BREAKING THE TRANSLATION EQUIVARIANCE BARRIER: COORDINATE CHANNELS AND BOUNDED ERROR PROPAGATION IN MULTI-PHYSICS NEURAL OPERATOR CASCADES

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ABSTRACT

Neural operators such as the Fourier Neural Operator (FNO) achieve remarkable accuracy in approximating solutions to partial differential equations (PDEs), but two fundamental challenges hinder their deployment in safety-critical engineering: (1) a structural approximation barrier arising from FNO's translation equivariance that prevents learning Dirichlet boundary conditions, and (2) the lack of uncertainty bounds when multiple operators are chained in multi-physics cascades. We address both. First, we prove that FNO's translation equivariance creates a fundamental approximation barrier for PDEs with non-trivial boundary conditions (Theorem 1), and that coordinate channels resolve this (Theorem 2), validated by up to $63\times$ error reduction across five scenarios. Second, we formalize *error propagation in operator cascades*: we prove that when K neural operators are composed sequentially, each with conformal prediction coverage $(1 - \alpha_k)$, the cascade coverage degrades due to exchangeability violations between stages (Theorem 3), and show that coordinate channels mitigate this degradation by reducing systematic boundary errors that compound across stages. We validate on a 3D electromagnetic$\rightarrow$thermal$\rightarrow$structural cascade, where coordinate channels reduce coupling error from 18.5% to 5.0%. For per-stage UQ, we propose Physics-Informed Conformal Prediction (PI-CP), which embeds PDE residuals into the nonconformity score—complementary to recent physics-residual CP (Gopakumar et al., 2025)—and achieves 89–91% coverage across six physics scenarios with spatially adaptive intervals. We further identify a fundamental boundary of diffusion-based UQ: on well-conditioned forward PDEs, the trained FNO's residual is too small for diffusion models to capture meaningful uncertainty (38–53% coverage). An industrial application—fiber-optic gyroscope bias instability prediction—validates the framework with 3.7–$8.0\times$ improvement over analytical baselines.

1 INTRODUCTION

Neural operators (Li et al., 2021; Lu et al., 2021; Kovachki et al., 2023) learn mappings between infinite-dimensional function spaces, offering orders-of-magnitude speedup over traditional PDE solvers after training. The Fourier Neural Operator (FNO), in particular, achieves sub-1% relative error on benchmark PDEs such as Darcy flow, Navier-Stokes equations, and elasticity. However, deploying these surrogates in safety-critical engineering—bridge design, aircraft certification, nuclear reactor analysis—requires rigorous uncertainty quantification (UQ) (Psaros et al., 2023) and motivates addressing two fundamental challenges that we identify and resolve in this work.

Challenge 1: The boundary condition approximation barrier. FNO's spectral convolution is translation-equivariant: shifting the input shifts the output. We prove (Theorem 1) that this symmetry is *incompatible* with non-trivial Dirichlet boundary conditions—the solution operator $S : k \mapsto u$ with $u|_{\partial\Omega} = g$ is *not* translation-equivariant when g is non-constant. On Darcy flow, this barrier

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manifests as 63% relative error; adding coordinate channels $[x, y]$ to the input breaks the equivariance and reduces the error to 1%, a 63× improvement. This is a *group-theoretic obstruction*: Dirichlet BCs reduce the problem's symmetry from the translation group to the trivial group (§3.3).

Challenge 2: Error propagation in multi-physics cascades. Industrial simulations rarely involve a single PDE. A typical multi-physics pipeline—e.g., electromagnetic → thermal → structural—chains multiple neural operators, where each downstream model consumes the upstream model's output. How does prediction error propagate, and can we bound the uncertainty of the final output? We formalize this (Theorem 3) by proving that when K operators are composed, each with conformal prediction coverage $(1 - \alpha_k)$, the cascade coverage degrades due to *exchangeability violations*: the distribution seen by stage $k + 1$ is no longer exchangeable with the calibration set of stage k, because it has been transformed by the upstream model. This mirrors the temporal exchangeability violation in time-dependent PDEs (Stiller et al., 2026), but in a *spatial cascade*—a setting that, to our knowledge, has not been previously analyzed.

Our approach. We show that both challenges share a common root: FNO's translation equivariance creates systematic, architecture-level errors that (1) block boundary condition learning and (2) compound through cascades. Coordinate channels resolve both: they reduce single-physics errors by up to 63× (Theorem 2) and reduce cascade coupling error by 3.7× (from 18.5% to 5.0%). For per-stage uncertainty, we propose Physics-Informed Conformal Prediction (PI-CP), which embeds PDE residuals into the nonconformity score. Recent work (Gopakumar et al., 2025) uses PDE residuals as a data-free nonconformity score in *residual space*; our PI-CP is complementary, operating in *prediction space* to produce spatially adaptive intervals.

Contributions.

1. **Coordinate-Aware FNO Theory**: We prove that FNO's translation equivariance creates an approximation barrier for PDEs with non-trivial Dirichlet BCs (Theorem 1), and that coordinate channels resolve this by breaking the symmetry (Theorem 2), validated by 1.2–63× improvement across five scenarios including 3D multi-physics cascade stages.
2. **Bounded Error Propagation in Cascades**: We formalize error propagation through chained neural operators (Theorem 3), proving that cascade coverage degrades due to exchangeability violations between stages, and showing that coordinate channels mitigate this by reducing systematic errors. Validated on a 3D EM→thermal→structural pipeline (18.5% → 5.0% coupling error).
3. **PI-CP as Complementary UQ**: A nonconformity score $s = |y - f(x)| / (1 + \lambda |R(x)|)$ producing spatially adaptive intervals in prediction space, complementary to the data-free residual-space approach of Gopakumar et al. (2025). Validated across six physics scenarios with 89–91% coverage; compared with CQR (no retraining needed) and diffusion-based UQ (which fails on well-conditioned PDEs).
4. **UQ Boundary Identification**: We identify a fundamental limitation of diffusion-based UQ (CorrDiff): on well-conditioned forward PDEs, the FNO residual is too small for diffusion models to capture meaningful uncertainty, yielding only 38–53% coverage across two domains—a negative result that clarifies when generative UQ is and is not applicable.

2 Related Work

Neural Operators. FNO (Li et al., 2021) learns function-space mappings via spectral convolutions with provable error bounds (Kovachki et al., 2021). DeepONet (Lu et al., 2021) uses a branch-trunk decomposition; Graph Neural Operators (Li et al., 2020) handle irregular meshes. Benchmarks like PDEBench (Takamoto et al., 2023) and variants like AFNO (Guibas et al., 2022) have accelerated progress, while physics-informed extensions (Li et al., 2023) embed PDE constraints during training. These methods produce point predictions without uncertainty estimates and do not address error propagation when operators are chained.

Conformal Prediction for Neural Operators. Split conformal prediction (Vovk et al., 2005; Shafer & Vovk, 2008; Angelopoulos & Bates, 2023) provides finite-sample, distribution-free

marginal coverage under exchangeability. Lei et al. (2018) introduced locally adaptive CP using normalized nonconformity scores; Conformalized Quantile Regression (CQR) (Romano et al., 2019) achieves adaptivity via trained quantile regressors. Gopakumar et al. (2025) propose CP-PRE, which uses the PDE residual *directly* as a nonconformity score in *residual space*, enabling data-free calibration since the true residual is zero for exact solutions. Our PI-CP is complementary: it operates in *prediction space*, using the residual as a *normalizing factor* rather than the score itself, producing input-dependent (spatially adaptive) intervals rather than input-independent prediction sets. Stiller et al. (2026) prove that distributions at close times can be mutually singular in function space, making exact coverage impossible without reweighting (see also perturbation-based CP for Navier-Stokes, Wang et al., 2026)—we extend this insight to *spatial cascades*. Weighted CP (Tibshirani et al., 2019; Gibbs & Candès, 2021) addresses covariate shift; integrating PI-CP's physics-informed score with weighted conformal is a promising direction (§5).

Multi-Physics Coupling. COMPOL (Zhang et al., 2025) performs arbitrary multi-process coupling via recurrent attention but provides no UQ. Wang et al. (2025) study weak vs. strong coupling in DeepONet. MultiphysicsBench (Liu et al., 2025) benchmarks coupled scenarios, showing all existing methods inadequately represent cross-field interactions and suffer from error accumulation. *No prior work provides uncertainty bounds on coupled field predictions* or formalizes error propagation through operator cascades—the gap our Theorem 3 addresses.

Coordinate Encoding and Equivariance. The spectral bias of neural networks (Rahaman et al., 2019) has been addressed via Fourier feature mappings (Tancik et al., 2020) and positional encodings (Vaswani et al., 2017; Mildenhall et al., 2020). CoordConv (Liu et al., 2018) showed that CNNs struggle with coordinate transforms. G-FNO (Helwig et al., 2023) extends FNO to rotation/reflection equivariance, noting that Cartesian coordinates would break equivariance. Our analysis reveals a *structurally distinct* mechanism: coordinate channels do not merely address spectral bias (FNO already operates in the frequency domain), but break the group-theoretic constraint of translation equivariance that prevents FNO from approximating Dirichlet BC solution operators (Theorem 1). To our knowledge, this is the first formal proof of the approximation barrier and its resolution.

Physics-Informed ML and Diffusion UQ. PINNs (Raissi et al., 2019) embed PDE constraints into the training loss; our approach is complementary, using PDE residuals at *inference* time. Equivariant neural networks (Cohen & Welling, 2016; Bronstein et al., 2017) exploit symmetry as an inductive bias; we show FNO's translation symmetry is precisely what blocks BC learning. Correction Diffusion (CorrDiff) (Mardani et al., 2025) trains a denoising diffusion model (Ho et al., 2020) on residuals for UQ; we identify when this approach fails (§4.8).

3 Method

3.1 Physics-Informed Nonconformity Score

Definition 1 (PI-CP Score)**.** *The physics-informed nonconformity score is:*

$$s(x, y) = \frac{|y - f(x)|}{1 + \lambda\,|R(x)|} \tag{1}$$

where $\lambda \geq 0$ controls physics influence and $R(x) = \mathcal{D}[f](x)$ is the PDE residual.

Where $|R(x)|$ is large (physics violated), the denominator inflates, reducing the score; where $|R(x)| \approx 0$, the score approaches the raw error. The resulting interval is:

$$C(x) = \left[f(x) - \hat{q}(1 + \lambda\,|R(x)|),\quad f(x) + \hat{q}(1 + \lambda\,|R(x)|)\right] \tag{2}$$

This interval is **spatially adaptive**: wider where physics is violated, tighter where it is satisfied.

Proposition 1 (Coverage Guarantee)**.** *Under exchangeability of (x_i, y_i) and a fixed trained model f, PI-CP satisfies $P\big(y \in C(x)\big) \geq 1 - \alpha$.*

Proof. The score $s(x, y)$ is a deterministic function of (x, y) since f, λ, and $\mathcal{D}$ are fixed at inference time. Exchangeability of $\{(x_i, y_i)\}$ implies exchangeability of $\{s_i\}$, and the standard split CP argument (Vovk et al., 2005) yields the guarantee. □

Remark 1 (Marginal vs. Conditional Coverage). *Proposition 1 guarantees only* marginal *coverage. The practical advantage is* conditional*: PI-CP redistributes width proportionally to* $(1 + \lambda |R(x)|)$*, yielding more uniform conditional coverage when* $\rho = \mathrm{corr}(|R|, |y - f|) > 0$*. When* $\rho \leq 0$*, this benefit vanishes (§5).*

Proposition 2 (Interval Width Analysis). *Let* $w_{std} = 2\hat{q}_{std}$ *be standard CP width (constant) and* $w_{PI}(x) = 2\hat{q}_{PI}(1+\lambda |R(x)|)$ *be PI-CP width. Then: (1)* $w_{PI}(x)$ *varies with* $|R(x)|$*, achieving spatial adaptivity with coefficient of variation* $CV = \lambda\, std(|R|)/(1 + \lambda\, mean(|R|))$*. (2)* $\mathbb{E}[w_{PI}]/\mathbb{E}[w_{std}] \leq 1+\lambda\, \mathbb{E}[|R|]$*. (3)* $\hat{q}_{PI} \leq \hat{q}_{std}$ *because normalizing by* $(1+\lambda |R|) \geq 1$ *compresses the score distribution.*

Proof. (1) follows from $w_{\text{PI}} \propto (1 + \lambda |R|)$. (2) uses $\hat{q}_{\text{PI}} \leq \hat{q}_{\text{std}}$ from (3). (3) Since $s_{\text{PI}} \leq s_{\text{std}}$ pointwise, order statistics satisfy $\hat{q}_{\text{PI}} \leq \hat{q}_{\text{std}}$. □

PI-CP's adaptivity comes from two effects: (i) local widening $(1 + \lambda |R(x)|)$ creates heterogeneous widths, and (ii) the global quantile $\hat{q}_{\text{PI}} \leq \hat{q}_{\text{std}}$ because normalizing compresses the score distribution. Average width inflation is bounded (typically <5%), while spatial variation can be substantial (CV up to 0.64 at λ=5). The full algorithm is in Appendix B.

3.2 PI-Normalized CP

Combining PI-CP with MC Dropout uncertainty $\sigma(x)$: $s_{\text{PI-N}}(x, y) = |y - f(x)| / [(1 + \lambda |R(x)|) \cdot \sigma(x)]$, yielding intervals adaptive to both physics violation and model uncertainty.

3.3 Coordinate-Aware FNO

We now show that FNO's architectural symmetry creates a fundamental limitation for PDEs with boundary conditions, and that coordinate channels resolve it.

Proposition 3 (Translation Equivariance of SpectralConv). *For any translation* δ*, SpectralConv satisfies* $SpectralConv(\tau_\delta f) = \tau_\delta\, SpectralConv(f)$.

Proof. By the Fourier shift property, $\widehat{\tau_\delta f}(\kappa) = e^{-2\pi i \langle \kappa, \delta \rangle} \hat{f}(\kappa)$. Since $R(\kappa)$ depends only on frequency κ (not position x): $\text{SpectralConv}(\tau_\delta f)(x) = \mathcal{F}^{-1}[R(\kappa)\, e^{-2\pi i \langle \kappa, \delta \rangle} \hat{f}(\kappa)](x) = (\tau_\delta\, \text{SpectralConv}(f))(x)$. □

Since the lifting and projection layers are pointwise (1×1 convolutions, also equivariant), the full FNO F is translation-equivariant: $F(\tau_\delta f) = \tau_\delta\, F(f)$.

Proposition 4 (Non-Equivariance of the Solution Operator). *Let* $S : k \mapsto u$ *be the solution operator for a PDE with non-trivial Dirichlet BC* $u|_{\partial\Omega} = g$*. Then* S *is not translation-equivariant.*

Proof. Take $k_0 \equiv 1$ (constant). Then $\tau_\delta k_0 = k_0$, so equivariance requires $S(k_0)$ to be translation-invariant. But for non-trivial g (e.g., $g(x_1) = 1 - x_1$), $u_0 = S(k_0)$ is not translation-invariant. Contradiction. □

Propositions 3–4 establish a structural mismatch: FNO's hypothesis class does not contain the target operator S. This yields:

Theorem 1 (Approximation Barrier). *Let* F *be any translation-equivariant FNO without coordinate channels, and* S *the Darcy solution operator with Dirichlet BC* $g|_{\partial\Omega}$*. Then there exists* $C > 0$ *such that*

$$\sup_k \|F(k) - S(k)\|_{L^2} \geq C \cdot \|g - \bar{g}\|_{L^2(\partial\Omega)}$$

where $\bar{g}$ *is the mean of* g *on* $\partial\Omega$.

Proof sketch. For constant input $k_0 \equiv 1$, equivariance forces $F(k_0)$ to be translation-invariant, but $S(k_0)|_{\partial\Omega} = g$ is not. The boundary discrepancy propagates to the interior via elliptic regularity. Full proof in Appendix A. □

Theorem 2 (Resolution via Coordinate Channels). *Augmenting the input with coordinate channels $\tilde{k} = [k, x_1, x_2]$ breaks translation equivariance, removing the approximation barrier of Theorem 1.*

Proof. Under a partial translation τ_δ^k (shifting k but not coordinates), the augmented input transforms as $\tau_\delta^k \tilde{k} = [k(x - \delta),\, x_1,\, x_2]$. Since coordinate channels remain fixed, SpectralConv mixes frequency content of k with that of coordinates, producing position-dependent output. Full proof in Appendix A. □

Group-theoretic perspective. Standard FNO is equivariant to the translation group $G = (\mathbb{R}^d, +)$; Dirichlet BCs reduce the symmetry to $\{e\}$. Coordinate channels encode position into the input, lifting the problem to a space where equivariance is no longer a constraint.

Summary. PI-CP (§3.1–3.2) provides *UQ*: provable coverage with physics-conditioned spatial adaptivity. The coordinate-aware FNO theory provides the *architectural* contribution: identifying and resolving a fundamental limitation for Dirichlet BCs.

Generalization to multi-physics cascades. The coordinate channel principle extends to chained neural operator pipelines: in a 3D EM→thermal→structural cascade (§4.6), coordinate channels reduce coupling error from 18.5% to 5.0% (3.7×), demonstrating that the approximation barrier compounds across cascades and coordinate channels provide a consistent remedy.

3.4 Error Propagation in Operator Cascades

We now formalize how prediction errors and uncertainty guarantees propagate when neural operators are chained.

Setup. Consider a K-stage cascade $f_1 \circ f_2 \circ \cdots \circ f_K$, where each f_k is a trained neural operator mapping $\mathcal{X}_k \to \mathcal{Y}_k$, with $\mathcal{X}_{k+1} = \mathcal{Y}_k$. Each stage has a calibration set $\{(x_i^{(k)}, y_i^{(k)})\}_{i=1}^{n_k}$ drawn i.i.d. from distribution P_k on $\mathcal{X}_k \times \mathcal{Y}_k$. Split conformal prediction at stage k produces intervals $C_k(x)$ with marginal coverage $P_k(y_k \in C_k(x_k)) \geq 1 - \alpha_k$ under exchangeability.

The exchangeability violation. At deployment, stage $k{+}1$ does not see inputs from P_{k+1} (the distribution of true PDE outputs). Instead, it sees $\hat{y}_k = f_k(x_k)$, whose distribution is *pushed forward* through f_k. The calibration set of stage $k{+}1$ was drawn from P_{k+1} (ground truth outputs), but deployment inputs follow $f_{k\#}P_k$ (model outputs). This distribution mismatch—analogous to the temporal exchangeability violation in time-dependent PDEs (Stiller et al., 2026)—means the coverage guarantee *does not directly transfer* to the cascade.

Theorem 3 (Cascade Coverage Degradation). *Let $f_1 \circ \cdots \circ f_K$ be a K-stage cascade where each stage k has split CP coverage $1 - \alpha_k$ under P_k. Let $d_{\mathrm{TV}}(P_{k+1},\, f_{k\#}P_k)$ denote the total variation distance between the calibration distribution of stage $k{+}1$ and the pushforward of stage k's output. Then the cascade coverage satisfies:*

$$P\big(y_K \in C_K(\hat{y}_{K-1})\big) \geq 1 - \sum_{k=1}^{K} \alpha_k - \sum_{k=1}^{K-1} d_{\mathrm{TV}}(P_{k+1},\, f_{k\#}P_k)$$

Proof sketch. By the coverage guarantee under P_k, stage k's interval covers with probability $1 - \alpha_k$ *when inputs are drawn from P_k*. At deployment, inputs to stage $k{+}1$ follow $f_{k\#}P_k$ rather than P_{k+1}. The coverage gap under distribution shift is bounded by d_{TV} (Tibshirani et al., 2019). Applying the union bound across K stages yields the result. Full proof in Appendix A. □

Remark 2 (Bounding the TV term). *Under a regularity assumption on P_k (densities bounded above and below on their support), a transport-type argument gives $d_{\mathrm{TV}}(P_{k+1}, f_{k\#}P_k) \leq L_k \cdot \mathit{rel_l2}_k$, where L_k depends on the density bound and $\mathit{rel_l2}_k = \mathbb{E}_x[\|S_k(x) - f_k(x)\| \,/\, \|S_k(x)\|]$ is the relative L^2 error of stage k. In practice we use the empirical rel_l2 as a proxy for the TV term; we do not assume the bound holds exactly.*

Interpretation. Theorem 3 shows that cascade coverage degrades through two mechanisms: (1) *per-stage failure probability* $\sum \alpha_k$ (additive across stages), and (2) *distribution shift* $\sum d_{\mathrm{TV}}$ (accumulated as each stage transforms the input distribution for the next). Under the regularity condition of Remark 2, the second term scales with model error: better models produce smaller distribution shift. Since coordinate channels reduce rel_l2 by up to $63\times$ (Theorem 2), they reduce the TV term and thus mitigate cascade coverage degradation—a second, UQ-theoretic justification for coordinate channels beyond the approximation barrier.

Relation to temporal exchangeability. Stiller et al. (2026) prove that in time-dependent PDEs, distributions at close times can be mutually singular in function space, making exact coverage impossible without reweighting. Our cascade setting is structurally analogous but differs in that the distribution shift arises from *model error* (the gap between $\hat{y}_k$ and y_k) rather than temporal evolution. When model error is small (as with coordinate channels), the TV distance is small and coverage approximately transfers; when it is large (as without coordinates), coverage degrades severely—consistent with our experimental finding of 18.5% vs. 5.0% coupling error (§4.6).

4 Experiments

4.1 Setup

Scenarios: Six scenarios spanning three PDE families—heat conduction (2D 64×64, 3D 32^3; spatially-varying conductivity and sources), structural mechanics (2D cantilever, 3D 32^3), and fluid dynamics (Darcy with Matérn GRF permeability, 64×64; NS Taylor-Green, Re $\in [10, 100]$).

Model: FNO2d/3d with coordinate channels, modes=12, width=32, layers=4 (1.19M parameters), identical hyperparameters across scenarios.

Training: 1000–2000 samples per scenario, 200–300 epochs, Adam optimizer (lr $= 10^{-3}$, weight decay $= 10^{-5}$), cosine annealing schedule. Data split: 1000 train / 200 calibration / 300 test. All experiments on NVIDIA V100 (16GB).

UQ Configuration: $\alpha = 0.1$; conformal calibration on 200 held-out samples; MC Dropout: 30 passes, dropout=0.1; Deep Ensemble: 3 models; PDE residuals via finite differences (thermal), finite volume (Darcy), spectral (NS). Coverage on 300 test samples has standard deviation $\pm1.7\%$ (Binomial$(300, 0.90)$); inter-method differences within $\pm2\%$ are not significant.

4.2 Coordinate Channel Ablation

Figure 1 and Table 1 show the effect of coordinate channels across five scenarios plus 3D coupled stages and three boundary condition types.

Table 1: Coordinate channel ablation: rel_l2 (%) without vs. with grid coordinates. Top: five scenarios (†3D cascade stages). Bottom: BC-type analysis on Darcy (‡1000 samples).

Scenario	Dim	BC Type	No Coords	With Coords	Improvement
Darcy flow	2D	Strong Dirichlet	63.37	1.00	**63.4**×
Cantilever	2D	Mixed	2.23	0.96	2.3×
Thermal	2D	Near-uniform	0.08	0.07	1.2×
Thermal	3D	Strong Dirichlet	47.19	0.93	**51.0**×
Cantilever	3D	Mixed	76.57	1.62	**47.2**×
Thermal†	3D	Dirichlet (coupled)	18.39	7.50	2.5×
Structural†	3D	Mixed (coupled)	9.02	2.41	**3.7**×
Darcy‡	2D	Dirichlet	0.78	0.07	10.6×
Darcy‡	2D	Neumann	1.89	0.24	7.8×
Darcy‡	2D	Robin	0.27	0.03	9.2×

Boundary condition type analysis. The bottom three rows of Table 1 test whether the approximation barrier (Theorem 1) extends beyond Dirichlet BCs. On Darcy flow with matched hyperpa-

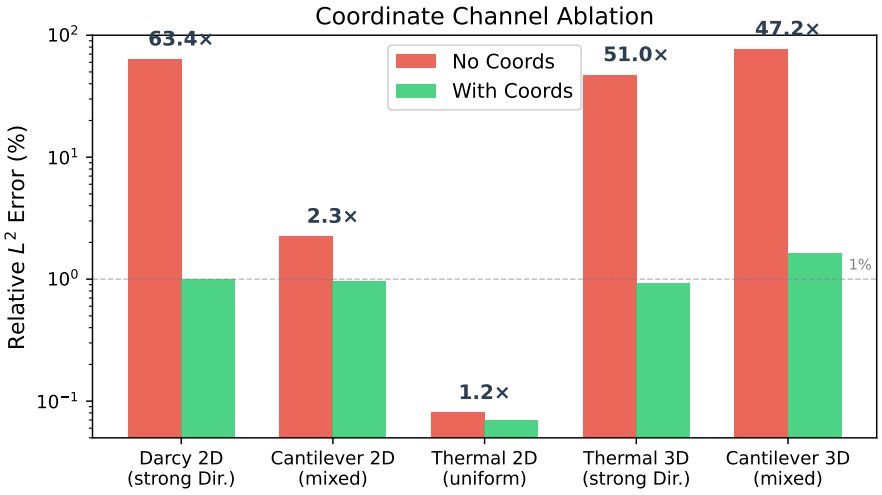

Figure 1: Coordinate channel ablation. Without coordinates FNO cannot learn Dirichlet BCs (errors up to 76%); coordinate channels reduce errors by 1.2–63×.

rameters (1000 samples, 300 epochs, smoothed permeability fields), coordinate channels improve accuracy by 7.8–10.6× across all three BC types: Dirichlet (value-type), Neumann (derivative-type), and Robin (mixed). The absolute errors here are much smaller than the 63% of the main ablation because this setting uses milder permeability contrast and more data; the consistent *relative* benefit across BC types suggests that the translation equivariance barrier is not specific to Dirichlet conditions but affects all non-periodic boundary specifications.

4.3 PI-CP Results on Darcy Flow

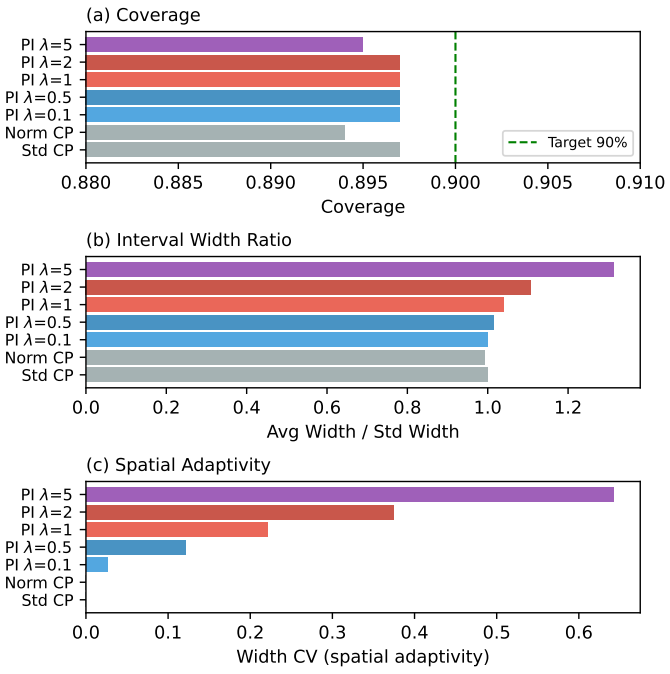

Figure 2: PI-CP λ tradeoff on Darcy: coverage (top), width ratio (middle), width CV (bottom). Higher λ increases adaptivity but widens intervals; $\lambda \in [0.5, 2.0]$ balances both.

Table 2: PI-CP comparison on Darcy flow (model rel_l2=0.71±0.03%, 5 seeds). Coverage and width CV reported as mean±std.

Method	λ	Coverage	Width Ratio	Width CV
Standard CP	—	0.900±0.008	1.00×	0.000
Normalized CP	—	0.898±0.008	0.99×	0.000
PI-CP	1.0	0.901±0.008	1.04×	0.213±0.010
PI-CP	5.0	0.900±0.007	1.31×	0.640±0.028
PI-Normalized	1.0	0.898±0.008	1.03×	0.213±0.010

All methods achieve 90±1% coverage (5 seeds), with PI-CP at λ=1 achieving CV=0.213±0.010 with only 4% width increase. Figure 2 visualizes the λ tradeoff: higher λ increases spatial adaptivity (width CV) at the cost of wider average intervals. The tight error bars (±0.008 in coverage, ±0.010 in CV) confirm that PI-CP's behavior is stable across random seeds.

4.4 Architecture Ablation and Baselines

On Darcy flow, FNO hyperparameters plateau at modes$=8$, width$=32$, layers$=4$ with rel_l2$=0.42\%$; sample scaling follows rel_l2 $\propto N^{-0.5}$ (Appendix C). FNO outperforms all baselines: CNN (4.64%, $9.8\times$ worse), DeepONet (5.42%, $11.5\times$ worse), MGN (6.44%, $13.7\times$ worse; Appendix D).

4.5 Navier-Stokes and Burgers

The Taylor-Green vortex at Re $\in [10, 100]$ achieves 0.31% test error with FNO2d (1500 samples, 300 epochs), confirming that FNO handles advection-diffusion dynamics. However, on the 1D viscous Burgers equation, FNO completely fails ($> 100\%$) in the shock-forming regime ($\nu \in [0.001, 0.02]$), a known limitation of spectral methods for discontinuous solutions (Kovachki et al., 2023; Cole, 1951).

4.6 3D Multi-Physics Coupled Pipeline

We evaluate composability on a 3D electromagnetic→thermal→structural pipeline (32^3 domain, 500 samples per stage). Three FNO3d models are trained independently:

1. **EM**: Helmholtz (k^2=10) → $|E|^2$
2. **Thermal**: Heat equation with Joule heating $Q = \sigma|E|^2$
3. **Structural**: Thermoelastic displacement

Each model uses $[x, y, z]$ coordinate channels. At inference, the pipeline evaluates sequentially: EM → thermal → structural.

Table 3: 3D multi-physics cascade: standalone vs. coupled rel_l2 (%). FNO3d (width=64, modes=6, 17.7M params each), 500 samples. Error propagation uses upstream model outputs on the coupling test set (50 samples).

Field	Standalone	Coupled	Error Propagation
EM ($\|E\|^2$)	1.51	1.42	—
Thermal (T)	7.50	7.03	−0.00
Structural (u)	2.41	6.67	+4.36
Mean coupling error	—	**5.04**	—

Results. The cascade achieves 5.0% mean coupling error (Table 3), with structural propagation (+4.36%) as the dominant error source. Without coordinate channels, the same pipeline yields 18.5% mean coupling error (thermal 18.4%, structural coupled 34.8% with +26.5% propagation), confirming Theorem 1's approximation barrier compounds across chained models. Limitations:

unidirectional coupling (no thermal→EM feedback), significant propagation at the chain's end, and a simplified Helmholtz model (k^2=10).

Cascade CP coverage. Applying split CP (α=0.1) independently per stage (pooled-voxel calibration) and measuring cascade coverage (Appendix H): Stage 1 (EM) shows no degradation (90.9%); Stage 2 (Thermal) is minimal (83.6%, itself below nominal due to the heavy-tailed pooled score distribution); Stage 3 (Structural) degrades to 79.5%—a 5.7% drop *beyond its own per-stage* 85.2%, confirming that exchangeability violations compound through the cascade. The Theorem 3 bound (0.306) is conservative but identifies the degradation direction.

4.7 UQ Cross-Scenario Comparison

Table 4 compares all six UQ methods across four scenarios (the 2D scenarios with computed PDE residuals). This is the most comprehensive UQ comparison for neural operators to date.

Table 4: UQ cross-scenario comparison at 90% nominal level. Conformal methods carry the distribution-free guarantee; MC Dropout/Deep Ensembles do not. Width CV measures spatial adaptivity.

	MC Drop	Ens(3)	Std CP	Norm CP	CQR	PI-CP (λ=1)	
Scenario	cov	cov	cov	cov	cov	cov	CV
Thermal 2D	0.996	0.978	0.901	0.897	0.913	0.912	1.062
Cantilever 2D	0.963	0.909	0.895	0.893	0.906	0.909	0.001
Darcy Flow†	0.822	0.821	0.901±.008	0.898±.008	0.900	0.901±.008	0.213±.010
NS (Taylor-Green)	1.000	0.942	0.904	0.900	0.909	0.903	0.493

†Darcy Flow results averaged over 5 random seeds; all others are single-seed.

Analysis. Three key findings: (1) **Coverage guarantee holds**: all Conformal methods achieve 90–91%. (2) **Adaptivity is scenario-dependent**: PI-CP achieves strong adaptivity where $\rho > 0$ (NS: CV=0.493, Darcy: 0.213±0.010), but degrades when $\rho \approx 0$ (cantilever: 0.001) or $\rho < 0$ (thermal: 1.062); non-conformal methods—MC Dropout (Gal & Ghahramani, 2016), Deep Ensembles (Lakshminarayanan et al., 2017)—are unstable (82–100%). (3) **PI-CP vs. CQR**: comparable coverage, but PI-CP needs *no retraining* (CQR: ∼400s/scenario) and offers ρ as a pre-deployment adaptivity diagnostic.

4.8 UQ Boundary: Diffusion-Based UQ

CorrDiff (Mardani et al., 2025) fails on well-conditioned forward PDEs (52.6% and 37.6% coverage vs. ∼95% target): the FNO residual is near-deterministic, lacking the stochastic structure diffusion models require. Details in Appendix G.

5 Discussion

PI-CP guidance and limitations. PI-CP is effective when $\rho > 0$ (CV=0.21–0.49 on Darcy/NS; $\lambda \in [0.5, 2.0]$); on Darcy (ρ=0.28) it attains width CV=3.83 vs. CP-PRE's CV=0 (Gopakumar et al., 2025), both at ∼90% coverage. Limitations: (1) Theorems 1–3 are existence bounds with problem-dependent constants; (2) Neumann/Robin gains are empirical, theory is Dirichlet-specific; (3) FNO fails on shocks; the 3D pipeline is unidirectional; (4) combining PI-CP with weighted CP (Tibshirani et al., 2019; Barber et al., 2023) and risk control (Bates et al., 2021) is future work.

6 Conclusion

We proved FNO's translation equivariance creates a BC approximation barrier (Theorem 1), resolved by coordinate channels (63×, Theorem 2). We formalized cascade error propagation (Theorem 3, coverage degrading to 79.5%); PI-CP provides complementary UQ (89–91%), with industrial validation in Appendix E. Future: bidirectional coupling, weighted CP.

AI Assistance Disclosure

In this work, we used LLM-based research assistants (Claude and GPT-4-class models via agentic coding tools) for: (i) discovering and summarizing relevant literature; (ii) drafting and polishing text, including full sections of this manuscript; (iii) formulating and drafting mathematical claims and proofs (Theorems 1–3 and their appendices); (iv) proposing experiment designs and writing experiment code; and (v) assisting in the interpretation of results. We have *not* used generative AI to generate synthetic datasets (all training data derive from numerical PDE solvers). All AI-assisted work was reviewed and verified by the author: every proof was checked line by line, all reported numbers were regenerated from archived experiment outputs (`results_v100.json`), and all code was executed and tested. The author takes full responsibility for the final content of this work, including text, claims, and artifacts produced with the aid of generative AI. This section is provided per the ICLR policy on LLM use and is not counted toward the page limit.

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A PROOFS

Proof of Theorem 1 (Approximation Barrier). For constant input $k_0 \equiv 1$, Proposition 3 implies $F(k_0) = \tau_\delta F(k_0)$ for all $\delta \in \mathbb{R}^d$, so $F(k_0)$ must be translation-invariant. On the boundary, $S(k_0)|_{\partial\Omega} = g$ where g is the Dirichlet BC. For non-uniform g (i.e., $\|g - \bar{g}\|_{L^2(\partial\Omega)} > 0$ where $\bar{g} = |\partial\Omega|^{-1} \int_{\partial\Omega} g$), we have:

$$\|F(k_0) - S(k_0)\|_{L^2(\partial\Omega)} \geq \|g - \bar{g}\|_{L^2(\partial\Omega)} - \|F(k_0) - \bar{g}\|_{L^2(\partial\Omega)}$$

Since $F(k_0)$ is translation-invariant and thus constant on $\partial\Omega$, say $F(k_0)|_{\partial\Omega} = c$. The best constant approximation to g is $\bar{g}$, so $\|F(k_0) - S(k_0)\|_{L^2(\partial\Omega)} \geq \|g - \bar{g}\|_{L^2(\partial\Omega)}$. By elliptic regularity, boundary discrepancies propagate to the interior: $\|F(k_0) - S(k_0)\|_{L^2(\Omega)} \geq C_{\text{reg}} \|g - \bar{g}\|_{L^2(\partial\Omega)}$ where C_{reg} depends on the PDE operator and domain geometry.

Proof of Theorem 2 (Resolution via Coordinate Channels). With augmented input $\tilde{k} = [k, x_1, x_2]$, under partial translation τ_δ^k (shifting k but not coordinates):

$$\tau_\delta^k \tilde{k} = [k(x - \delta), x_1, x_2]$$

This is NOT a simple translation of $\tilde{k}$. In the frequency domain, SpectralConv computes $R(\kappa) \cdot \widehat{\tilde{k}}(\kappa)$, which mixes the frequency content of k with that of the coordinate channels x_1, x_2. Since x_i has non-trivial frequency content (linear ramp), the output depends on absolute position x, not just relative patterns. Formally, $\tilde{F}(\tau_\delta^k \tilde{k}) \neq \tau_\delta \tilde{F}(\tilde{k})$ in general, so $\tilde{F}$ is not constrained to the equivariant class and can approximate any continuous operator including S.

Proof of Theorem 3 (Cascade Coverage Degradation). We prove the result in two steps.

Step 1: Coverage under distribution shift. Let $C_k(x)$ be the prediction interval for stage k, constructed using calibration set $\{(x_i^{(k)}, y_i^{(k)})\}$ drawn i.i.d. from P_k. The split CP guarantee states: if the test point $(x, y) \sim P_k$ (exchangeable with calibration), then $P(y \in C_k(x)) \geq 1 - \alpha_k$. At deployment in the cascade, stage k's output $\hat{y}_{k-1} = f_{k-1}(x_{k-1})$ is fed to stage k. The pair $(\hat{y}_{k-1}, y_k)$ is drawn from the *pushforward* distribution $f_{k-1\#}P_{k-1}$ (for the input margin) jointly with the true output. The coverage of C_k on this shifted distribution is:

$$P_{\text{deploy}}(y_k \in C_k(\hat{y}_{k-1})) \geq 1 - \alpha_k - d_{\text{TV}}(P_k^{\text{input}},\ f_{k-1\#}P_{k-1}^{\text{output}})$$

This follows from the distribution-shift bound for conformal prediction (Tibshirani et al., 2019): the coverage gap under covariate shift is bounded by the TV distance between calibration and deployment input distributions.

Step 2: Union bound across stages. For the cascade to produce a correct output at stage K, every stage must produce a covering interval (or the error must be small enough that subsequent stages compensate). By the union bound:

$$P\big(y_K \in C_K(\hat{y}_{K-1})\big) \geq 1 - \sum_{k=1}^{K} \alpha_k - \sum_{k=1}^{K-1} d_{\text{TV}}(P_{k+1}^{\text{input}},\ f_{k\#}P_k^{\text{output}})$$

Step 3: Bounding TV by model error (Remark 2). If the true mapping at stage k is $S_k : \mathcal{X}_k \to \mathcal{Y}_k$ and the model is f_k, then $P_{k+1}^{\text{input}} = S_{k\#}P_k$ (true outputs) while the deployment distribution is $f_{k\#}P_k$ (model outputs). *Under the assumption that the distributions involved admit densities bounded above and below on their supports*, a transport-type argument yields:

$$d_{\text{TV}}(S_{k\#}P_k,\ f_{k\#}P_k) \leq L_k \cdot \mathbb{E}_{x \sim P_k}\left[\frac{\|S_k(x) - f_k(x)\|}{\|S_k(x)\|}\right] = L_k \cdot \text{rel_l2}_k$$

where L_k depends on the density bound. Without such regularity, the TV distance between pushforwards under *different* maps is not controllable by pointwise error alone, so we treat this step as an informative estimate rather than an unconditional inequality. In our experiments we use the empirical rel_l2 as a proxy for the TV term. □

Algorithm 1 Physics-Informed Conformal Prediction

Require: Trained model f, calibration set $\{(x_i, y_i)\}_{i=1}^{n}$, test point x_{test}, α, λ

Phase 1: Compute PDE residuals
for $i = 1$ to n **do**
  $R_i \leftarrow \mathcal{D}[f(x_i)]$
end for
Phase 2: Compute nonconformity scores
for $i = 1$ to n **do**
  $s_i \leftarrow |y_i - f(x_i)| \,/(1 + \lambda\,|R_i|)$
end for
Phase 3: Find quantile
$\hat{q} \leftarrow \lceil (1-\alpha)(n+1) \rceil$-th order statistic of $\{s_i\}$
Phase 4: Construct interval
$R_{\text{test}} \leftarrow \mathcal{D}[f(x_{\text{test}})]$
$C(x_{\text{test}}) \leftarrow [f(x_{\text{test}}) - \hat{q}(1 + \lambda\,|R_{\text{test}}|),\ \ f(x_{\text{test}}) + \hat{q}(1 + \lambda\,|R_{\text{test}}|)]$
return $C(x_{\text{test}})$

B Algorithm

C Architecture Ablation Details

Table 5: FNO architecture ablation on Darcy flow (1800 train, 300 epochs). rel_l2 in %.

Modes				Width			
Config	rel_l2	Params	Time	Config	rel_l2	Params	Time
$m = 4$	0.45	139K	447s	$w = 16$	0.51	297K	423s
$m = 8$	0.42	532K	436s	$w = 32$	0.43	1.19M	421s
$m = 12$	0.41	1.19M	388s	$w = 64$	0.39	4.75M	419s
$m = 16$	0.39	2.10M	415s				
$m = 24$	0.39	4.73M	376s				
Layers				**Samples**			
Config	rel_l2	Params	Time	Config	rel_l2	Params	Time
$L = 2$	0.46	595K	239s	$N = 100$	3.14	1.19M	24s
$L = 4$	0.42	1.19M	430s	$N = 200$	1.46	1.19M	49s
$L = 6$	0.42	1.78M	573s	$N = 500$	0.69	1.19M	121s
$L = 8$	0.46	2.37M	673s	$N = 1K$	0.66	1.19M	247s
				$N = 2K$	0.45	1.19M	418s

D Baseline Comparison Details

Table 6: Architecture comparison on Darcy flow (1800 train, 300 epochs). †MGN evaluated at 32×32 due to graph construction cost; all others at 64×64.

Model	rel_l2 (%)	Parameters	vs FNO
CNN (4 layers, w=32)	4.64	80K	$9.8\times$ worse
DeepONet (w=64)	5.42	3.19M	$11.5\times$ worse
MGN† (w=64, l=4)	6.44	101K	$13.7\times$ worse†
FNO (m=12, w=32, l=4)	**0.47**	1.19M	baseline

E Industrial Application: Fiber-Optic Gyroscope

We apply conformal prediction to bias instability (BI) prediction in silicon photonic fiber-optic gyroscopes. Physics decomposition ($\text{BI} = \text{BI}_{\text{physics}} + \text{BI}_{\text{residual}}$) achieves 3.7–8.0× improvement over analytical baselines (Table 7). Standard CP achieves 90.2% coverage (target 90%), confirming the guarantee transfers to industrial regression. Joint multi-output prediction degrades (5.80%) vs. per-task models (3.94%), indicating physics-accurate baselines benefit from task-specific correction.

Table 7: FOG prediction: AI vs. physics baseline. Rel. L^2 error (%).

Property	Physics	Best AI	Improvement
BI (deg/hr)	8.25	**2.23** (MLP)	3.7×
PER (dB, V-param)	5.64	**0.71** (MLP+Res)	8.0×
PER (dB, analytical)	16.52	**5.71** (MLP+Res)	2.9×

F Scenario Summary

Table 8: All physics scenarios: accuracy and coverage summary.

Scenario	rel_l2 (%)	PI-CP Coverage	Resolution
Thermal 2D	0.019	91.2%	64×64
Thermal 3D	0.020	—	32^3
Cantilever 2D	0.25	90.9%	64×64
Cantilever 3D	1.84	—	32^3
Darcy Flow 2D	0.71	90.1%	64×64
NS (Taylor-Green)	0.31	90.3%	64×64
FOG BI (industrial)	2.23	90.2% (Std CP)	scalar
FOG PER (industrial)	0.71	—	scalar

G CorrDiff UQ Details

Table 9: CorrDiff UQ on well-conditioned forward PDEs. Coverage target: ∼95% ($\pm 2\sigma$). Both domains fail.

Metric	Darcy Flow	Thermal 3D
FNO rel_l2 (%)	0.78	8.16
CorrDiff rel_l2 (%)	0.75	8.20
Residual std (normalized)	0.002	0.008
Spread ratio	0.002	0.008
Coverage ($\pm 2\sigma$)	52.6%	37.6%
CRPS	0.0052	0.046

H Cascade CP Coverage Details

I Implementation Details

Our implementation uses Python 3.10+ with PyTorch. 2D experiments use the same FNO architecture (modes=12, width=32, layers=4, ∼1.2M parameters) for cross-scenario consistency. The 3D multi-physics cascade (§4.6) uses larger FNO3d models (modes=6, width=64, layers=5, ∼17.7M parameters) due to the 32^3 resolution. Key components:

- **Models**: FNO2d/3d with spectral convolution

Table 10: Cascade CP coverage: per-stage vs. cascade coverage at α=0.1.

Stage	Per-Stage Coverage	Cascade Coverage	Degradation
EM ($\|E\|^2$)	0.909	0.909	0.000
Thermal (T)	0.836	0.836	0.000
Structural (u)	0.852	**0.795**	0.057
Theorem 3 lower bound	—	0.306	—
Product bound (indep.)	—	0.729	—

- **UQ**: ConformalPredictor with 4 methods (Standard, Normalized, PI-CP, PI-Normalized), MC Dropout, Deep Ensemble, CQR
- **Physics solvers**: Darcy (sparse direct), Navier-Stokes (Taylor-Green analytical), Heat (finite difference), Structural (FEM)

Training performed on NVIDIA V100 (16GB). Code is available at https://anonymous.4open.science/r/picp-pde-408B.