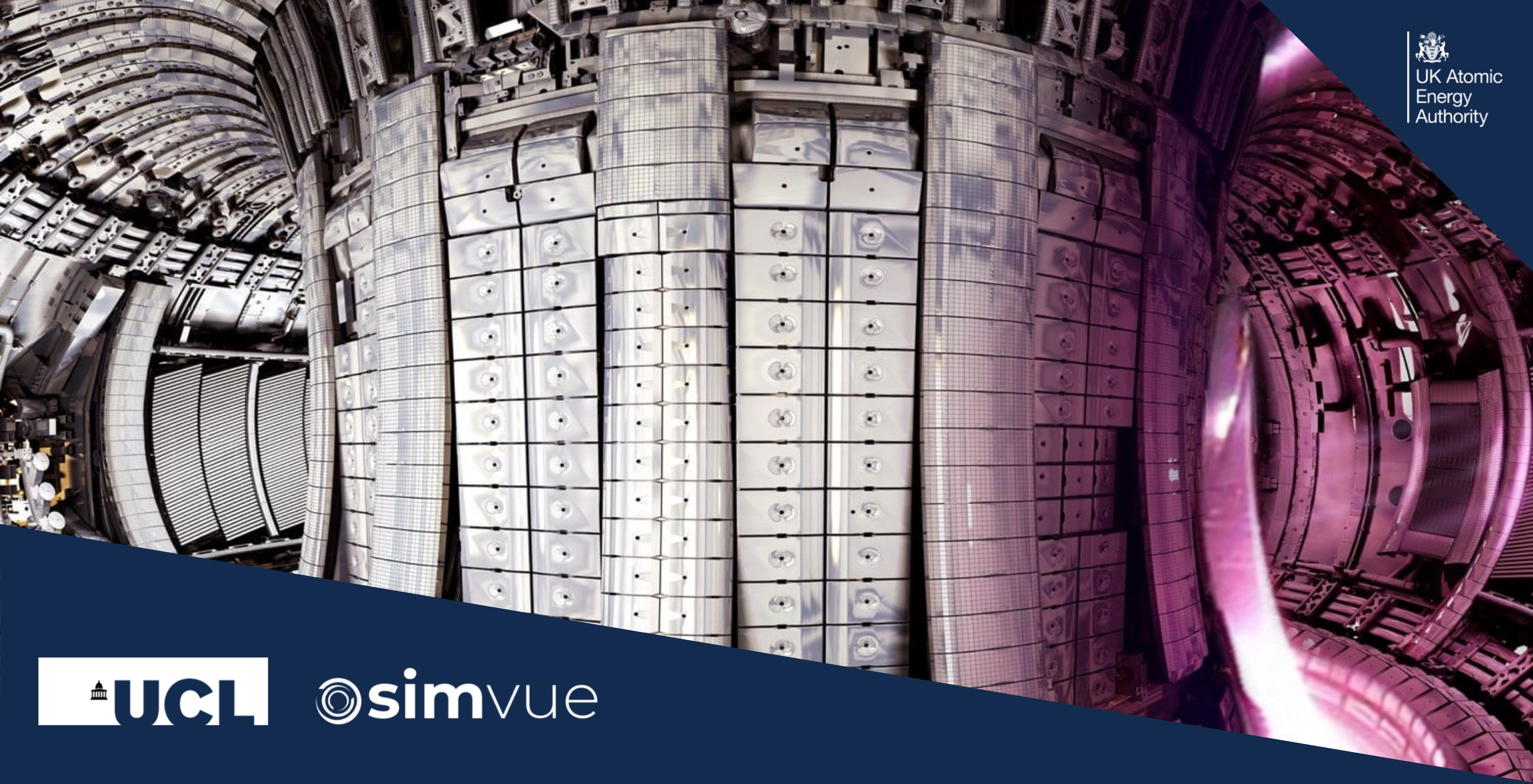

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UCL simvue

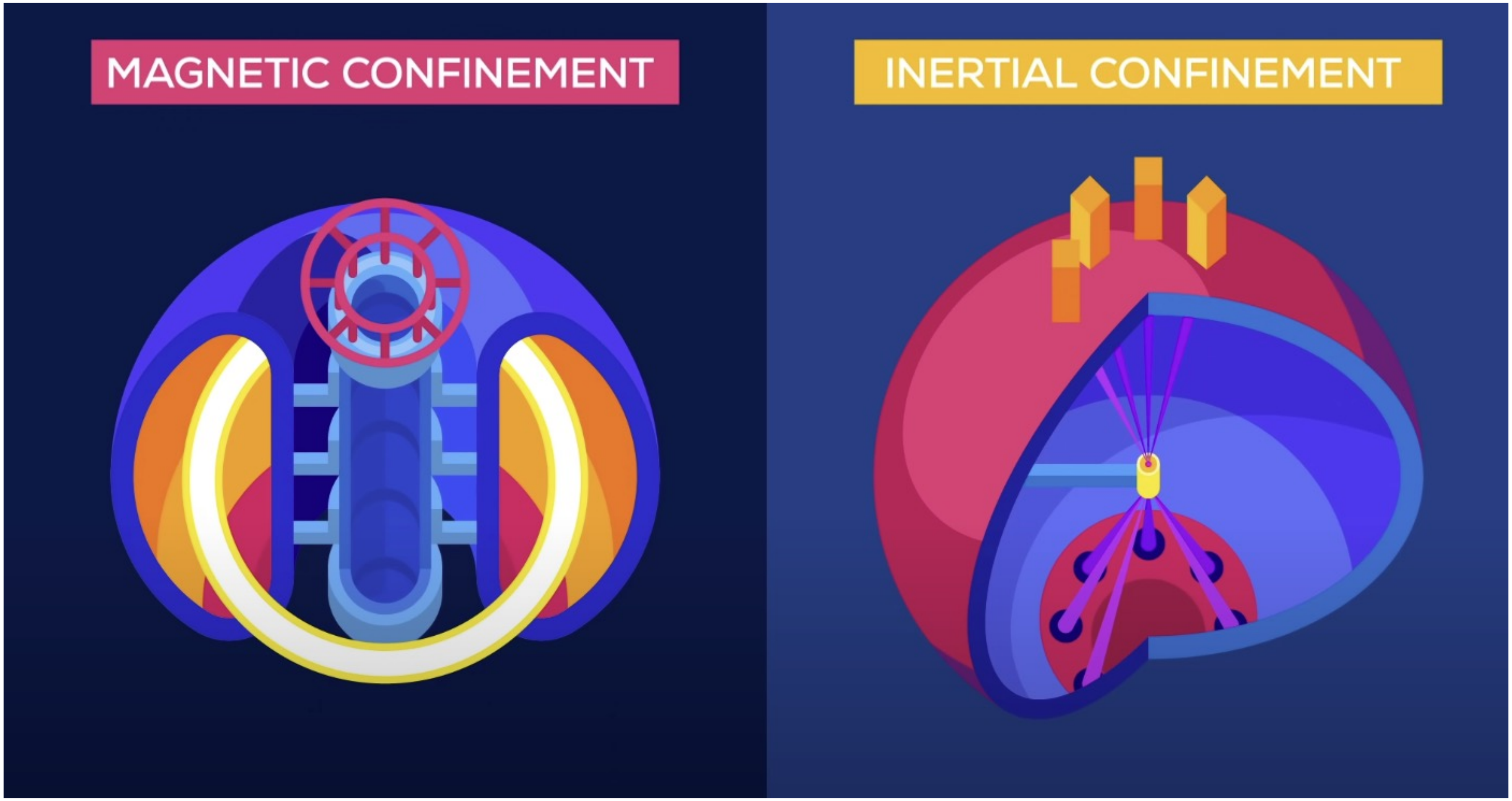
On Surrogate Modelling for Fusion

Invited Talk at PhysicsX
19th July, 2024 - London

Vignesh Gopakumar
AI Research Scientist

The only working Fusion "Reactor"

Types of Fusion Devices



Tokamak

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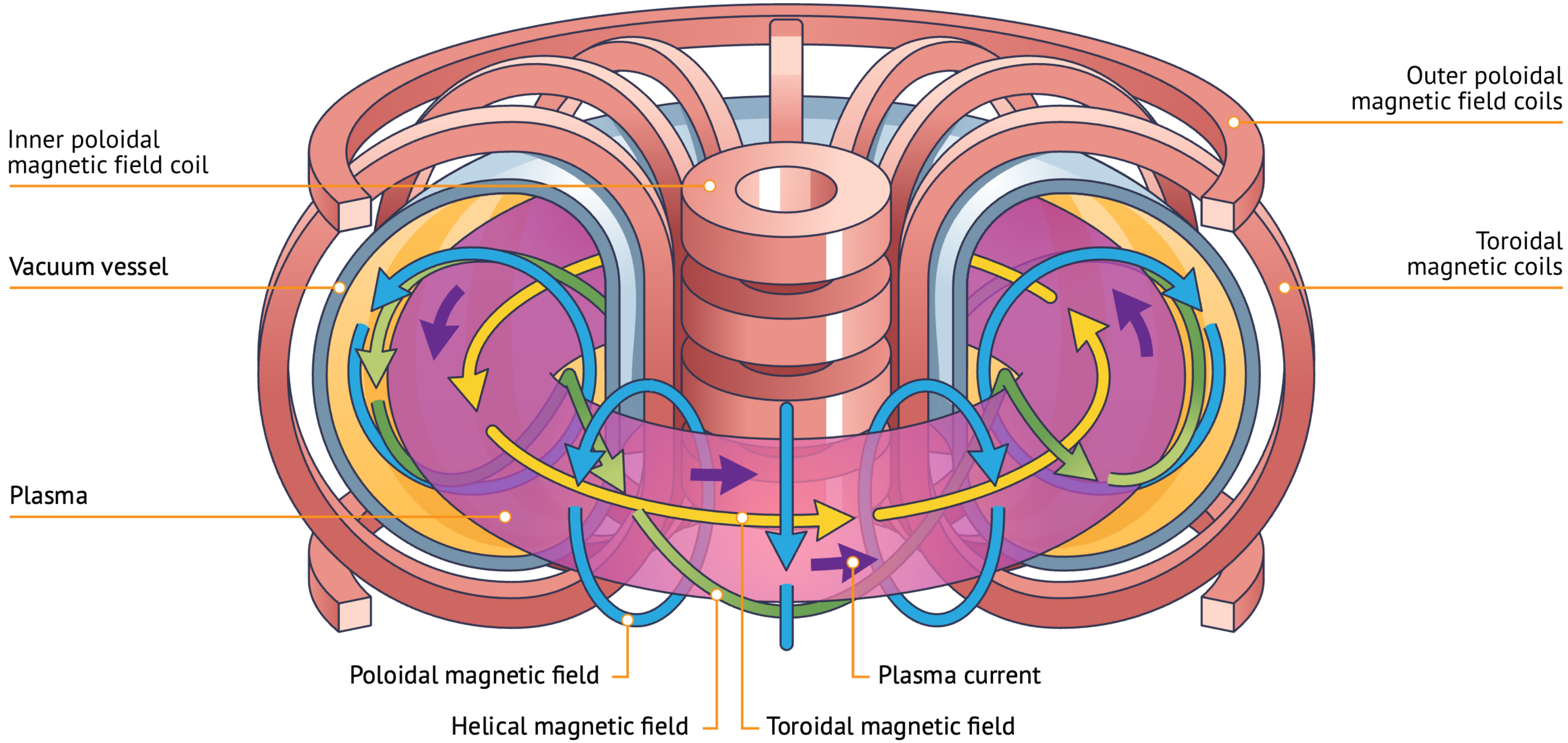

Q1. What makes Fusion so hard ?

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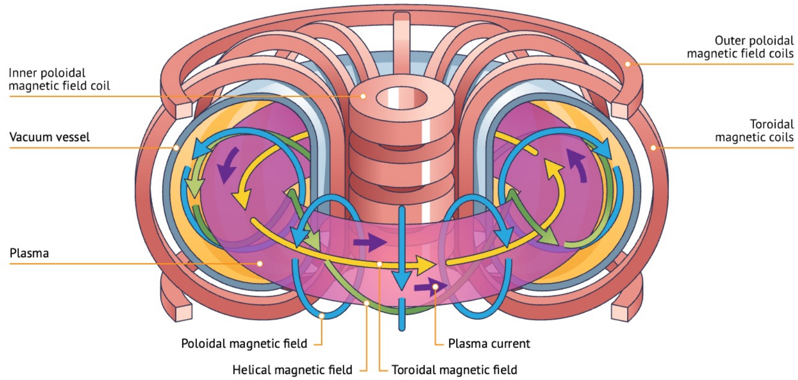


Confinement

- Sharp Temperature and Pressure gradients
- Exhausts to remove impurities

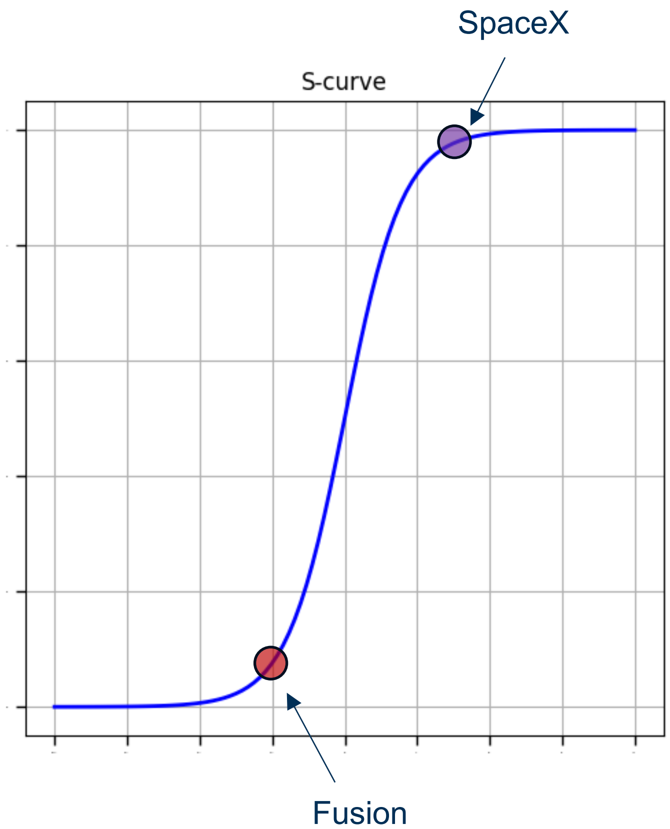
Materials

- Excessive Heat Load on Plasma Facing Components
- Breeding Blankets for Fuel Cycle

Turbulence

- Complex Multi-Scale Multi-Physics:
- Navier-Stokes + Maxwells Equations + Neutrals + Boltzmann Equation.

State of Fusion Research



- Cannot “afford” iterative test-based engineering design.
- In-silico design at the Exascale
- Simulations and Digital Twins

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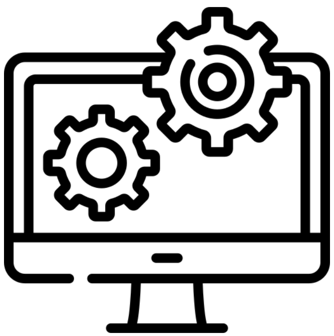
Q2. What are the challenges of simulations ?

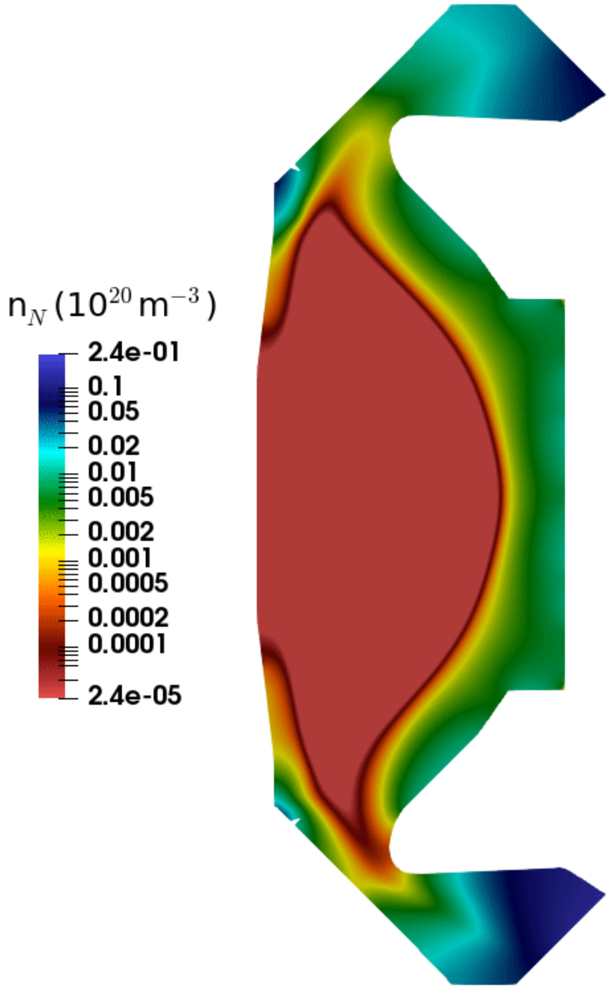


Computational Complexity

Latency

Unknown unknowns

Q2. What are the challenges of simulations ?



Simulating 14 ms of plasma instabilities takes:

> 2 months & > 2000 nodes.

Source:
ELM Instabilities in MAST-U. Smith et al., 2021.

Neural Operators: Operator Learning using Neural Networks

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Traditional Neural Networks (MLPs, CNNs, RNNs …) map from the **input vector space** to the **output vector space**, **learning the function** that performs the required transformation.

Vector Space

$$NN : H_\theta : \boxed{A} \rightarrow \boxed{U}$$

Neural Operators map the **input function space** to the **output function space, learning the operator** that performs the function transformation.

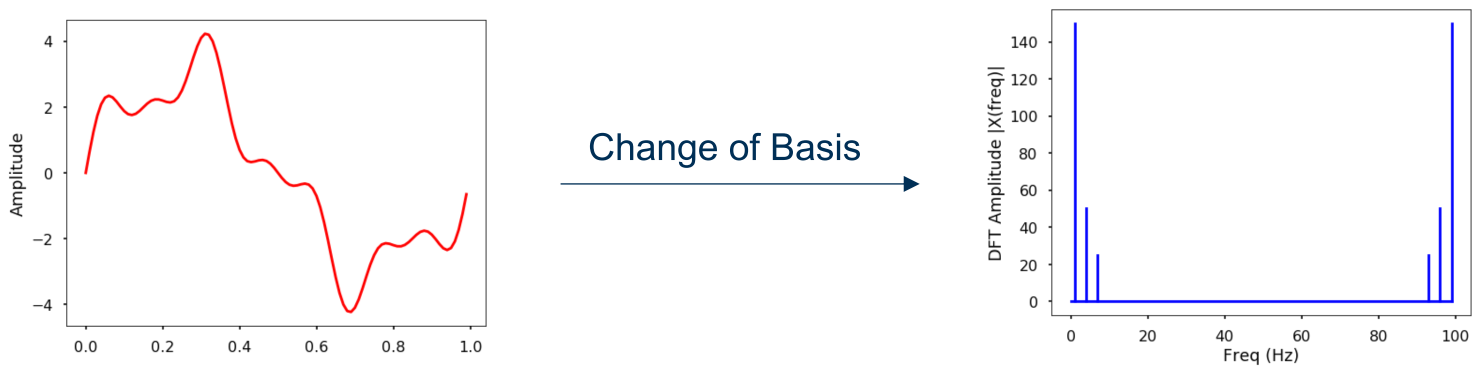
Function Space

$$NO : G_\theta : \boxed{A} \rightarrow \boxed{U}$$

Neural Operators: Operator Learning using Neural Networks

But learning in the function space means learning the continuous operators ?
How does one do that numerically ?

Basis Functions



Network is composed of Kernels that learn within the basis decomposition and point-wise operations allowing us to learn continuous representations on arbitrary discretised inputs and outputs.

Neural Operators for PDEs

Differential Operator in Space

$$\frac{\partial u}{\partial t} = \boxed{D(u, X)}$$

$$\frac{\partial u}{\partial t} = \boxed{G_\theta(u, X)}$$

Neural Operator in Space

Point-wise

Kernel Operator

$$\nu_{t+1} = \sigma\left(W \, \nu_t(x) + \kappa(a; \phi) \, \nu_t(x) \right)$$

Output

Input

Choose your Basis

Wavelet Decomposition	→	Wavelet Neural Operator[1]
Laplace Transform	→	Laplace Neural Operator [2]
Complex Transform	→	Complex Neural Operator [3]
Polynomial Basis	→	DeepONet [4]
Fourier Decomposition	→	Fourier Neural Operator [5]

[1] Tripura et al. – Wavelet neural operator: a neural operator for parametric partial differential equations
[2] Cao et al. – LNO: Laplace Neural Operator for Solving Differential Equations
[3] Tiwari et al. – CoNO: Complex Neural Operator for Continuous Dynamical Systems
[4] Lu et al. – DeepONet: Learning nonlinear operators for identifying differential equations based on the universal approximation theorem of operators
[5] Li et al. – Fourier Neural Operator for Parametric Partial Differential Equations

Fourier Neural Operator

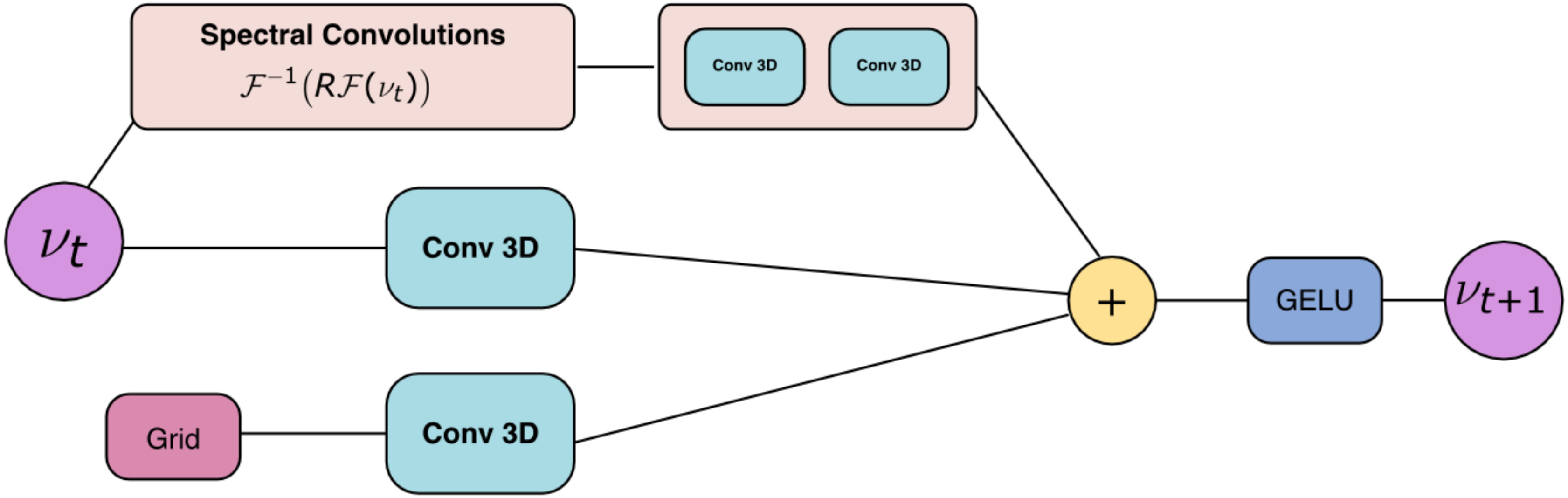
General Neural Operator Framework:

$$\underbrace{\nu_{t+1}}_{\text{Output}} = \sigma\left(\overbrace{W}^{\text{Point-wise}}\,\underbrace{\nu_t(x)}_{\text{Input}} + \overbrace{\kappa(a;\phi)}^{\text{Kernel Operator}}\,\underbrace{\nu_t(x)}_{\text{Input}}\right)$$

Fourier Neural Operator Framework:

$$\underbrace{\nu_{t+1}}_{\text{Output}} = \sigma\left(\overbrace{W}^{\text{Point-wise}}\,\underbrace{\nu_t(x)}_{\text{Input}} + \overbrace{\mathcal{F}^{-1}(R\mathcal{F}}^{\text{Kernel Operator}}\left(\underbrace{\nu_t(x)}_{\text{Input}}\right))\right)$$

Fourier Layer



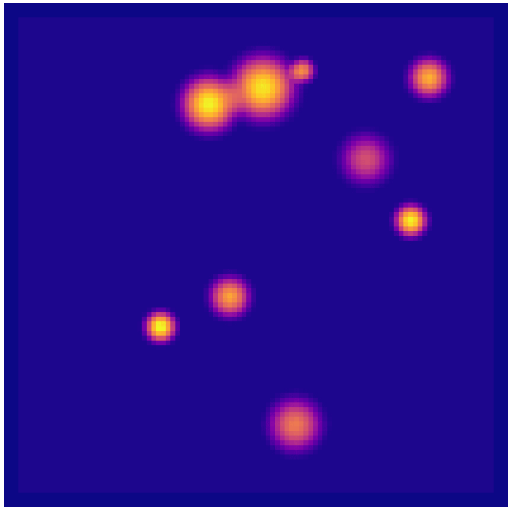
Multi-variable FNO : FNO modified with additional channel to accommodate multiple variables associated with a family of PDEs.

Source:
Plasma Surrogate Modelling using Fourier Neural Operator. Gopakumar et al., 2023.

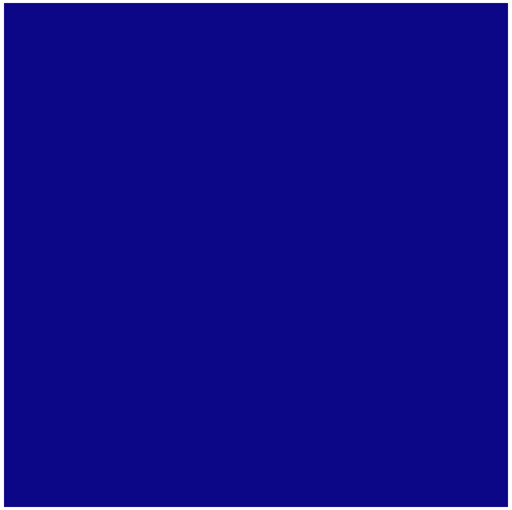
Reduced-MHD

Radial Convection of plasma blobs in toroidal geometry using JOREK

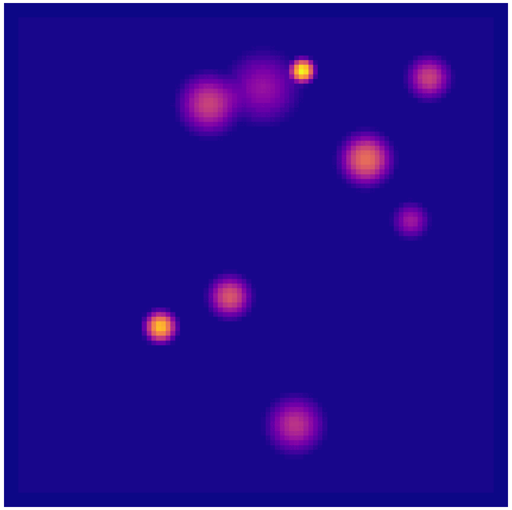
Absence of a plasma current equilibrium generates a buoyancy effect, causing the blob to move outwards towards the edge.



Density



Electric Potential

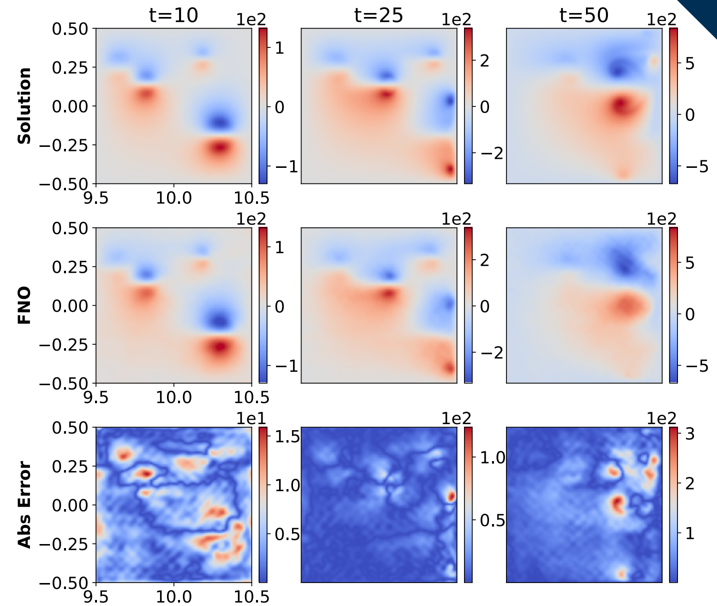


Temperature

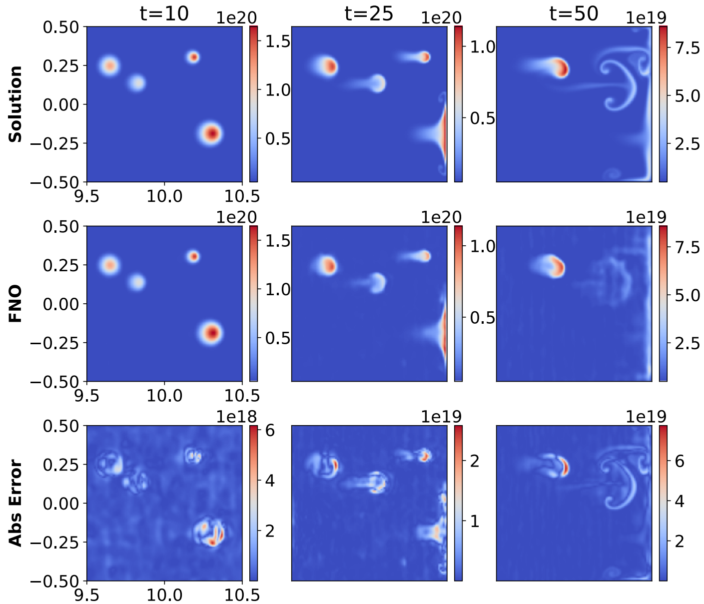
2000 simulations built by varying the initial conditions of the plasma blobs: number, position, width and amplitude

FNO over MHD

FNO: 6 orders of magnitude faster than JOREK

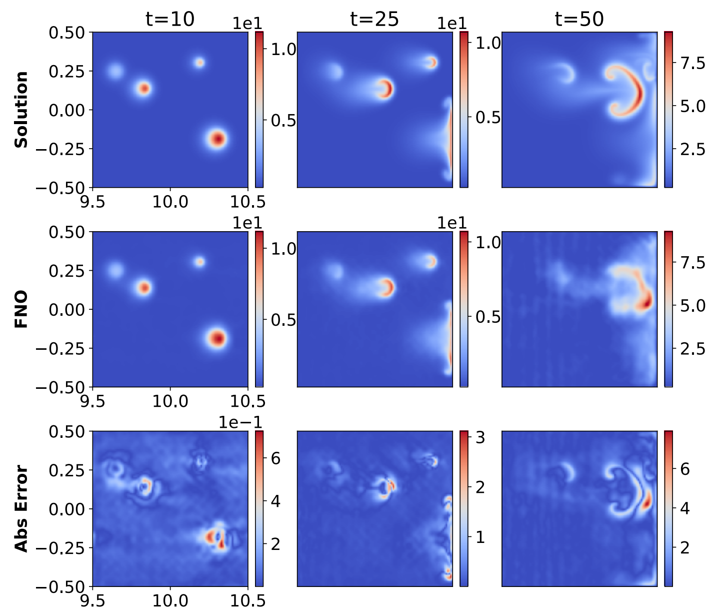


Electric Potential



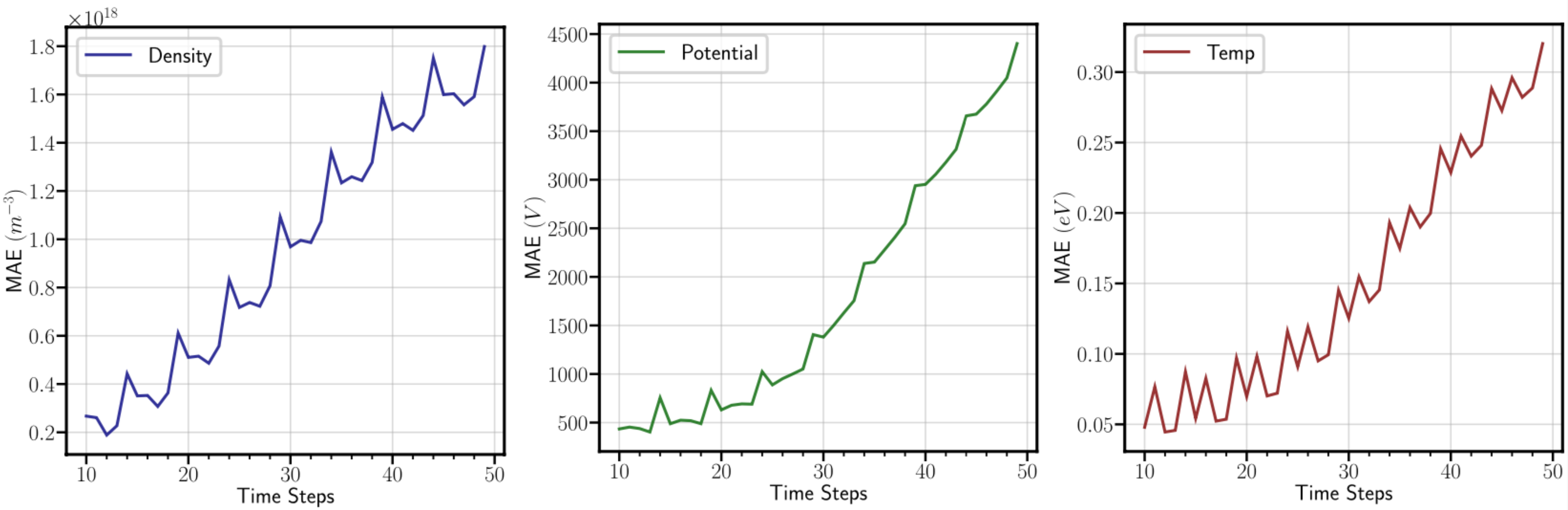
Density

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



Temperature

Error Growth



Super-Resolution

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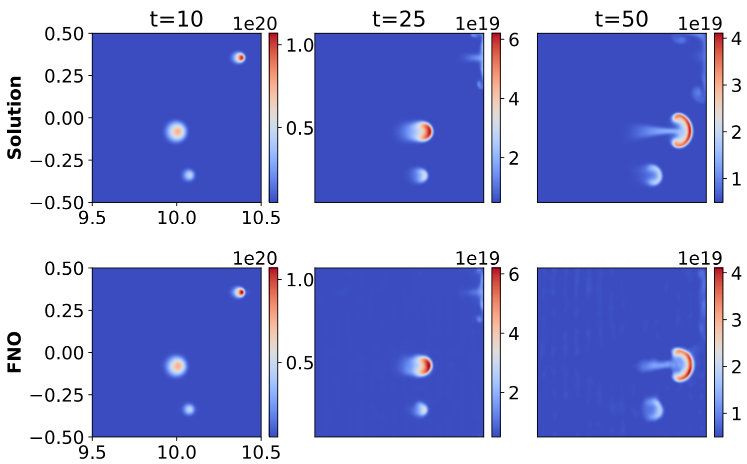
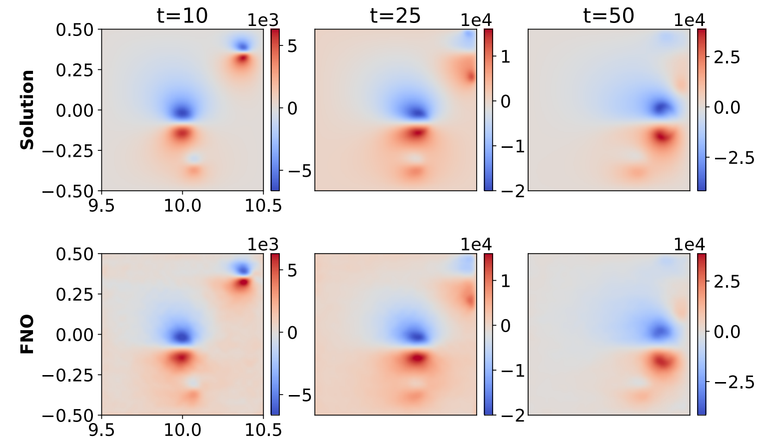
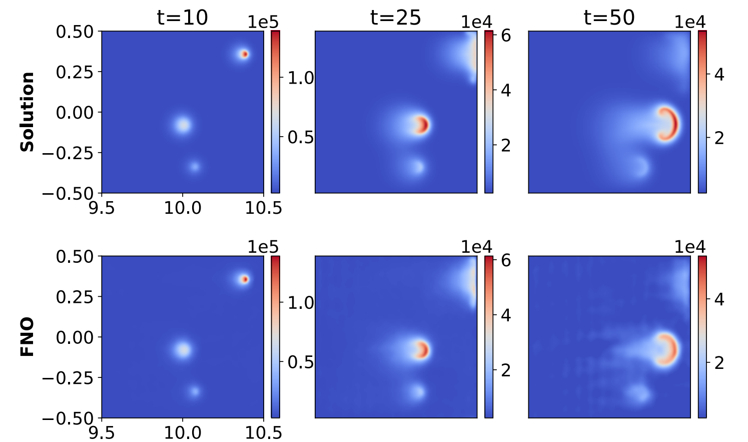


Density



Potential

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

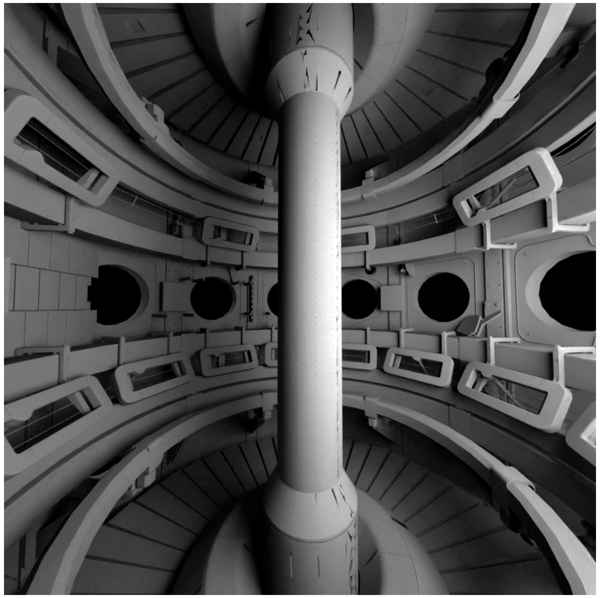


Temperature

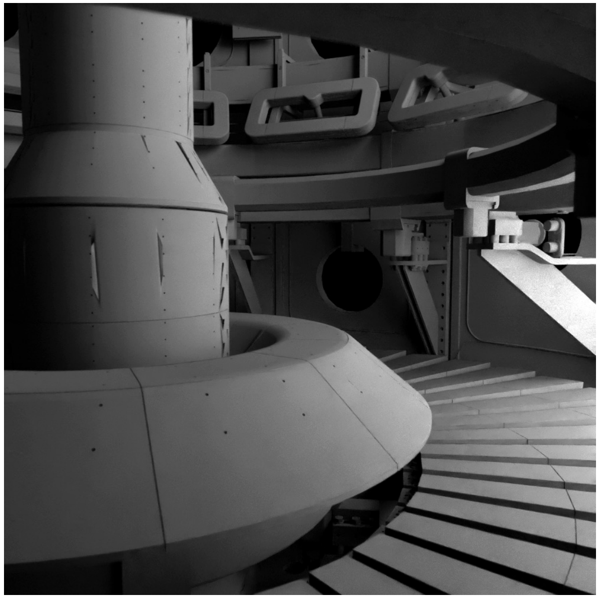
FNO Over Camera

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)



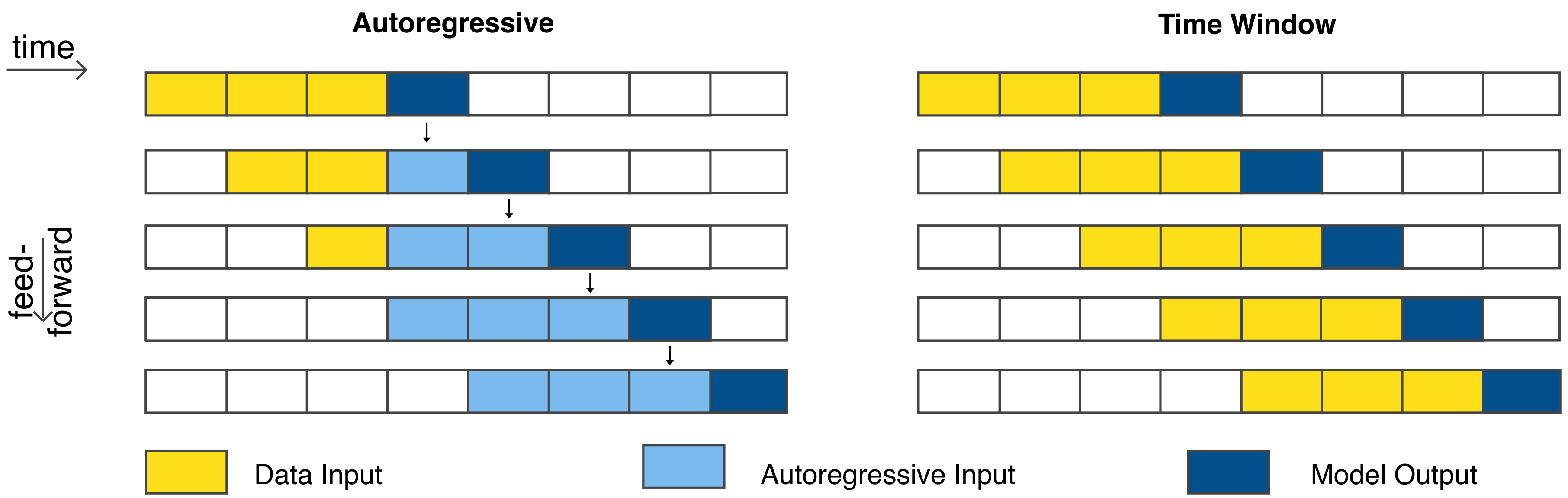
Camera viewing the central solenoid (rbb)[1]



Camera viewing the divertor (rba) [1]

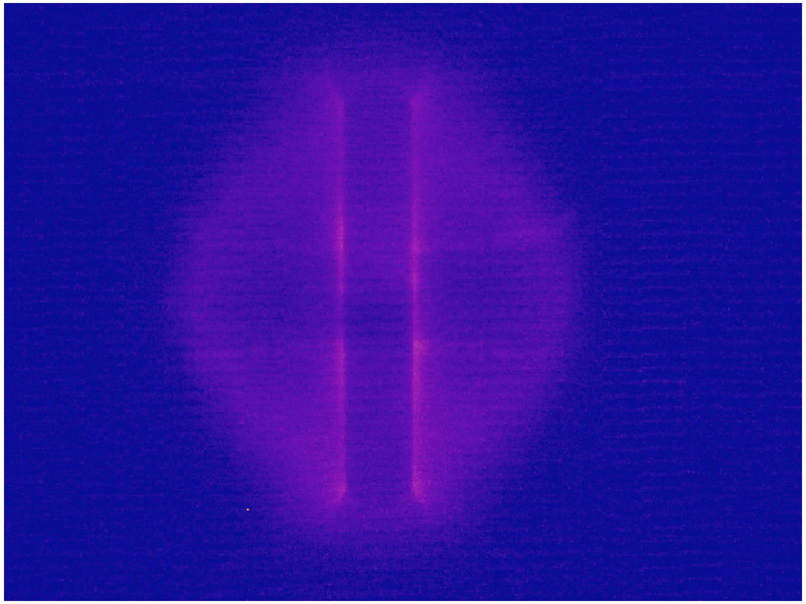
[1] Synthetic renders of the camera views created using the CAD model of MAST and Nvidia Omniverse.

Autoregressive vs Time Window

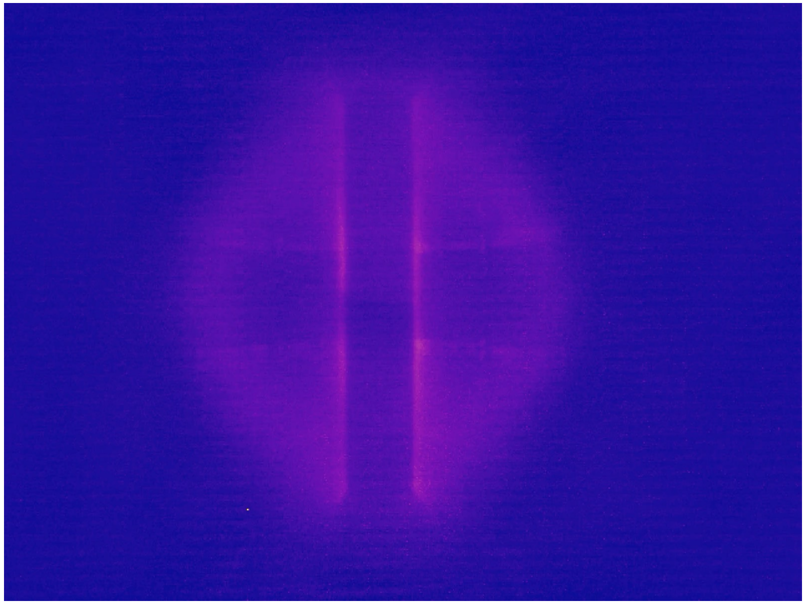


Camera viewing the central solenoid (rbb)

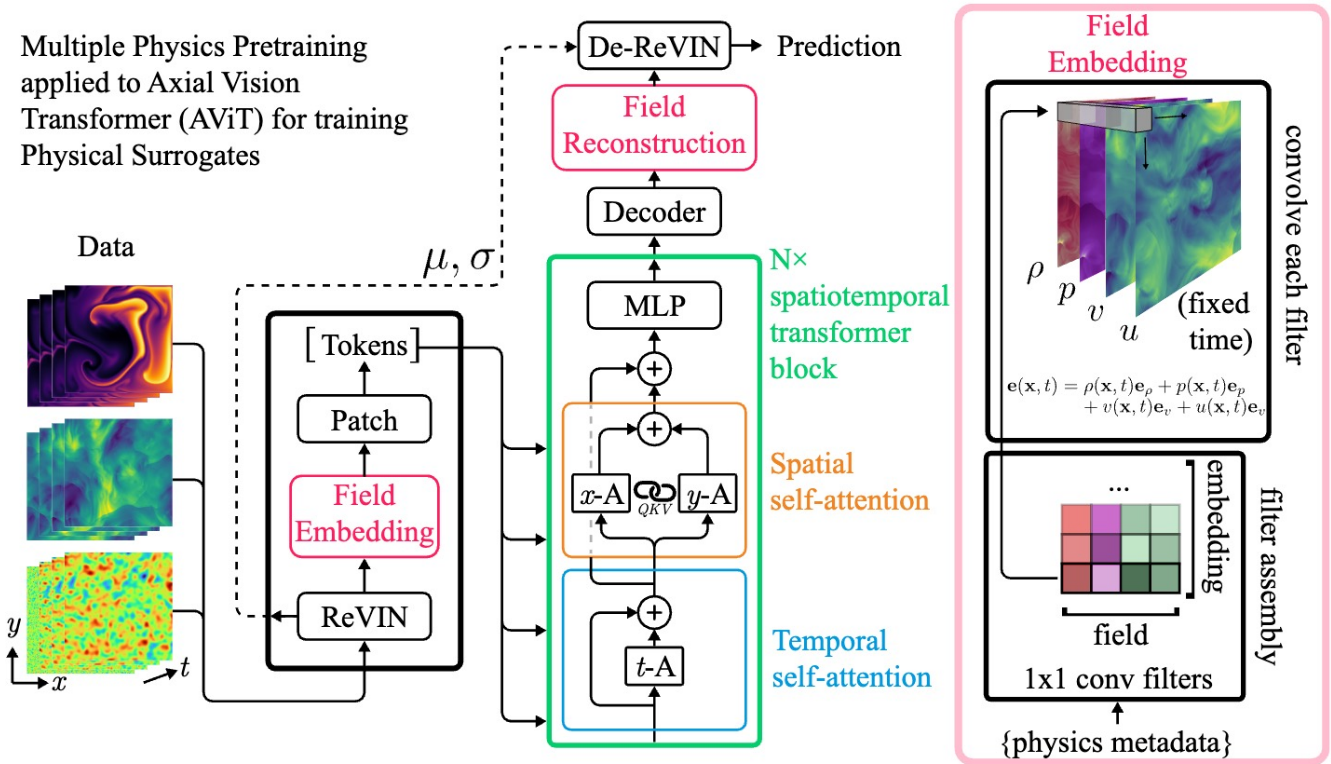
Camera



FNO

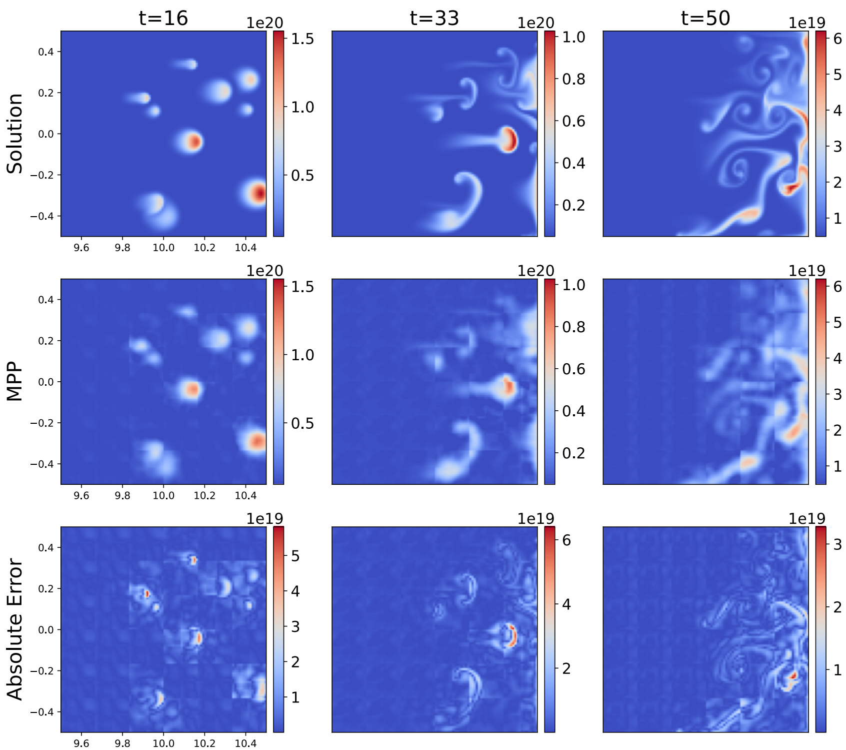


Foundation Physics Models

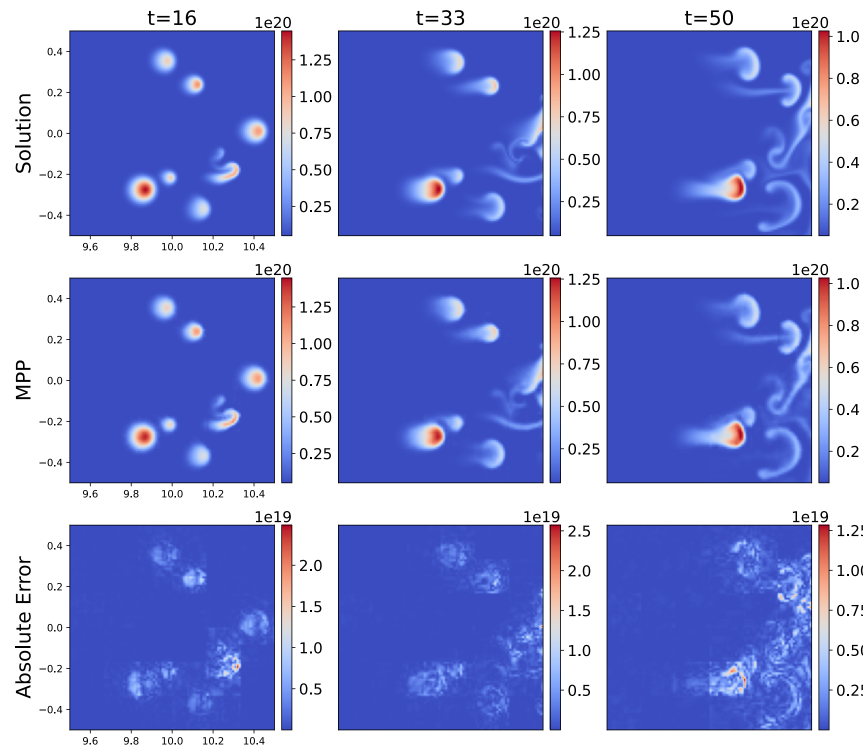


Source:
Multiple Physics Pretraining for Physical Surrogate Models. McCabe et al., 2023

Foundation Physics Models

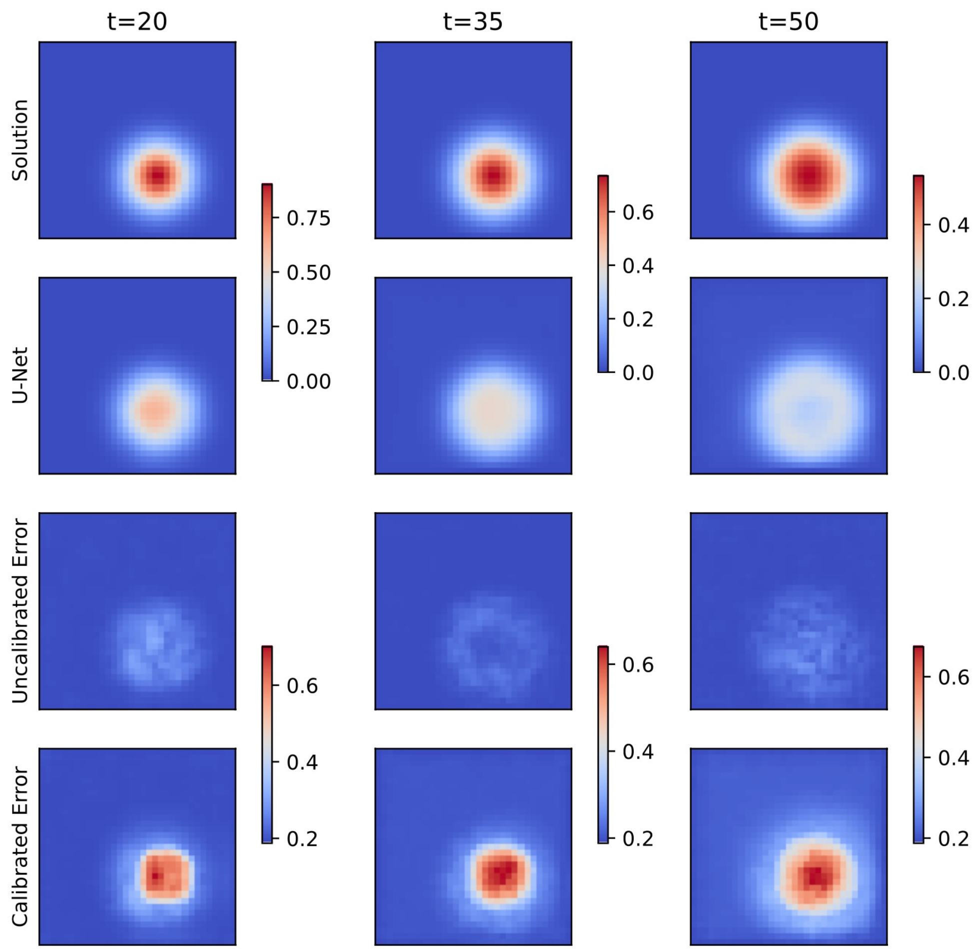


Zero-Shot



Fine-tuned: using only 10% of data.

Uncertainty Quantification via Conformal Prediction



Inductive Conformal Prediction

$$\hat{s} = |y_c - \tilde{y}_c|$$

Calibration

$$\longrightarrow$$

$$\hat{q} = F_{\hat{s}}^{-1}\left(\frac{\lceil (n+1)(1-\alpha) \rceil}{n}\right)$$

Quantile Estimation

$$\longrightarrow$$

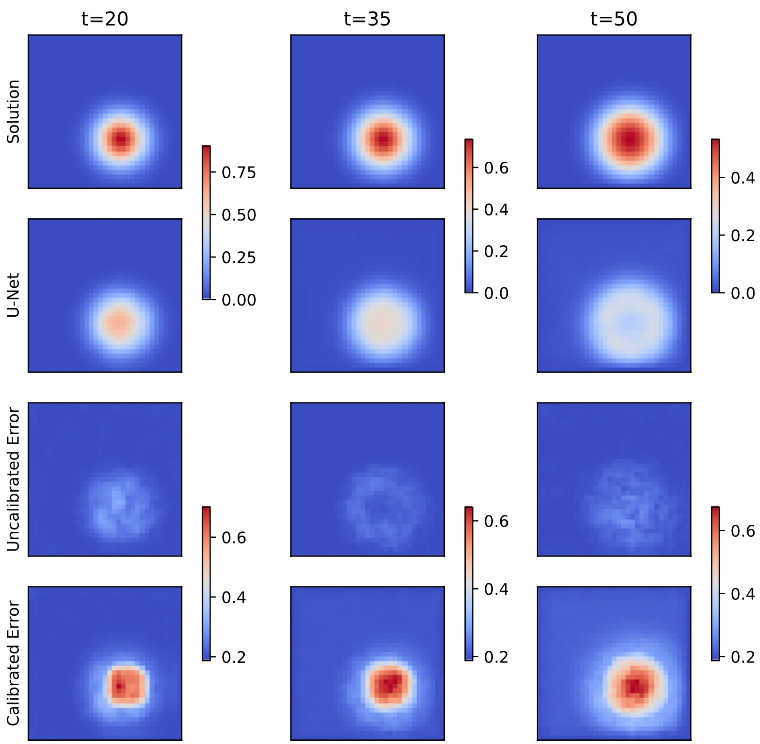
$$\hat{y_p} = \tilde{y}_p \pm \hat{q}$$

Prediction Sets

$$\mathbb{P}(y_p \in \hat{y}_p^{\alpha}) \geq 1 - \alpha.$$

Conditional validity of inductive conformal predictors – Vladimir Vovk 2012.

Uncertainty Quantification via Conformal Prediction



Cell-wise *Marginal Coverage* across the Spatio-Temporal Domain of interest.

CP over the FNO-MHD

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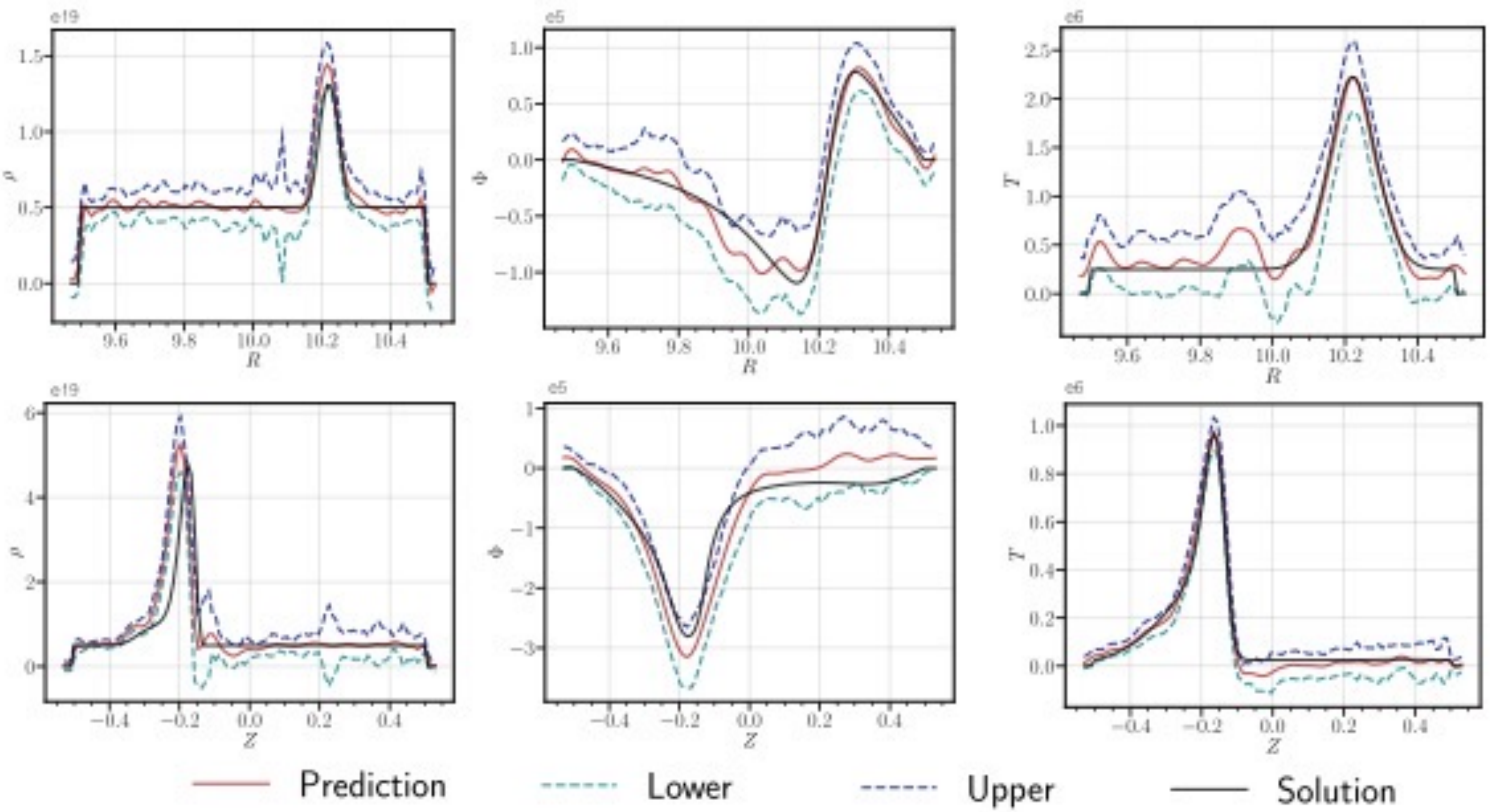

UQ for Neural Weather Models with CP

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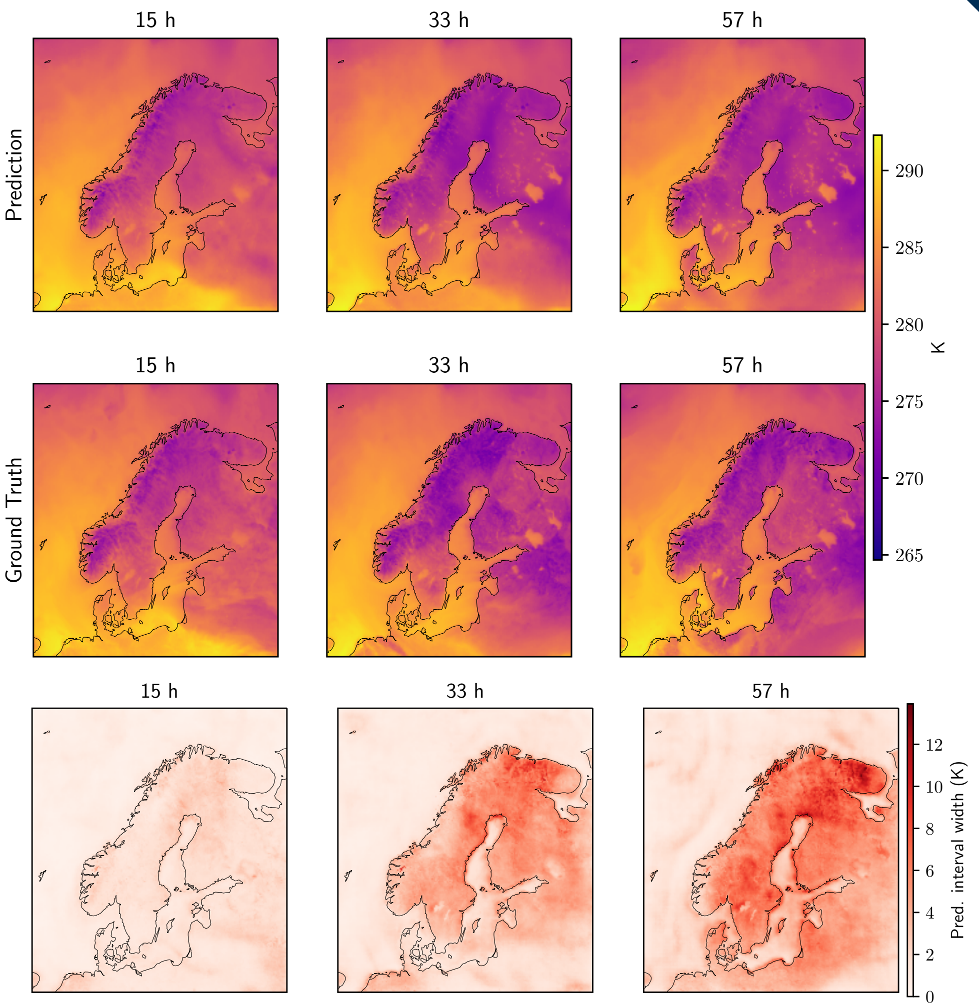
GraphCast modified for limited area model across the Nordic region.

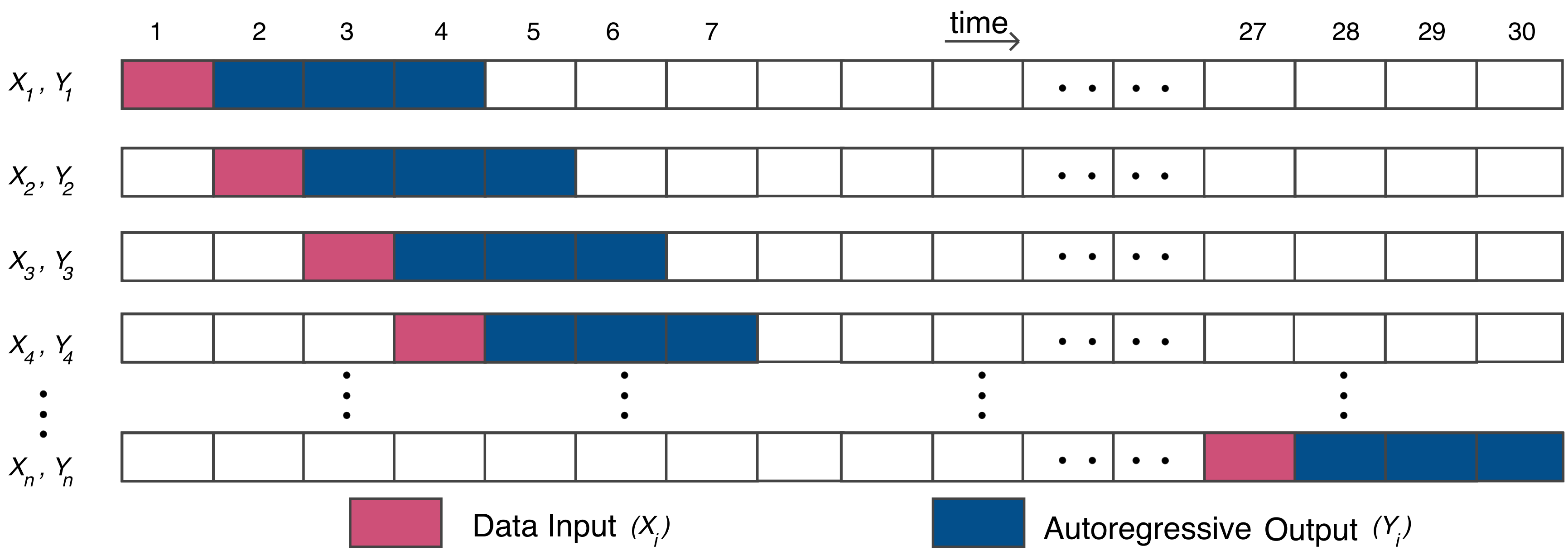
Calibrated using weather data from **Sept. 2021** to predict over **Sept. 2022.**

Plots for Temp. 2m above the surface.



Source:
Valid Error Bars for Neural Weather Models using Conformal Prediction. Gopakumar et al., 2024.

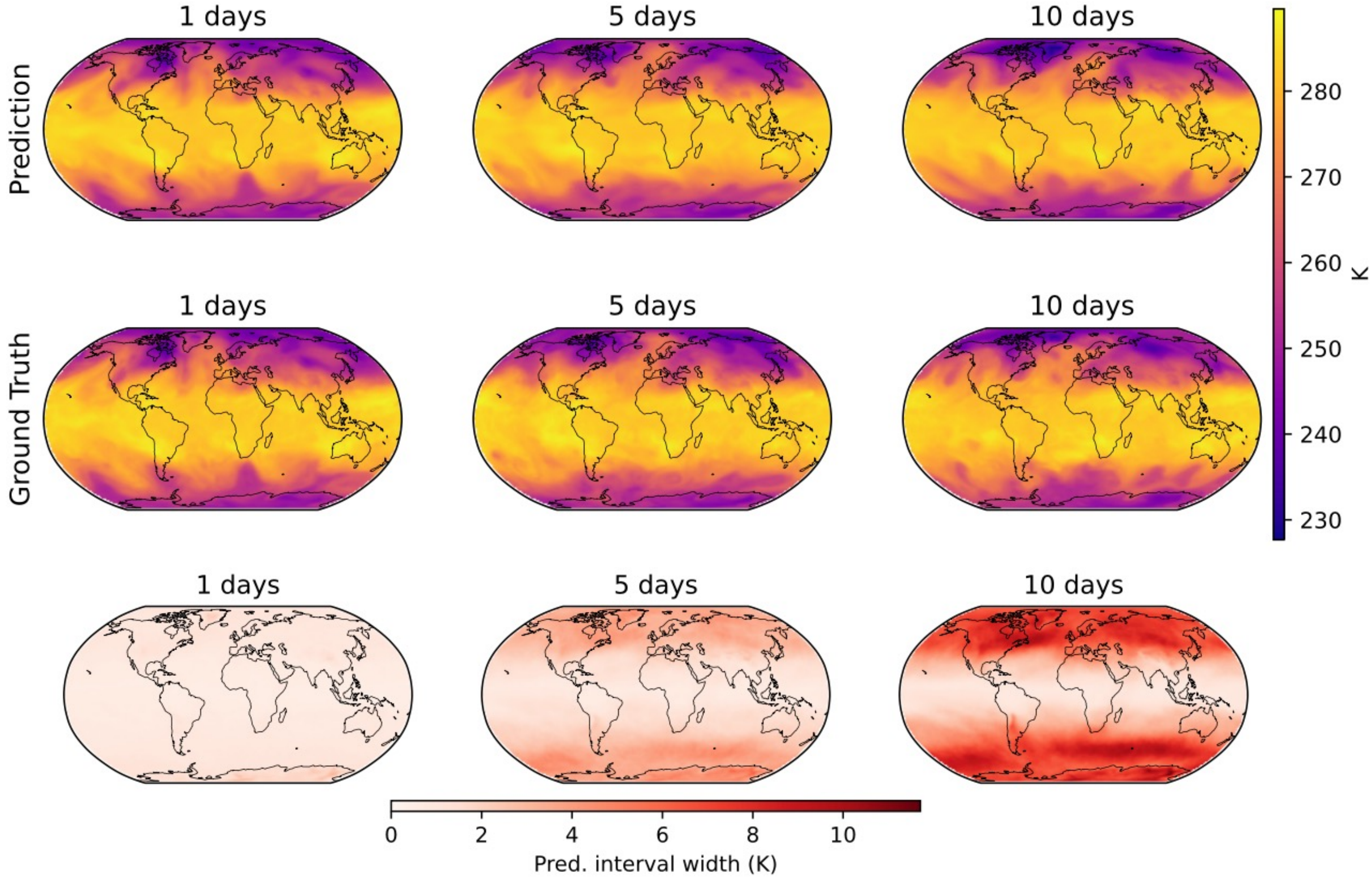
"Exchangeable Time Series"



By treating the modelling task and thus the input-output pairs as an **initial value problem** with a **fixed time horizon** of interest.

Global forecasts :

Calibrated over 2018 and Predicted over 2019



Temperature at 2000 ft

Major Challenges for Surrogate Modelling

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Models	Uncertainty Quantification
Physics Obedience	Calibrated and Statistical Guarantees
Multi-physical Interactions	Physics based Validation
Long-term Time Evolution	Out-of-Distribution effectiveness
Input Dependence	

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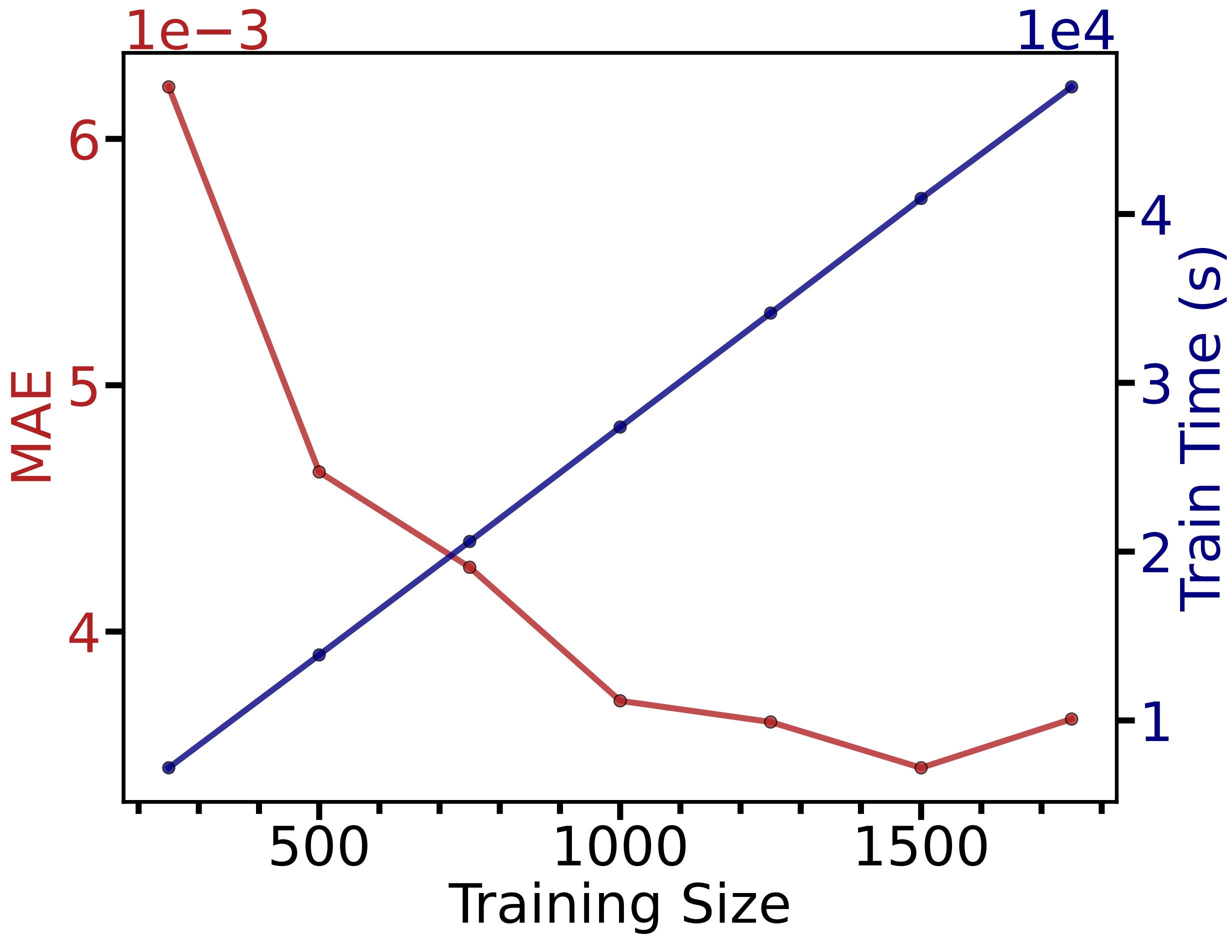
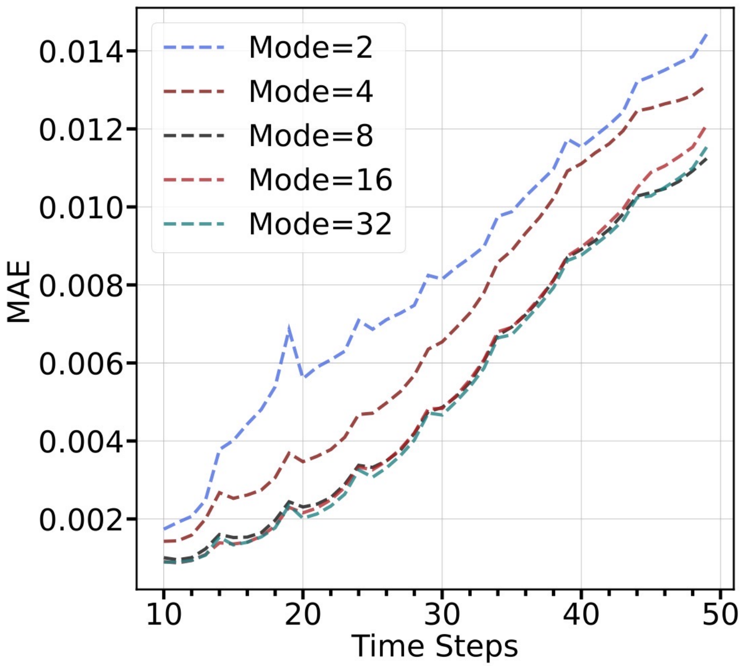
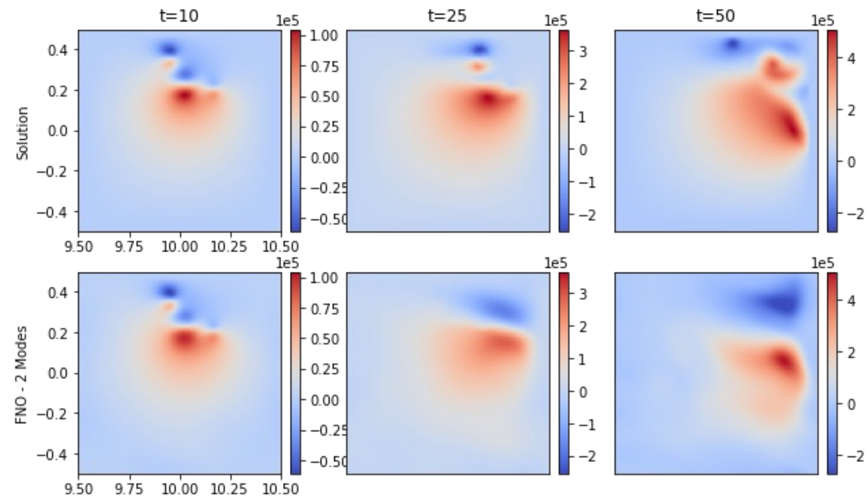
Supplementary Slides

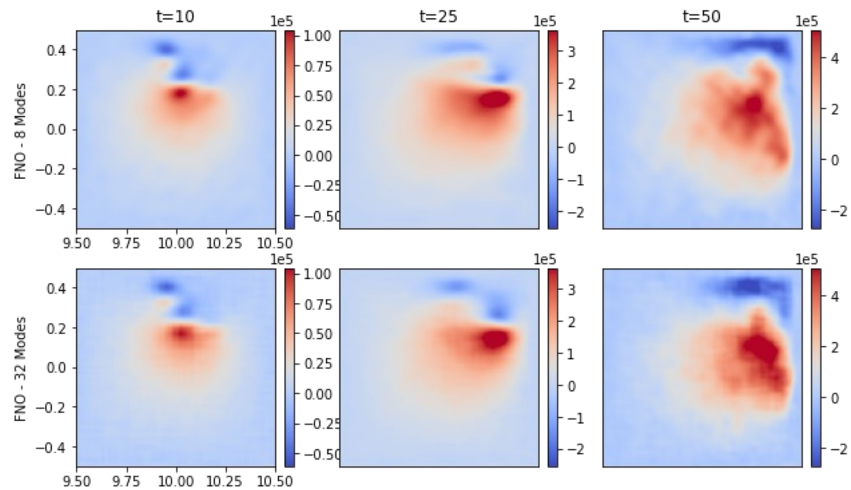
Impact of Training Data



Mode Ablation Study







Individual FNO vs Multi-variable FNO

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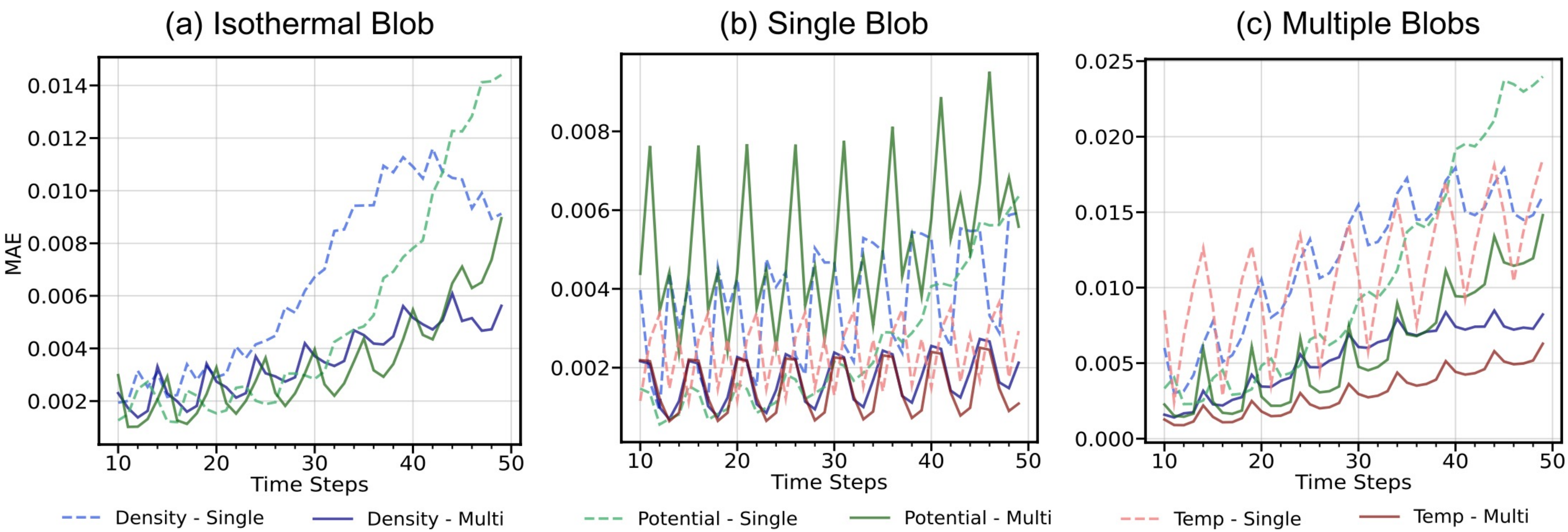
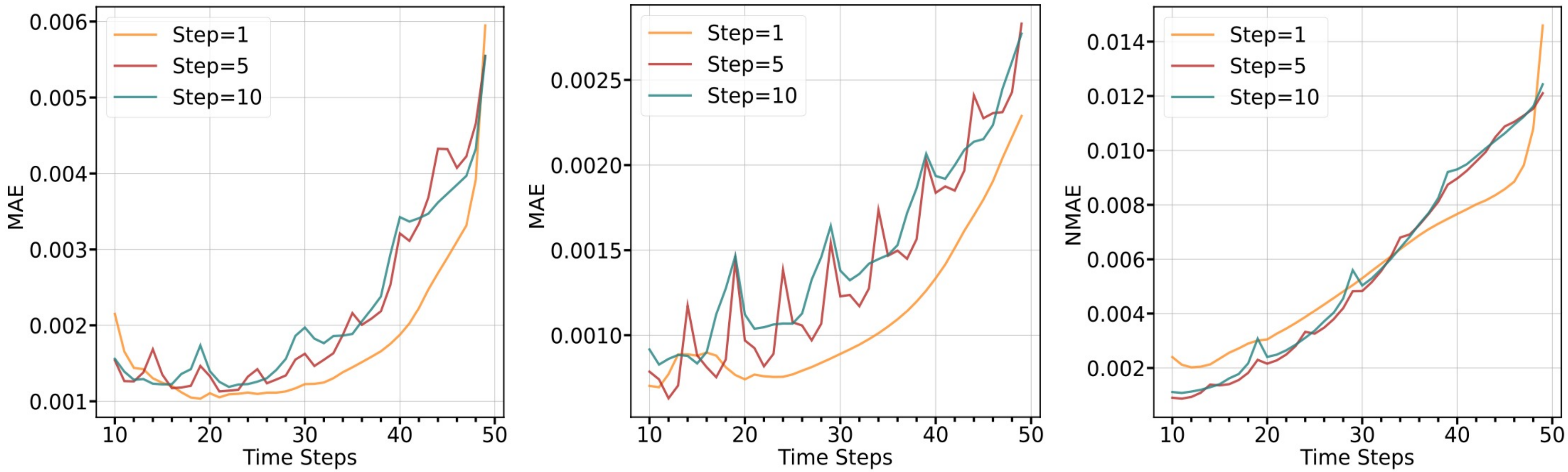
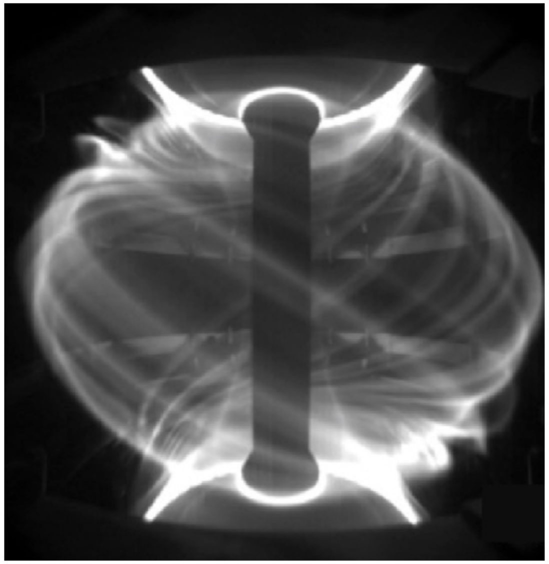


Impact of Step Size

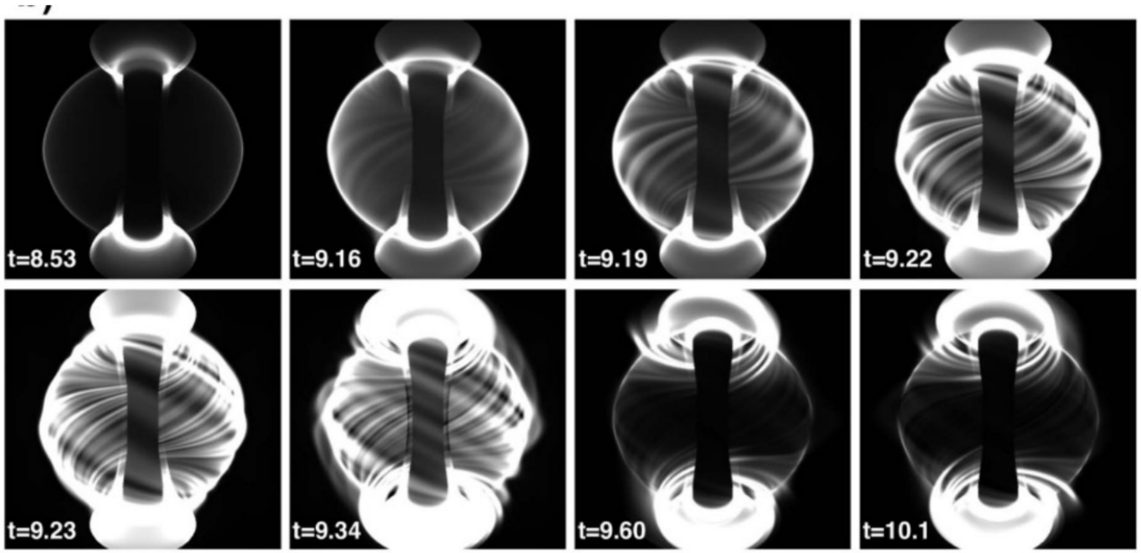


(a) Isothermal Blob (b) Single Blob (c) Multi-blobs

Sim2Real Gap – Concepts



(a) Experiment



(b) Simulation