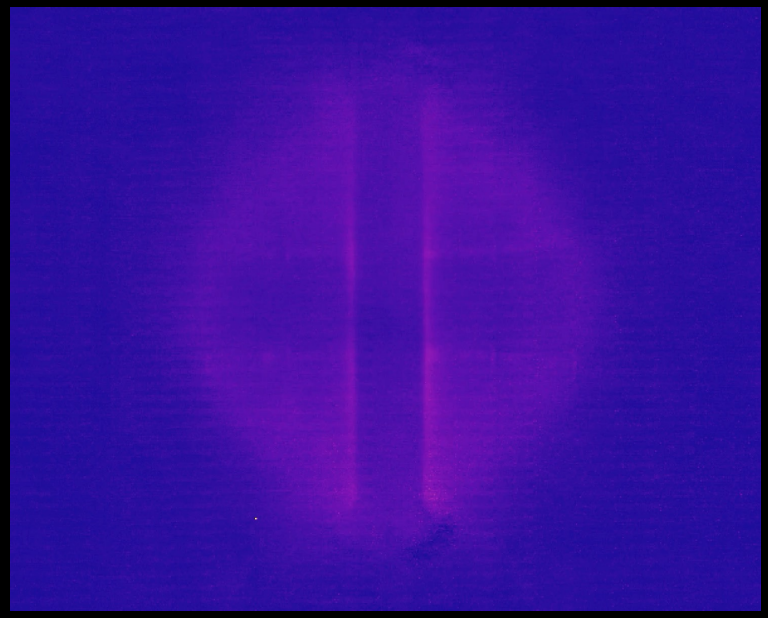
Our AI (FNO) enables larger ensembles and **better risk assessment**

NEURAL OPERATORS (FNO) - SIMULATION

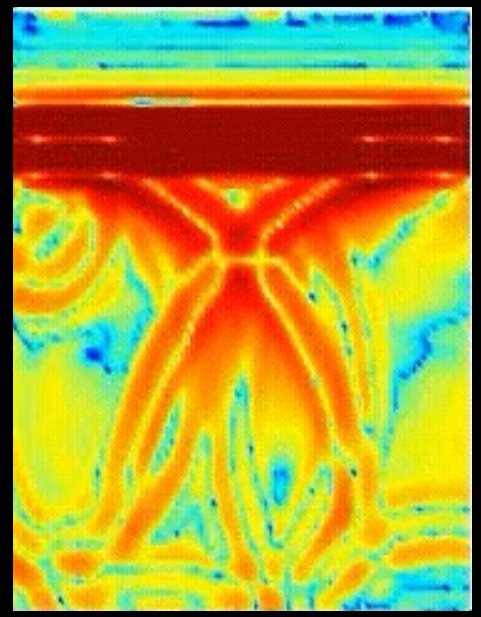
Deformation



Fusion



Ultrasound

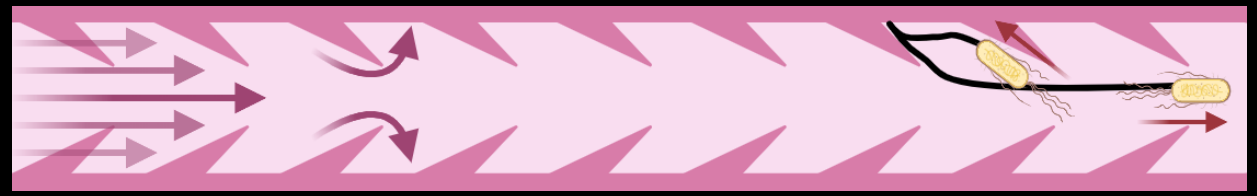


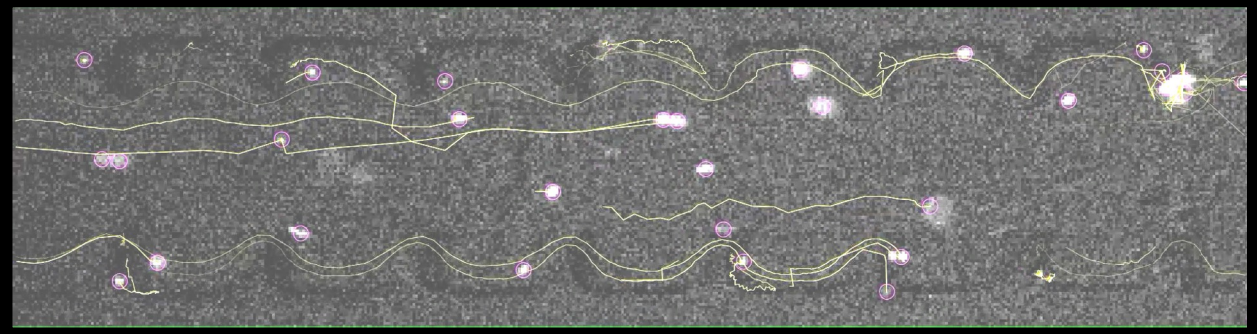
Our AI (FNO) is ~**100,000 times** faster

Gopakumar, Vignesh, et al. "Fourier Neural Operator for Plasma Modelling." *arXiv preprint arXiv:2302.06542* (2023).

NEURAL OPERATORS (FNO) - DESIGN

Catheter

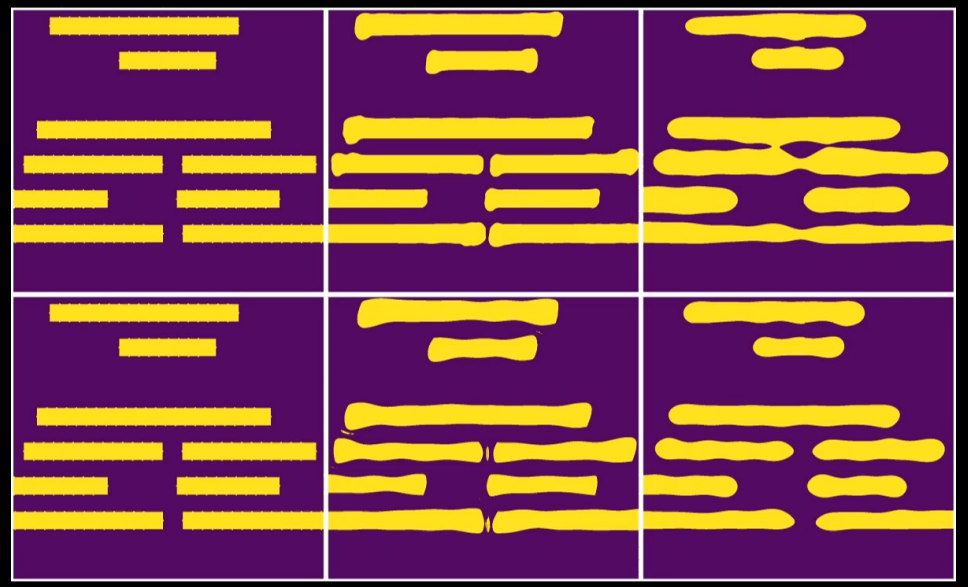




Lithography

Epoch 1
AI: MSE 920798 EPE 382
ILT: MSE 717711 EPE 123

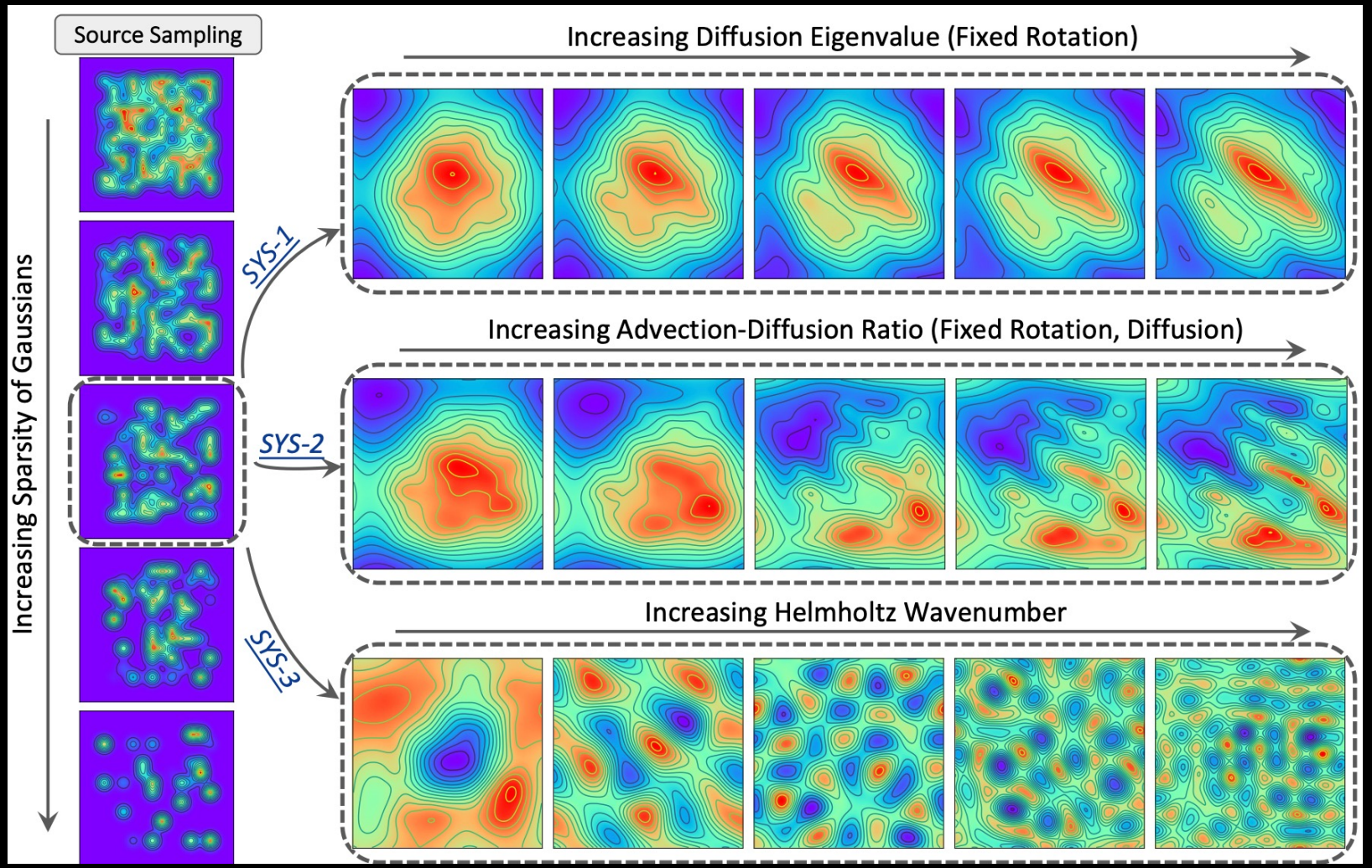
Design Mask Resist



Our AI (FNO) is **differentiable** and can do **inverse design**

Zhou, Tingtao, et al. "AI-aided Geometric Design of Anti-infection Catheters." *arXiv preprint arXiv:2304.14554* (2023).

NEURAL OPERATORS (FNO) - FOUNDATION MODEL



FNO trained on multiple different PDE systems

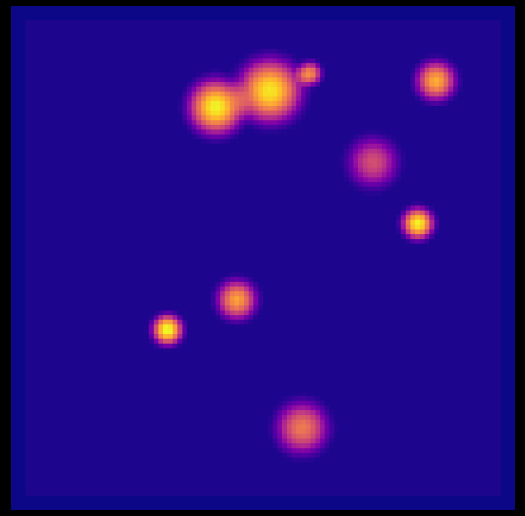
Subramanian, Shashank, et al. "Towards Foundation Models for Scientific Machine Learning: Characterizing Scaling and Transfer Behavior." *arXiv preprint arXiv:2306.00258* (2023).

APPLICATION TO FUSION

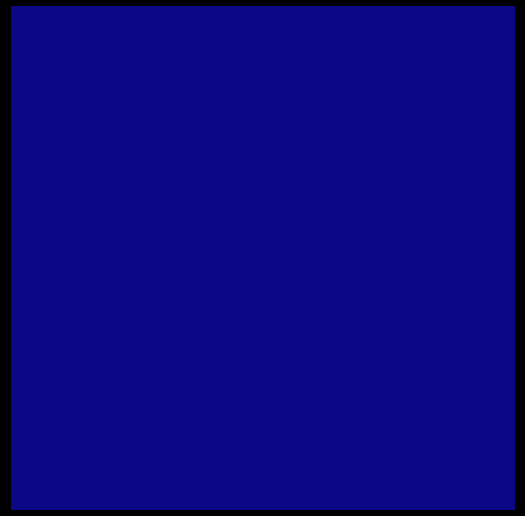
REDUCED-MHD

Radial Convection of plasma blobs in toroidal geometry using JOREK

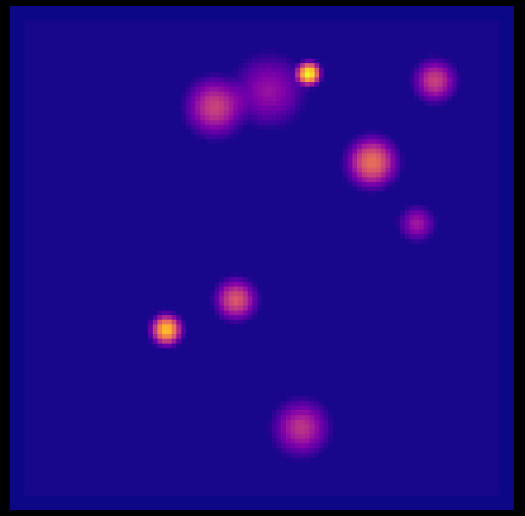
Absence of a plasma current equilibrium generates a buoyancy effect, causing the blob to move outwards towards the edge.



Density



Electric Potential

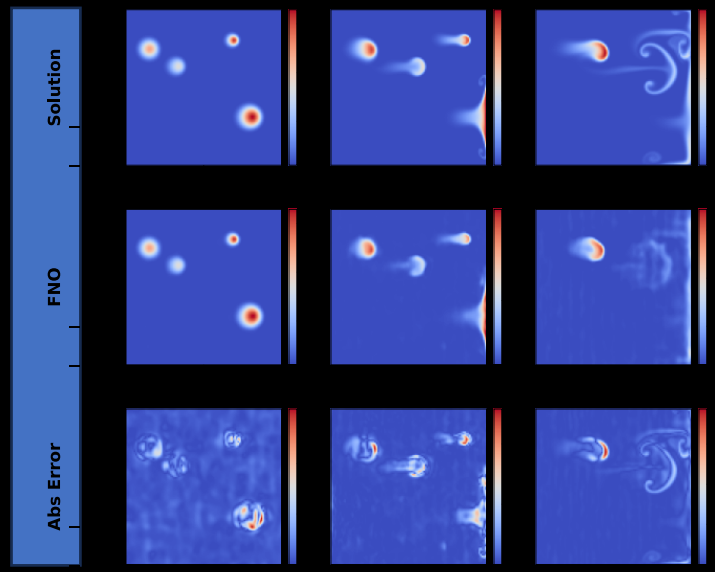


Temperature

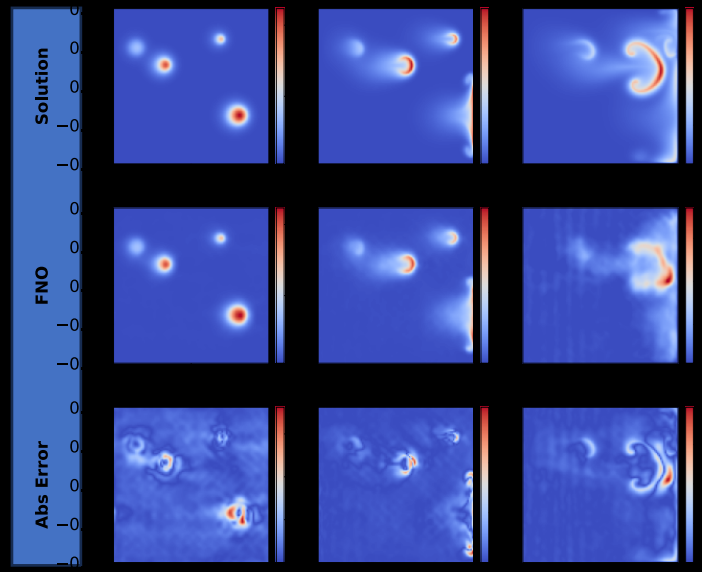
2000 simulations built by varying the initial conditions of the plasma blobs: number, position, width and amplitude

FNO OVER MHD

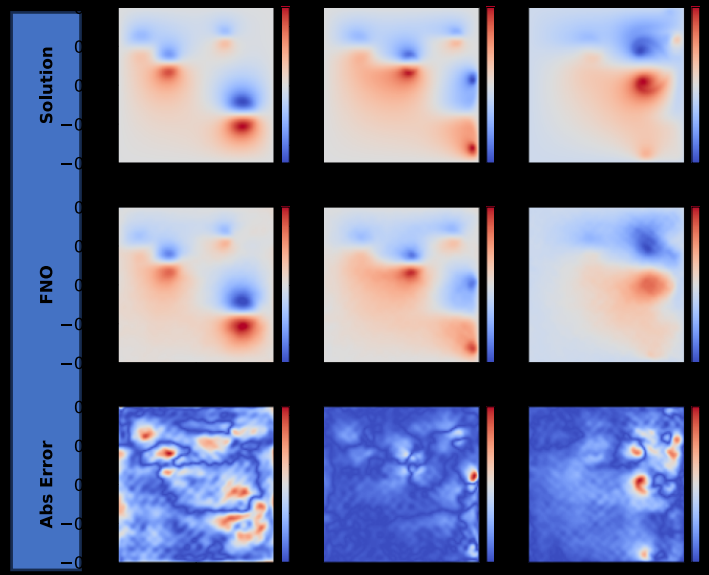
FNO: 6 orders of magnitude faster than JOREK



Density



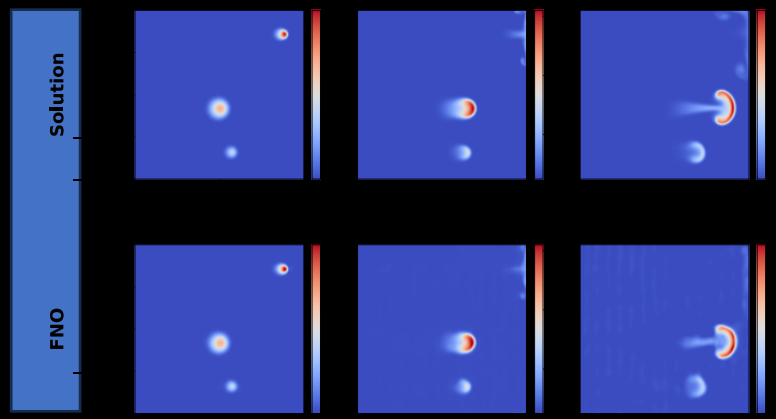
Temperature



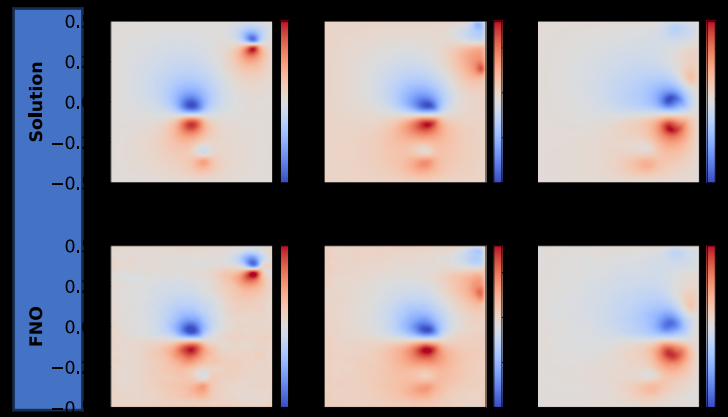
Electric Potential

T_{in} = 10
Step = 5
T_{out} = 40

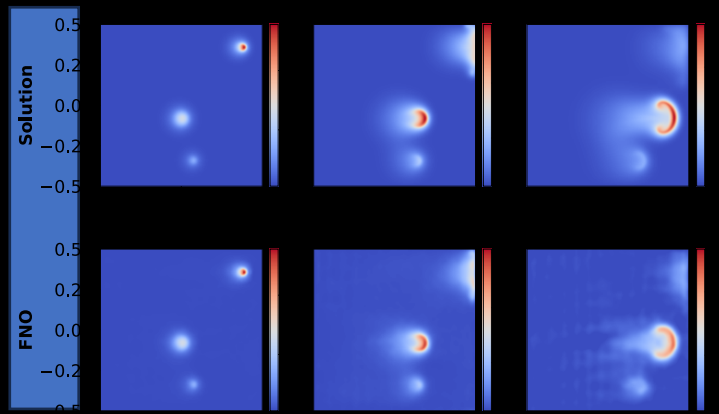
SUPER-RESOLUTION



Density



Potential



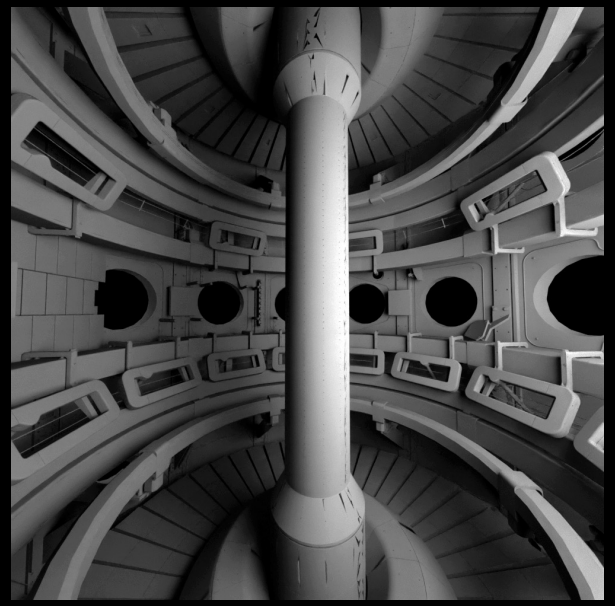
Temperature

Being discretisation-invariant,
FNO trained on coarser grids *(100x100)*,
can be deployed for finer grids *(500x500)*.

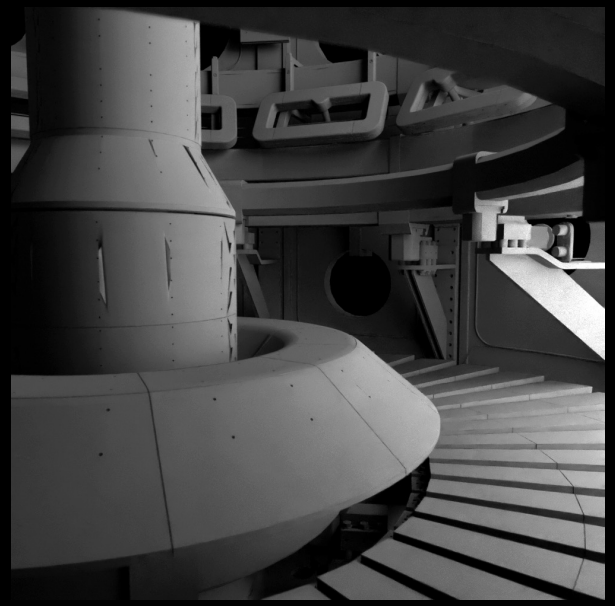
FNO OVER CAMERA

Modelling the plasma as diagnostically captured by the Fast Cameras on MAST

Modelled over the entire shot duration of 55 shots from the last campaign on MAST (M9)



Camera viewing the central solenoid (rbb)[1]



Camera viewing the divertor (rba) [1]

Motivation:

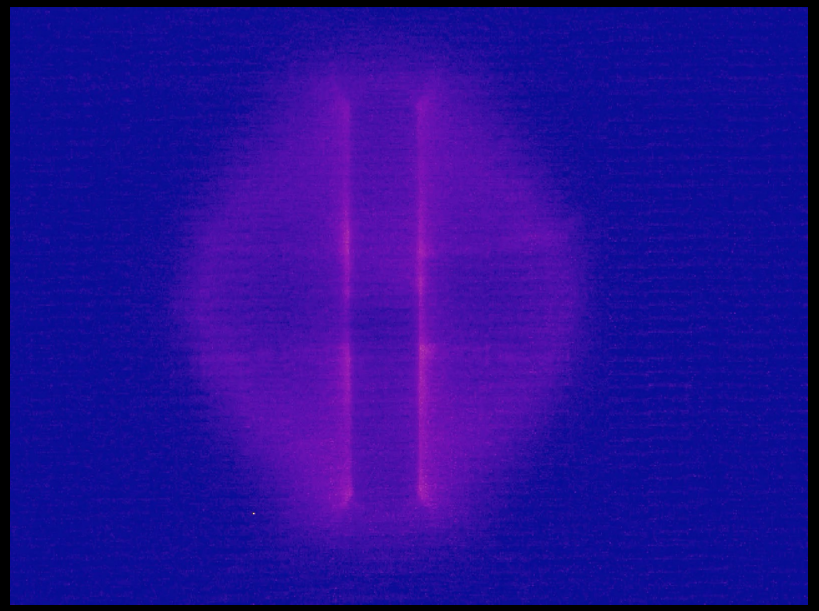
Real-time forecasting of fast camera images to track

- plasma evolution,
- predict L-H transition,
- build further unto disruption prediction.
- data assimilation (Sim2Real)

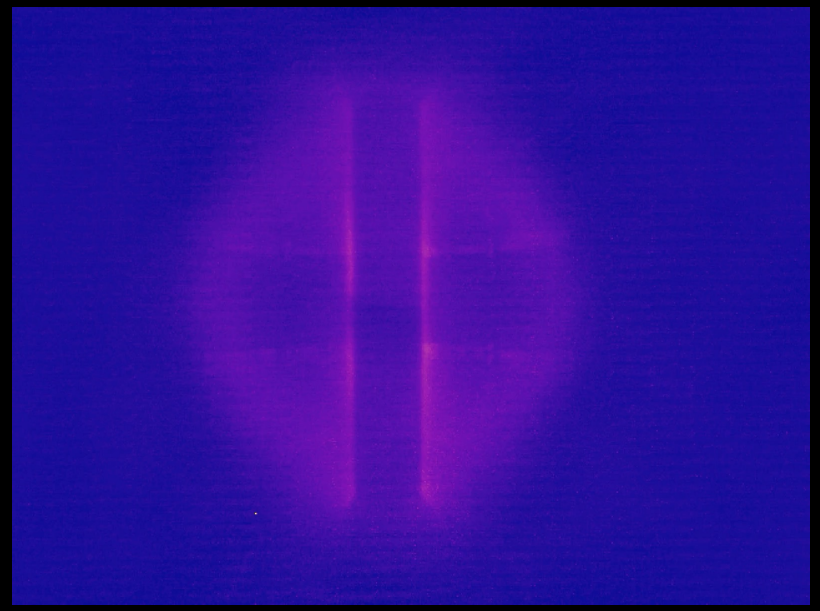
[1] Synthetic renders of the camera views created using the CAD model of MAST and Nvidia Omniverse.

CAMERA VIEWING THE CENTRAL SOLENOID (RBB)

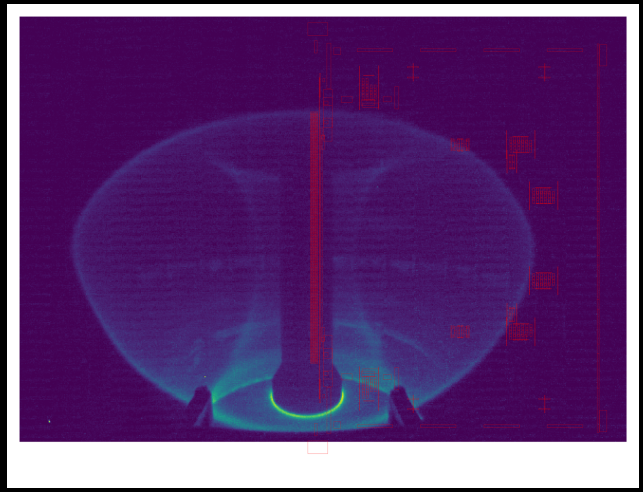
Camera



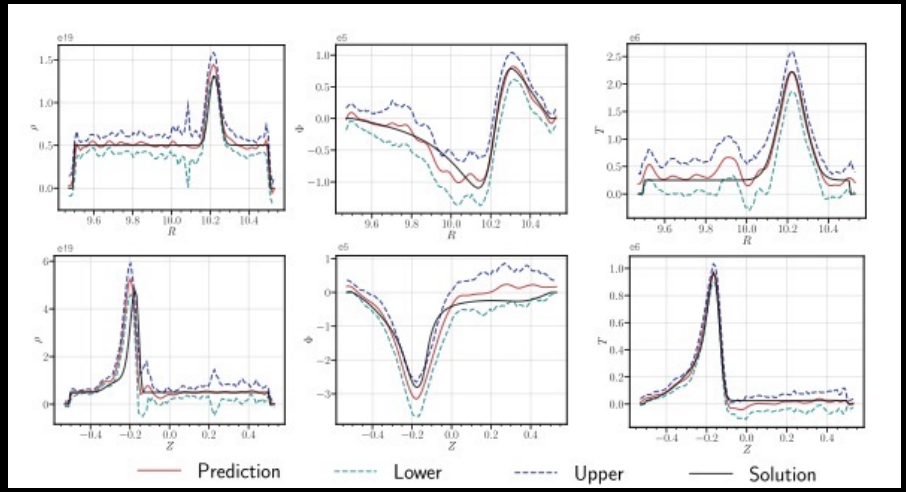
FNO



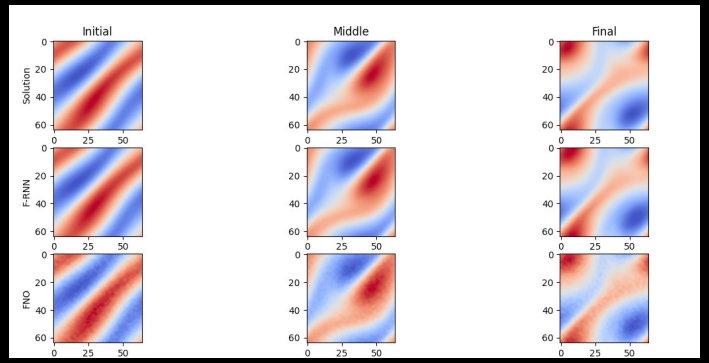
ONGOING WORK



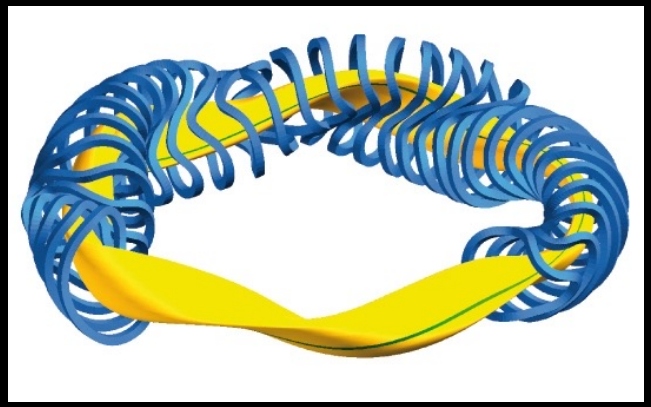
Provision of Control Signals to the Camera Digital Twin - LH Classifier



Uncertainty Quantification for Neural Operators using Conformal Prediction



Further development of state space models (Fourier-RNNs) for long time roll-outs



High-fidelity Digital Models for Fusion Pilot Plant Design (stellarator)

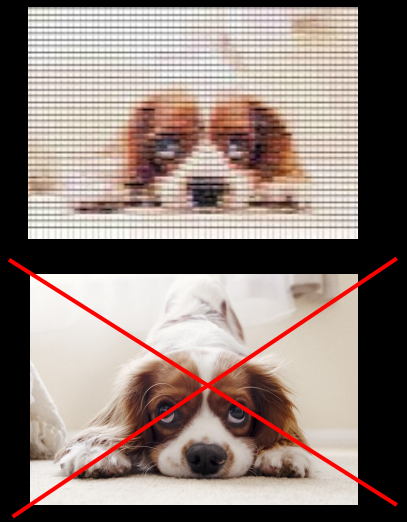
NEURAL OPERATORS

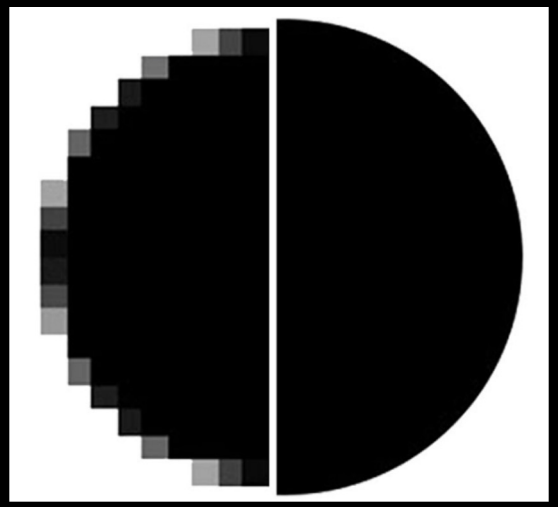
CAPTURING THE CONTINUUM: NEURAL OPERATORS

Our AI model predicts at any discretization

Neural Network

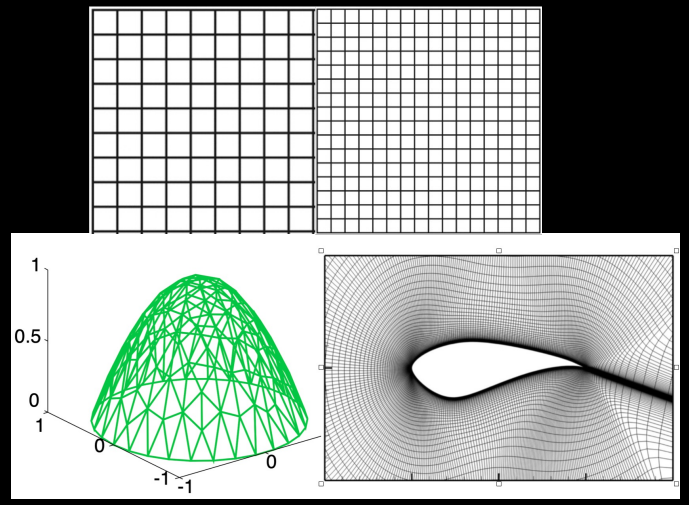
Input and output at fixed resolution



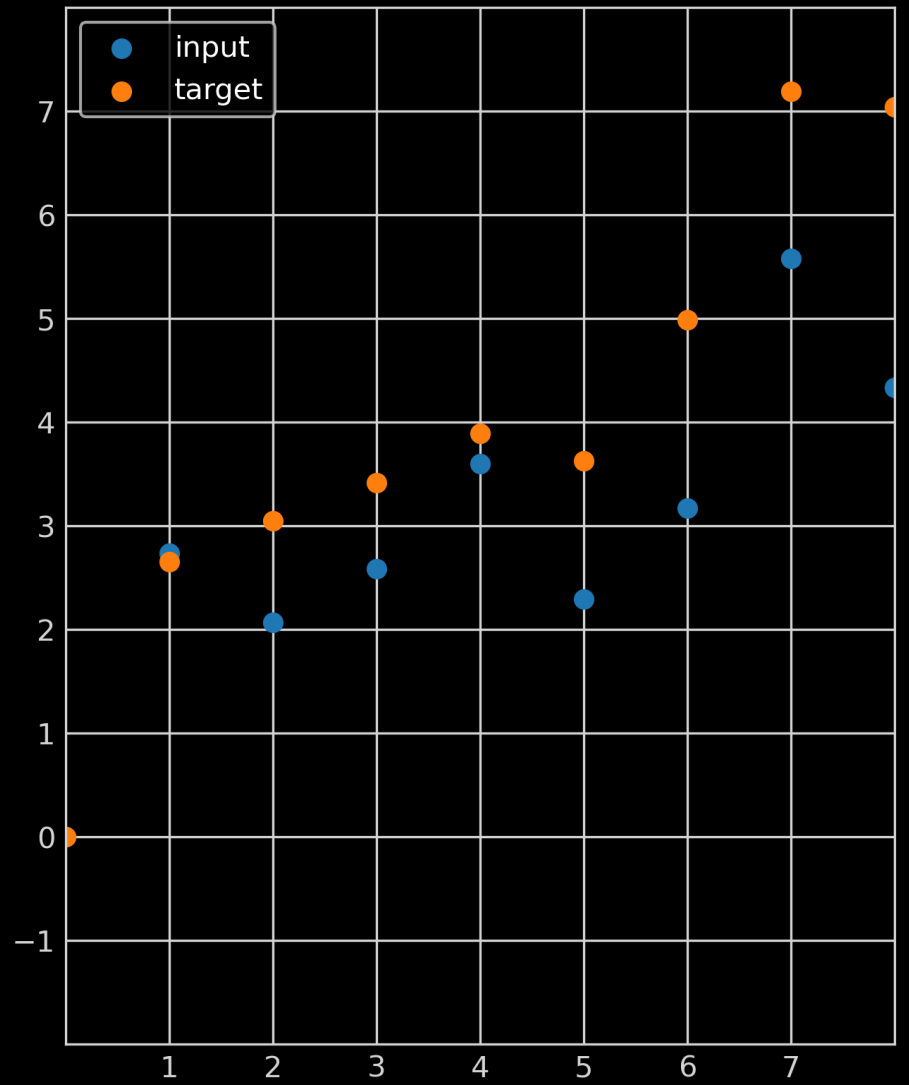


Neural Operator

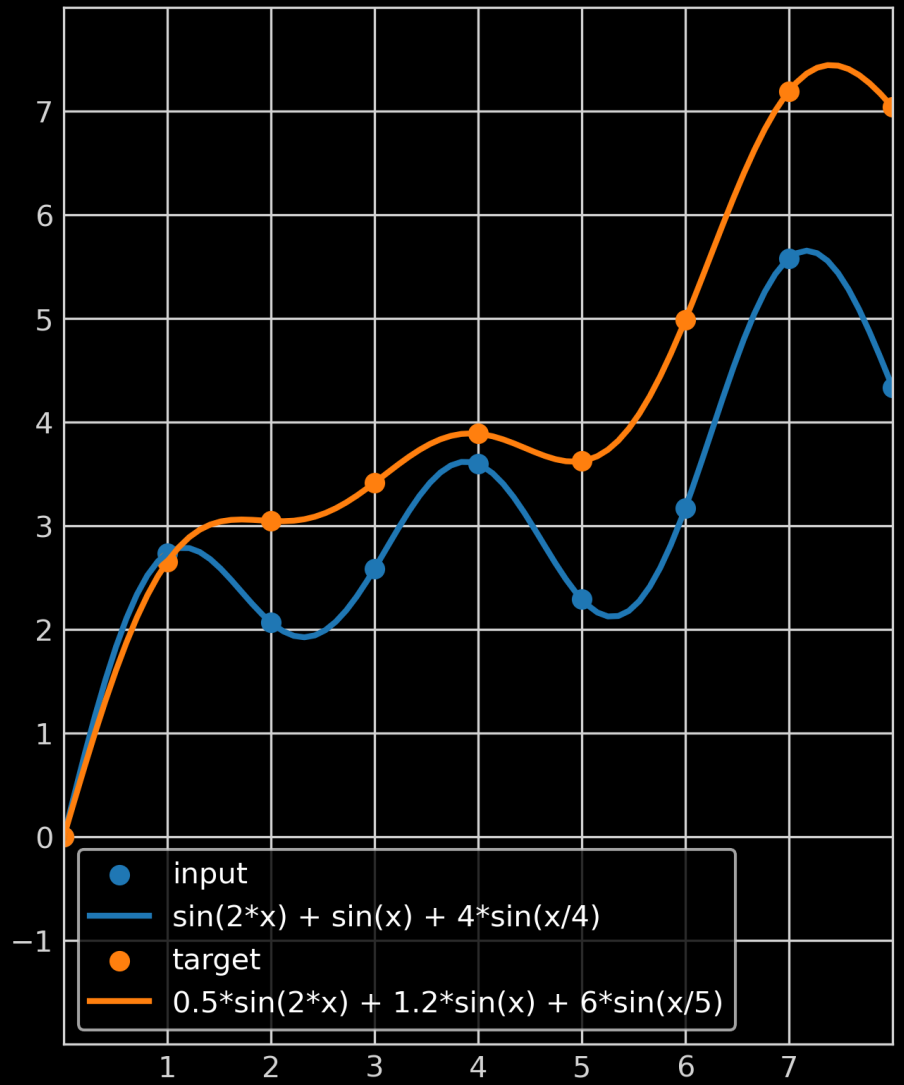
Input and output at any points in domain



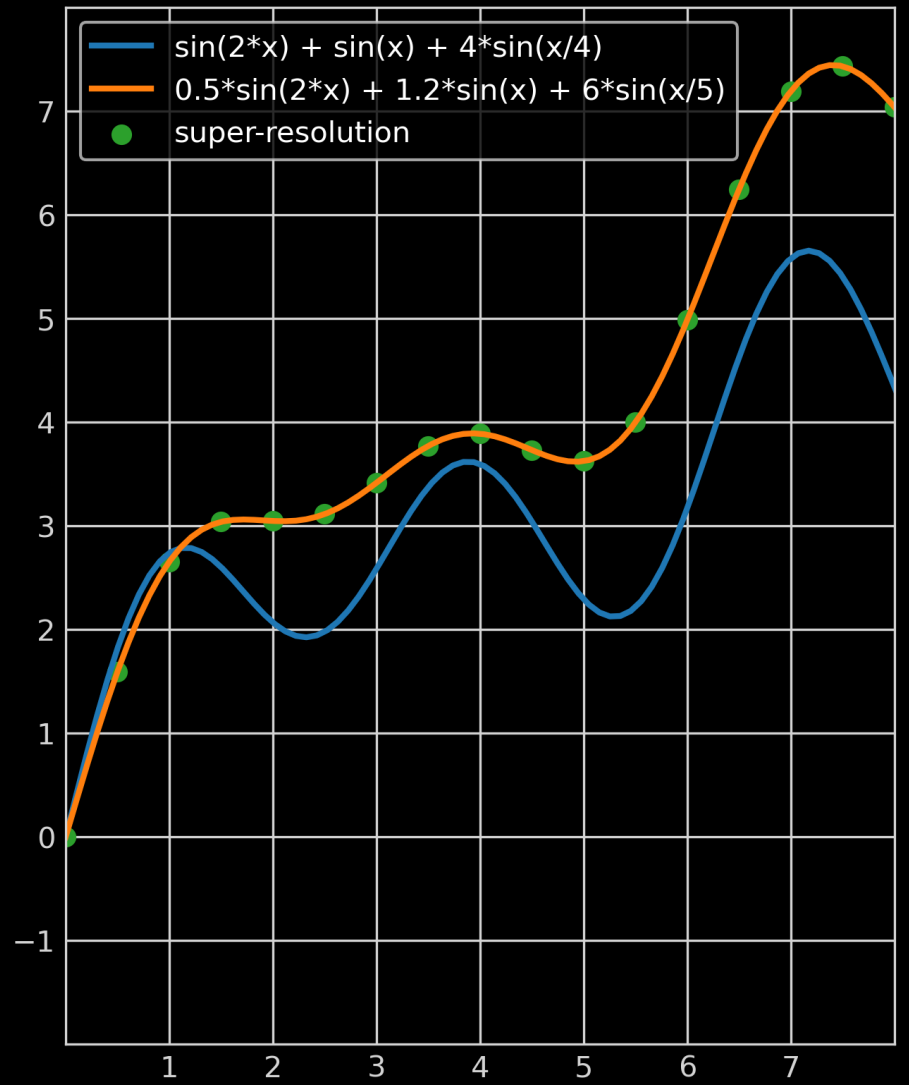
FOURIER NEURAL OPERATOR



FOURIER NEURAL OPERATOR



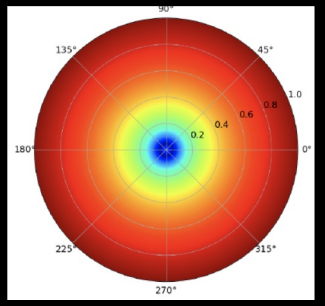
FOURIER NEURAL OPERATOR



LINEAR PDE : INTEGRAL SOLUTION OPERATOR

Input → Integral Linear Operator → Output

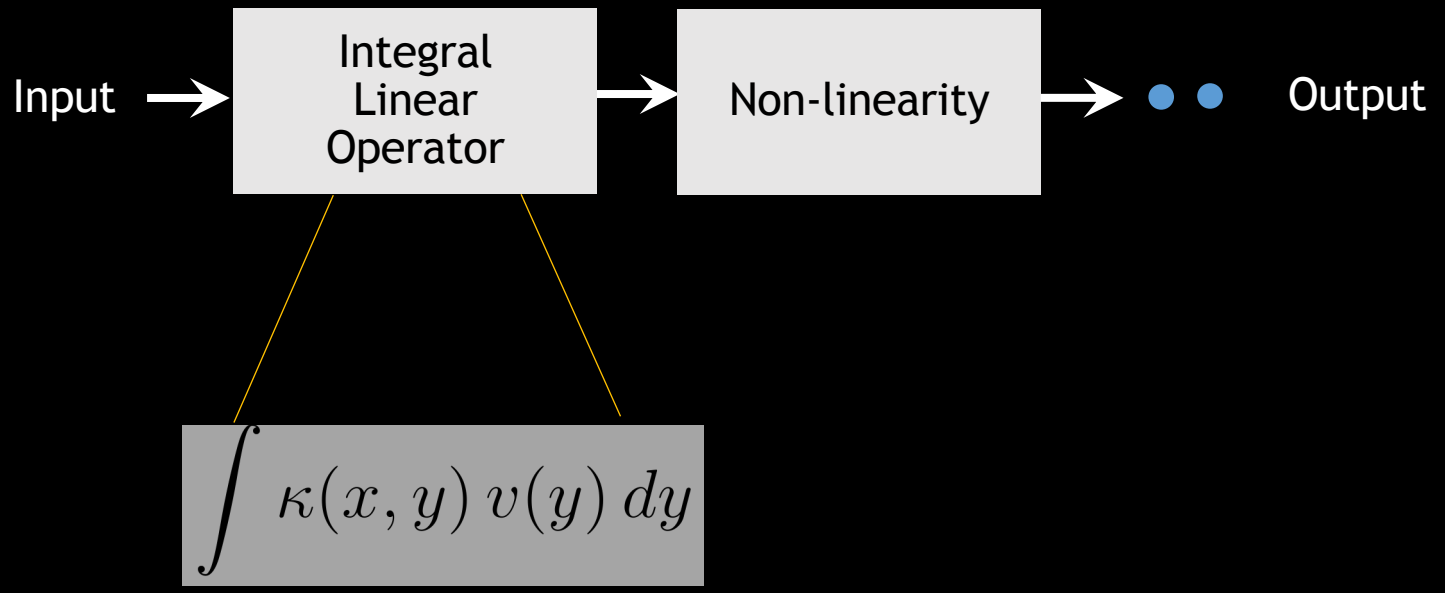
$$\int \kappa(x,y)\, v(y)\, dy$$

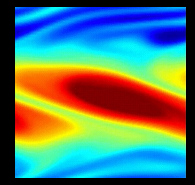


$K\ (x, y)$

Kernel of integral operator
For heat diffusion

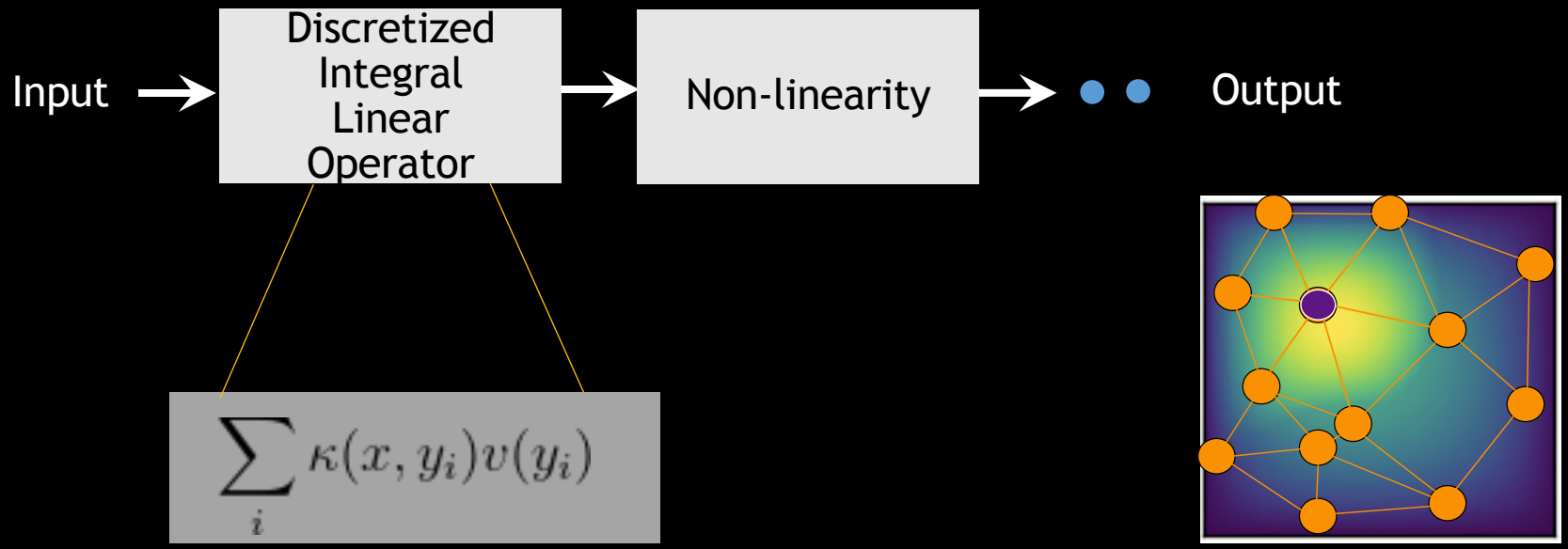
NEURAL OPERATOR: A GENERAL FRAMEWORK



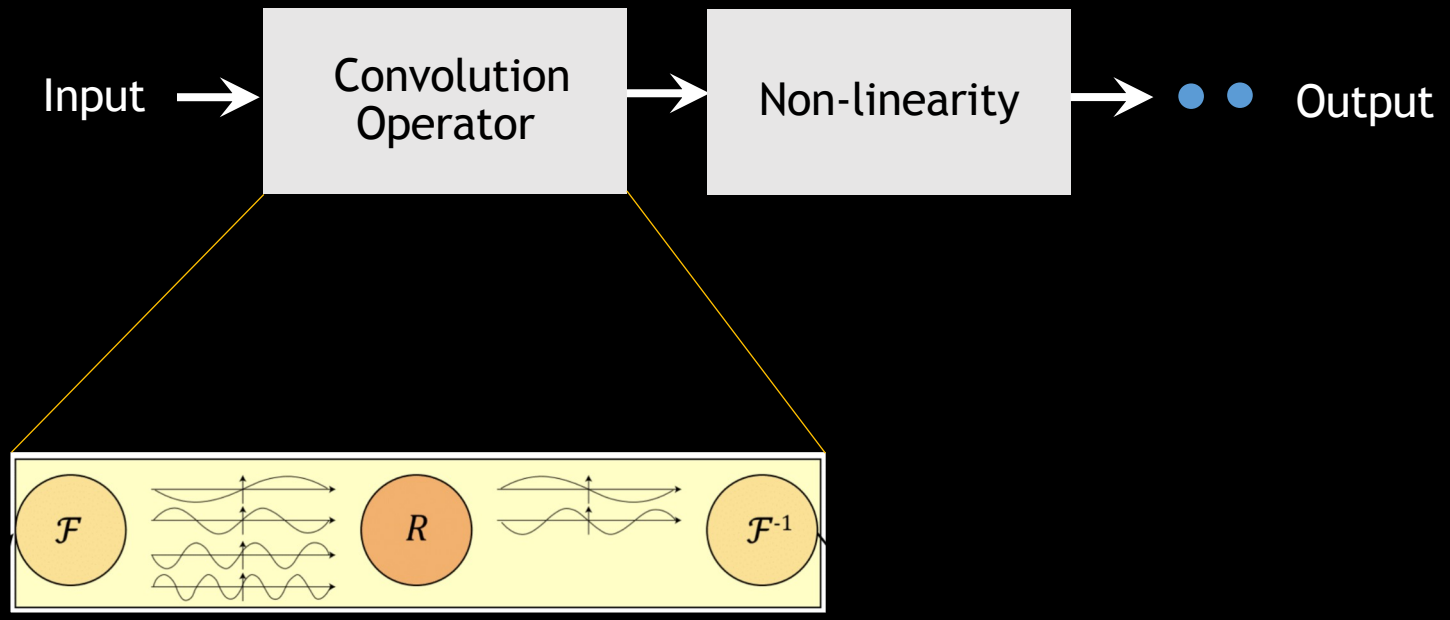


Solution operator
of fluid flows
is non-linear

GRAPH NEURAL OPERATOR



FNO: FOURIER NEURAL OPERATOR



Li, Zongyi, et al. "Fourier neural operator for parametric partial differential equations." ICLR, 2021.

FOURIER TRANSFORM FOR GLOBAL CONVOLUTION

Integral linear operator

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

Convolution operator
(special case of integral operator)

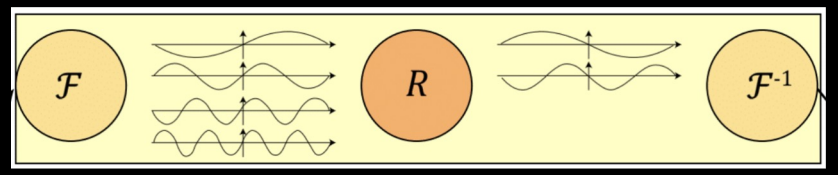
$$\int \kappa(x - y)\, v(y)\, dy$$

Solving convolution in Fourier domain

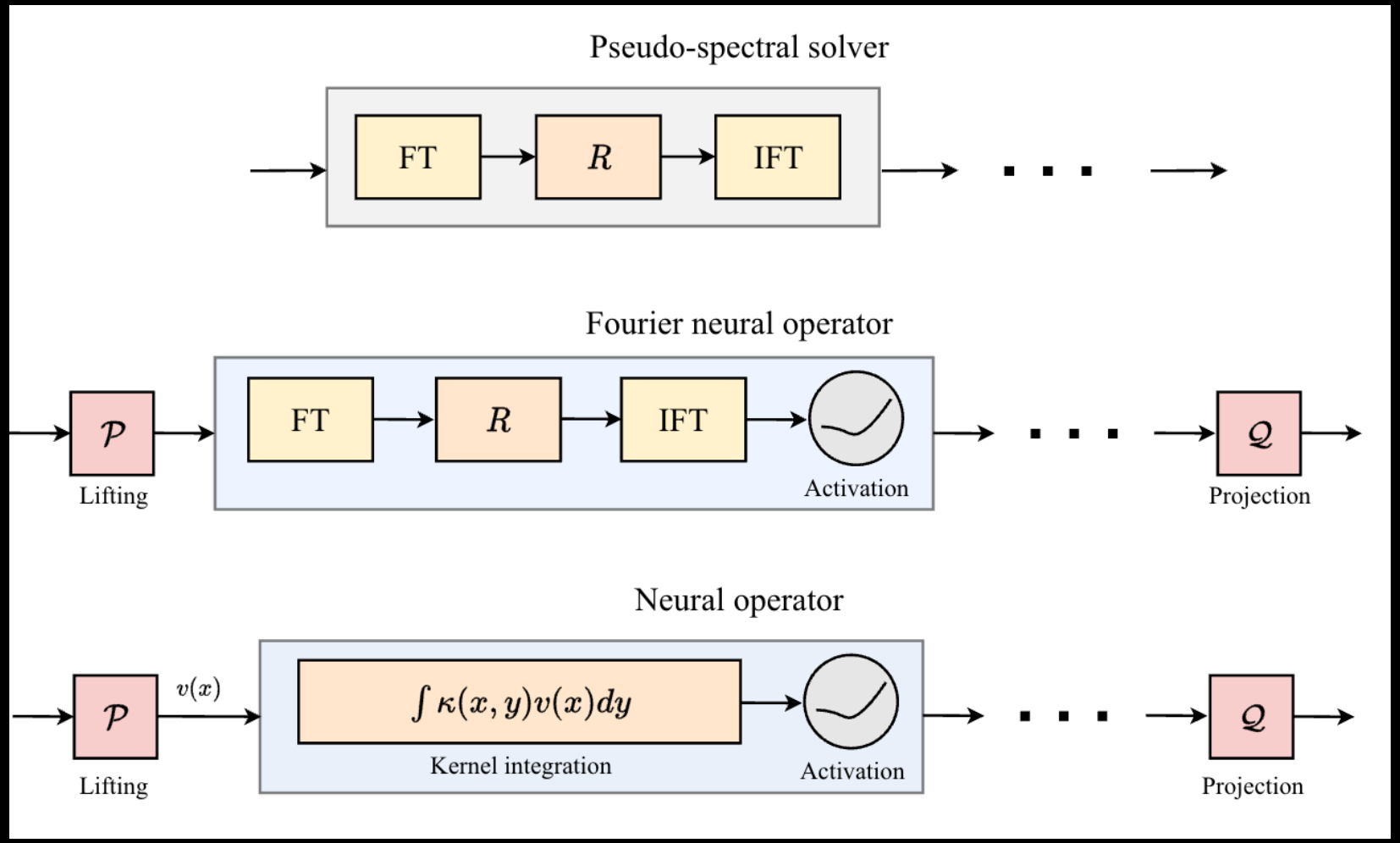
$$\mathcal{F}^{-1}(\, \mathcal{F}(\kappa)\, .\, \mathcal{F}(v)\,)$$

$$R := \mathcal{F}(\kappa)$$

Learn weights *R* in Fourier Domain



FROM PSEUDO-SPECTRAL SOLVER TO FNO: FOURIER NEURAL OPERATOR

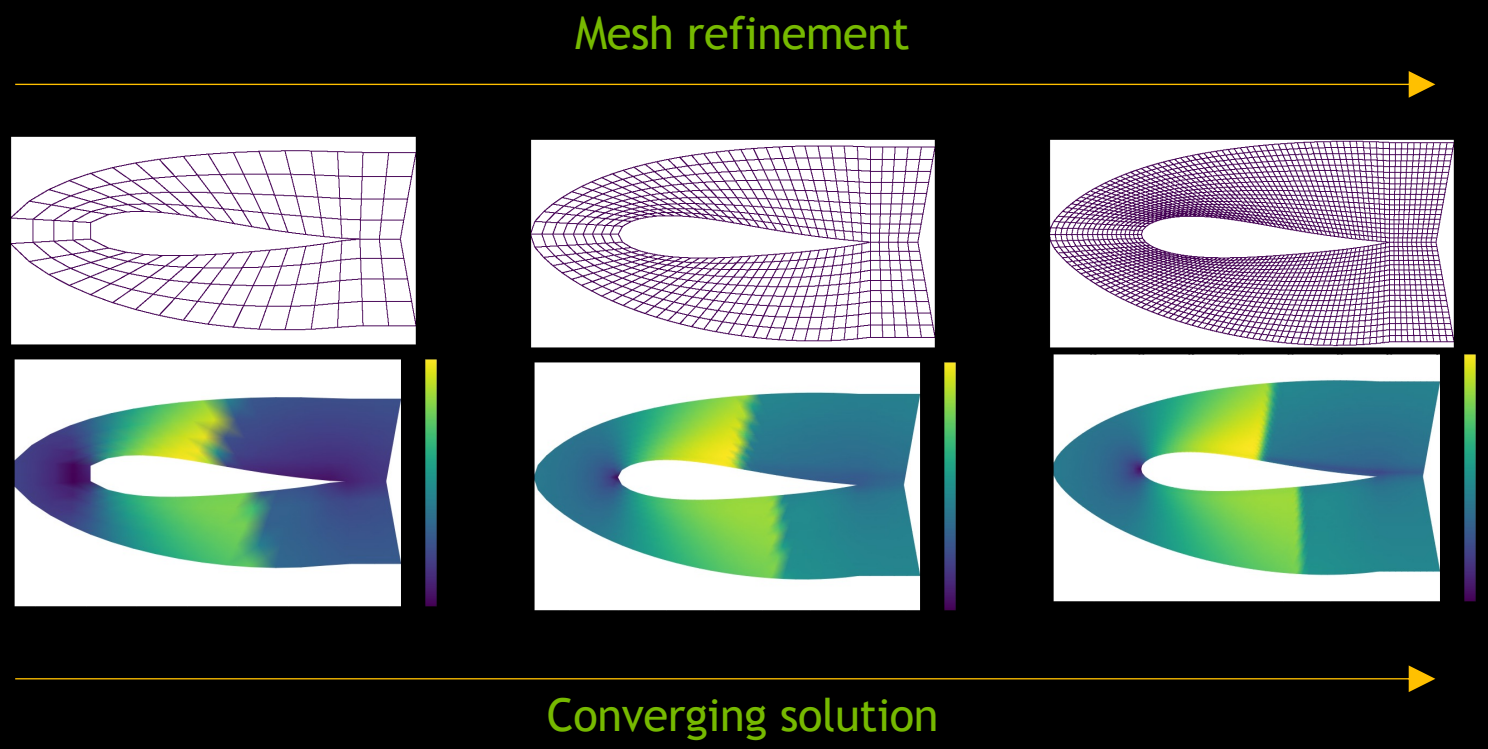


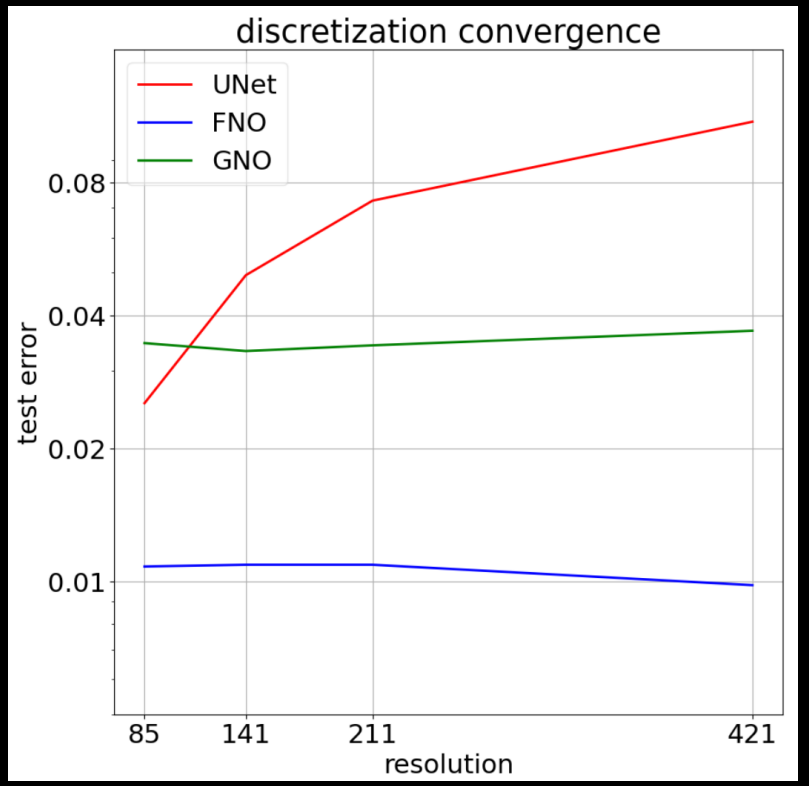
Li, Zongyi, et al. "Fourier neural operator for parametric partial differential equations." ICLR, 2021.

CAPTURING THE CONTINUUM: NEURAL OPERATORS

With neural operators, we can:

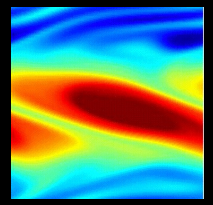
- We can query at any point in the domain (not limited to training grid.
- Converges upon mesh refinement to a limit (continuum).



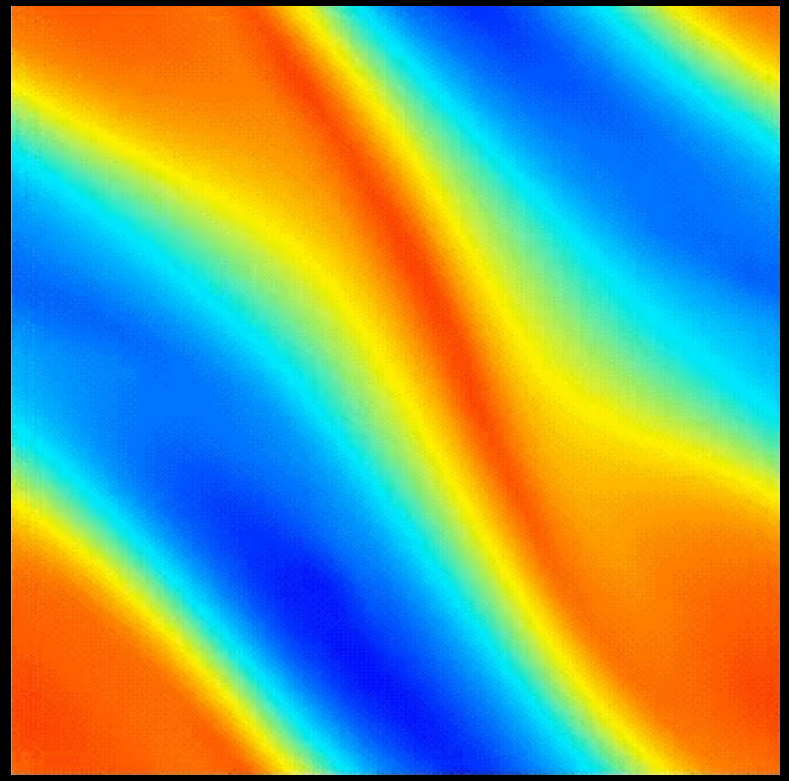


LEARNING ACROSS RESOLUTIONS WITH NEURAL OPERATORS

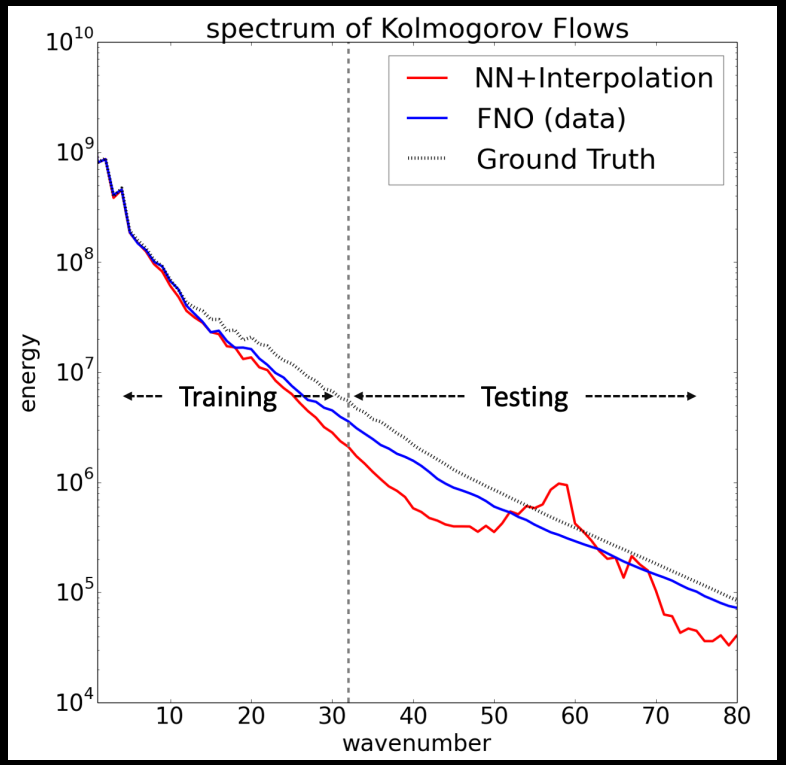
training data
(64x64)



prediction
(256x256)

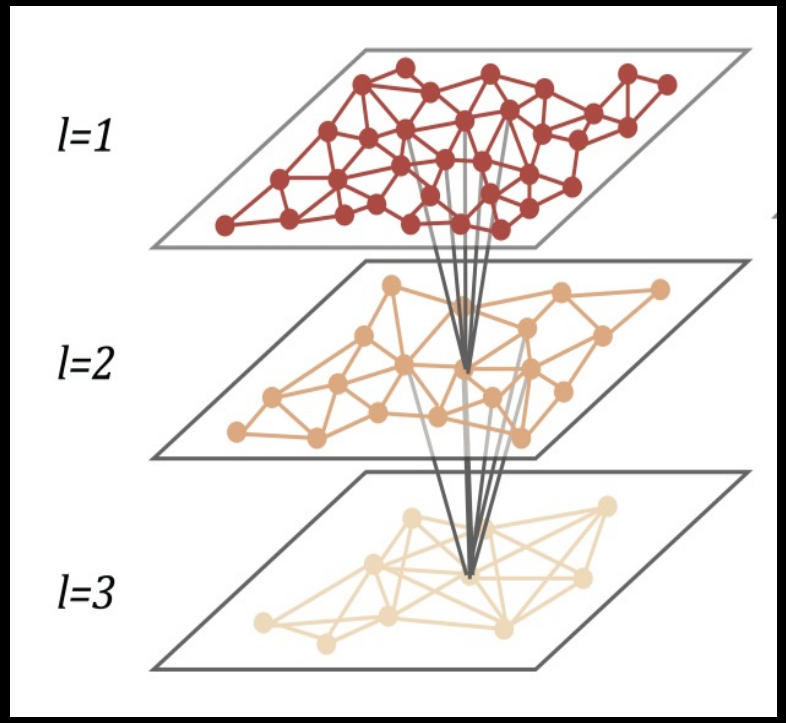


https://github.com/neuraloperator

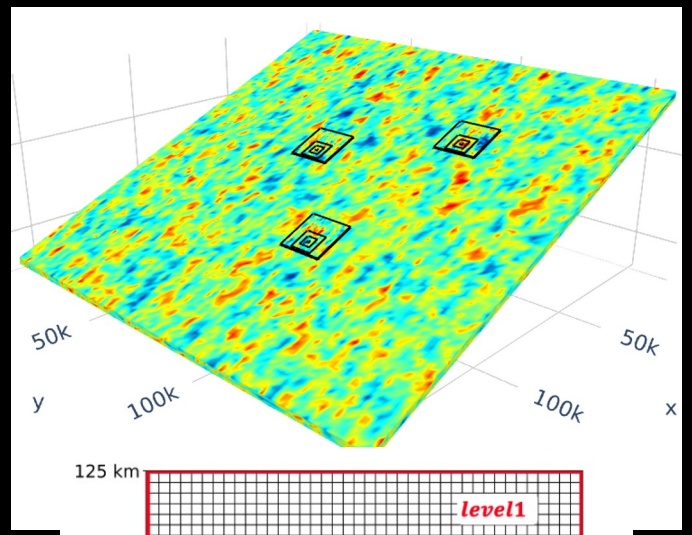


Our AI model (FNO) captures physical effects at all scales

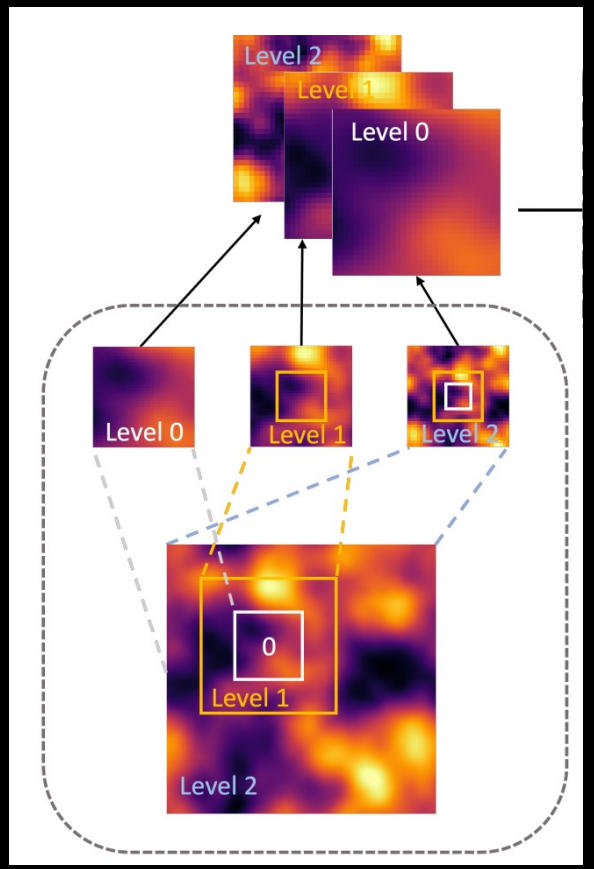
MULTI-SCALE NEURAL OPERATOR



Multi-level Graph Neural Operator



Nested Fourier Neural Operator



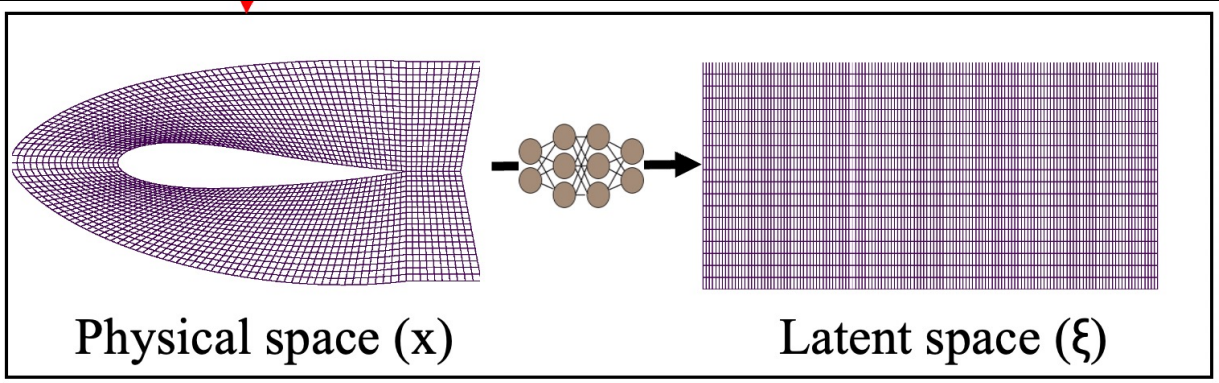
Multi-grid domain decomposition

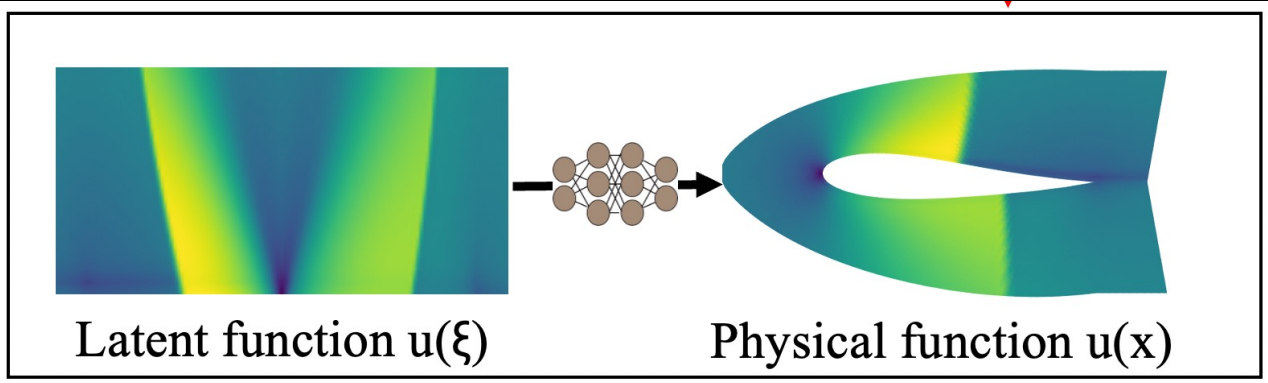
IRREGULAR GEOMETRY

GEOMETRIC-FNO

Previous FNO can be only applied to rectangular domains with a uniform grid.

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





PREDICTING DEFORMATION IN MATERIALS

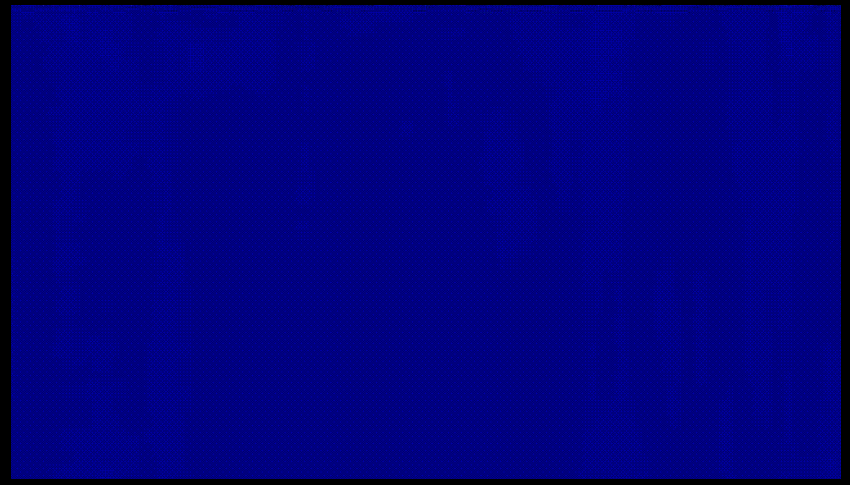
Plastic forging problem: a block of material is impacted by a frictionless, rigid die from top.

10^5 faster.

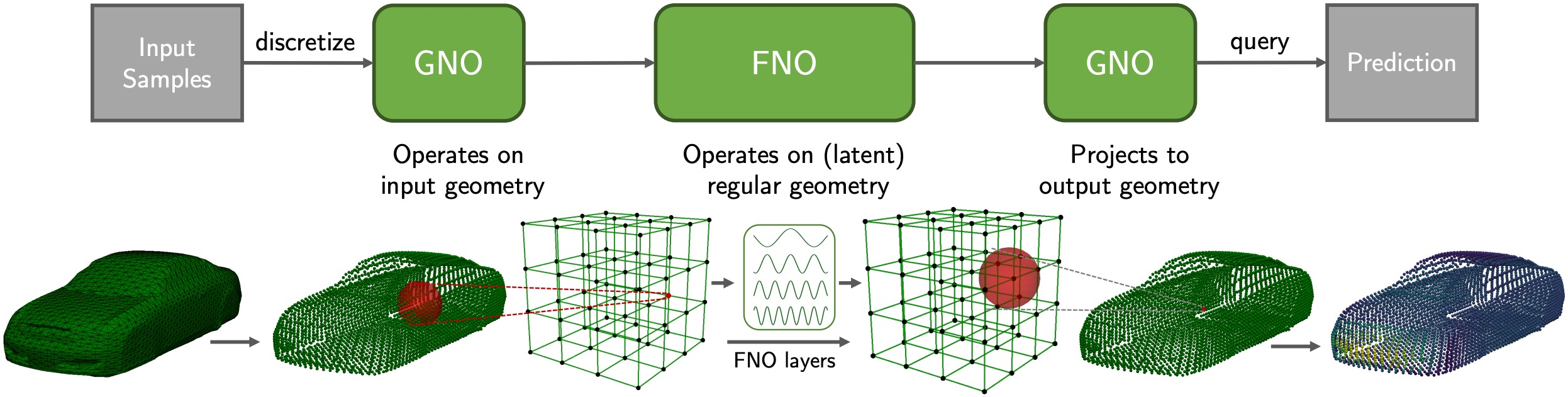
Ground Truth



Prediction

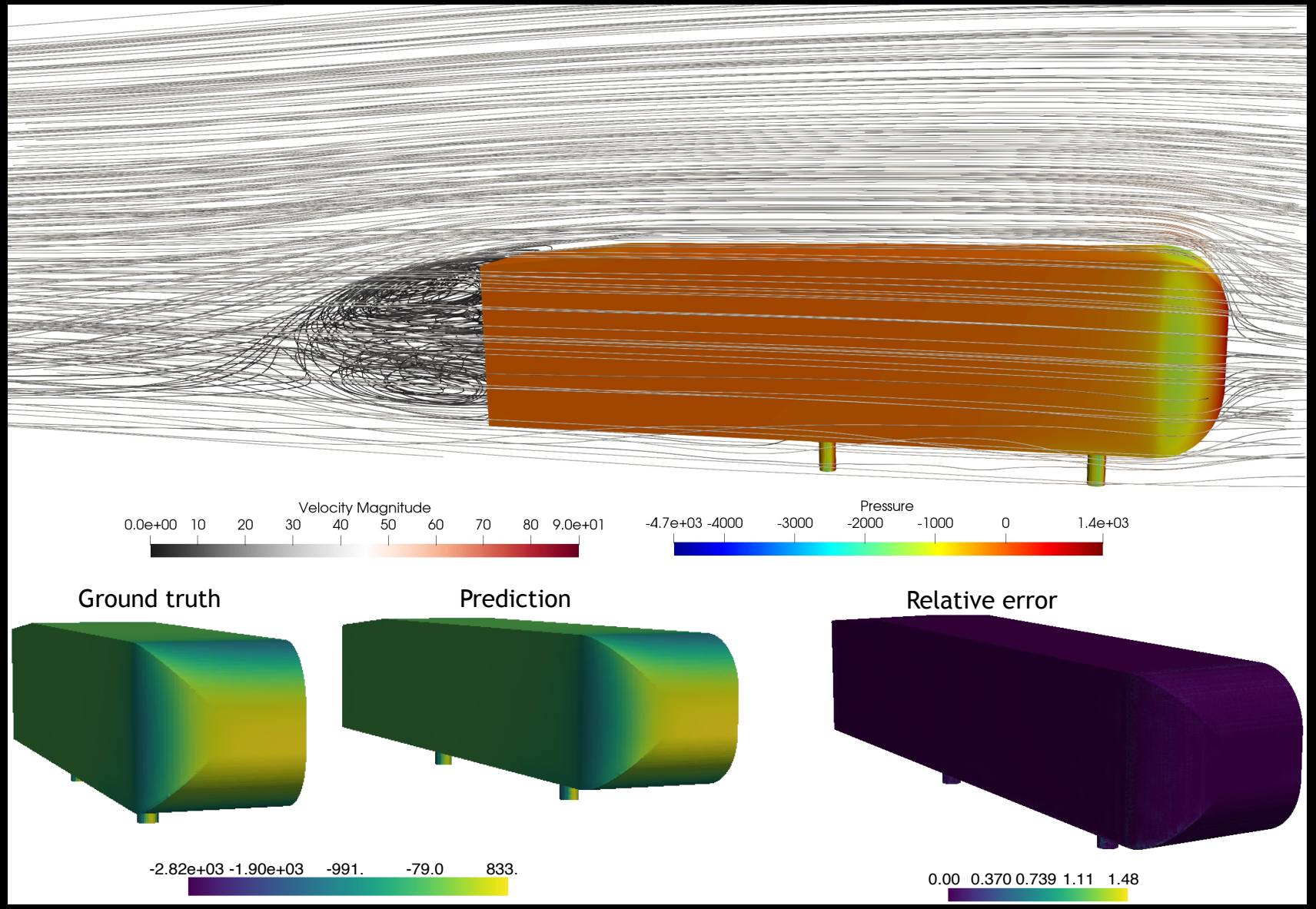


SDF + FOURIER + GRAPH NEURAL OPERATOR

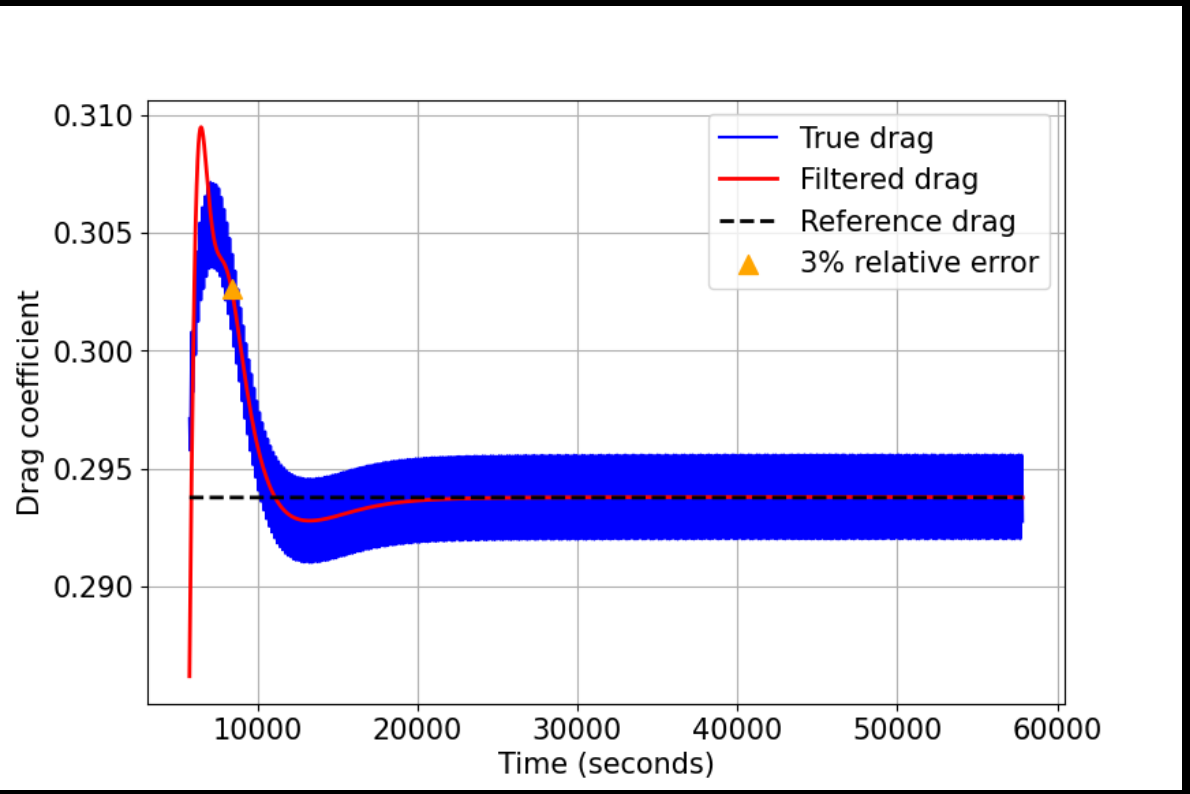


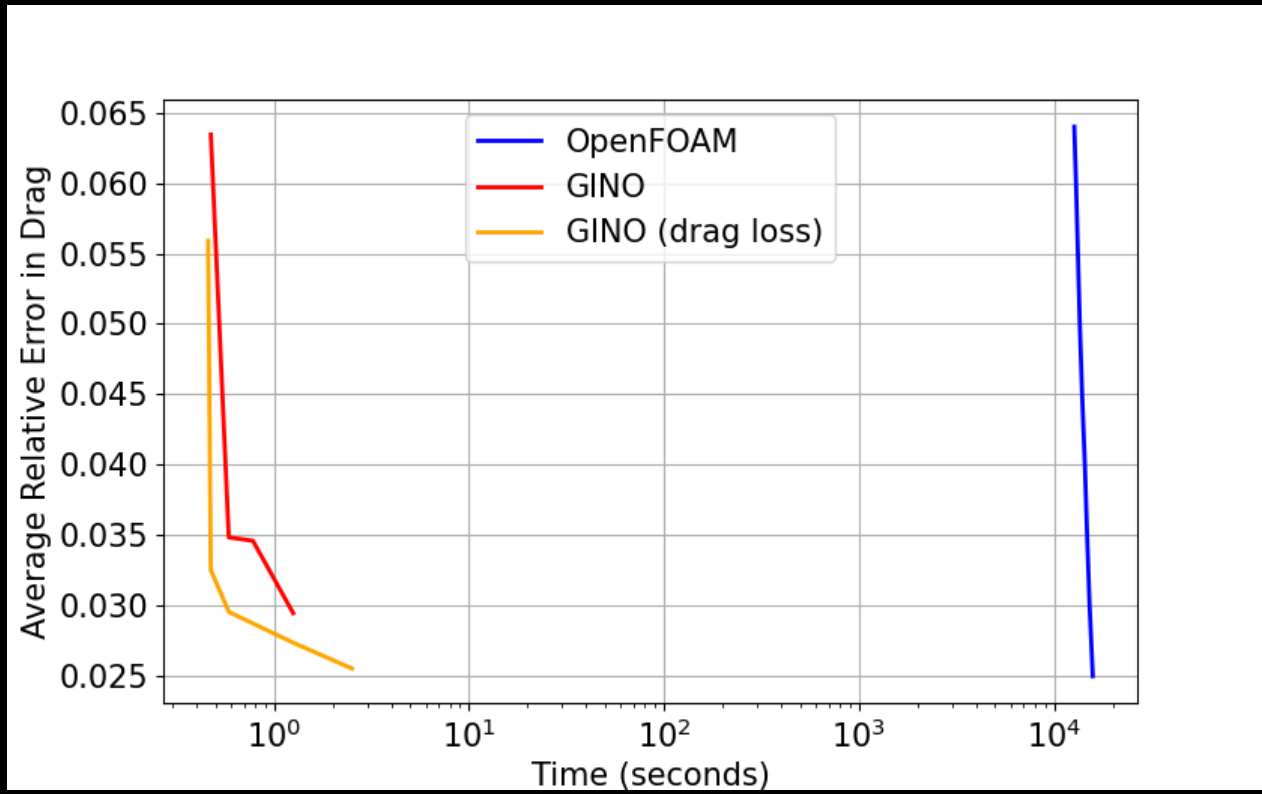
Li, Zongyi, et al. "Geometry-Informed Neural Operator for Large-Scale 3D PDEs." *arXiv preprint arXiv:2309.00583* (2023).

3D REALISTIC AUTOMOTIVE AERODYNAMICS



DRAG COEFFICIENT



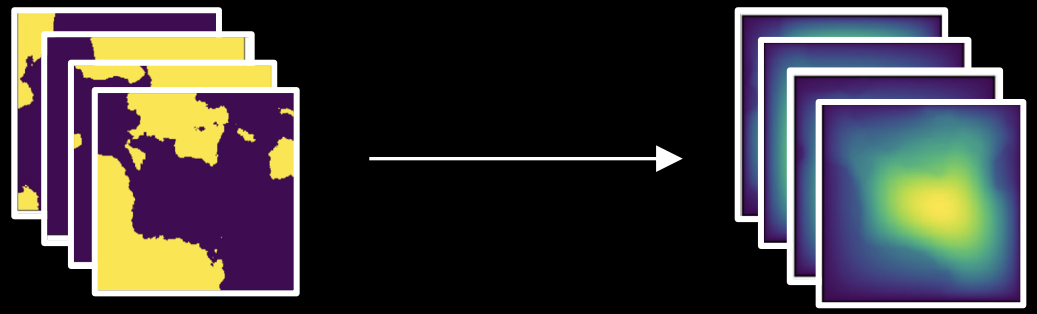


PHYSICS INFORMED LEARNING

PINO: PHYSICS-INFORMED NEURAL OPERATOR

PINO can learn solution operator for a family of equations and fine-tune on an instance

Operator learning



Instance-wise finetuning



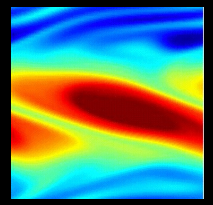
SOLVING PDE VS OPERATOR LEARNING

- Solving a PDE through numerical solvers or physics informed neural networks (PINN).
- Uses only PDE and no data.
- Solving from scratch is usually a difficult optimization.

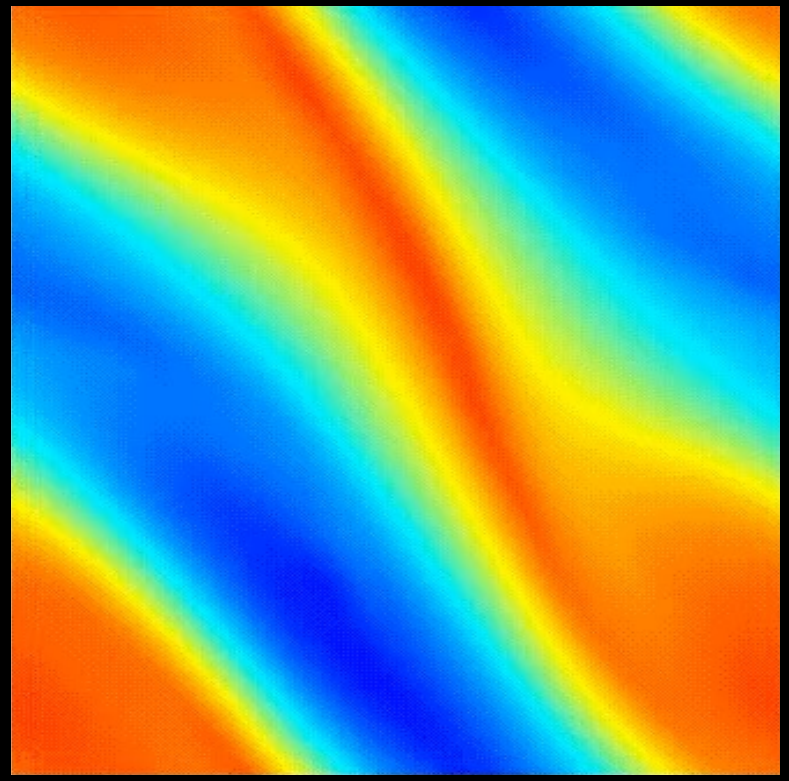
- Supervised learning solution mapping through operator learning.
- Can use data and/or PDE constraints.
- Data helps overcome optimization challenges.

PHYSICS INFORMED NEURAL OPERATORS

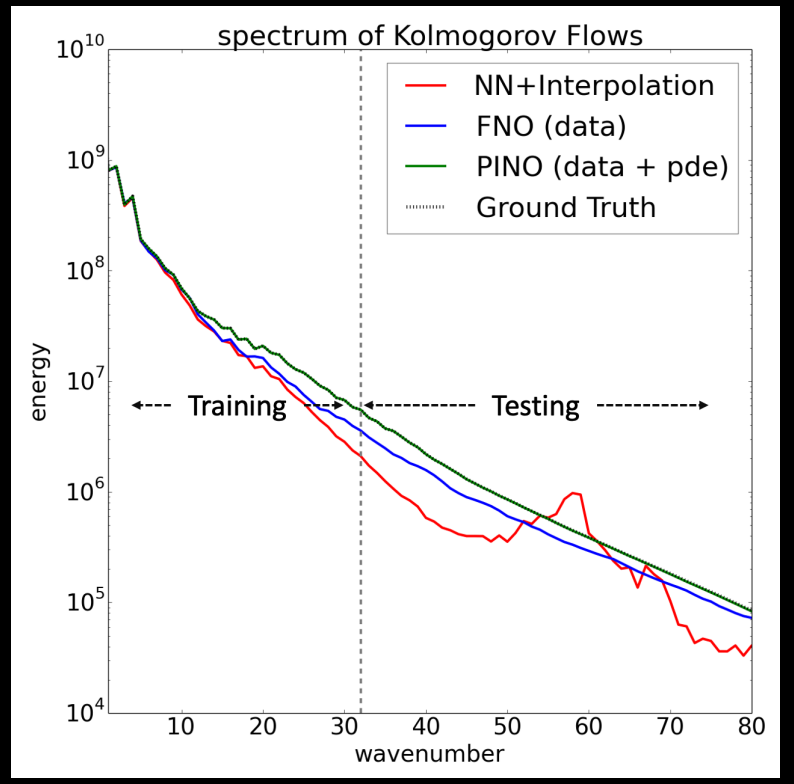
training data
(64x64)



prediction
(256x256)



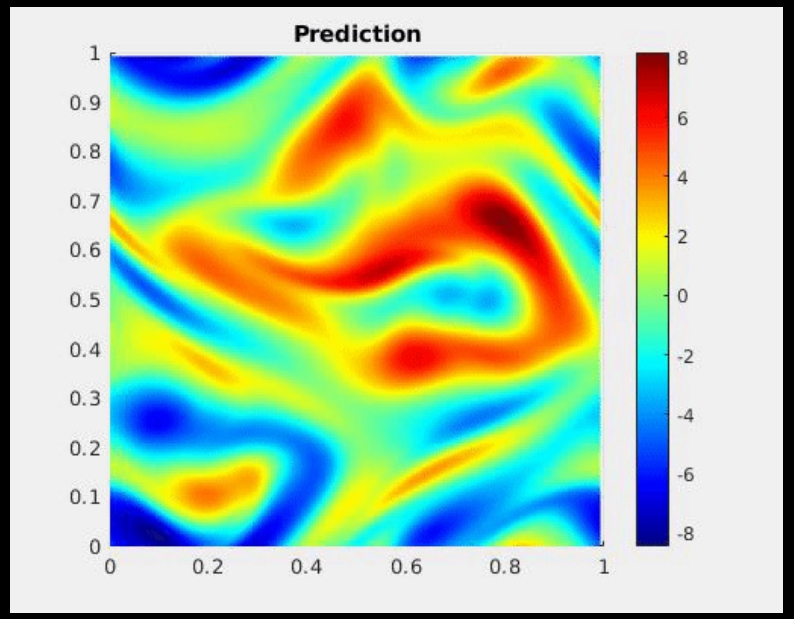
https://github.com/neuraloperator



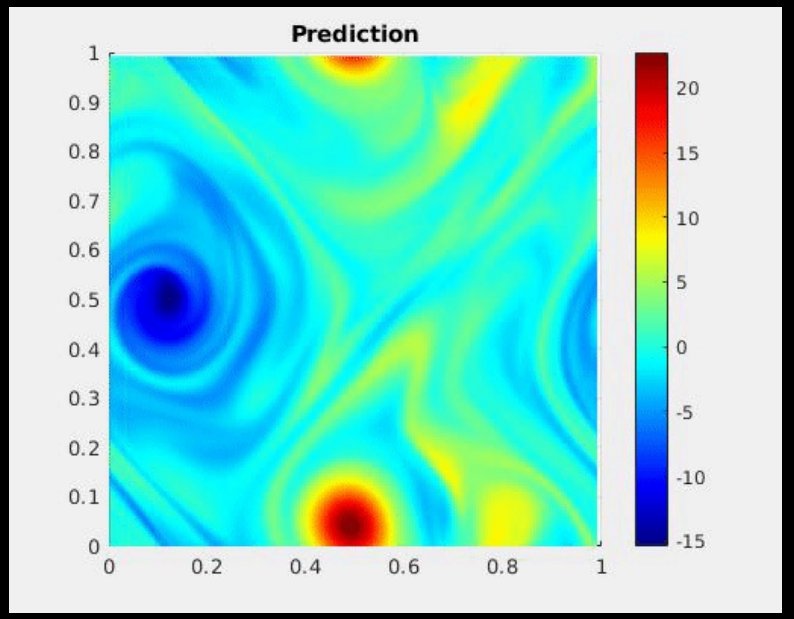
Our AI model (PINO) perfectly learns physical effects at all scales

TRANSFER LEARNING WITH PINO

Operator learned on Reynolds number 100, fine-tune to 500.
Converges 3x faster.



Re100



Re500

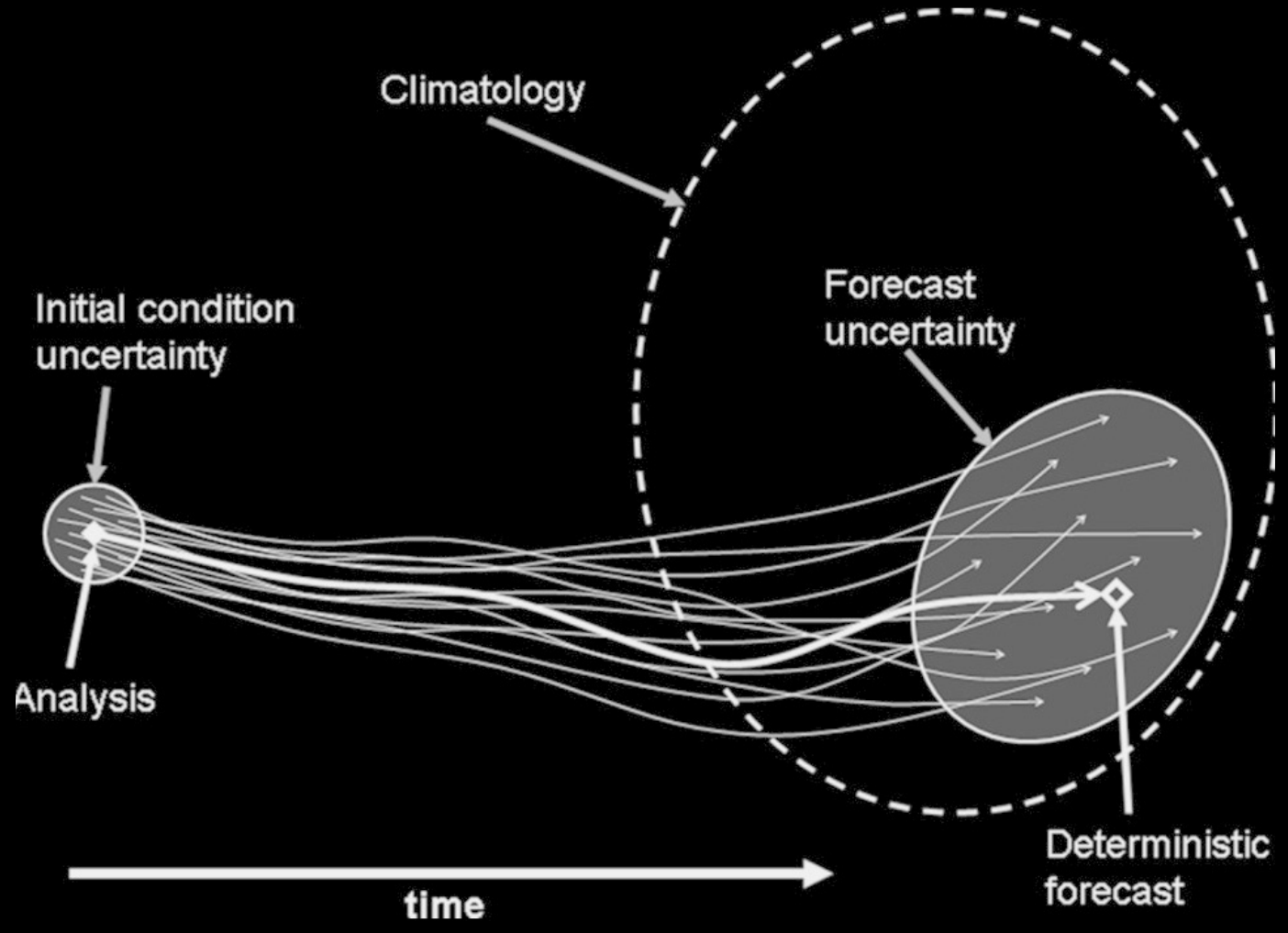
CHAOTIC SYSTEMS

CHAOTIC SYSTEMS

Chaotic systems are intrinsically unstable.

Small errors accumulate and trajectories unpredictable.

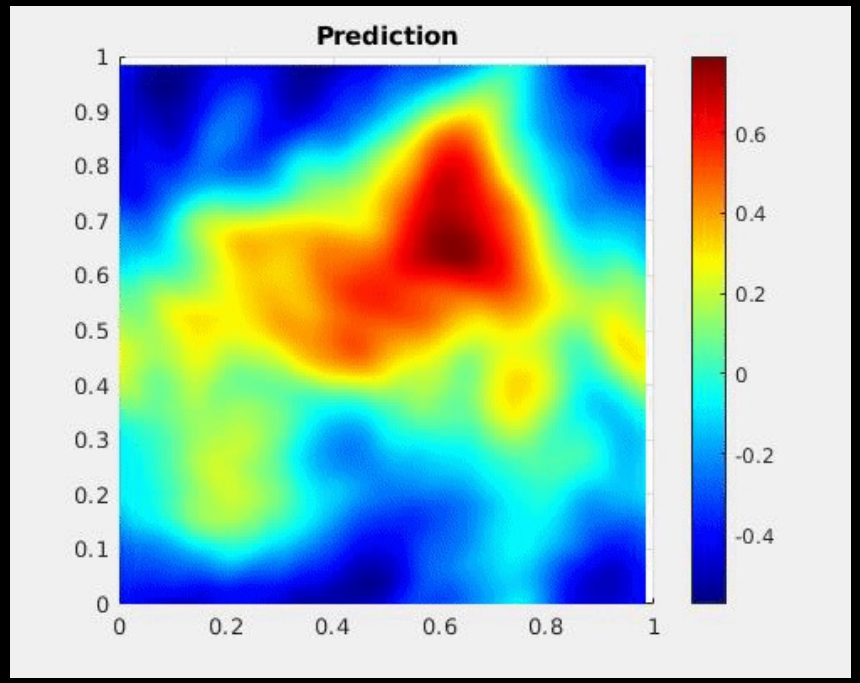
Can we recover the (**attractor**) and its **statistical properties**?



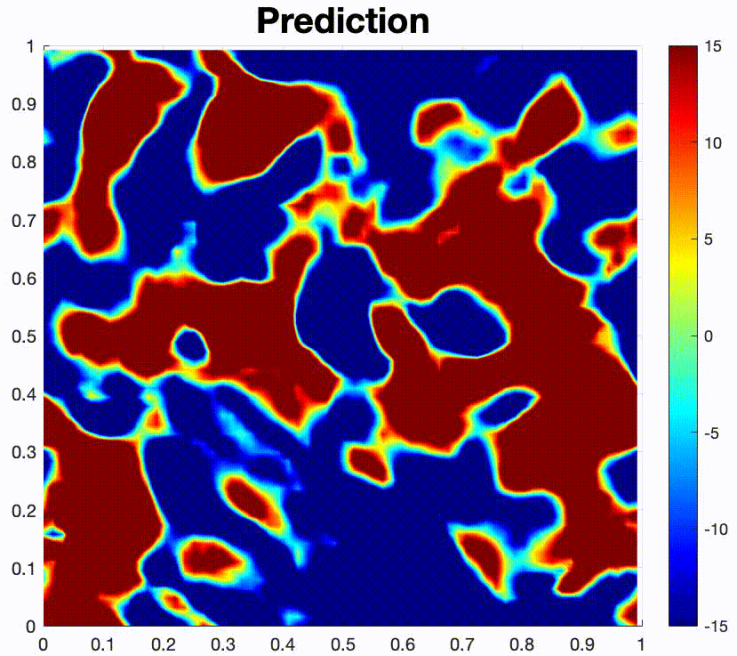
ENFORCING DISSIPATIVITY: MOTIVATIONS

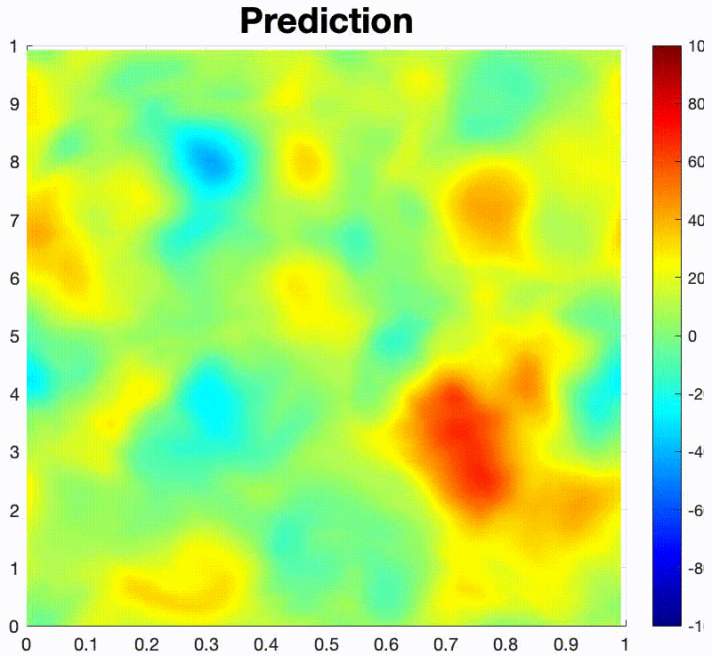
Many chaotic systems have the **dissipative** property, which pushes the dynamics back to the attractor.

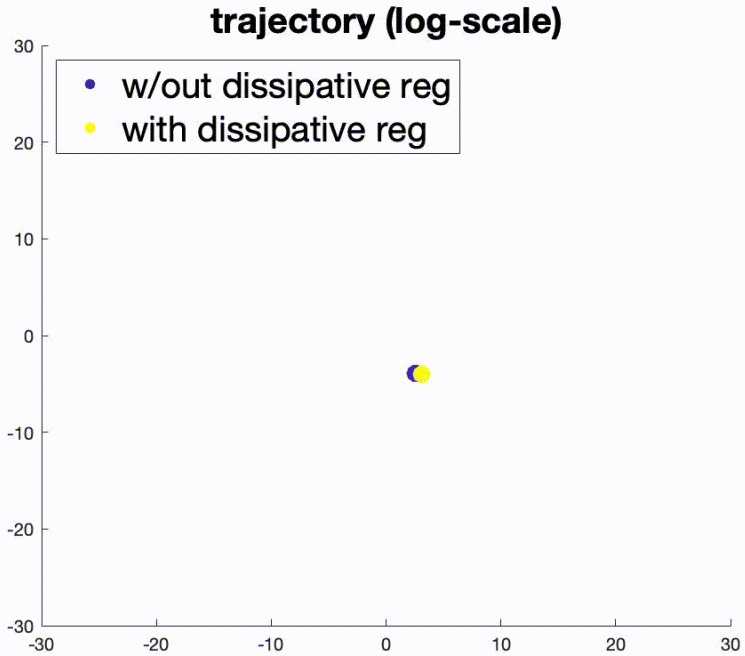
Without such dissipativity, the model is prone to blow up.



KOLMOGOROV FLOW WITH ENFORCED DISSIPATIVITY







With dissipative regularization

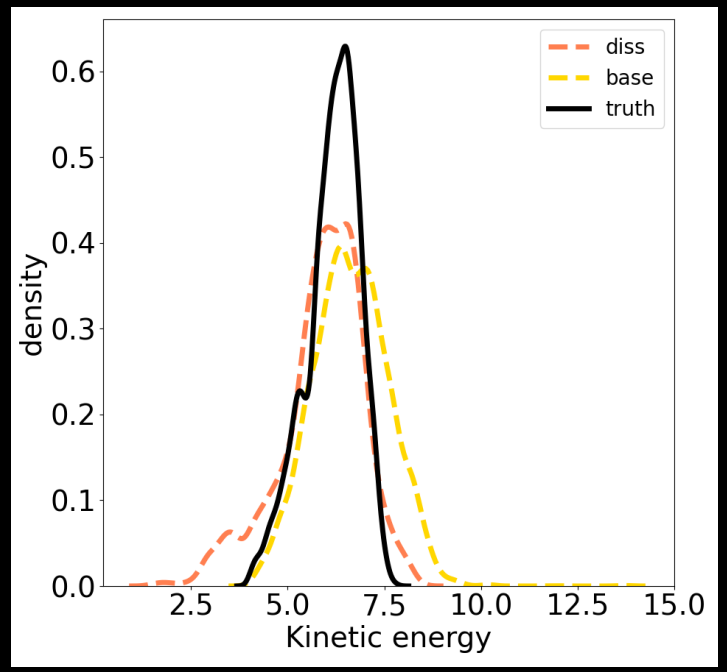
Without dissipative regularization

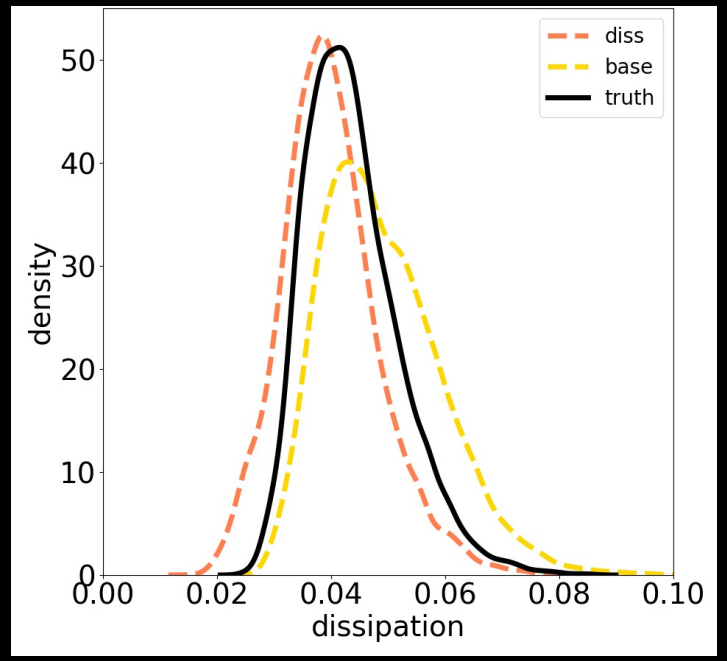
Trajectory visualization

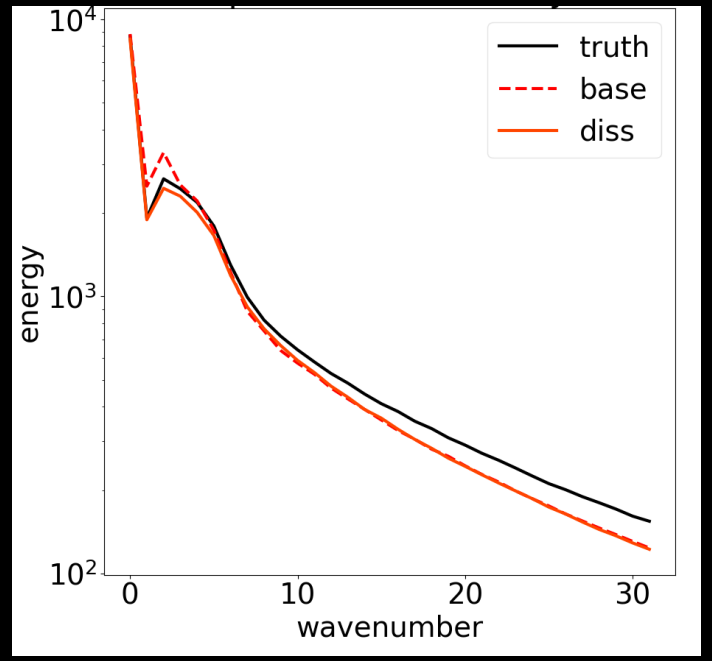
Initial condition outside the attractor

Li, Zongyi, et al. "Learning chaotic dynamics in dissipative systems." *Advances in Neural Information Processing Systems* 35 (2022)

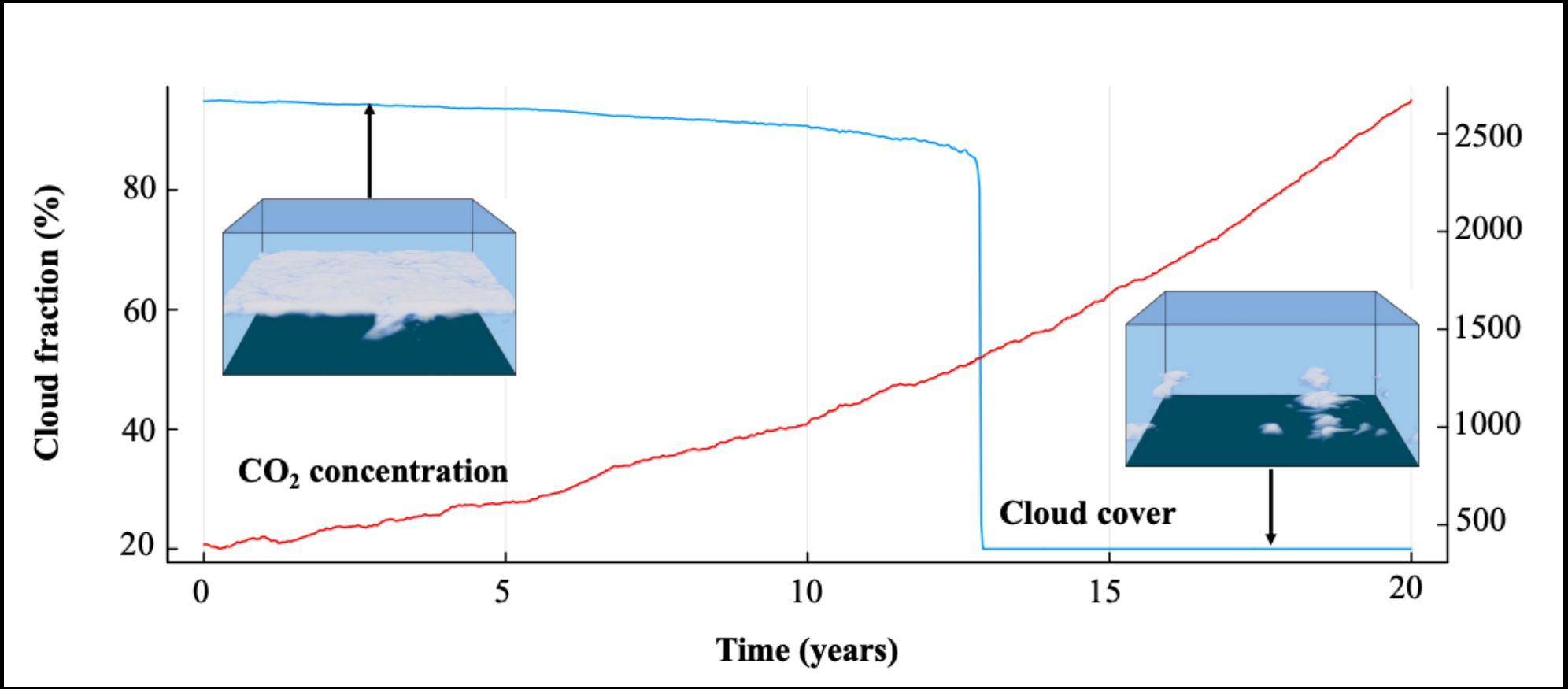
KOLMOGOROV FLOW WITH ENFORCED DISSIPATIVITY





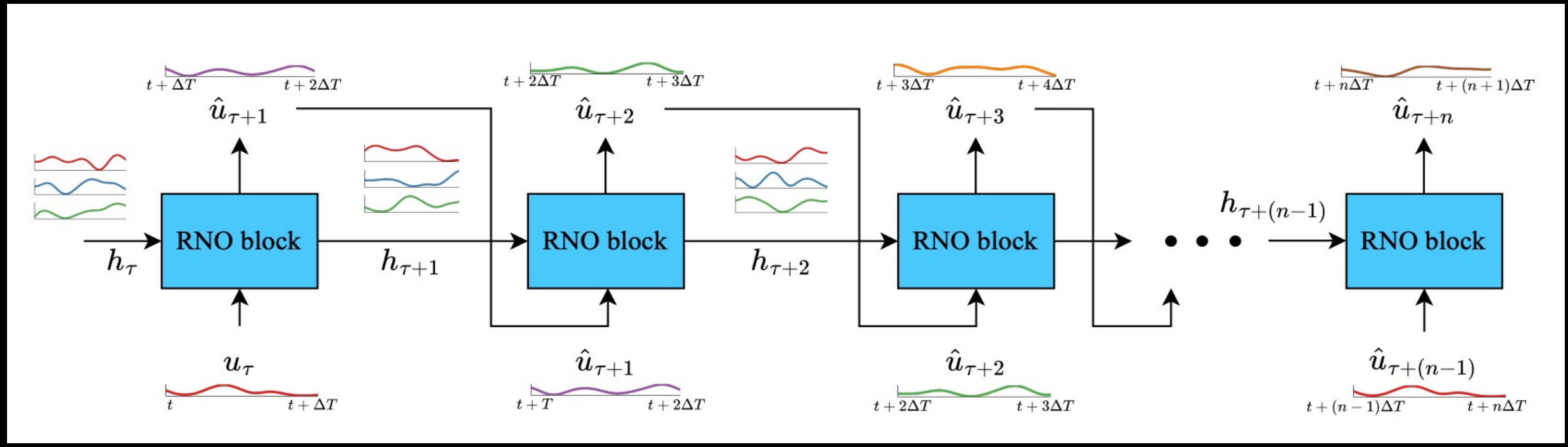


TIPPING POINT DETECTION IN NON-STATIONARY SYSTEMS

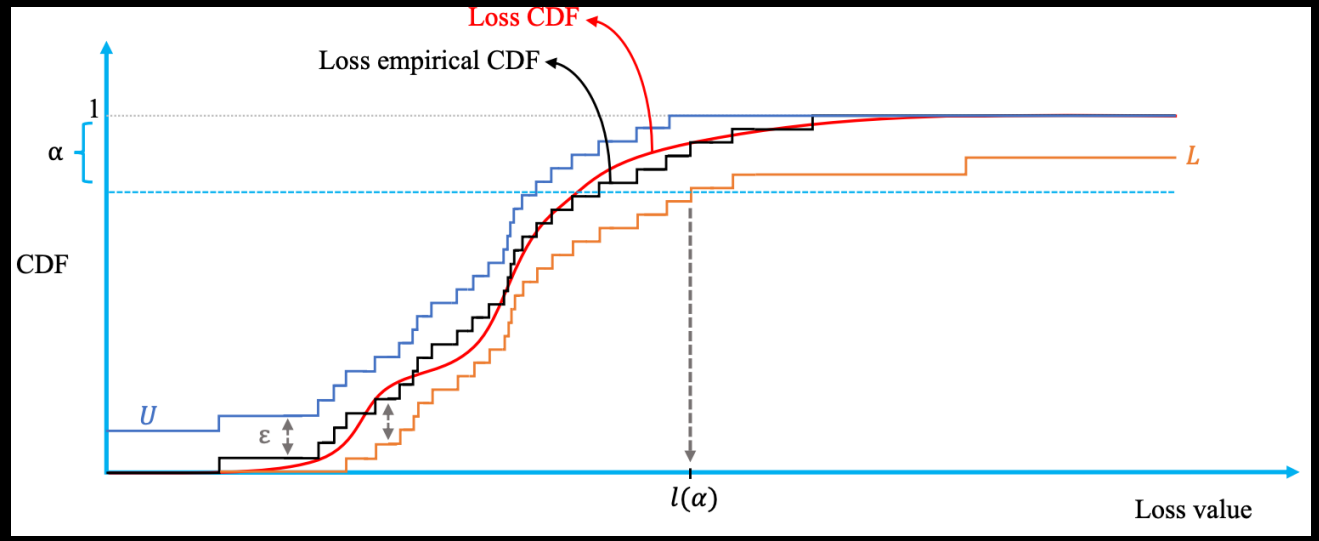


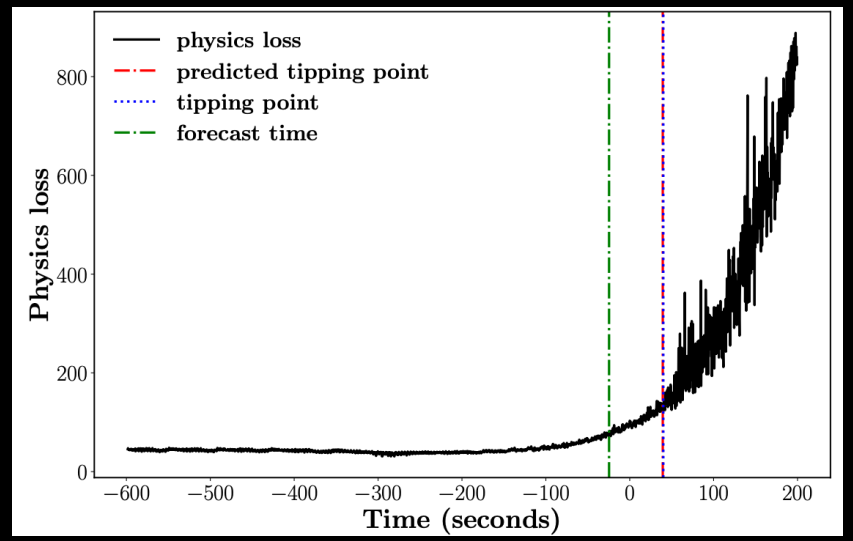
Liu-Schiaffini, Miguel, et al. "Tipping Point Forecasting in Non-Stationary Dynamics on Function Spaces." arXiv preprint arXiv:2308.08794 (2023).

RECURRENT NEURAL OPERATOR



TIPPING POINT DETECTION THROUGH CONFORMAL PREDICTION

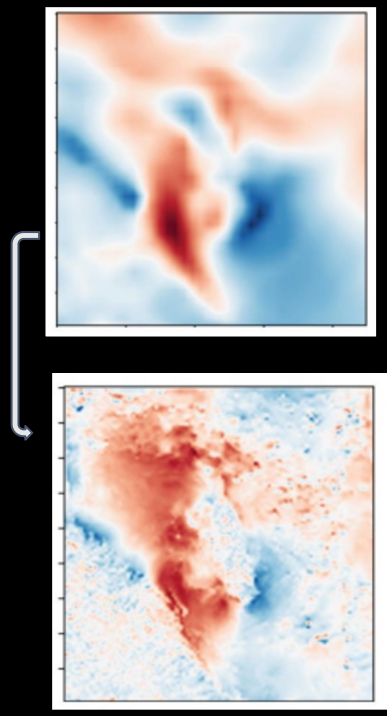




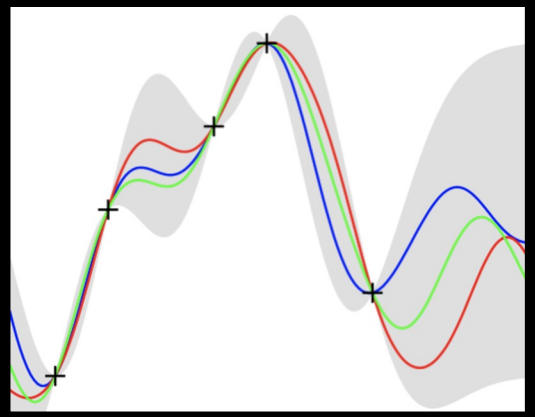
RNO forecasting 64 seconds ahead an ODE system

GENERATIVE AI FOR SCIENCE

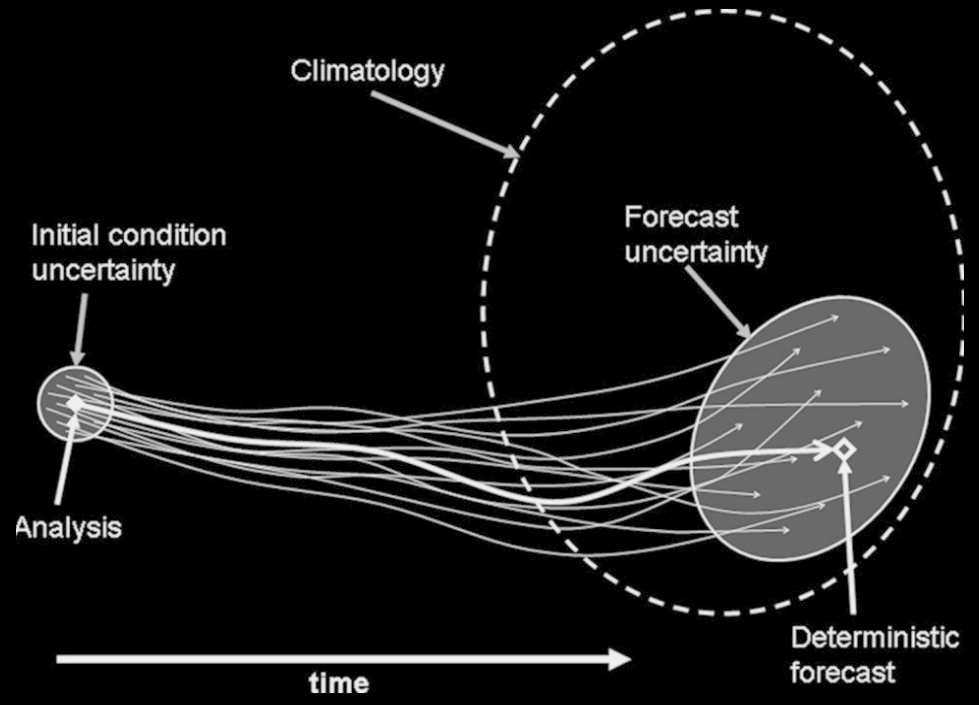
SCIENTIFIC COMPUTING REQUIRES PROBABILISTIC MODELING



INVERSE PROBLEMS

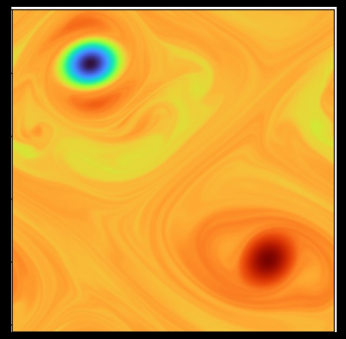


UNCERTAINTY QUANTIFICATION

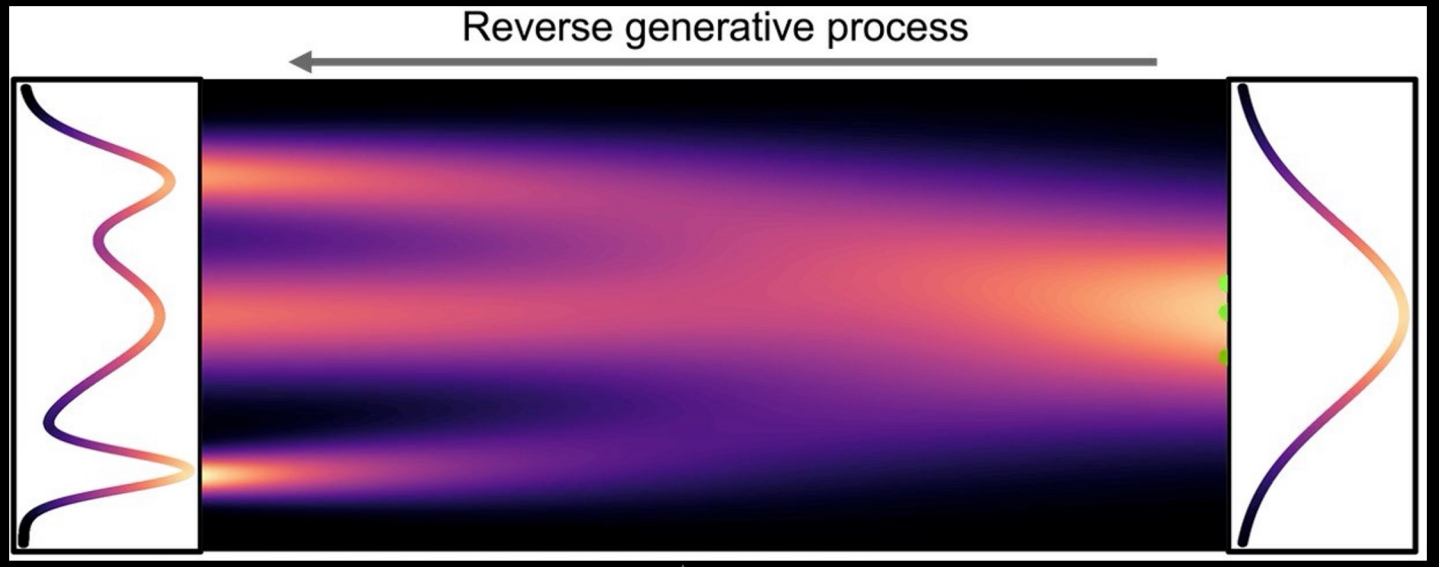


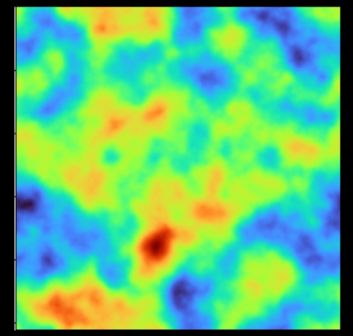
CHAOTIC DYNAMICS

DIFFUSION NEURAL OPERATOR

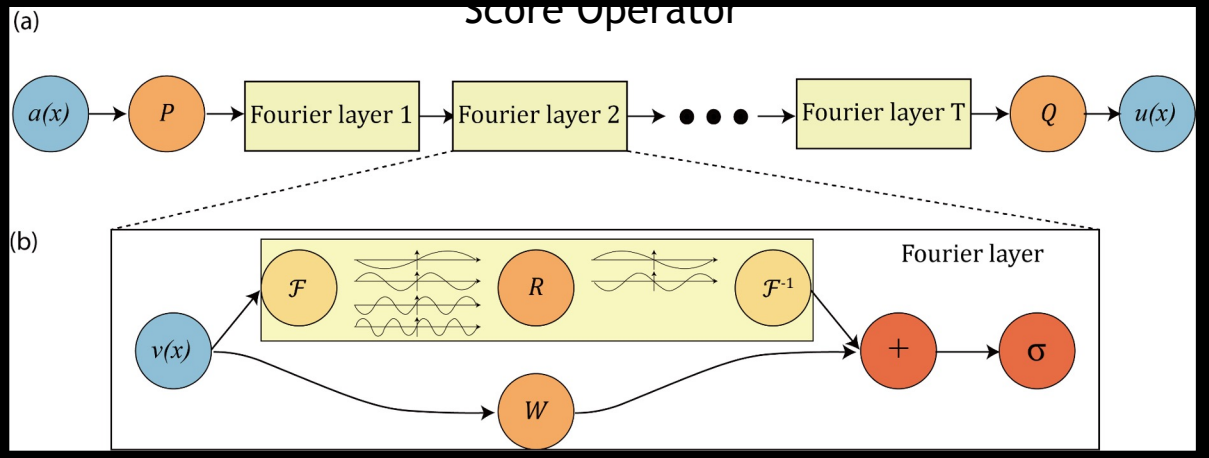


ATTRACTOR



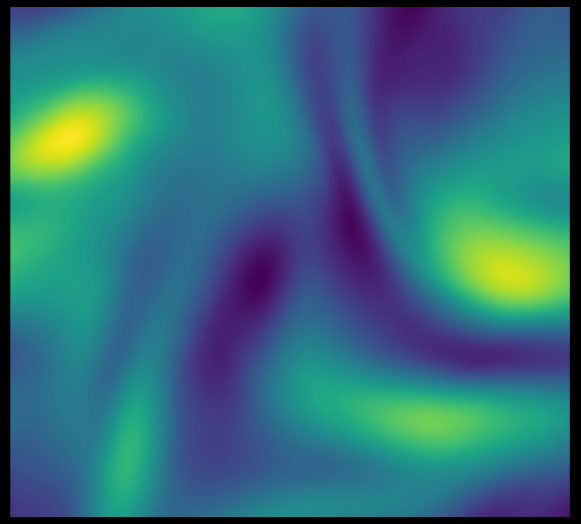


GRF



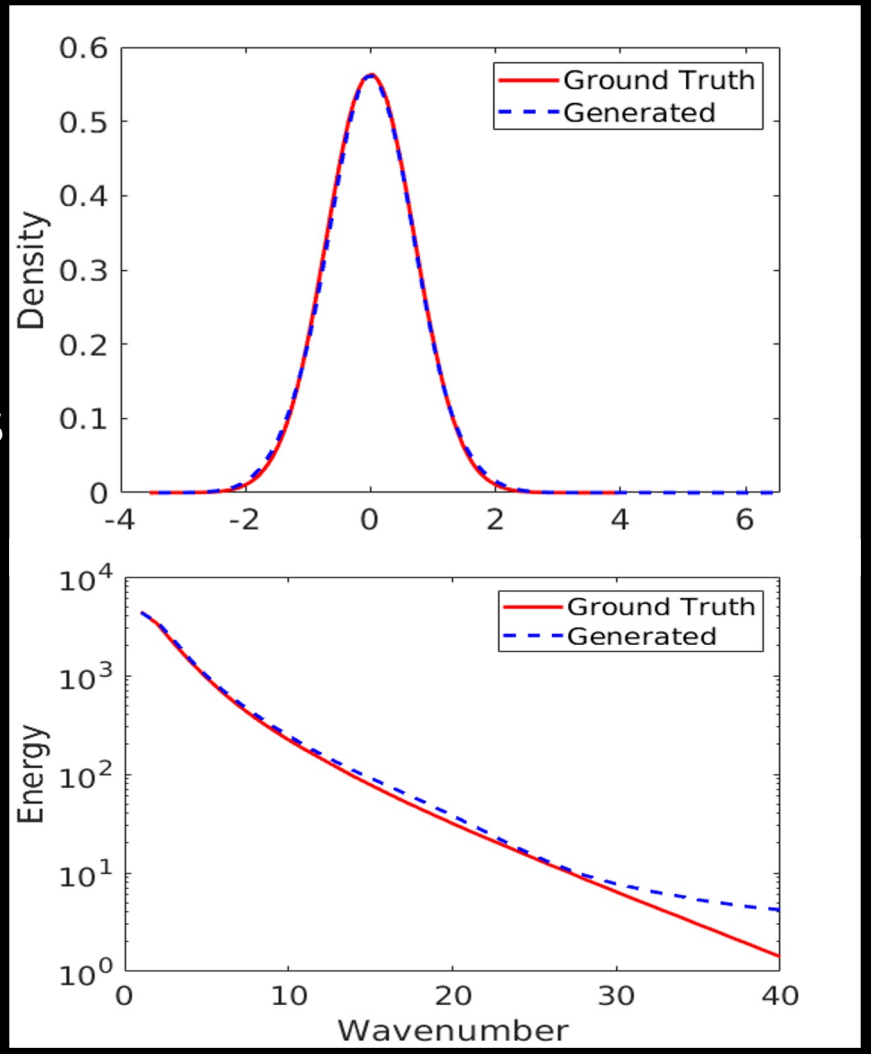
Lim, Jae Hyun, et al. "Score-based diffusion models in function space." *arXiv preprint arXiv:2302.07400* (2023).

ZERO-SHOT SUPER RESOLUTION SAMPLING



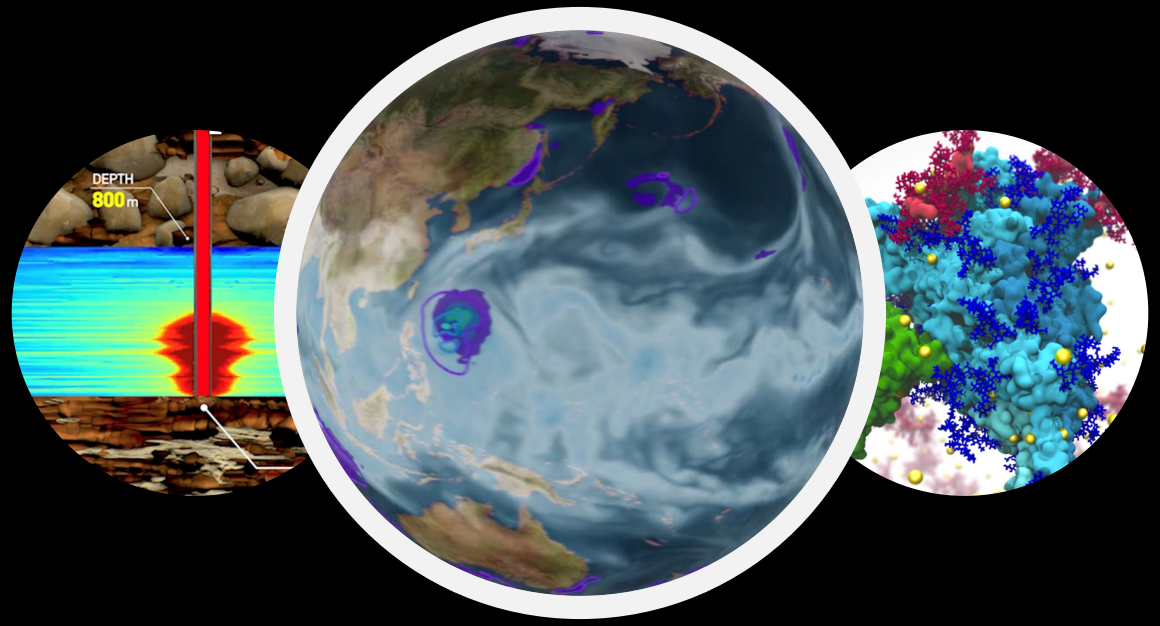
GENERATION: 1024x1024
TRAINING: 128x128

HIGH-RES STATISTICS



CONCLUSION

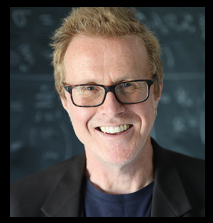
- AI+ Science is the future of science
- Principled algorithms for zero-shot generalization
- Operator learning extends neural networks to learning in infinite dimensional spaces
- Orders of magnitude speedup while maintaining accuracy



Caltech



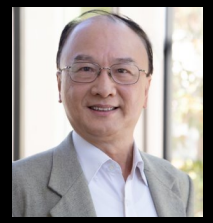
Anima Anandkumar



Andrew Stuart



Kaushik Bhattacharya



Thomas Y. Hou



Oscar P. Bruno



Morteza Gharib



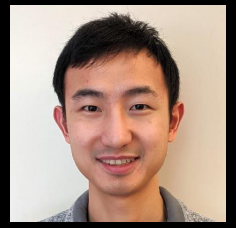
Chiara Daraio



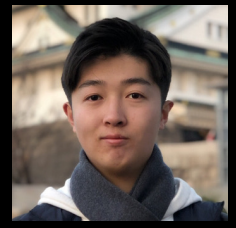
Kamyar Azizzadenesheli



Nikola B. Kovachki



Daniel Zhengyu Huang



Jiawei Zhao



Hongkai Zheng



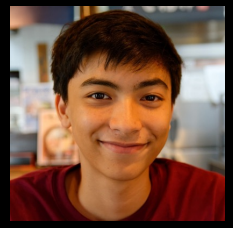
Sahin Lale



Yixuan Wang



Daniel Leibovici



Miguel Liu-Schiaffini



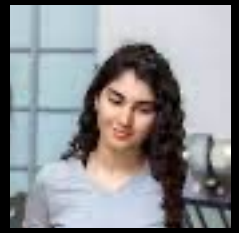
David Jin



Derek Qin



Haydn Maust



Kimia Hasabi



Vansh Tibrewal

NVIDIA



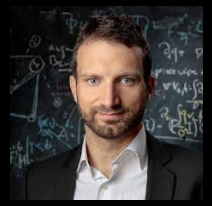
Kamyar Azizzadenesheli



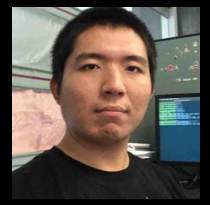
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Thorsten Kurth

Stanford



Sally M. Benson



Gege Wen

UC San Diego



Yuanyuan Shi



Miroslav Krstic

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UNIVERSITY OF CAMBRIDGE



Arvind Ramanathan



Austin Clyde



Sanjeev Raja



Burigede Liu