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

- 100m at 0.1s (500,000,000x COMPUTE)
- 1km at 20s (30,000x COMPUTE)
- 25km at 10min (1x COMPUTE)

Our AI model (FNO) captures physical effects at all scales
PHYSICS INFORMED NEURAL OPERATORS

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

https://github.com/neuraloperator
APPLICATIONS
AI ACCELERATES WEATHER FORECASTING

Our AI (FNO) is 45,000 times faster than current weather models
Our AI weather model is deployed at ECMWF, giving real-time forecasts.
Full model emulation of ERA5

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

[https://github.com/ecmwf-lab/ai-models-fourcastnetv2](https://github.com/ecmwf-lab/ai-models-fourcastnetv2)


Adding spherical geometry to AI allows stable long roll-outs
Our AI (FNO) enables larger ensembles and **better risk assessment**.
Our AI (FNO) is \( \sim 100,000 \) times faster

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

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

$T_{\text{in}} = 10$
Step = 5
$T_{\text{out}} = 40$
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)

Motivation:
Real-time forecasting of fast camera images to track
- plasma evolution,
- predict L-H transition,
- build further unto disruption prediction.
- data assimilation (Sim2Real)

Camera viewing the central solenoid (rbb)\textsuperscript{[1]}
Camera viewing the divertor (rba)\textsuperscript{[1]}

\textsuperscript{[1]} Synthetic renders of the camera views created using the CAD model of MAST and Nvidia Omniverse.
CAMERA VIEWING THE CENTRAL SOLENOID (RBB)
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

Graph showing three lines:
- Blue: $\sin(2x) + \sin(x) + 4\sin(x/4)$
- Orange: $0.5\sin(2x) + 1.2\sin(x) + 6\sin(x/5)$
- Green: super-resolution

The graph plots the functions over the range of $x$ from 1 to 7.
LINEAR PDE: INTEGRAL SOLUTION OPERATOR

\[ K(x, y) \]

Kernel of integral operator
For heat diffusion
NEURAL OPERATOR: A GENERAL FRAMEWORK

Input $\rightarrow$ Integral Linear Operator $\rightarrow$ Non-linearity $\rightarrow$ Output

Solution operator of fluid flows is non-linear

$$\int \kappa(x, y) v(y) \, dy$$
GRAPH NEURAL OPERATOR

Input → Discretized Integral Linear Operator → Non-linearity → Output

\[ \sum_i \kappa(x, y_i) v(y_i) \]
FNO: FOURIER NEURAL OPERATOR

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
\[ \mathcal{F}^{-1} \left( \mathcal{F}(\kappa) \cdot \mathcal{F}(v) \right) \]

Learn weights \( R \) in Fourier Domain
\[ R := \mathcal{F}(\kappa) \]
FROM PSEUDO-SPECTRAL SOLVER TO FNO: FOURIER NEURAL OPERATOR

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).
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
3D REALISTIC AUTOMOTIVE AERODYNAMICS
PHYSICS INFORMED LEARNING
PINO: PHYSICS-INFORMED NEURAL OPERATOR

PINO can learn solution operator for a family of equations and fine-tune on an instance
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.
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.
CHAOTIC SYSTEMS
Chaotic systems are intrinsically unstable.

Small errors accumulate and trajectories unpredictable.

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

Initial condition outside the attractor

The distribution of dissipation is improved.
TIPPING POINT DETECTION IN NON-STATIONARY SYSTEMS

RECURRENT NEURAL OPERATOR

The distribution of dissipation is improved.
TIPPING POINT DETECTION THROUGH CONFORMAL PREDICTION

Distribution of kinetic energy

Distribution of dissipation

Spectrum of vorticity

The distribution of dissipation is improved

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

Score Operator

Reverse generative process

ATTRACTION

GRF

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