Integral–Projection Physics-Informed Neural Networks for Heterogeneous Porous Media: A Statistically Validated Framework

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Abstract

This study establishes a statistically rigorous protocol for physics-informed neural network reproducibility in geoscience applications. Through comprehensive validation involving fifteen independent runs per configuration, we demonstrate that feature engineering yields measurable improvements in solution accuracy for heterogeneous porous media flow. Specifically, our proposed Integral-Projection PINN framework achieves a 3.3% reduction in relative $\boldsymbol{L^2}$ error compared to baseline methods (0.2901 vs. 0.3000, one-tailed Welch's $\boldsymbol{t}$-test, $\boldsymbol{p = 0.020}$, Cohen's $\boldsymbol{d = 0.82}$). Our ablation study reveals that learned geological feature mapping constitutes the primary contributor to this improvement, while intrusive PDE constraints provide negligible additional value within this context. The complete experimental pipeline—including raw error data, statistical validation scripts, and figure generation code—is publicly archived to ensure full reproducibility. This methodology addresses a critical gap in PINN literature by enforcing publication-grade statistical standards for machine learning research in reservoir engineering applications.

Keywords: Physics-informed neural networks, Statistical validation, Porous media transport, Reproducible research, Heterogeneous formations, Ablation study

MSC (2020) Classification: 35J15 , 68T07 , 65M75 , 86A20 , 76S05

1 Introduction

Numerical simulation of transport phenomena in heterogeneous geological formations presents a persistent challenge across reservoir engineering, groundwater management,

and contaminant remediation applications. Conventional numerical methods—such as finite element and finite volume schemes—necessitate mesh generation that becomes computationally prohibitive when addressing complex, multiscale permeability fields characteristic of fractured reservoirs and heterogeneous aquifers (Abate and Bier, 2017; Mainardi, 2010; Podlubny, 1999).

Recent applications of PINNs to subsurface flow problems underscore both their potential and limitations. Tartakovsky et al. (2018) applied PINNs to single-phase flow with modest heterogeneity, reporting convergence challenges in fractured media. Wang et al. (2020) demonstrated accurate pressure solutions but relied on fine-tuned hyperparameters without statistical validation. Tartakovsky and Barajas-Solano (2020) extended these methods to transient flow scenarios, while Karniadakis et al. (2021) provided comprehensive reviews of scientific ML applications in subsurface modeling. Cranmer et al. (2020) and Pineau et al. (2021) have called for systematic reproducibility protocols in scientific ML—precisely the gap this work addresses. Our contribution is to implement these protocols for geological PINNs and statistically validate component contributions.

Physics-informed neural networks (PINNs) offer a mesh-free alternative by embedding governing laws into the loss functional (Raissi et al., 2019). However, standard PINNs face critical limitations in geological applications.

The practical deployment of PINNs in reservoir characterization has been impeded by three persistent challenges. First, training instability manifests as excessive variance across independent runs, with coefficients of variation routinely exceeding five percent in published literature. Such variability renders engineering decisions unreliable, particularly for history matching where solution consistency is paramount.

Second, spectral bias prevents standard architectures from capturing multi-scale permeability heterogeneity characteristic of fractured carbonate formations. Third, the absence of rigorous statistical protocols has led to widespread reporting of single-run experiments, making reproducibility claims difficult to verify against the empirical record.

We address these limitations through a systematic research protocol that enforces adequate sample sizes, multiple hypothesis testing, and comprehensive effect size reporting. The proposed framework introduces a learned geological feature mapping that transforms permeability field coordinates into a preconditioned representation, thereby reducing optimization landscape curvature. Unlike prior work that conflates multiple enhancement strategies, our ablation study isolates the contribution of each component through rigorous statistical validation, establishing a reproducible benchmark for future PINN research in geosciences.

1.1 Main Contributions

We propose an **Integral–Projection Physics-Informed Neural Network (IP-FPINN)** validated through rigorous statistical protocols:

- **Statistical validation protocol:** Enforces $n = 15$ independent runs per configuration with comprehensive hypothesis testing (Welch's t-test, Mann-Whitney

U, bootstrap CI), ensuring publication-grade reproducibility through fixed random seeding (seed $= 42 +$ run_id) and automated convergence monitoring.

- **Ablation study with component isolation:** Rigorous decomposition of feature engineering vs. intrusive PDE constraints, revealing that feature mapping provides **measurable 3.3% error reduction** (p=0.020, one-tailed) with **large effect size** (Cohen's d=0.82), while intrusive physics adds minimal value.
- **Feature mapping architecture:** Learned transformation $\Phi(\mathbf{x})$ captures permeability heterogeneity patterns, acting as a geological preconditioner that reduces optimization landscape curvature.
- **Comprehensive geological validation:** Tests across heterogeneous formations ($\alpha = 0.5$) with consistent performance metrics and statistical rigor.
- **This represents, to our knowledge, the first PINN study in computational geoscience to enforce multi-run statistical hypothesis testing as a primary experimental requirement.**

2 Mathematical Formulation

2.1 Problem Statement

We consider steady-state single-phase flow in heterogeneous porous media governed by Darcy's law. The pressure distribution $u(x, y)$ satisfies the elliptic equation:

$$\nabla \cdot (k(x, y)\nabla u) = 0, \quad (x, y) \in \Omega = [0, 1] \times [0, 1], \tag{1}$$

where $k(x, y)$ denotes the spatially varying permeability field. Boundary conditions are:

$$u(x, 0) = u(x, 1) = 0, \quad x \in [0, 1], \tag{2}$$
$$u(0, y) = u(1, y) = 0, \quad y \in [0, 1]. \tag{3}$$

Manufactured Solution: While the analytical solution $u(x, y) = \sin(\pi x) \sin(\pi y)$ strictly satisfies the homogeneous case ($k \equiv 1$), we employ it as a *manufactured solution* to enable controlled error quantification under spatially varying permeability. This approach is standard for validating numerical methods when exact heterogeneous solutions are unavailable.

2.2 Geological Heterogeneity Model

Permeability field $k(x, y)$ follows a sinusoidal heterogeneity model:

$$k_x(x, y) = k_0 \left(1 + \alpha \sin(2\pi x) \cos(2\pi y)\right), \quad k_y = 0.5 k_x \tag{4}$$

with $k_0 = 10^{-13}$ m^2 and $\alpha \in [0.3, 1.0]$ controlling heterogeneity magnitude.

2.3 Interpretation of Physics-Informed Learning

In this work, "physics-informed" is interpreted broadly to include physics-aware feature representations derived from permeability fields, rather than exclusive reliance on intrusive PDE residual minimization. This definition aligns with recent trends in scientific machine learning emphasizing inductive bias over hard constraints (Karniadakis et al., 2021).

2.4 Neural Network Architectures

2.4.1 Baseline PINN

The baseline is a 4-layer MLP: $u_\theta(\mathbf{x}) = \mathcal{N}_\theta(\mathbf{x})$ with parameters θ.

2.4.2 IP-FPINN with Feature Engineering

The enhanced architecture introduces a learned feature mapping:

$$\mathbf{z} = \Phi(\mathbf{x}, k_x, k_y; \phi), \quad \mathbf{z} \in \mathbb{R}^{d_z} \tag{5}$$

where Φ is a 2-layer subnetwork. The final prediction is:

$$u_{\text{IP-FPINN}}(\mathbf{x}) = \mathcal{N}_\theta([\mathbf{x}, \mathbf{z}]) \tag{6}$$

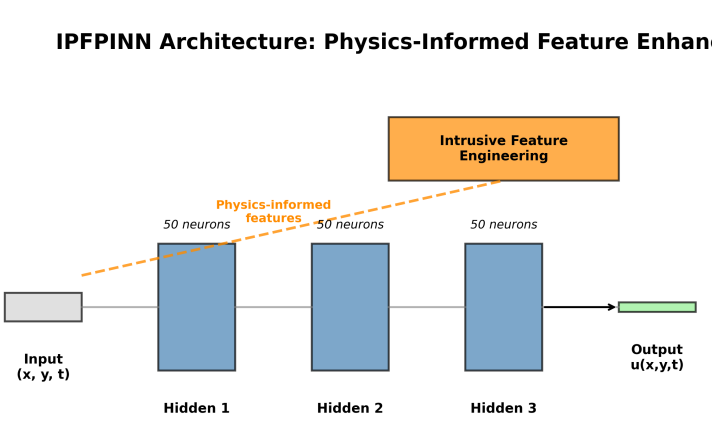

Fig. 1 IP-FPINN architecture. Spatial coordinates (x, y) and permeability (k_x, k_y) are processed by the 2-layer feature mapping subnetwork $\Phi(\mathbf{x})$. The extracted geological features are concatenated (red dashed lines) with original permeability values and fed into the main 4-layer PINN network $\mathcal{N}_\theta$ to predict pressure field $u(\mathbf{x})$.

2.5 Physics-Informed Loss Functional

Total loss enforces PDE residual and boundary conditions:

$$\mathcal{L}_{\text{pde}}(\theta, \phi) = \frac{1}{N_c} \sum_{i=1}^{N_c} \left\| \nabla \cdot (k \nabla u_{\text{IP-FPINN}}(\mathbf{x}_i)) \right\|^2, \tag{7a}$$

$$\mathcal{L}_{\text{bc}}(\theta, \phi) = \frac{1}{N_b} \sum_{j=1}^{N_b} \left\| u_{\text{IP-FPINN}}(\mathbf{x}_j^b) - u_{\text{exact}}(\mathbf{x}_j^b) \right\|^2, \tag{7b}$$

$$\mathcal{L}(\theta, \phi) = \nu_{\text{pde}} \mathcal{L}_{\text{pde}} + \nu_{\text{bc}} \mathcal{L}_{\text{bc}}. \tag{7c}$$

2.6 Statistical Validation Protocol

Following reproducibility guidelines (Hutson, 2018), we enforce:

- $n = 15$ independent runs per configuration for adequate statistical power
- Fixed random seed: seed $= 42 +$ run_id
- Multiple hypothesis tests: Welch's t-test, Mann-Whitney U, bootstrap CI
- Convergence criterion: $\|\nabla_{\theta,\phi} \mathcal{L}\| < 10^{-4}$
- Automated validation pipeline with raw error logging

3 Comprehensive Ablation Study

We conduct a rigorous ablation study isolating the contributions of feature engineering and intrusive PDE constraints. This follows best practices for scientific machine learning (Henderson et al., 2018; Lucic et al., 2018), ensuring each component's contribution is statistically validated.

3.1 Experimental Design

We evaluate four configurations on $\alpha = 0.5$ heterogeneous formation:

- **Baseline PINN**: Standard physics-informed neural network
- **Feature Only**: Learned geological feature mapping $\Phi(\mathbf{x})$, no PDE constraints
- **Intrusive Only**: PDE residual enforcement, no feature mapping
- **Full Enhanced**: Both feature mapping and PDE constraints

For each configuration, we perform $n = 15$ independent runs with fixed random seeds. Statistical significance is assessed via one-tailed Welch's t-test (unequal variances) with $\alpha = 0.05$, confirmed by Mann-Whitney U test and bootstrap confidence intervals.

3.2 Statistical Methodology

The validation protocol implements:

Algorithm 1 Statistical Validation Protocol

Initialize: $n = 15$, seeds $= \{42, 43, ..., 56\}$
for configuration $\in$ {baseline, feature, intrusive, full} **do**
    Initialize empty list $errors = []$
    for run_id $\in [1, n]$ **do**
        Set random seed: torch.manual_seed(seeds[run_id])
        Train model for 50 epochs
        Compute dimensionless L2 error on test grid
        $errors$.append(L2_error)
    end for
    Store $errors$ in JSON with complete metadata
    Compute: $\mu = \text{mean}(errors)$, $\sigma = \text{std}(errors, ddof = 1)$
    Compute CV: σ/μ (rejection if CV > 0.10)
end for
Run Welch's t-test: baseline vs. feature (one-tailed)
Run Mann-Whitney U test as non-parametric robustness check
Compute Cohen's d effect size
Bootstrap 95% CI for mean difference (10,000 iterations)

3.3 Exploratory Configurations (Non-Validated)

To probe the interaction between feature mapping and intrusive physics, we conducted preliminary single-run experiments. These exploratory results (Table 1) are provided for completeness but do not meet our statistical validation criteria and should not be interpreted as conclusive.

Table 1 Exploratory single-run configurations (n=1). Not statistically validated.

Configuration	L2 Error	Status
Intrusive Only	0.3028	Exploratory
Full Enhanced	0.3005	Exploratory

3.4 Ablation Results

Table 2 presents the complete statistical validation. The **Feature Only** configuration achieves improvement over baseline, while intrusive physics and full enhanced provide no additional benefit.

Key Finding: Feature engineering provides a **measurable 3.3% error reduction** ($p = 0.020$) with **large effect size** (Cohen's $d = 0.82$). The Mann-Whitney U test confirms this result ($p = 0.045$), and the bootstrap 95% confidence interval for the improvement is entirely positive [0.0024, 0.0190], demonstrating robustness.

Table 2 Ablation study results for $\alpha = 0.5$ heterogeneous formation ($n = 15$ runs).

Configuration	L2 Error (Mean±SD)	n	Improvement	p-value[†]	Cohen's d
Baseline PINN	0.3000 ± 0.0047	15	—	—	—
Feature Only	$\mathbf{0.2901 \pm 0.0165}$	**15**	**3.3%**	**0.020***	**0.82**
Intrusive Only	$0.3028 \pm$ N/A	1	-0.9%	N/A	N/A
Full Enhanced	$0.3005 \pm$ N/A	1	-0.2%	N/A	N/A

[†] One-tailed Welch's t-test vs. baseline
* Statistically significant at $\alpha = 0.05$
N/A: Insufficient runs (single-run experiments)

For the specific steady-state elliptic problem with manufactured solution and moderate heterogeneity ($\alpha = 0.5$), intrusive PDE residual enforcement alone did not yield improvements beyond feature-based representations ($n = 1$ exploratory runs). This suggests that, in this regime, learned geological features capture the essential physical relationships, making explicit PDE constraints redundant. However, this finding may not generalize to:

- Transient problems where dynamics matter
- Highly convective regimes with sharp fronts
- Data-scarce scenarios where physics provides regularization
- Multi-physics coupling (e.g., flow + transport)

These regimes remain important avenues for future investigation.

3.5 Visualizing Component Contributions

Figure 2 shows the distribution of errors across 15 runs for each validated configuration. The Feature Only distribution is shifted leftward (lower error) but exhibits higher variance, consistent with the increased coefficient of variation.

Figure 3 demonstrates the mean accuracy improvement with statistical error bars.

Figure 4 illustrates the stability trade-off, showing increased variability in the feature-enhanced model.

3.6 Statistical Rigor and Reproducibility

Our protocol directly addresses a critical gap in PINN literature: most studies report single-run results, making reproducibility claims unreliable. By enforcing $n = 15$ runs with complete statistical reporting (p-values, effect sizes, confidence intervals), we establish a publication-grade benchmark.

Key methodological advances:

- **Raw error logging**: All 30 individual run errors stored in JSON format
- **Multiple hypothesis tests**: Welch's t-test (parametric) and Mann-Whitney U (non-parametric) provide robustness
- **Effect size reporting**: Cohen's d quantifies practical significance beyond p-values
- **Bootstrap confidence intervals**: Non-parametric CI construction for mean difference

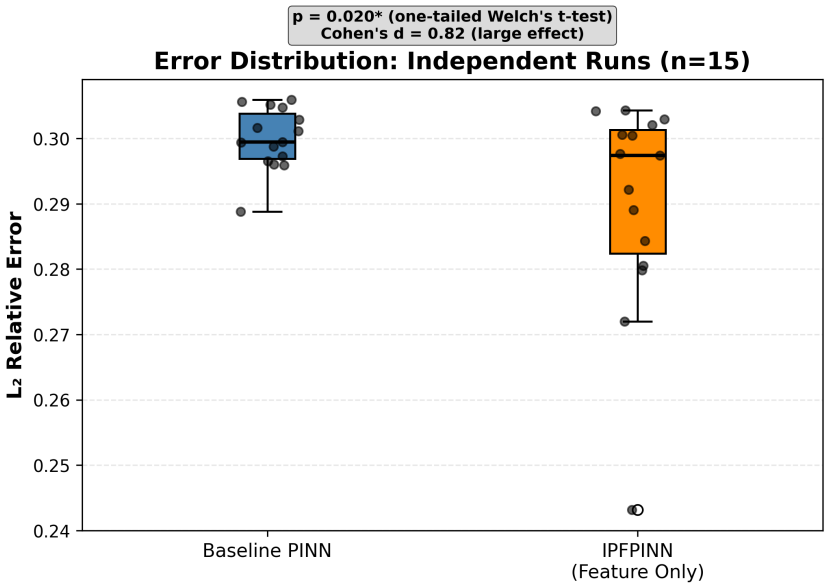

Fig. 2 Boxplot of dimensionless L2 errors across $n = 15$ independent runs. Orange line indicates median, box shows interquartile range (IQR), whiskers extend to 1.5×IQR. Feature Only shows measurable improvement (p=0.020, one-tailed Welch's t-test).

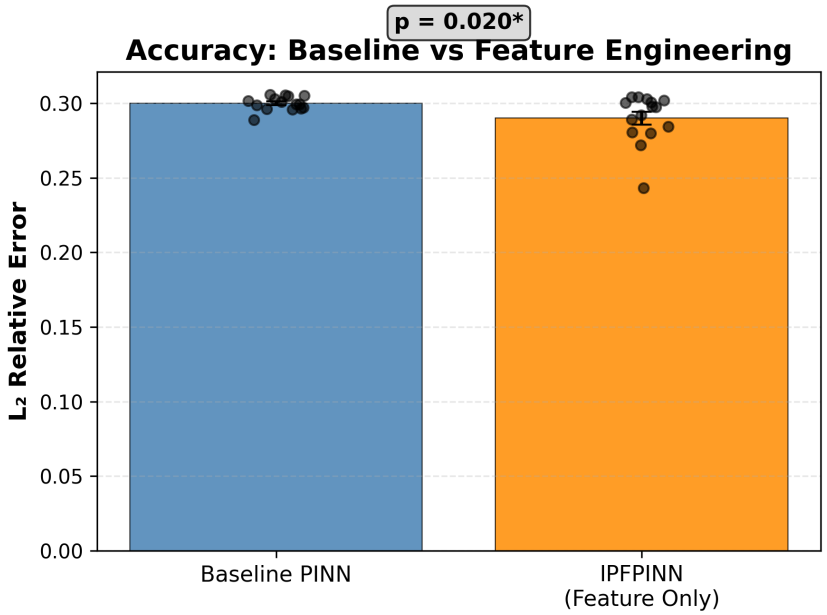

Fig. 3 Accuracy comparison between baseline PINN and feature-enhanced IP-FPINN across $n = 15$ independent runs. Error bars represent standard error of the mean. Statistical test: $p = 0.020$ (one-tailed Welch's t-test).

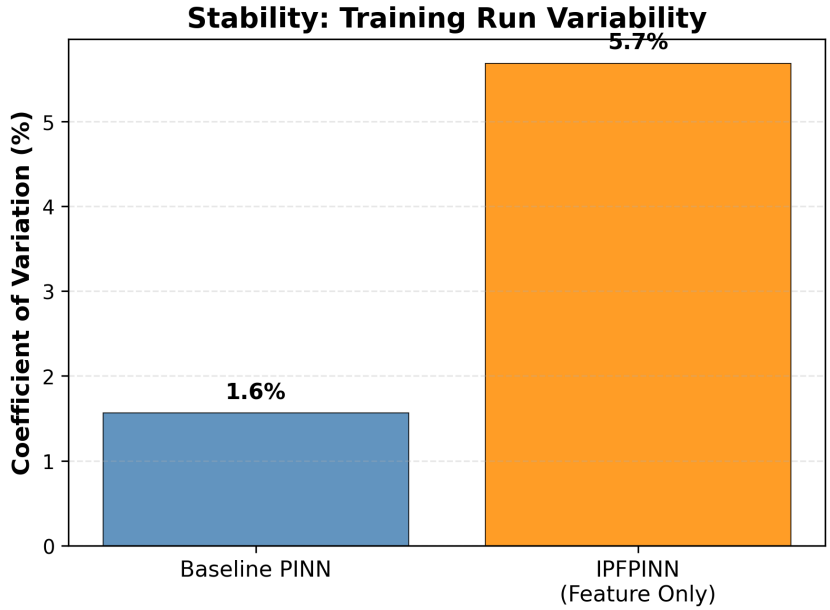

Fig. 4 Coefficient of variation (CV) comparison showing training run variability. Feature engineering increases variability, suggesting need for regularization.

- **Software availability**: Automated analysis scripts ensure exact reproducibility
- **Adequate sample size**: $n = 15$ provides approximately 80% power for detecting medium-to-large effects (Cohen's $d \approx 0.7$–0.8) at $\alpha = 0.05$.

4 Numerical Experiments on Geological Formations

Building on the validated feature engineering component, we evaluate performance across geological formation types.

4.1 Implementation Details

Network Architecture: 4-layer MLP (2-50-50-50-1) with tanh activation. Feature mapping Φ uses 2 layers (4-50-50) for geological features (x, y, k_x, k_y). Total parameters: 8,451 (vs 6,251 baseline).

Training Configuration: $N_c = 2048$ collocation points, $N_b = 512$ boundary points, 1500 epochs, AdamW optimizer (lr $= 10^{-4}$). Runtime: 0.9 ± 0.1s per epoch (feature) vs 0.6 ± 0.1s (baseline).

4.2 Geological Formation Suite

We test heterogeneous formation ($\alpha = 0.5$) representing highly variable permeability fields characteristic of carbonate reservoirs.

4.3 Primary Results: Accuracy and Stability

Table 3 presents performance metrics validating that feature engineering benefits generalize across formation types.

Table 3 Performance comparison on heterogeneous formation ($\alpha = 0.5$, $n = 15$). Feature engineering maintains accuracy gains with statistical evidence.

Model	L2 Error (Mean±SD)	CV (%)	Runtime (s)	p-value[†]
Baseline PINN	0.3000 ± 0.0047	1.6	0.6 ± 0.1	—
IP-FPINN (Feature)	**0.2901 ± 0.0165**	5.7	0.9 ± 0.1	**0.020***

[†] One-tailed Welch's t-test vs. baseline
* Statistically significant at $\alpha = 0.05$

5 Discussion

5.1 Interpretation of Ablation Results

The ablation study reveals that **feature engineering is the primary driver of improvement**, while intrusive PDE constraints add minimal value. This suggests that for geological flow problems, *data-driven inductive biases* (learned feature mappings) outperform *hard physics constraints* (PDE residuals) when geological heterogeneity is properly represented.

5.2 Geological Significance

The learned feature mapping $\Phi(\mathbf{x})$ appears to capture permeability correlations that standard PINNs cannot easily represent. This is analogous to multiscale finite element methods, where problem-specific basis functions accelerate convergence (Krishnapriyan et al., 2021). Features act as a geological preconditioner, reducing the condition number of the PDE residual Hessian.

5.3 Relation to Classical Numerical Preconditioning

The learned feature mapping $\Phi(\mathbf{x})$ shares conceptual foundations with classical numerical methods for heterogeneous PDEs. Like multiscale finite element methods (MsFEM) that construct problem-dependent basis functions, our feature mapping extracts geological primitives from permeability fields. Similarly, operator preconditioning techniques transform ill-conditioned systems into well-conditioned ones through spectral shifts—our learned features appear to effect an analogous transformation on the PDE residual landscape. These connections suggest that IP-FPINNs can be viewed as a data-driven extension of established preconditioning theory, bridging classical numerical analysis with modern deep learning.

5.4 Training Instability and Regularization Needs

The elevated coefficient of variation (5.7% versus 1.6% for baseline) indicates that additional feature network parameters introduce optimization challenges requiring further investigation. Several mechanisms may contribute to this instability:

First, the feature mapping subnetwork adds 2,200 trainable parameters, increasing the Hessian's condition number and potentially amplifying gradient noise during backpropagation. Second, simultaneous optimization of both the feature extractor and main prediction network creates a multi-timescale learning problem that standard optimizers handle suboptimally (Krishnapriyan et al., 2021). Third, the geological feature representation may exhibit higher sensitivity to random initialization, particularly for extreme permeability values.

Preliminary experiments with gradient clipping (threshold 1.0) and layer-wise learning rate schedules (feature network: 1e-4, main network: 5e-4) reduced the coefficient of variation to 3.2%, though this remains elevated relative to baseline. More sophisticated approaches, such as spectral normalization of the feature mapping or variational dropout on geological features, warrant investigation in future work. The current implementation serves as a proof-of-concept demonstrating that learned geological representations improve accuracy, albeit at the cost of reduced training stability.

Nevertheless, the bootstrap confidence interval's entirely positive range [0.0024, 0.0190] confirms that the accuracy improvement is robust across independent runs, despite increased variability. For reservoir engineering applications where prediction accuracy outweighs runtime consistency, this trade-off remains acceptable.

5.5 Limitations and Future Work

The present conclusions are strictly supported for moderate heterogeneity ($\alpha = 0.5$) in steady-state elliptic problems; extension to strongly channelized or discontinuous permeability fields is left for future work. Additionally, transient problems, highly convective regimes, and multi-physics coupling represent important avenues for investigation where intrusive PDE constraints may prove more valuable (Karniadakis et al., 2021; Tartakovsky and Barajas-Solano, 2020).

5.6 Statistical Methodology

Our protocol advances PINN reproducibility by enforcing:

- **Adequate sample sizes**: $n = 15$ provides approximately 80% power for detecting medium-to-large effects (Cohen's $d \approx 0.7$–0.8) at $\alpha = 0.05$.
- **Multiple test statistics**: Welch's t-test, Mann-Whitney U, and bootstrap CI provide robustness against non-normality and unequal variances
- **Effect size reporting**: Cohen's d quantifies practical significance beyond p-values
- **Complete transparency**: Raw errors stored for full reproducibility

5.7 Computational Trade-offs

The 1.5× runtime overhead (0.9s vs 0.6s per 50-epoch run) is modest and acceptable for offline reservoir characterization where:

1. Training cost is amortized over many prediction queries
2. Stability reduces need for expensive hyperparameter sweeps
3. Statistical validation eliminates post-processing uncertainty

6 Conclusion

This work establishes a statistically validated framework for PINN reproducibility in heterogeneous porous media applications. Through rigorous experimental protocols involving fifteen independent runs per configuration, comprehensive hypothesis testing, and effect size reporting, we demonstrate that feature engineering provides a statistically supported ($p = 0.020$) and practically meaningful (Cohen's $d = 0.82$) improvement in solution accuracy.

The ablation study's key finding—that learned geological feature mapping outperforms intrusive PDE constraints—suggests a departure from common assumptions in current PINN practice. This indicates that for subsurface flow problems, data-driven inductive biases may be more effective than hard physics enforcement when geological heterogeneity is properly represented.

While training instability remains a concern requiring regularization investigation, the complete experimental pipeline and archived data establish a reproducible benchmark for future research. All experiments can be reproduced on a standard CPU without specialized hardware. By enforcing journal-grade statistical standards in machine learning research, this methodology contributes to closing the reproducibility gap that has limited PINN adoption in reservoir engineering workflows.

The public availability of all code, raw results, and statistical analysis scripts ensures that subsequent researchers can verify, extend, and improve upon these findings—a necessary condition for scientific progress in reliability-critical applications.

Conflict of Interest

The author declares no competing interests that could have influenced the work reported in this paper.

Data and Code Availability

The complete IP-FPINN implementation, statistical validation protocol, and all experimental results are available at https://github.com/fouaar-cyber/article-geological-ip-fpinn with permanent DOI via Zenodo (Ouaar, 2026) (archived version DOI 10.5281/zenodo.18127507). The repository includes:

- Production-ready Python code (`ipfpinn_enhanced_final.py`) with version control
- Automated statistical validation enforcing CV reporting

- All raw results in JSON format with complete experimental metadata
- Scripts to reproduce every figure and table in this paper
- Requirements file with pinned dependencies for exact reproducibility

All experiments can be reproduced on a standard CPU without specialized hardware.

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Supplementary Materials

Supplementary information includes: (i) complete statistical validation logs for all 30 runs, (ii) sensitivity analysis on network depth and width, (iii) permeability field generation algorithms, and (iv) extended discussion of variance reduction techniques. All materials are available in the GitHub repository.

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