UK Atomic
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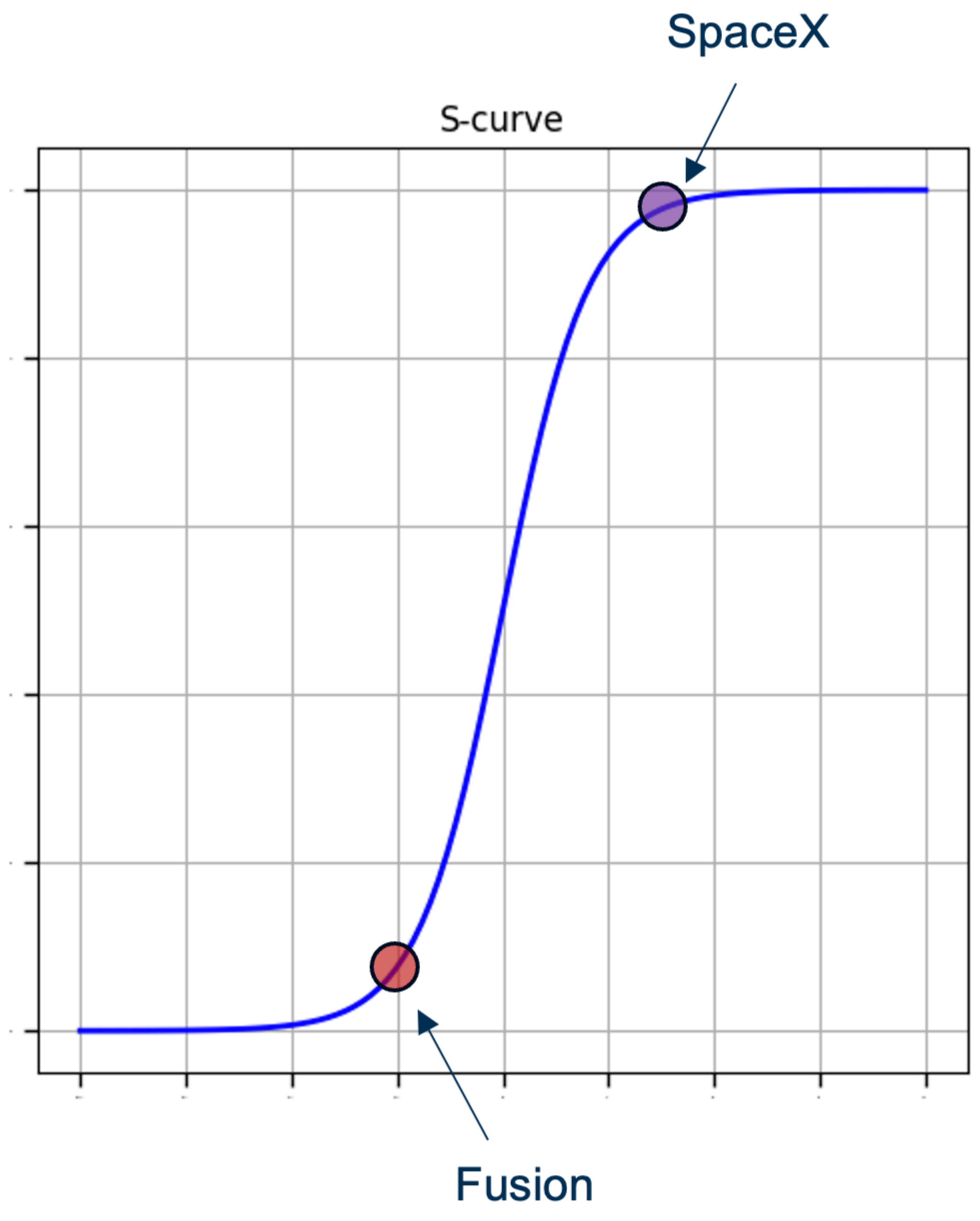
Calibrated Physics-Informed Uncertainty Quantification

Workshop on calibrating prediction uncertainty
University of Cambridge

Vignesh Gopakumar

June 6, 2025

Need for Surrogates
Motivation



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

Need for Surrogates

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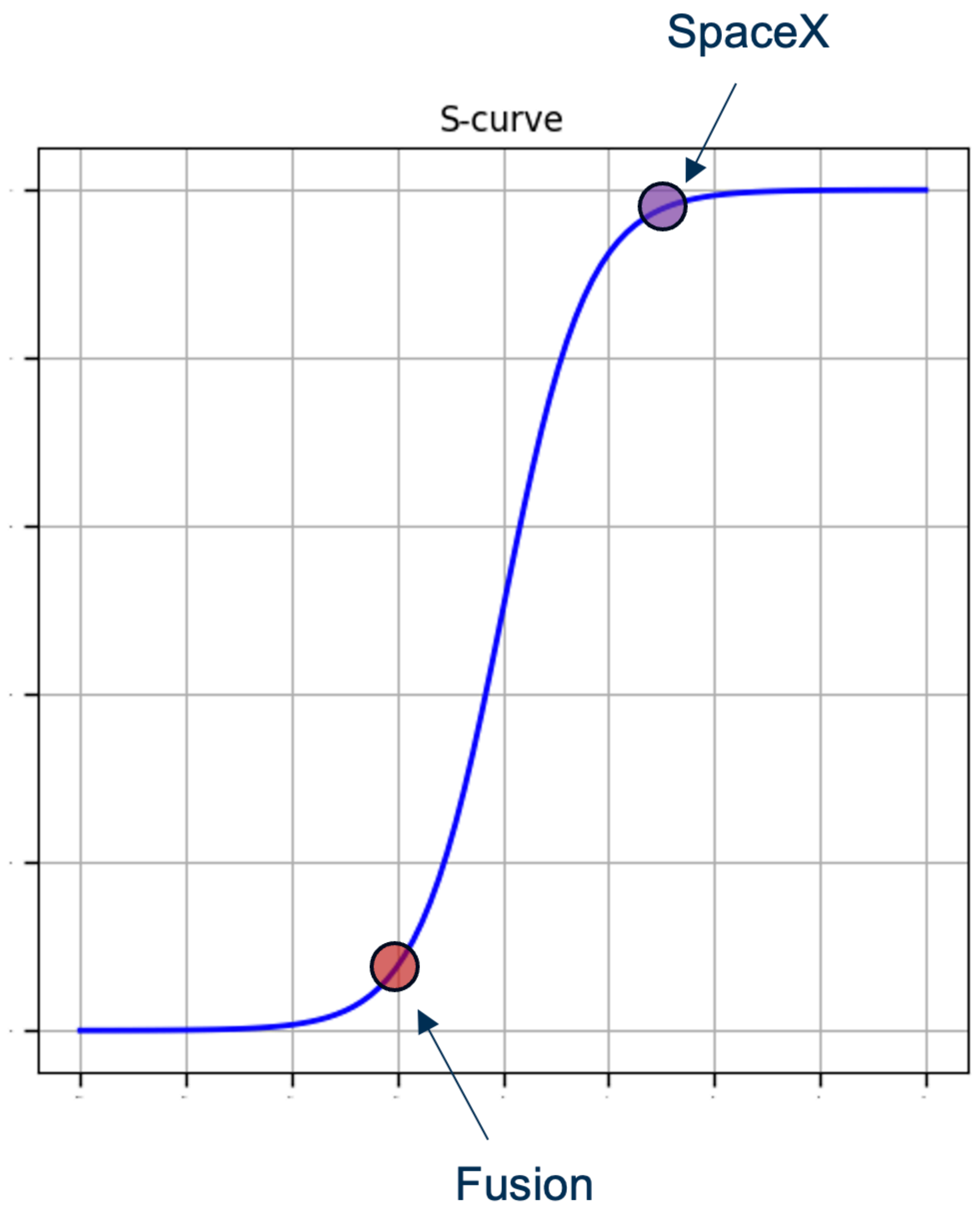
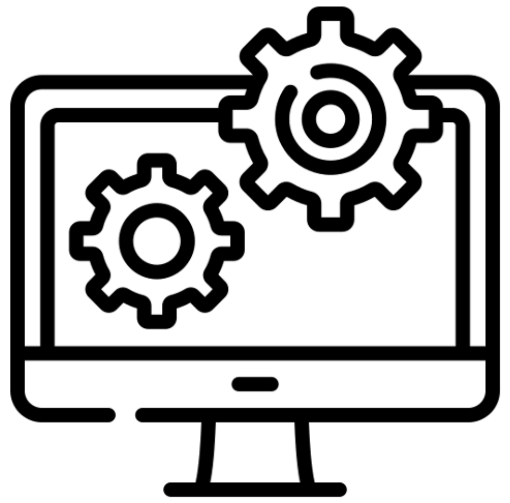
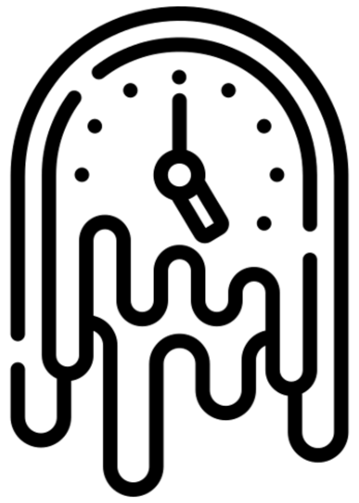




Computational Complexity

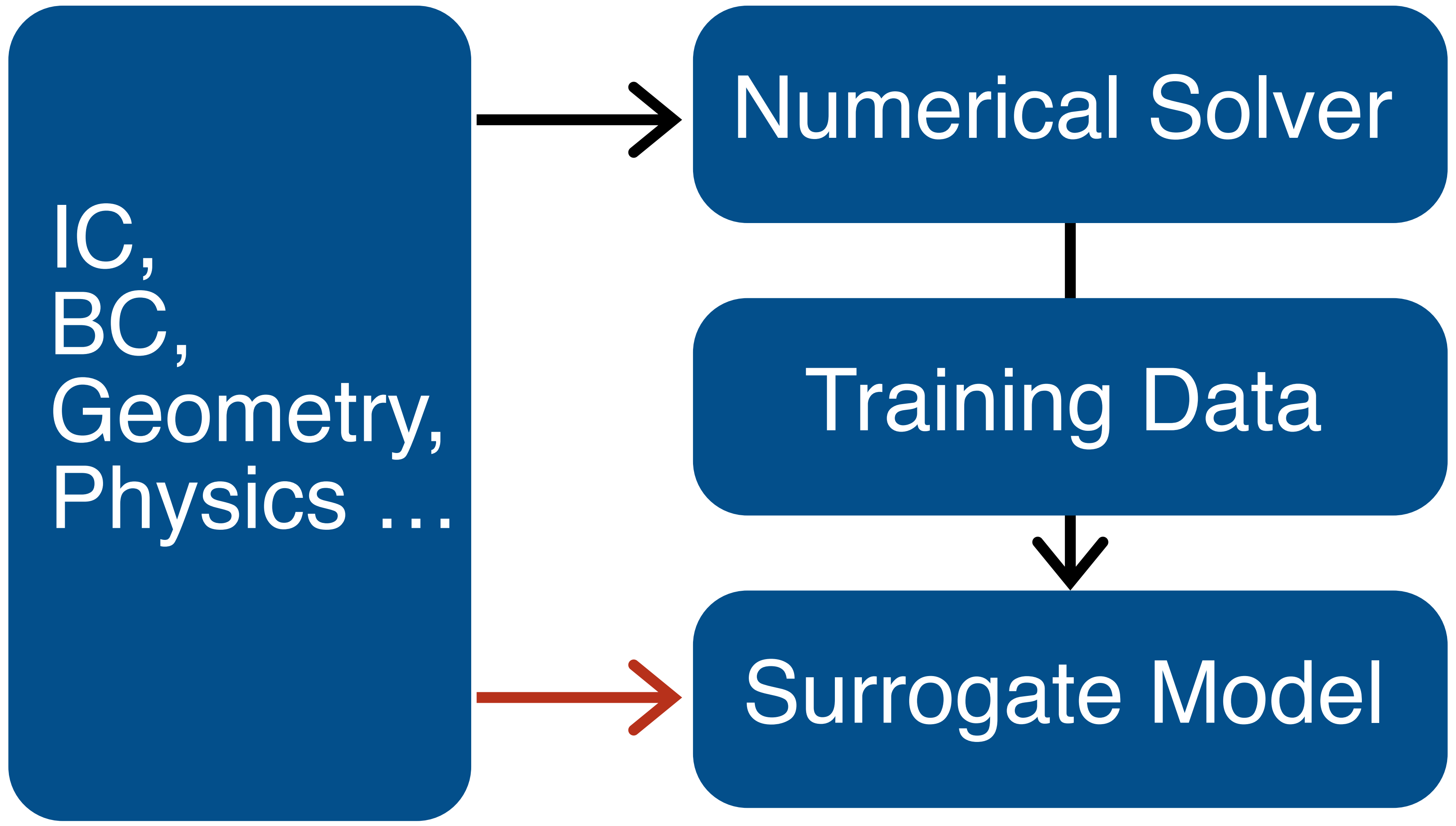


Latency

Unknown unknowns

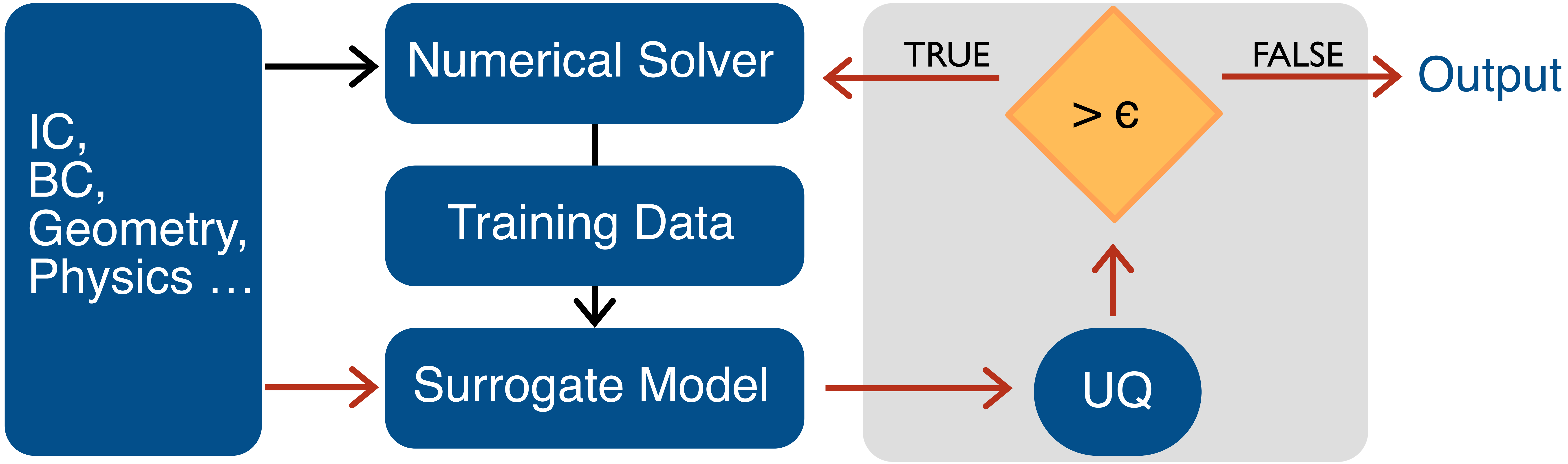
- Cannot “afford” iterative test-based engineering design.
- In-silico design at the Exascale
- Simulations and Digital Twins

Surrogate Model Ecosystem



Surrogate Model here refers to a data-driven method such as a neural network

Surrogate Model Ecosystem



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The Issue with current UQ methods

Validity and Guaranteedness

Traditional NN architectures are deterministic

Fails to scale to high dimensions

Requires extensive sampling

Unable to capture out-of-distribution

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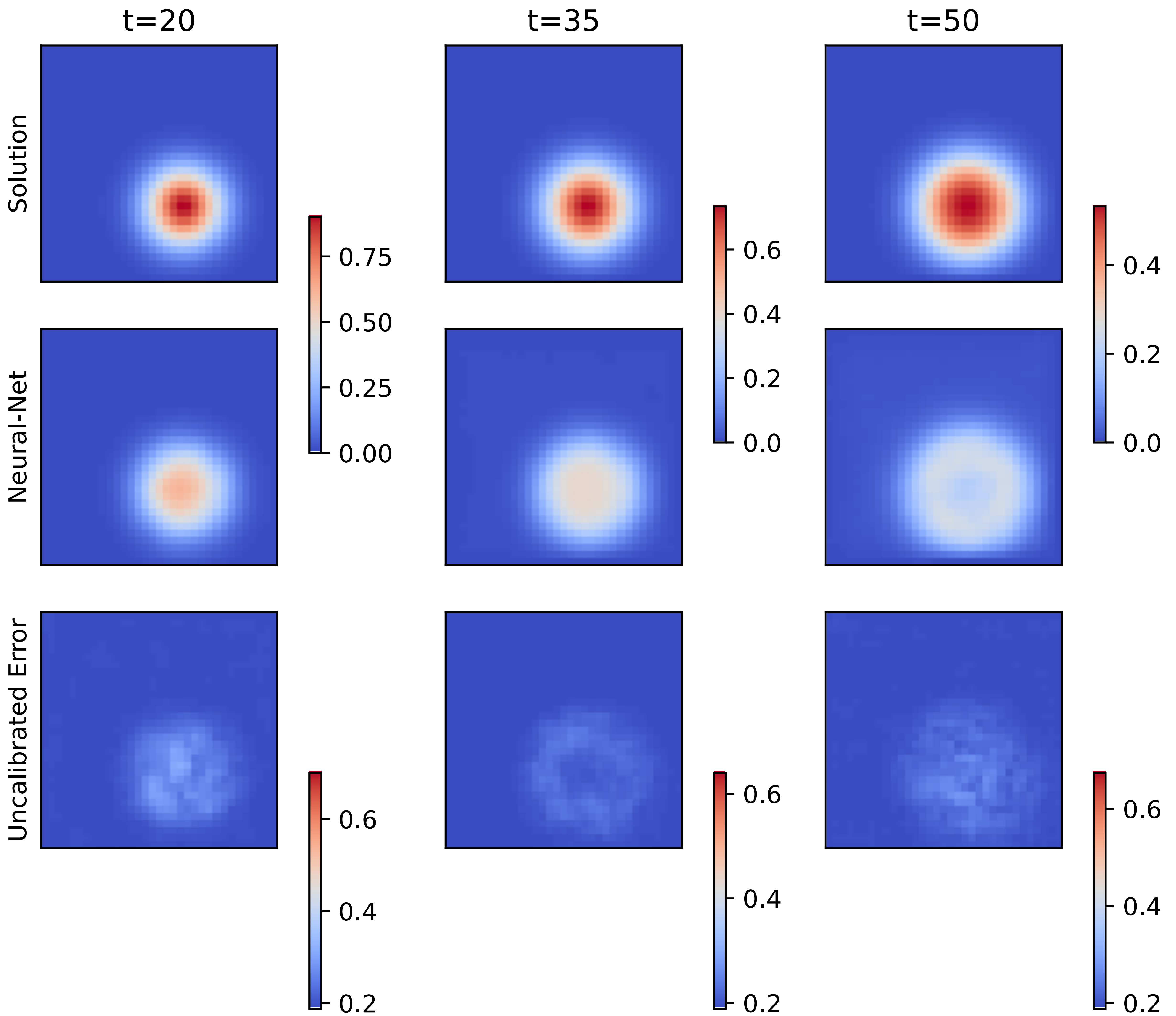


Multivariate CP

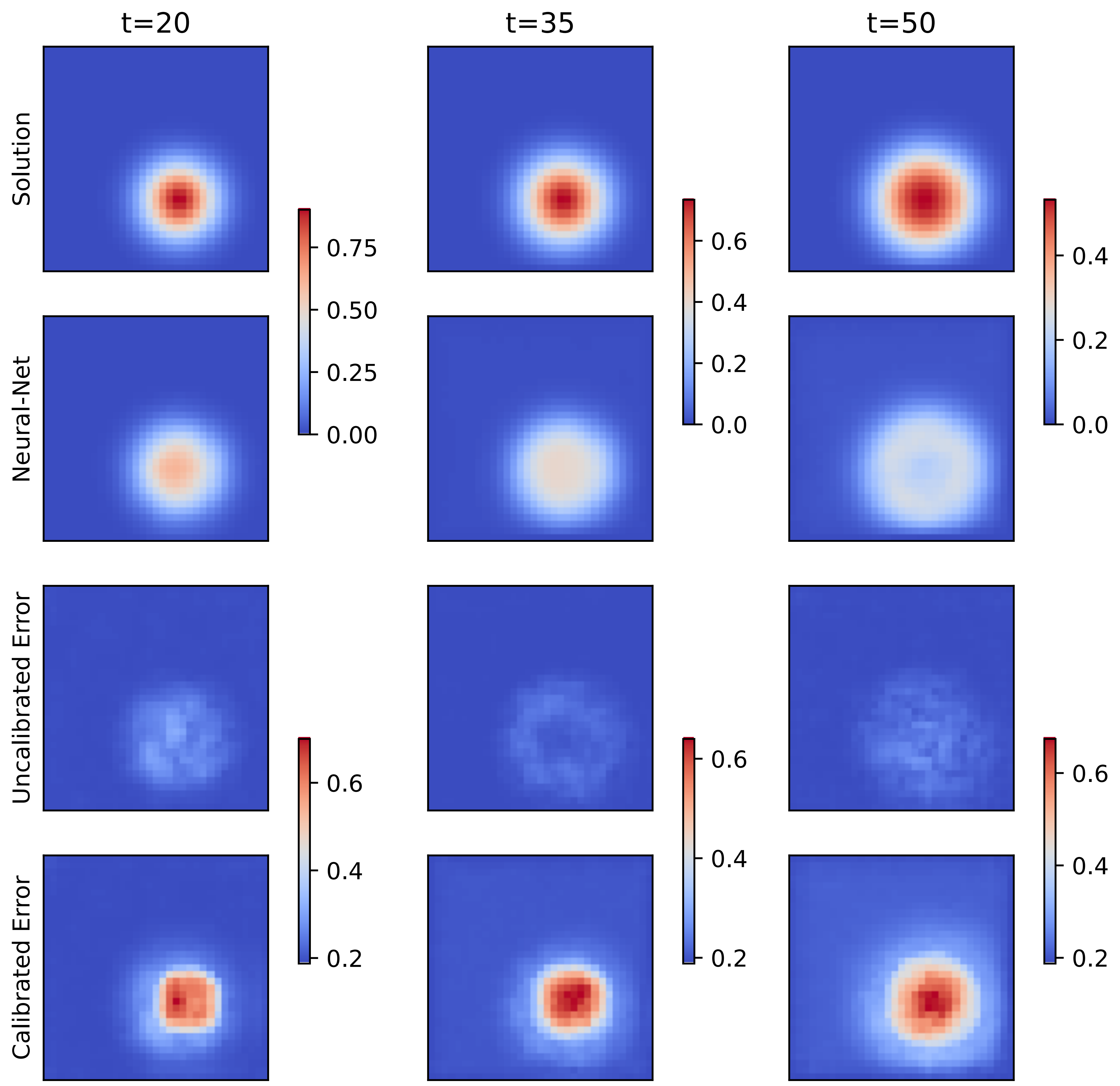
Cellwise Marginal CP

As long as the calibration and prediction data is exchangeable:

✓ Statistically valid coverage guarantees

✓ Model agnostic

✓ Infinite dimensions



Uncertainty Quantification of Surrogate Models using Conformal Prediction - Gopakumar et al

Multivariate CP

Cellwise Marginal CP

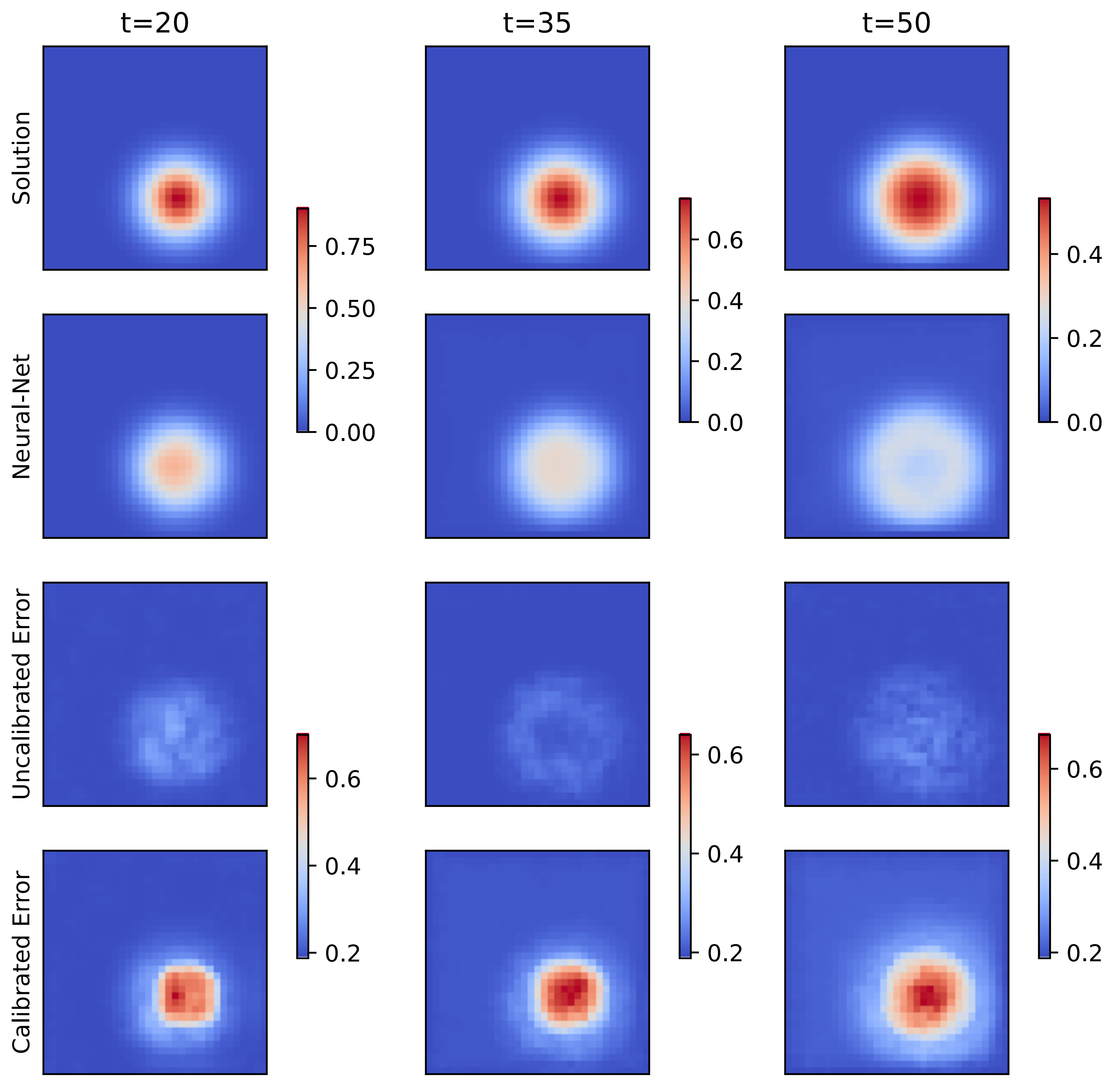
As long as the calibration and prediction data is exchangeable:

✓ Statistically valid coverage guarantees

✓ Model agnostic

✓ Infinite dimensions

✳ Requires sufficient calibration data for each prediction regime



Uncertainty Quantification of Surrogate Models using Conformal Prediction - Gopakumar et al

Residual Errors

Dynamical physical systems are solved by minimising the residual error.

Dynamics in the Standard Canonical Form: $Ax = b$

A: Discrete dynamics operator
x: State of the system
b: Externals

Prediciton errors are quantified as the residual: $r = Ax - b$

For a well-defined PDE this takes the form: $D(u) - b = 0$

A: Differential Operator
u: physical field
b: Externals

Physics Residual Errors (PRE)

PDE Residuals as a measure of surrogate performance=

Consider the 2D Wave Equation :

$$\frac{\partial^2 u}{\partial t^2} = c^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

Physics Residual Error over prediction $\hat{u}$:

$$D = \frac{\partial^2 \hat{u}}{\partial t^2} - c^2\left(\frac{\partial^2 \hat{u}}{\partial x^2} + \frac{\partial^2 \hat{u}}{\partial y^2}\right)$$

CP-PRE

Implicit knowledge of the PDEs as the nonconformity score function

Method	Score Function	Prediction Set
Absolute Error Residual (AER)	$\left(\lvert f_\theta(X_i) - Y_i \rvert \right)_{i=1}^{n}$	$f_\theta(X_{n+1}) \pm \hat{q}^\alpha$

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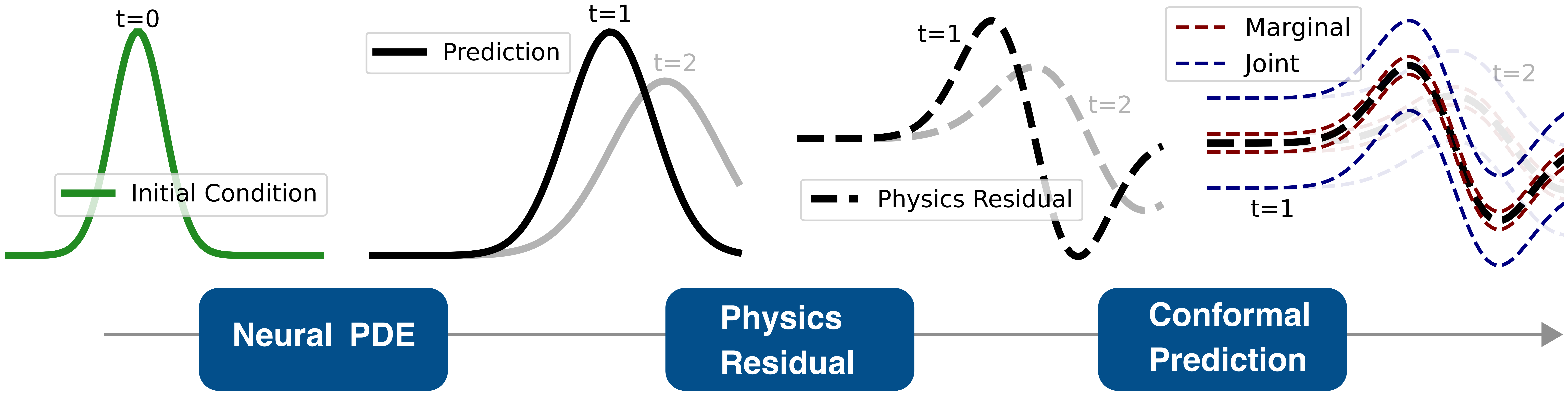
Physics Residual Error (PRE)	$\left(\lvert D(f_\theta(X_i)) - 0 \rvert \right)_{i=1}^{n}$	$0 \pm \hat{q}^\alpha$

CP-PRE Framework

Overview



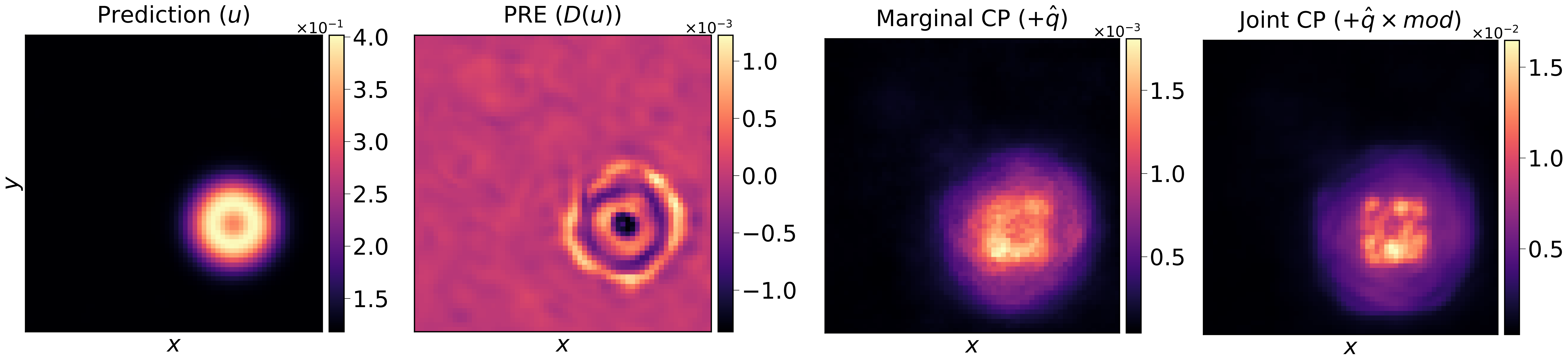
Joint CP-PRE for spatio-temporal coverage

Helps identify entire predictions that are unfeasible

Score Function (Marginal): $$\hat{s} = |D(f_\theta(X))|$$

Score Function (Joint): $$\mathcal{S} = \sup_{X \in \Omega,\, t \in [0,T]} \left(\frac{\hat{s}}{\sigma(\hat{s})} \right)$$

CP-PRE



✓ Guaranteed Coverage

✓ Model Agnostic

✓ Modification-Free

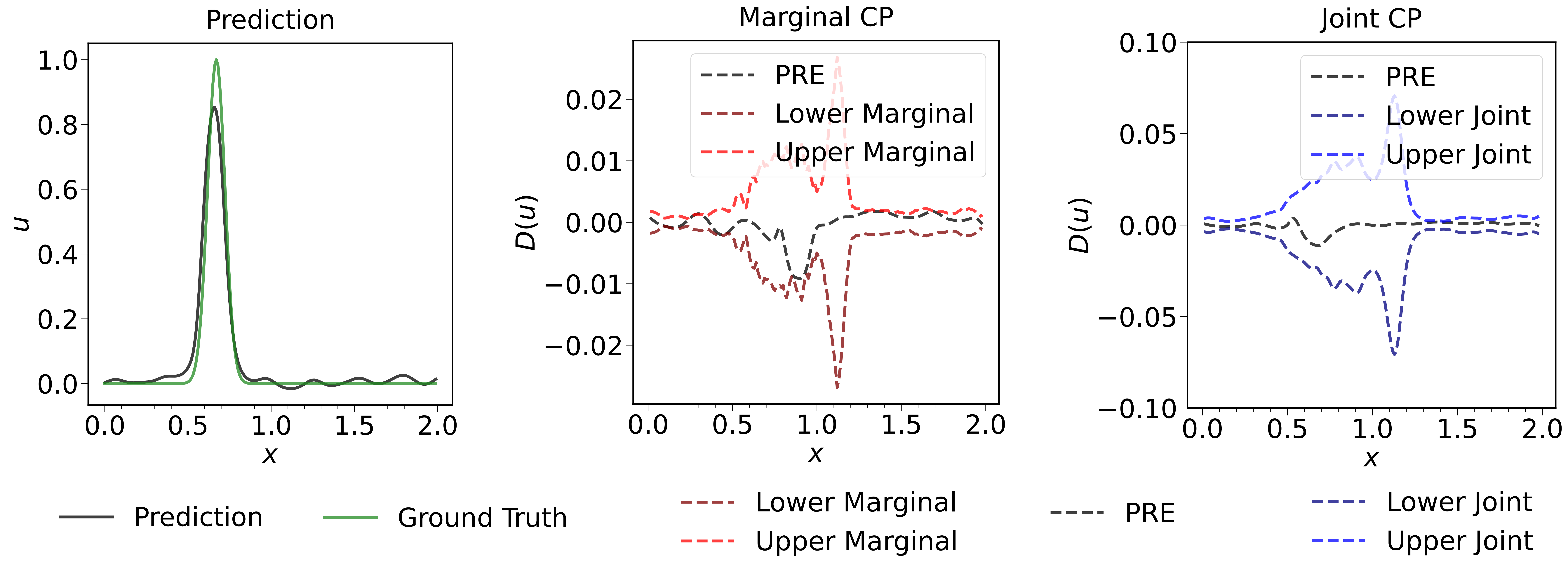
✓ Sampling-Free

✓ Data-Free

✓ Physics-Informed

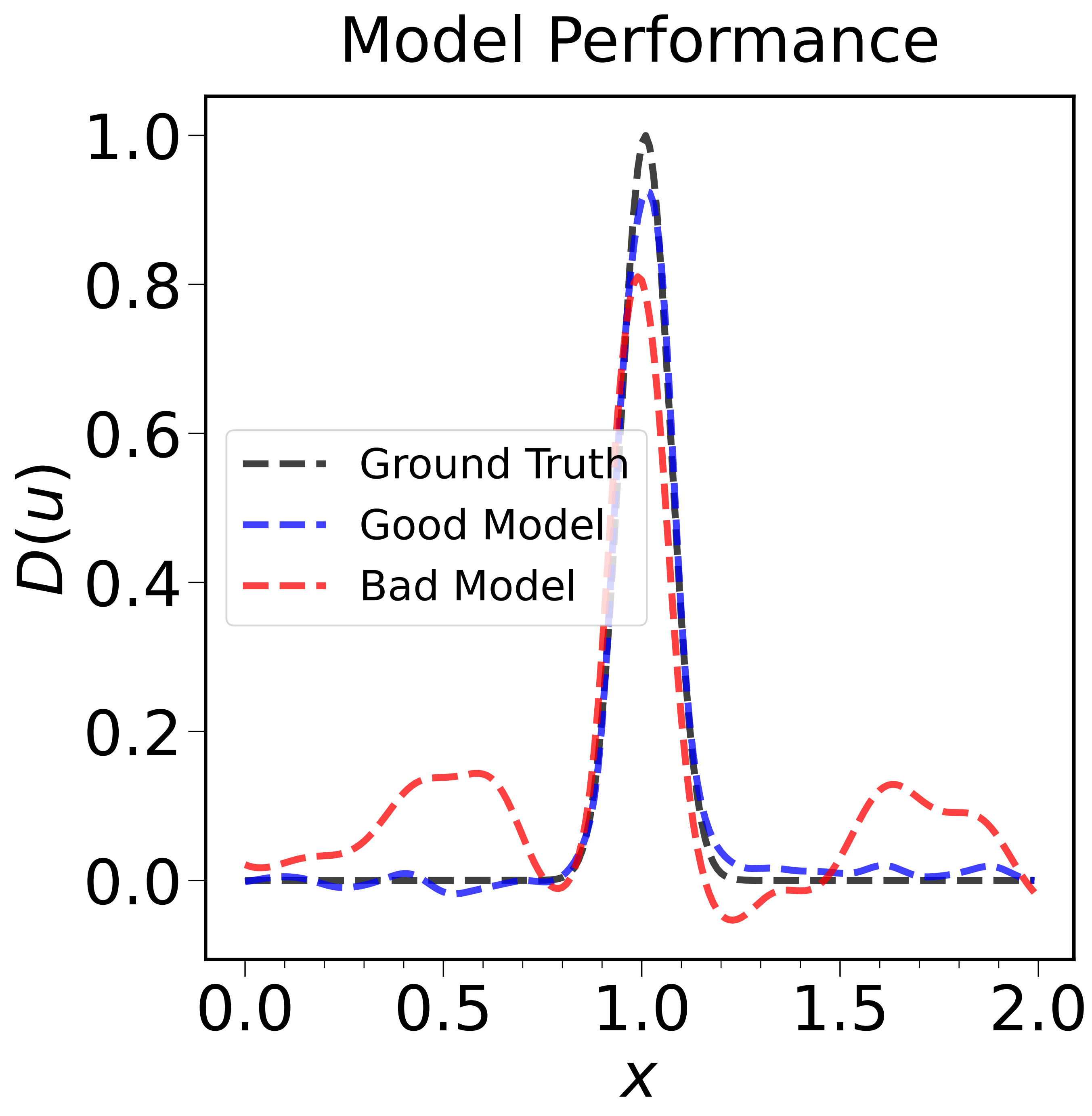
Example: 1D Advection

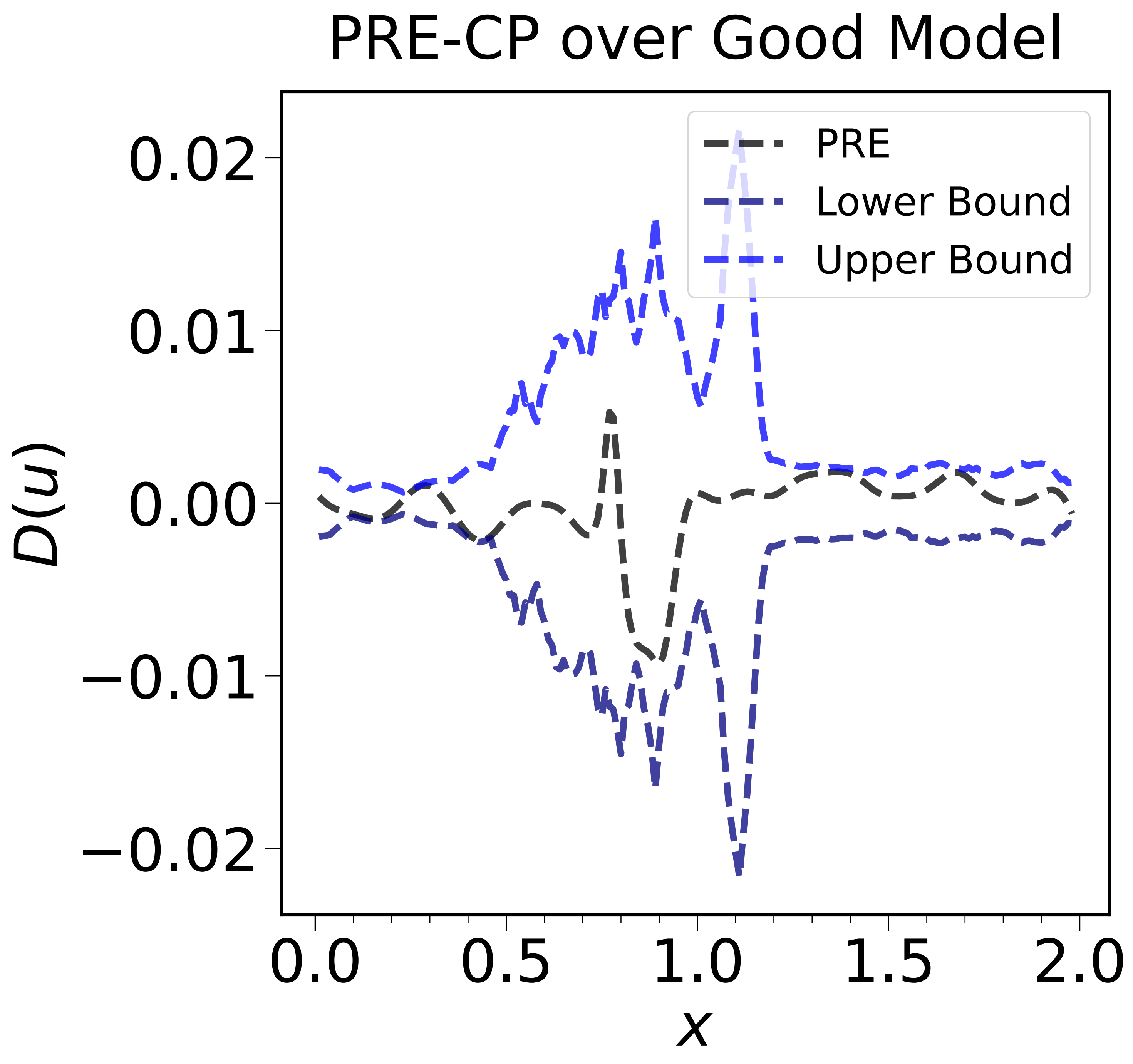
$$\frac{\partial u}{\partial t} + \nu \frac{\partial u}{\partial x} = 0$$

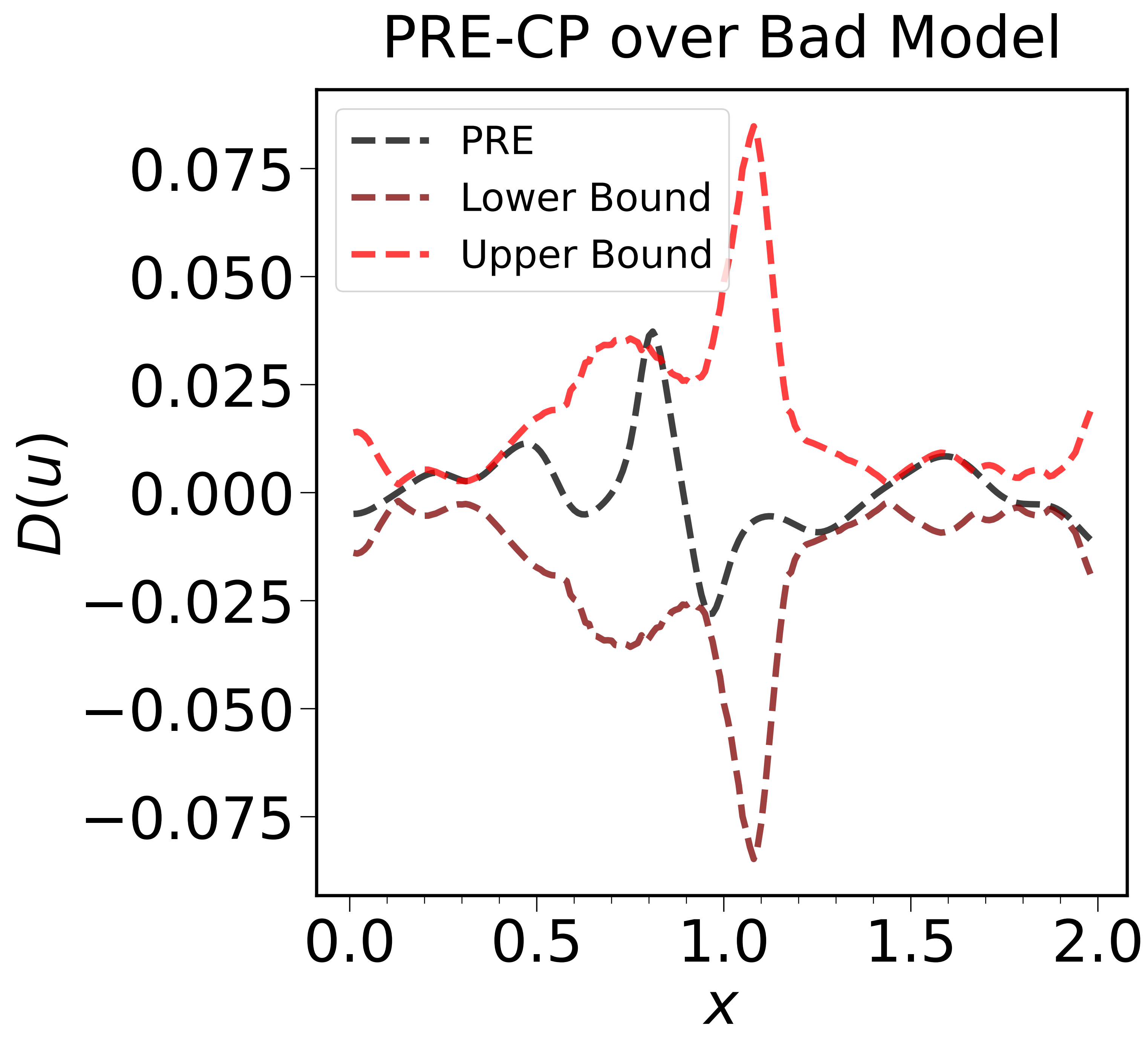


CP-PRE as a measure of model quality

Only marginal CP visualised

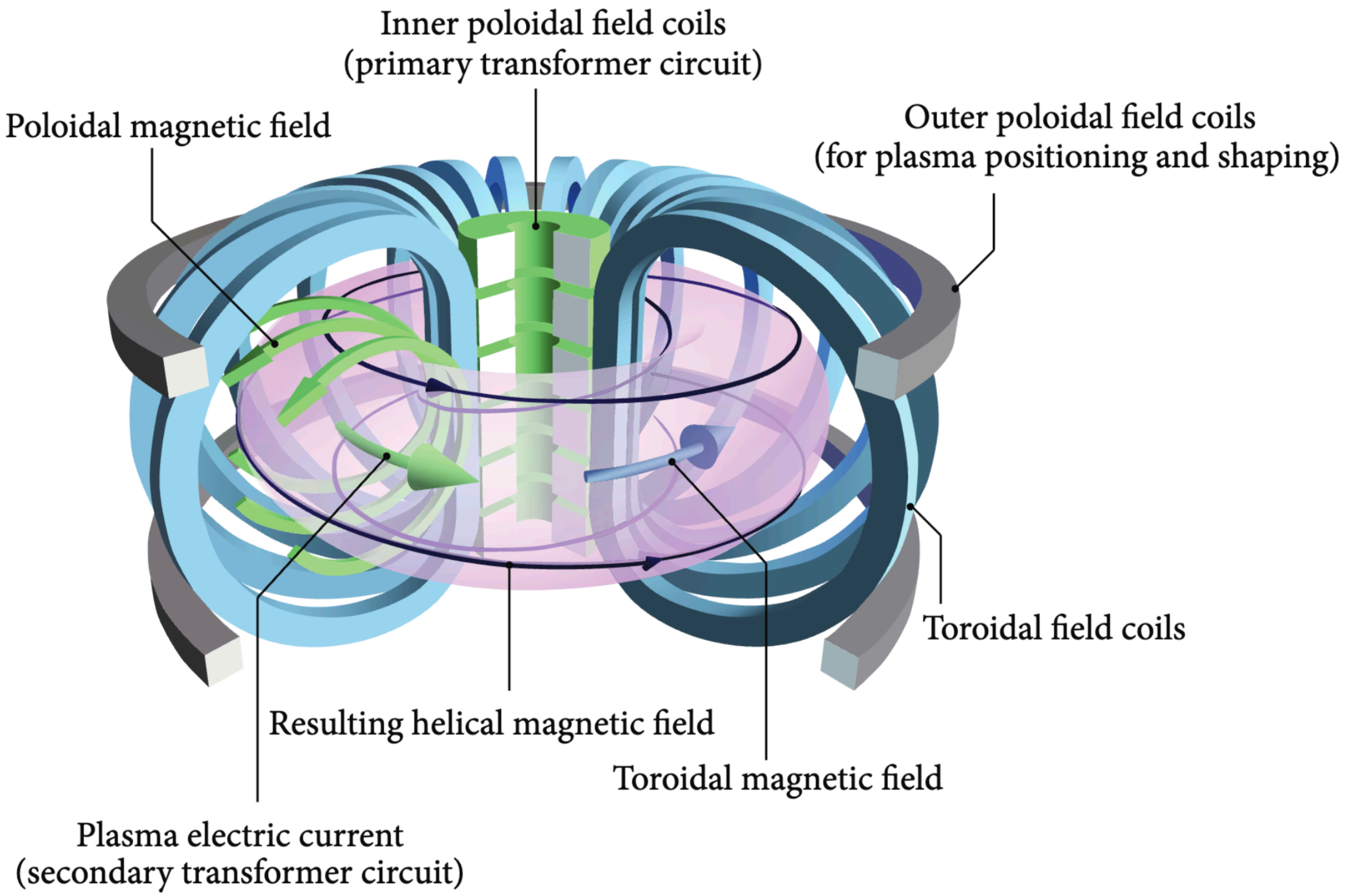






Tokamak Design

Optimal placement of poloidal field coils for Magnetic Equilibrium



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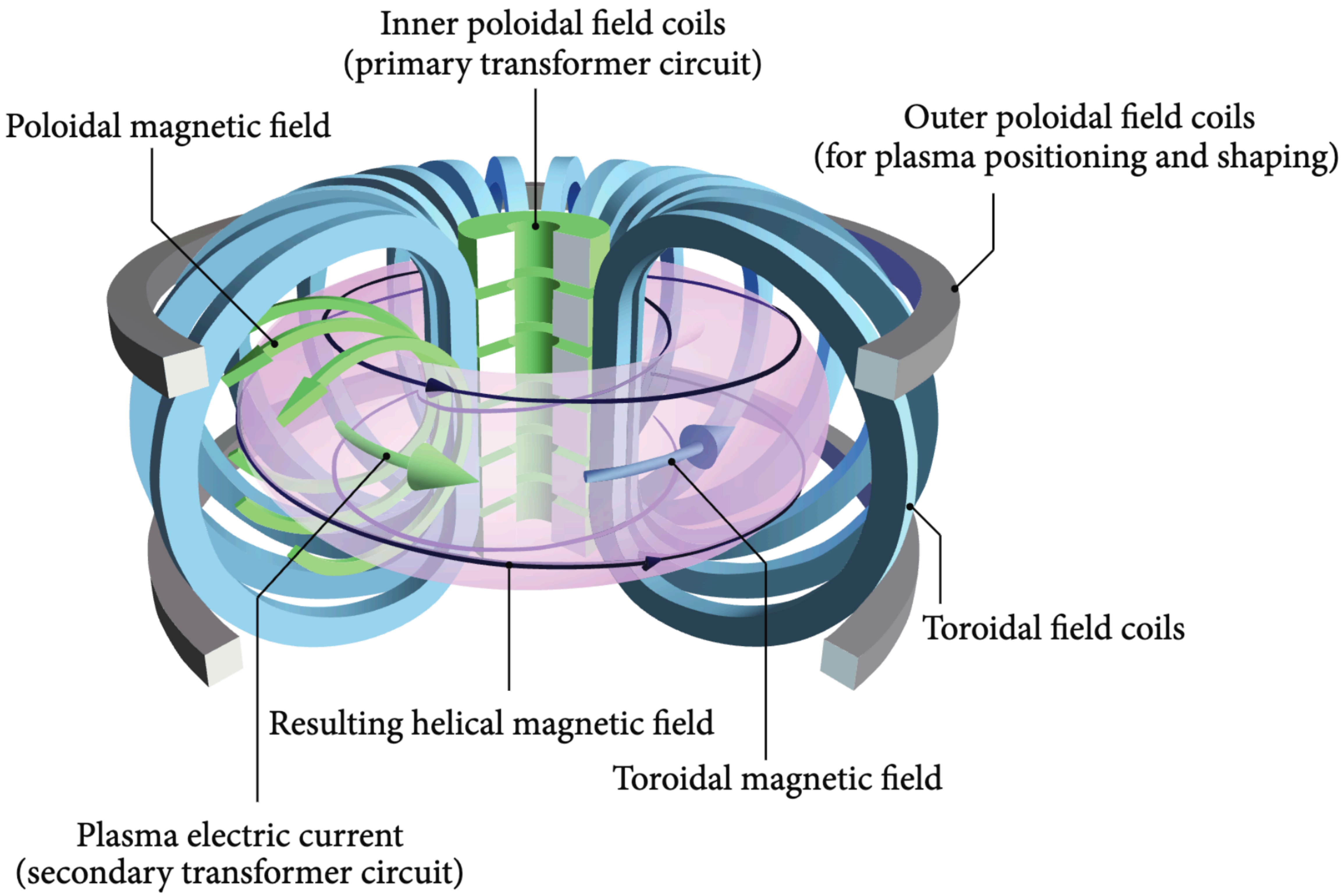
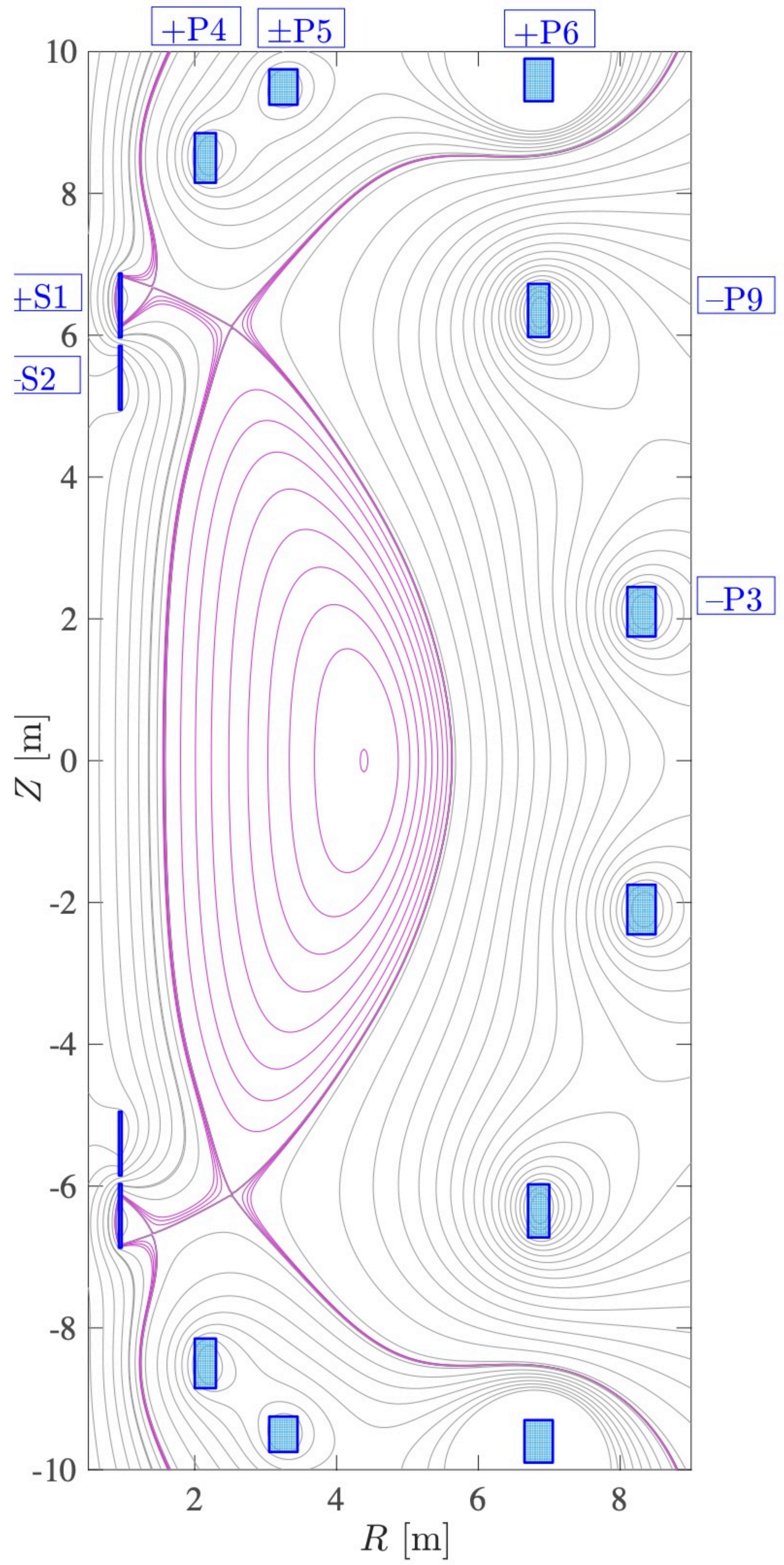
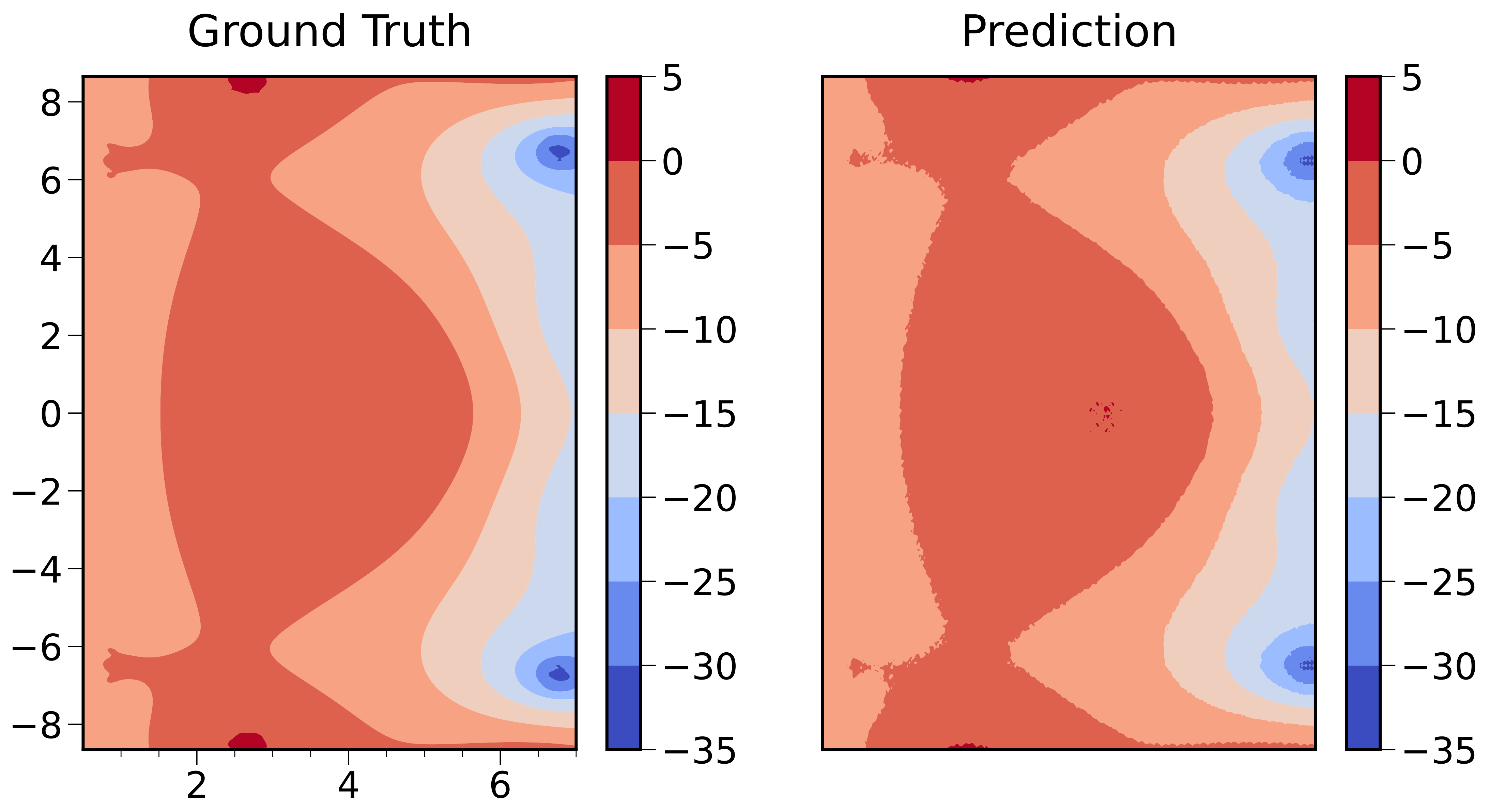




Example: Magnetic Equlibrium in a Tokamak

Bounds over the PRE of the Grad-Shafranov Equation

$$\frac{\partial^2 \psi}{\partial r^2} - \frac{1}{r}\frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial z^2} = -\mu_0 r^2 \frac{dp}{d\psi} - \frac{1}{2}\frac{dF^2}{d\psi}$$



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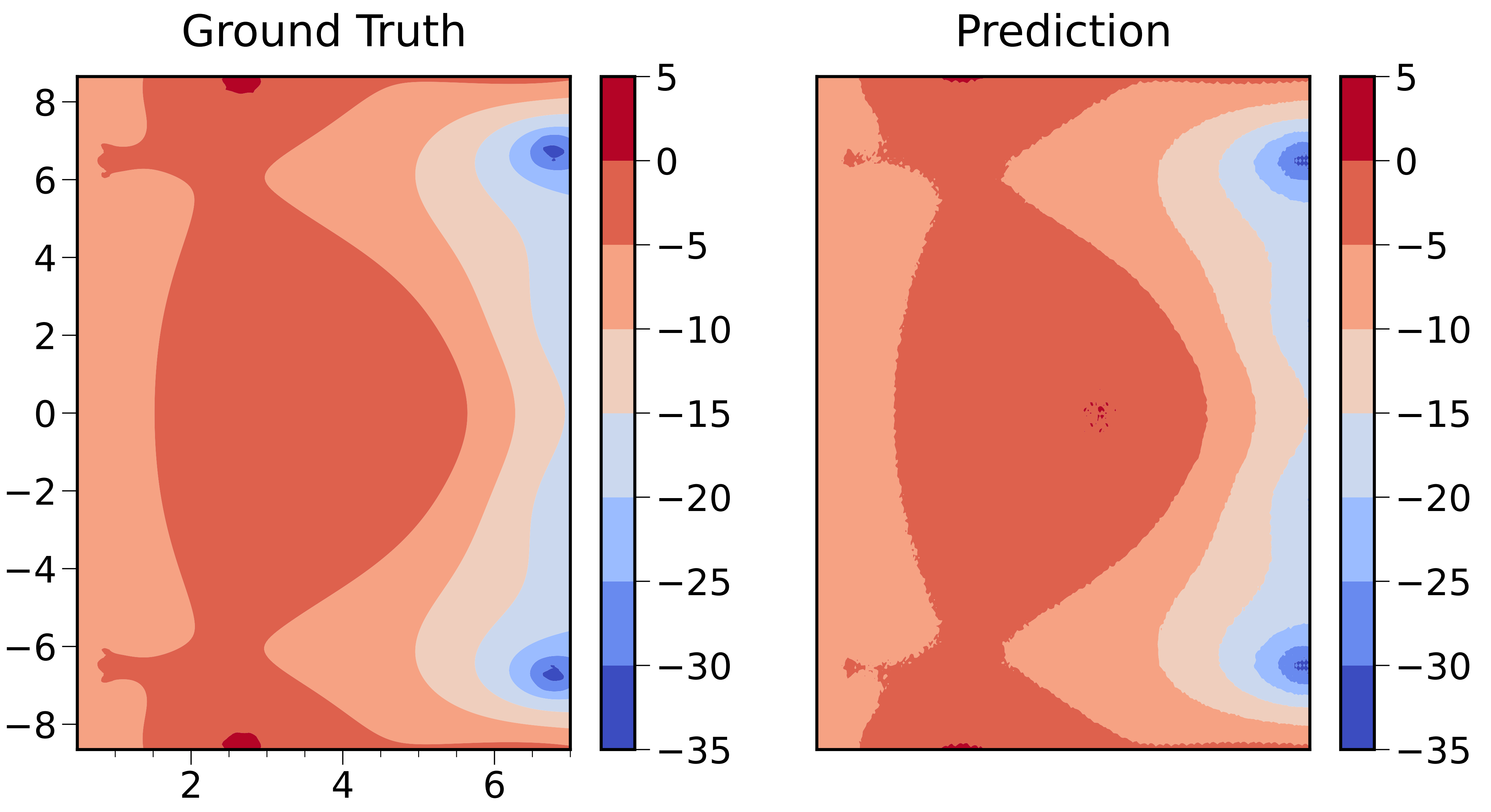

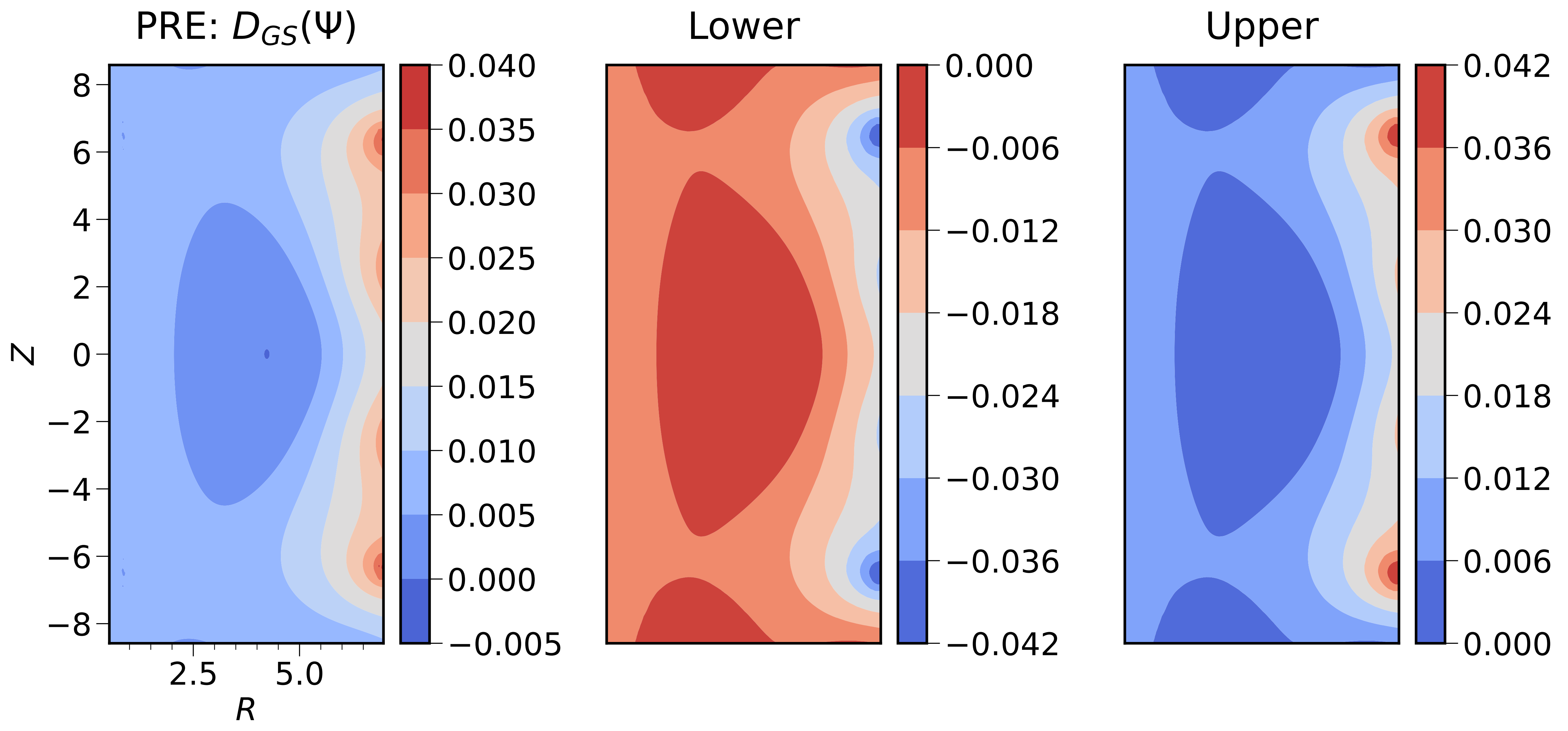

Conclusion

- Valid, guaranteed bounds over the conservative space for Neural PDE solvers
- Data-free, physics-informed and model-agnostic UQ method
- Marginal-CP for identifying erroneous regions within the spatio-temporal domain
- Joint-CP for identifying erroneous predictions across the entire spatio-temporal domain
- Extends to predictive cases with an equality constraint expressed in the standard canonical form: $D(u) - b = 0$

Paper

Accepted at ICML 2025

Calibrated Physics-Informed Uncertainty Quantification

Authors:

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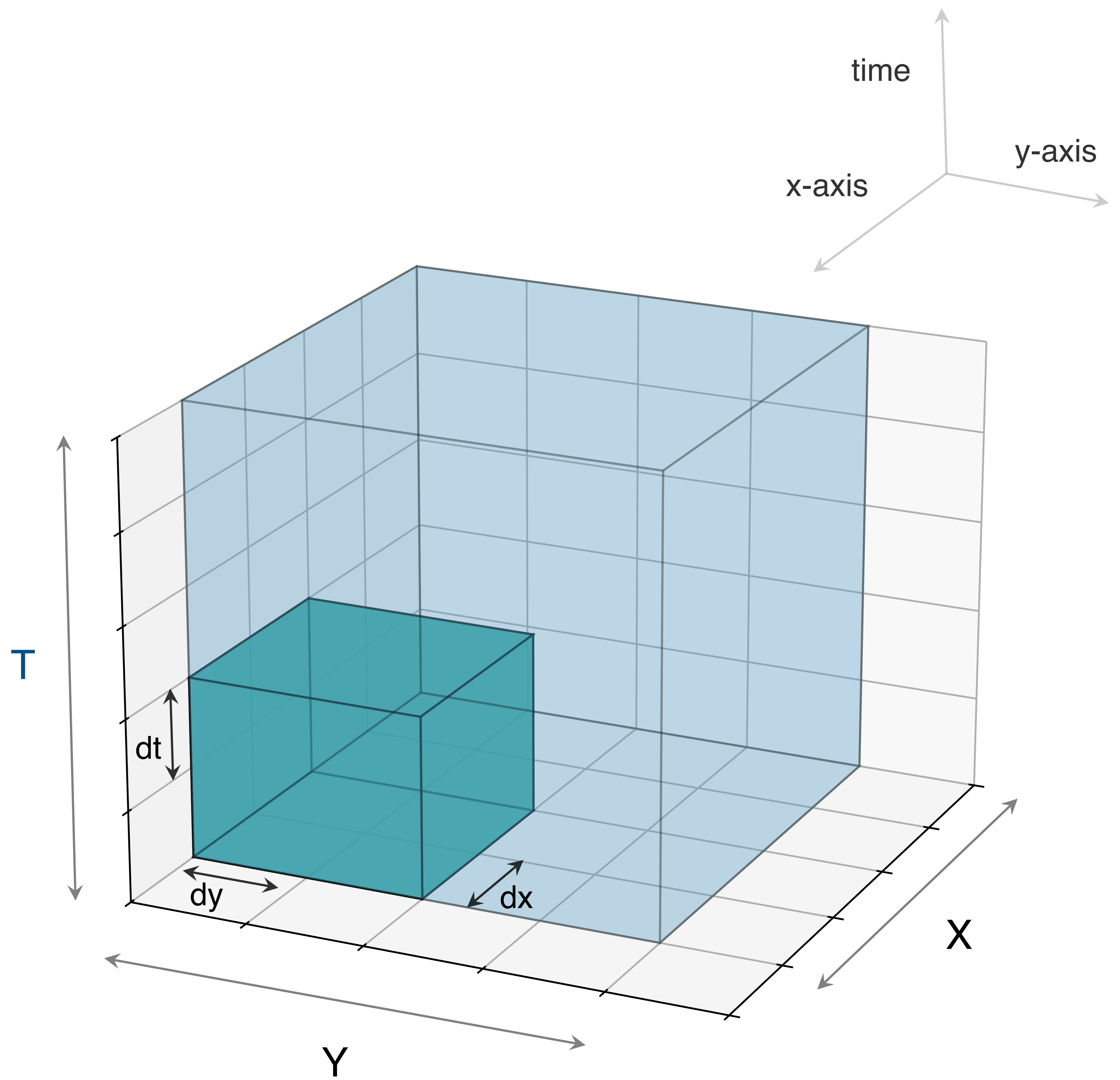
Estimating Differential Operators

Finite-Difference Stencils as Convolutional Kernels



$$\nabla^2 \approx \frac{1}{h^2}\begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

ConvOps for PRE

```
from ConvOps_2d import ConvOperator

# Define each operator within the PDE
D_tt = ConvOperator(domain='t', order=2) #time-derivative
D_xx_yy = ConvOperator(domain=('x','y'), order=2) #Laplacian

# Setting up additive kernels for PRE
c =  0.5  # wave speed
D = ConvOperator()
D.kernel = D_tt.kernel - c**2 * D_xx_yy.kernel

#Estimating PRE over model prediction
y_pred = model(X)
PRE = D(y_pred)
```

CP-PRE: Gist

The prediction set for a given nonconformity score function is given as:

$$\mathbb{C}^{\alpha}(X_{n+1}) = \{y : S(X_{n+1}, y) \leq \hat{q}^{\alpha}\}$$

The score function while using AER is expressed as:

$$S_{AER}(X, Y) = |f_{\theta}(X) - Y|$$

Where the prediction set that defines the coverage is:

$$\mathbb{C}^{\alpha}_{AER}(X_{n+1}) = [f_{\theta}(X_{n+1}) - \hat{q}^{\alpha}, f_{\theta}(X_{n+1}) + \hat{q}^{\alpha}]$$

Similarly, the score function while using PRE actually has a target:

$$S_{PRE}(f_{\theta}(X)) = |D(f_{\theta}(X)) - 0|$$

Leading to a prediction set that is independent of the input:

$$\mathbb{C}^{\alpha}_{PRE} = [-\hat{q}^{\alpha}, \hat{q}^{\alpha}]$$