Calibrated Physics-Informed Uncertainty Quantification

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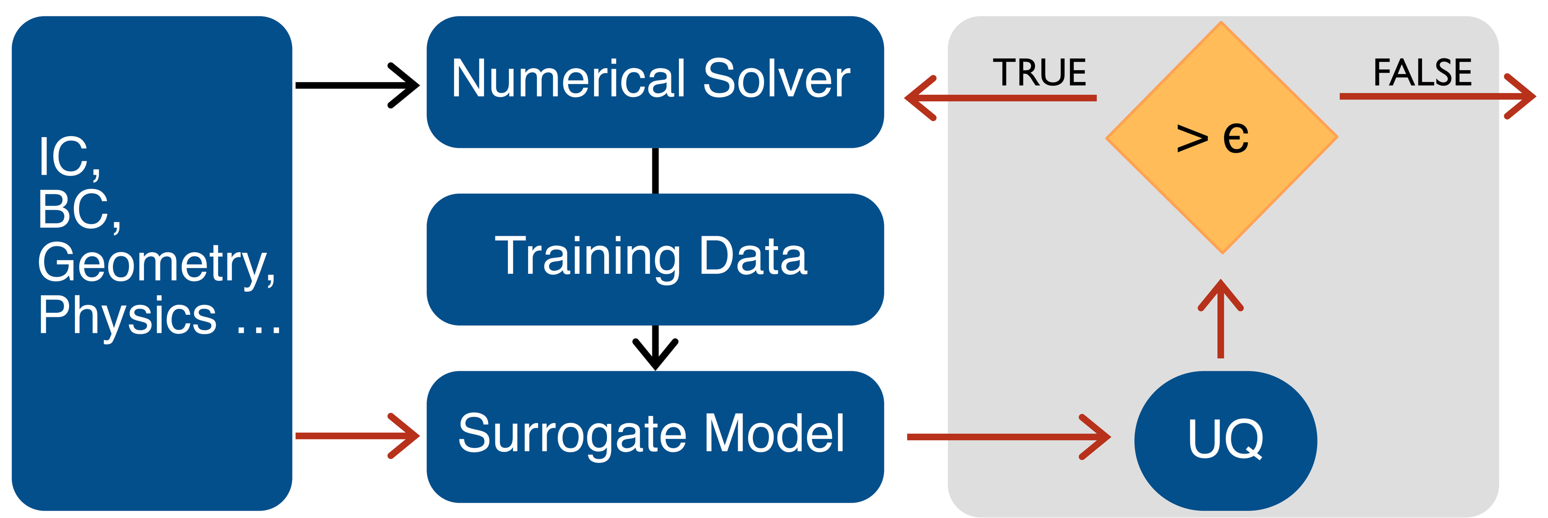
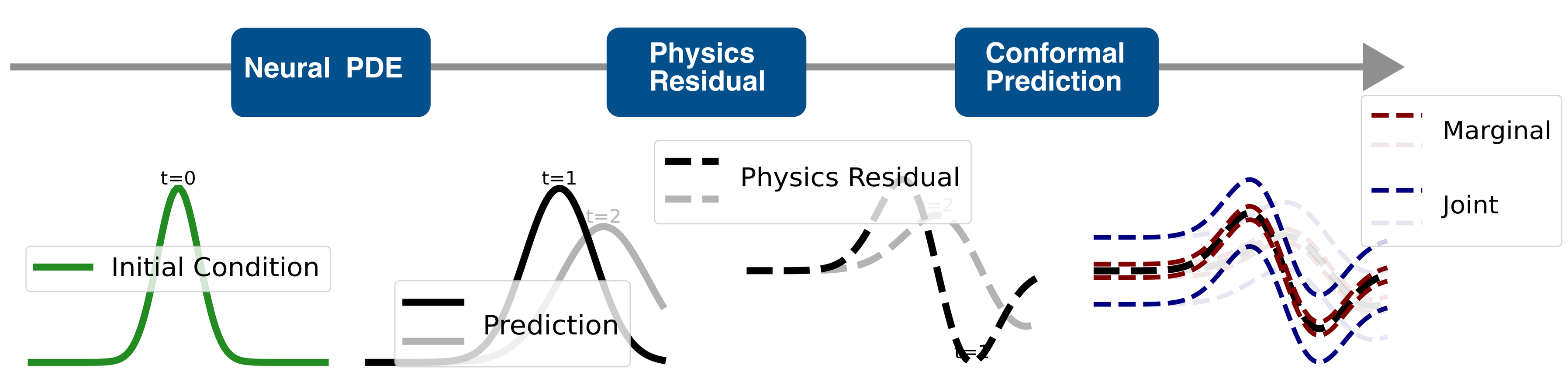
TLDR: Calibrated uncertainty quantification of neural PDE solvers using physics residual errors as non-conformity scores for data-free conformal prediction

Motivation



Surrogate models approximating PDE solutions need to be be made "actionable" using **valid** UQ methods

Method: CP-PRE



➡ **CP-PRE** provides bounds to a model's adherence to the governing physics equations.

➡ Performs conformal prediction using Physics Residual Errors as a nonconformity score for calibrated measures of physical misalignment.

➡ The error bars are over the residual space associated with the PDE, bounding the model's violation of the conservation equations.

Physics Residual Error (PRE):

PDE residual estimated over the discretised solution predicted by the surrogate model.

$$\text{PRE} = D(u) - b \sim 0$$

D - Composite spatio-temporal differential operator characterising the PDE

u - Prediction, **b** - External forcing

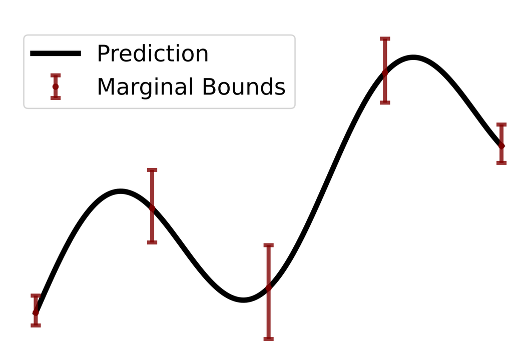
Contributions

Novel UQ method for neural-PDE solvers that

- 👍 provides coverage guarantees
- 👍 is model-agnostic
- 👍 requires no calibration data
- 👍 is sampling Free
- 👍 provides physics-informed uncertainty bounds

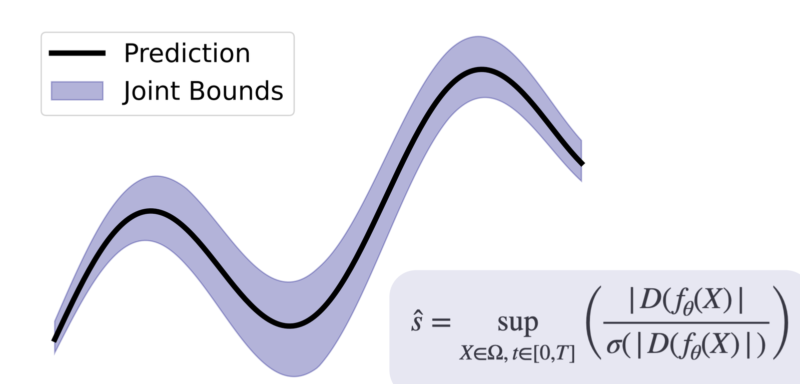
Marginal Coverage

Cell-wise coverage
Identify erroneous regions within the spatio-temporal domain, tagging unphysical features within the domain by providing point-wise uncertainty.



Joint Coverage

Spatio-temporal coverage
Identifies erroneous predictions across the spatio-temporal domain, tagging unphysical predictions. Domain-wise confidence enables rejection of physically inconsistent predictions.



$$\hat{s} = \sup_{X\in\Omega,\, t\in[0,T]} \left(\frac{|D(f_\theta(X))|}{\sigma(|D(f_\theta(X)|)}\right)$$

Method	Score Function	Prediction Set
Absolute Error Residual (Traditional CP)	$\left(\lvert f_\theta(X_i) - Y_i \rvert\right)_{i=1}^{n}$	$f_\theta(X_{n+1}) \pm \hat{q}^\alpha$
Physics Residual Error (Ours)	$\left(\lvert D(f_\theta(X_i)) - 0 \rvert\right)_{i=1}^{n}$	$0 \pm \hat{q}^\alpha$

Experiments

Navier-Stokes Equations

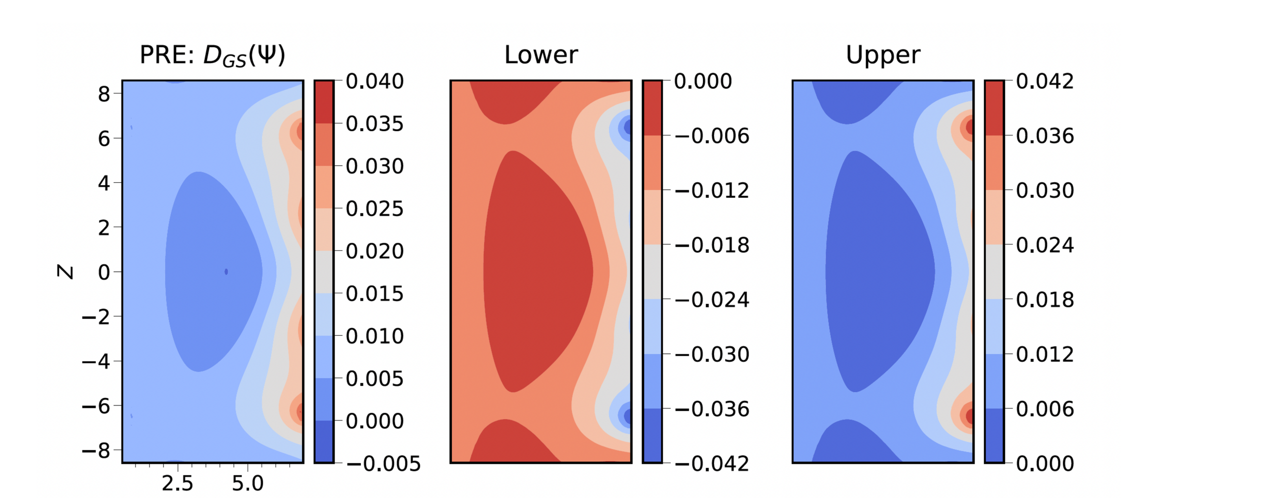
🔵 Baseline comparison of our method against other methods of UQ for neural PDE surrogates modelling the incompressible Navier-Stokes equations.

🔵 We obtain guaranteed coverage for both in-distribution and out-of-distribution evaluations while being the most computationally efficient.

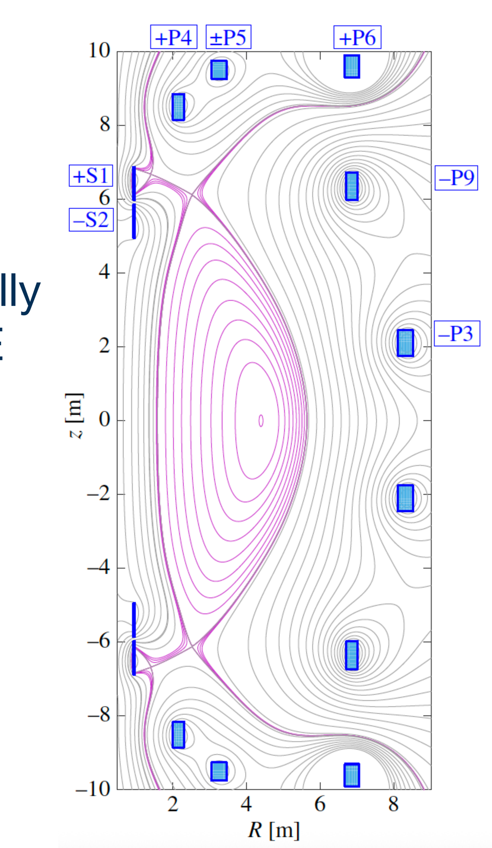
	in-distribution		out-of-distribution		Time	
UQ	MSE	Coverage (95%)	MSE	Coverage (95%)	Train (hr)	Eval (s)
Deterministic	1.05e-04 ± 6.91e-06	-	3.67e-03 ± 5.30e-05	-	3:22	25
MC Dropout	5.96e-04 ± 2.30e-05	82.21 ± 0.22	4.30e-03 ± 8.05e-05	44.05 ± 0.26	3:34	153
Deep Ensemble	1.22e-04 ± 3.95e-06	91.31 ± 0.08	3.67e-03 ± 3.52e-05	30.74 ± 0.19	16:22	147
BNN	6.90e-03 ± 1.31e-04	89.91 ± 0.20	6.95e-03 ± 1.31e-04	85.19 ± 0.23	3:39	152
SWA-G	1.96e-04 ± 1.15e-05	84.22 ± 2.37	3.63e-03 ± 1.37e-04	31.00 ± 2.85	3:28	146
CP-AER	1.05e-04 ± 6.58e-06	**95.56 ± 0.40**	3.66e-03 ± 2.81e-05	**95.54 ± 0.15**	3:22	20026
CP-PRE (Ours)	1.07e-04 ± 5.18e-06	**95.44 ± 0.22**	3.70e-03 ± 4.23e-05	**95.57 ± 0.14**	3:22	**134**

Magnetic Equilibrium in a Fusion Reactor

Grad-Shafranov Equation
Position of field coils (blue rectangles) determines the quality of equilibrium (contour lines) in a fusion reactor. During the design phase, it is infeasible to solve the equilibrium equation numerically for a million iterations. Surrogate models equipped with CP-PRE provides an actionable model that allows us to explore the proposed design space with confidence.



PRE over the predicted equilibrium with the lower and upper bounds



Coils and Magnetic Equilibrium

Paper

Extensions beyond PDEs:

Our method can be extended to provide valid error bounds for any predicitve model that is governed by an equality constraint as given in the standard canonical form: $Ax - b = 0$