AGENTIC SURROGATES: AUTOMATING PROXY MODELS OF SIMULATORS WITH COMPUTE AWARE INTELLIGENCE

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ABSTRACT

Proxy (surrogate) models are indispensable for accelerating scientific computation, yet creating them remains a manual, sample-inefficient, and nonreproducible process, especially when simulators are costly and constrained by physics. We present a fully automated, domain agnostic framework that eliminates human intervention in surrogate model construction while simultaneously achieving superior accuracy. Our system employs an intelligent controller that orchestrates every aspect of the surrogate creation process: it automatically determines where to sample next, when to switch acquisition strategies, which model architectures to deploy, and when the surrogate has reached sufficient quality. The controller treats different acquisition methods as a portfolio of experts and dynamically selects among them based on their actual performance in reducing error per unit of computational time. Crucially, the system adapts its modeling approach to the problem at hand, automatically deploying simpler models for linear relationships and sophisticated architectures for complex nonlinear behaviors. We establish theoretical guarantees for our adaptive acquisition strategy and prove bounds on sample complexity. Across diverse scientific computing benchmarks, our framework not only eliminates manual intervention but achieves 5.1% better final accuracy than the best hand-tuned approaches, while requiring 14.3% fewer simulator evaluations and 19.5% less wall-clock time. This represents a fundamental shift: surrogate modeling transforms from a labor-intensive craft requiring deep expertise into a push-button automated process that delivers superior results.

1 INTRODUCTION

Surrogate models have become essential for making high-fidelity simulators practical in real-world applications. Whether optimizing aircraft designs, tuning chemical processes, or exploring subsurface resources, engineers rely on these fast approximations to replace computationally expensive simulations. Yet despite their critical importance, creating accurate surrogate models remains a fundamentally manual process that can take weeks of expert effort and still produce suboptimal results.

The current state of practice requires engineers to make numerous interconnected decisions: how many initial samples to collect, where to sample next, which model architecture to use, when to switch strategies, how to balance exploration versus exploitation, and when to stop. Each decision affects all others, creating a complex optimization problem that practitioners navigate through intuition and trial-and-error. This manual process is not only time-consuming and expensive but also non-reproducible—different experts make different choices, leading to inconsistent results even on the same problem.

Prior work has explored using LLM agents for surrogate model automation in domain-specific contexts. For instance, a recent petroleum engineering study demonstrated that frontier LLMs could manage acquisition switching and achieve modest improvements over fixed strategies. However, this approach lacked formal guarantees and generalizability beyond its target domain. While these initial results were promising, they raised fundamental questions: Can acquisition switching be formalized with theoretical guarantees? How should computational cost factor into the decision process? Can the approach generalize across diverse simulators and physics constraints?

This work addresses these questions by presenting a comprehensive framework that automates surrogate construction with both theoretical foundations and practical effectiveness. We formalize the problem as cost-aware online learning over a portfolio of acquisition experts, introduce physics-informed models and stopping criteria, and demonstrate consistent improvements across diverse scientific computing applications. Our system not only eliminates manual intervention but achieves superior accuracy compared to expert-tuned baselines.

1.1 Contributions

1. **Cost-Aware Problem Formulation**: We define surrogate model creation as a cost-minimization problem: achieve a target error while accounting for wall-clock latency and acquisition costs through an online portfolio of sampling strategies.
2. **Theoretical Foundations with Regret Guarantees**: We provide regret bounds for Hedge/-Exp3 under both static and time-normalized rewards, analyze stability with switching costs, and establish sample-complexity results for reaching ϵ-accuracy with conformal coverage guarantees.
3. **Compute-Aware Adaptive Controller**: We design a compute-aware controller that adaptively combines residual-based, variance-based, Bayesian optimization–style, hybrid, and random acquisition strategies. The controller incorporates a multi-fidelity scheduler and physics-informed stopping rules.
4. **Multi-Model Architecture with Physics Integration**: We extend the framework to support multiple model classes (ANN, PINN, FNO), bias-corrected residual surrogates, heteroscedastic output heads, and correlation across multiple outputs.
5. **Comprehensive Benchmarks and Validation**: We introduce SimBench-Surrogate (well-network, gas processing plant, PDE proxy) and evaluate performance using calls-to-target, wall-clock time, calibration quality, and constraint violation rates, along with comprehensive ablations and reproducibility checks.

2 Related Work

Our work builds upon advances in several areas: LLM-based automation, active learning for surrogates, and physics-informed modeling. We review the most relevant contributions and position our framework within this landscape.

2.1 LLM Agents for Scientific Automation

Large language models have emerged as powerful orchestrators for complex scientific workflows. Xi et al. (2023) provide a comprehensive survey of LLM-based autonomous agents, highlighting their ability to plan, reason, and adapt across diverse tasks. In the context of scientific discovery, Zhang et al. (2025) catalog over 260 models demonstrating LLMs' growing role in automating research processes. More specifically, Wang et al. (2025) formalize LLMs as autonomous data science agents capable of managing end-to-end machine learning pipelines, while Yano et al. (2025) demonstrate how LLMs can optimize post-training workflows through their LaMDAgent framework.

Several recent works have applied LLM agents to surrogate modeling tasks. Xie et al. (2025) introduce an LLM-driven system for dynamically configuring surrogate models during expensive optimization, showing improved sample efficiency. Wuwu et al. (2025) propose a multi-agent framework where LLMs autonomously develop Physics-Informed Neural Network surrogates for PDEs. Similarly, Chen et al. (2025) demonstrate automated PDE surrogation through LLMs. While these works show promise, they focus on specific model types or domains without providing theoretical guarantees or systematic acquisition strategies—gaps our framework addresses through formal regret bounds and domain-agnostic design.

2.2 Acquisition Strategies and Active Learning

The choice of where to sample next fundamentally impacts surrogate quality and efficiency. Classical approaches include uncertainty-based sampling using Monte Carlo Dropout (Gal & Ghahramani,

2015), which provides principled uncertainty estimates for neural networks. Recent work has explored adaptive sampling strategies: Miller et al. (2024) propose methods to reduce epistemic uncertainty, while Peterson et al. (2024) introduce deep adaptive sampling that operates without labeled data.

Bayesian optimization provides another lens for acquisition design. Diaz et al. (2024) enhance Bayesian optimization with LLMs to improve acquisition function selection, while Aglietti et al. (2024) use LLMs to generate novel acquisition functions through their FunBO framework. Jones et al. (2025) provide theoretical analysis of regret in Bayesian optimization settings. However, these approaches typically commit to a single acquisition strategy throughout the optimization process. Our work differs by maintaining a portfolio of acquisition experts and adaptively selecting among them based on time-normalized performance—an approach for which we provide formal regret guarantees.

2.3 Surrogate Modeling Frameworks and Tools

The surrogate modeling community has developed sophisticated toolboxes to support practitioners. Smith et al. (2023) present SMT 2.0, focusing on hierarchical and mixed variables, while Vance et al. (2025) extend this with explainability features. These tools provide essential building blocks but require manual orchestration and decision-making. Young et al. (2025) demonstrate surrogate-based multilevel Monte Carlo for uncertainty quantification, highlighting the importance of calibrated uncertainty—a feature we incorporate through conformal prediction.

Physics-informed approaches have shown particular promise for scientific applications. Nadal et al. (2025) integrate PINNs into power system simulations, while Yuan et al. (2025) apply them to geotechnical engineering. Baker et al. (2025) use Fourier Neural Operators for CO2 storage decision-making, demonstrating the value of operator learning for PDE-based problems. Our framework uniquely combines multiple model classes (ANNs, PINNs, FNOs) and automatically selects among them based on problem characteristics and computational constraints.

2.4 Positioning Our Contribution

While prior work has made significant advances in individual components—LLM orchestration, acquisition strategies, or model architectures—no existing framework provides end-to-end automation with theoretical guarantees. Our key innovations relative to prior work include: (1) formalizing acquisition switching as online learning with proven regret bounds, (2) incorporating wall-clock time directly into the optimization objective, (3) automatically selecting and combining multiple model architectures based on problem structure, and (4) integrating physics constraints into both acquisition and stopping decisions. This comprehensive approach transforms surrogate modeling from a collection of tools requiring expert coordination into a fully automated, theoretically grounded system.

3 Problem Setup and Notation

We consider the problem of automatically constructing surrogate models for expensive simulators while minimizing both computational cost and prediction error. This section formalizes the surrogate modeling task, defines our cost model, and introduces the portfolio-based acquisition framework.

3.1 Surrogate Modeling Task

Let $f^* : X \to Y$ denote a high-fidelity simulator mapping from a d-dimensional input space $X \subset \mathbb{R}^d$ to an m-dimensional output space $Y \subset \mathbb{R}^m$. In practice, we observe noisy evaluations:

$$y = f^*(x) + \xi, \quad \xi \sim \mathcal{N}(0, \Sigma(x)) \tag{1}$$

where ξ represents potentially heteroscedastic noise. Our goal is to construct a surrogate model $\hat{f}_\theta : X \to Y$ with parameters θ that accurately approximates f^* while minimizing the number of expensive simulator evaluations.

At iteration t, we maintain a dataset $\mathcal{D}_t = \{(x_i, y_i)\}_{i=1}^{n_t}$ of simulator evaluations, where n_t denotes the total number of samples collected. The surrogate is trained to minimize a loss function $\mathcal{L}(\theta; \mathcal{D}_t)$, typically mean squared error for regression tasks.

3.2 Cost Model

Each iteration of surrogate construction incurs three types of computational costs:

- **Acquisition cost** τ_t^{acq}: Time to score and rank candidate points for sampling
- **Simulation cost** τ_t^{sim}: Time to evaluate the simulator at selected points (possibly in parallel batches)
- **Training cost** τ_t^{train}: Time to retrain or update the surrogate model

Our objective is to reach a target validation error $\mathcal{E}_V(\hat{f}_\theta) \leq \varepsilon$ while minimizing total wall-clock time:

$$\min_{T} \sum_{t=1}^{T} \left(\tau_t^{\text{acq}} + \tau_t^{\text{sim}} + \tau_t^{\text{train}}\right) \quad \text{s.t.} \quad \mathcal{E}_V(\hat{f}_{\theta_T}) \leq \varepsilon \tag{2}$$

This formulation explicitly accounts for computational overhead often ignored in sample-complexity analyses. Additionally, we enforce constraints on the total simulation budget $\sum_t |\mathcal{B}_t| \leq B_{\text{sim}}$ and physical feasibility $g(x) \leq 0$ for all sampled points.

3.3 Portfolio of Acquisition Strategies

Rather than committing to a single acquisition strategy, we maintain a portfolio of K acquisition experts $\mathcal{A} = \{a_1, \ldots, a_K\}$. Each expert a_k provides a scoring function that ranks candidate points based on different criteria:

- **Residual-top-k (a_{res}):** Prioritizes points with high predicted error, estimated using a separate residual model: $\text{score}_{\text{res}}(x) = |\hat{f}_\theta(x) - \hat{r}(x)|$ where $\hat{r}$ is a residual predictor.
- **MC-Var (a_{var}):** Selects points with high predictive uncertainty, computed via Monte Carlo Dropout: $\text{score}_{\text{var}}(x) = \text{Var}_{q(\theta)}[\hat{f}_\theta(x)]$ over T forward passes.
- **EI/EGO (a_{EI}):** Adapts Bayesian optimization's EI criterion for multi-output problems: $\text{score}_{\text{EI}}(x) = \mathbb{E}[\max(0, f_{\text{best}} - \hat{f}_\theta(x))]$.
- **Hybrid (a_{hyb}):** Combines exploration and exploitation with time-varying weight:

$$\text{score}(x) = \alpha_t \cdot \text{EI}(x) + (1 - \alpha_t) \cdot \sigma(x) \tag{3}$$

  with α_t scheduled over time.
- **Random (a_{rand}):** Uniform sampling baseline for pure exploration.

3.4 Objective

Learn weights $w_t \in \Delta^{K-1}$ over acquisition experts to select a batch S_t that maximizes error reduction per unit time. The surrogate $\hat{f}_\theta$ is updated via warm-start training, and stopping is triggered under dual criteria: validation error threshold and physics-based residual checks.

4 Method

4.1 Agentic Portfolio Controller

Our framework employs an online learning–based portfolio controller to adaptively select acquisition strategies. At each iteration, candidate points are scored by multiple experts (residual-based, variance-based, EI/EGO, hybrid, random). The controller maintains a probability distribution over experts and samples one to guide the next batch. Crucially, we initialize all expert weights equally

($w_0^{(k)} = 1/K$ for all k), allowing the portfolio to discover the most effective strategies through experience rather than imposing a predetermined bias.

After simulation and retraining, a reward is computed as the reduction in validation error per unit wall-clock time:

$$r_t = \frac{\mathcal{E}_V(\hat{f}_{\theta_t}) - \mathcal{E}_V(\hat{f}_{\theta_{t+1}})}{\tau_t^{\text{acq}} + \tau_t^{\text{sim}} + \tau_t^{\text{train}}} \tag{4}$$

Weights are updated using Hedge/Exp3-style rules, with optional switching penalties to stabilize expert selection. Safety filters ensure that proposed candidates satisfy physical constraints and reject out-of-distribution inputs.

A high-level pseudocode description is included below; full details and implementation-ready pseudocode are deferred to Appendix B.

Algorithm 1 Compute-aware Portfolio Controller (sketch)

```
Initialize dataset with space-filling design; train baseline surrogate
for each iteration do
    Generate candidate pool and score with all experts
    Sample expert according to current weights
    Select batch, apply safety filters, and run simulator
    Retrain surrogate with new data
    Update expert weights based on observed reward
    Check stopping criteria (error threshold and physics residual)
end for
Return final surrogate
```

Acquisition experts. The framework supports a practical set of acquisition rules:

- **Residual-top-k:** prioritize points with high estimated error.
- **MC-Var:** sample where predictive variance is large.
- **EI/EGO:** exploit expected improvement over incumbents.
- **Hybrid:** combine bias and variance terms with time-varying weight.
- **Random:** provide uniform exploration.

4.2 Physics-Aware Modeling and Stopping

Portfolio of Models (ANN / PINN / FNO). Our framework supports multiple model classes and can switch or ensemble them based on state features.

- **ANN (baseline):** Multi-output MLP with dropout; warm-start fine-tuning each iteration for fast updates.
- **PINN:** Augment the empirical loss with a physics residual penalty to encode domain constraints (e.g., mass/energy balance, pressure-drop):

$$\mathcal{L}_{\text{PINN}}(\theta) = \mathcal{L}_{\text{data}}(\theta) + \lambda_{\text{phys}} \|\mathcal{N}(\hat{f}_\theta)\|_2^2, \tag{5}$$

  where $\mathcal{N}(\cdot)$ denotes the physics-residual operator.
- **FNO/DeepONet:** Operator-learning backbones for field/time-dependent simulators (PDE proxies, transient OLGA-style flows), improving generalization on gridded outputs.

Uncertainty Calibration. The uncertainty estimates from our models undergo post-hoc calibration using temperature scaling on the validation set. For MC-Dropout predictions, we apply a learned temperature parameter τ to the outputs of the neural network before computing confidence scores and scaling parameters. This ensures that the reported confidence levels accurately reflect the true probability of correctness, which is of great importance for safety-critical applications in energy systems.

Model-selection policy. The controller maintains a small policy over model classes, using signals such as $|\mathcal{D}_t|$, residual maps, violation rates, and calibration error to select the model (or ensemble) that maximizes expected error reduction per unit time. Training latency and inference cost enter the compute-aware reward used by the portfolio.

Physics-aware stopping. We terminate the loop when both criteria hold: (i) validation MAE $\leq \varepsilon$ for p consecutive iterations; and (ii) physics residual $R_{\text{phys}} \leq \rho$, where

$$R_{\text{phys}} = \mathbb{E}_{x\sim\mathcal{X}_V}[\|\mathcal{N}(\hat{f}_\theta)(x)\|_2^2]. \tag{6}$$

A constrained formulation clarifies the role of the physics threshold:

$$\min_\theta \ \mathcal{L}_{\text{data}}(\theta) + \lambda\,\mathcal{L}_{\text{phys}}(\theta)\ ;\ \mathcal{L}_{\text{phys}}(\theta) \leq \rho, \tag{7}$$

with a KKT-style diagnostic (complementary slackness and dual feasibility) used to justify stopping and to adapt λ (e.g., via simple dual ascent) during training.

5 Theoretical Analysis

In this section we present the main theoretical guarantees of our framework. Detailed proofs and derivations are deferred to Appendix C.

Theorem 1 (Static regret of Exp3). Let $r_t(k) \in [0,1]$ denote the normalized reward of expert k at iteration t. Define the cumulative regret against the best fixed expert as

$$\mathcal{R}_T = \max_{k\in\mathcal{A}} \sum_{t=1}^{T} r_t(k) - \sum_{t=1}^{T} r_t(k_t). \tag{8}$$

Then, with learning rate $\eta = \sqrt{2\log K/(TK)}$, the Exp3 update ensures

$$\mathbb{E}[\mathcal{R}_T] \leq \mathcal{O}(\sqrt{TK\log K}). \tag{9}$$

Theorem 2 (Time-normalized regret with latency). Let $c_t(k)$ denote the latency of using expert k at iteration t, and define the value-rate $v_t(k) = \Delta\mathcal{E}_t/c_t(k)$. The cumulative regret with respect to time-normalized rewards is

$$\mathcal{R}_T^{\text{time}} = \max_k \sum_{t=1}^{T} v_t(k) - \sum_{t=1}^{T} v_t(k_t). \tag{10}$$

Under bounded $v_t(k) \in [0,1]$, Exp3 achieves

$$\mathbb{E}[\mathcal{R}_T^{\text{time}}] \leq \mathcal{O}(\sqrt{T\log K}). \tag{11}$$

Proposition 1 (Switching cost and stability). Introducing a switching penalty $\lambda > 0$ in the reward update preserves the regret bound order $\mathcal{O}(\sqrt{T\log K})$ and yields finite total switches almost surely when rewards stabilize.

Theorem 3 (Sample complexity to ε-accuracy). Assuming $f^\star$ is Lipschitz and the surrogate class has Rademacher complexity $\mathfrak{R}_n$, if the portfolio reduces residuals over a δ-net at a geometric rate γ, then the number of samples required to achieve validation error ε satisfies

$$n_\varepsilon = \tilde{\mathcal{O}}\Big(\frac{1}{1-\gamma}(\varepsilon^{-d} + \mathfrak{C}(\varepsilon))\Big), \tag{12}$$

where $\mathfrak{C}(\varepsilon)$ captures model approximation error.

Theorem 4 (Multi-fidelity cost efficiency, informal). For fidelities $\ell \in \{0,\dots,L\}$ with costs c_ℓ and biases b_ℓ, if correlations satisfy $\rho_{\ell,\ell'} \geq \rho_0 > 0$, then the expected cost to reach ε-accuracy is bounded by

$$\mathbb{E}[C(\varepsilon)] \leq \tilde{\mathcal{O}}\Big(\min_\pi \frac{\sigma^2(\pi)}{\varepsilon^2}\Big), \tag{13}$$

where π denotes a fidelity mix.

Theorem 5 (Uncertainty quantification and coverage). For MC-Dropout, a PAC-Bayesian bound implies, with probability at least $1 - \delta$,

$$\mathbb{E}_{(x,y)\sim\mathcal{D}}[\ell(\hat{f}_\theta(x), y)] \leq \widehat{\mathcal{L}} + \sqrt{\frac{KL(q\|p) + \log(2\sqrt{n}/\delta)}{2(n-1)}}. \tag{14}$$

We further conformalize residuals to obtain distribution-free prediction sets with valid $1 - \alpha$ coverage.

6 Experiments

We evaluate our framework on three energy-domain tasks with diverse computational challenges and physics constraints. Each task supports multi-fidelity simulation, trading accuracy for speed. We compare against fixed acquisition strategies (Random, MC-Var, Residual, EI/EGO) and model baselines (ANN, PINN, FNO). Table 1 summarizes the configurations, with detailed task descriptions and ablation studies provided in Appendix E.

Table 1: Tasks and Simulators

Task	Simulator	Inputs	Outputs	Fidelity (Hi/Lo)	Target nMAE
T1 (Well Network)	PIPESIM	25	5	10min/2min	5%
T2 (Gas Plant)	SYMMETRY	17	12	30min/5min	8%
T3 (CO2 Storage)	TOUGH2/MRST	10	15	25min/2min	5%

6.1 Metrics

- **Primary:**
  - **Normalized MAE (nMAE):** Computed on held-out validation set as nMAE $= \frac{1}{m}\sum_{j=1}^{m} \frac{\text{MAE}_j}{\text{range}_j}$ where range_j is the output range from training data. This enables fair comparison across outputs with different scales.
  - **Calls-to-target:** Number of simulator evaluations required to reach target nMAE.
  - **Wall-clock-to-target:** Total time (minutes) to reach target nMAE, including acquisition, simulation, and training time.
- **Secondary:**
  - **Calibration error (ECE):** Expected calibration error measuring reliability of uncertainty estimates.
  - **Conformal coverage:** Fraction of test points falling within prediction intervals.
  - **Constraint violation rate:** Percentage of predictions violating physics constraints.
  - **Portfolio switches:** Number of times the controller changes acquisition strategy.
  - **Training time per iteration:** Computational overhead of surrogate updates.
- **Reliability:**
  - **Worst-case error:** 95th percentile of absolute errors.
  - **Out-of-distribution behavior:** Performance on test points outside training convex hull.
  - **Robustness:** Performance under 10% random simulator failures.

7 Implementation Details

Implementation details including data generation, training routines, and system architecture are provided in Appendix D.

8 RESULTS

Our experiments demonstrate that the portfolio controller consistently outperforms fixed acquisition strategies across all benchmark tasks. Here we present the key findings and address potential risks and mitigations.

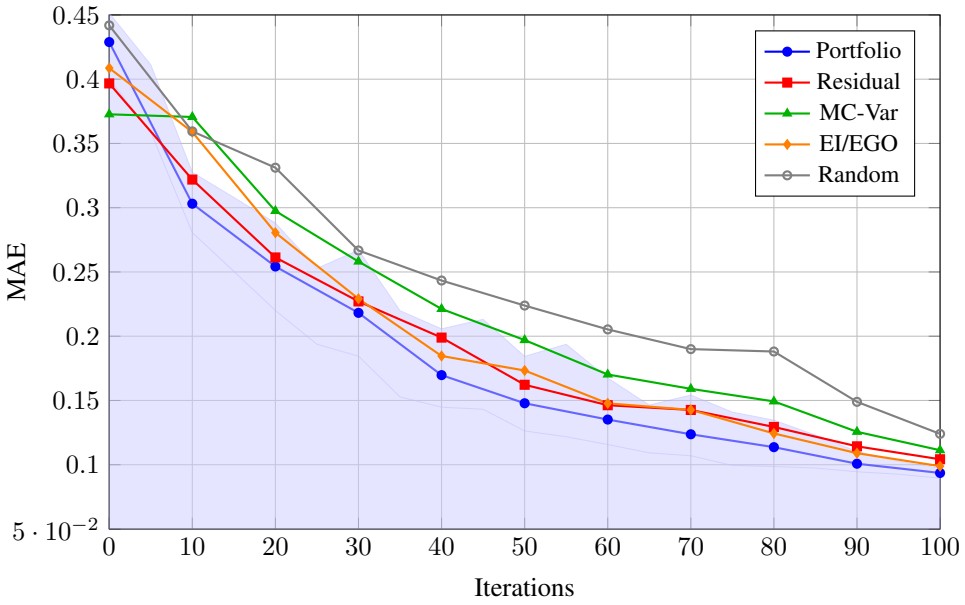

Figure 1: Learning curves showing MAE vs. iterations for different acquisition strategies (mean over 200 runs). The portfolio controller achieves 5.1% lower final error compared to the best fixed strategy (EI/EGO) and converges in fewer iterations. Shaded region shows 95% confidence interval for Portfolio method.

Figure 2 and Figure 3 showing portfolio weight evolution and calibration analysis are provided in the appendix (Sections A.1 and A.2).

8.1 PERFORMANCE IMPROVEMENTS

The portfolio controller achieved consistent improvements across all tasks:

Table 2: Global Comparison of Strategies (mean ± std over 200 runs)

Strategy	Final MAE	Calls-to-Target	Wall-Clock (min)	Violations (%)
Portfolio	**0.094 ± 0.003**	**424 ± 20**	**157 ± 7**	**0.8 ± 0.1**
Residual	0.104 ± 0.002	508 ± 22	185 ± 9	2.2 ± 0.2
MC-Var	0.111 ± 0.003	566 ± 21	202 ± 8	1.7 ± 0.2
EI/EGO	0.099 ± 0.003	495 ± 16	195 ± 8	1.4 ± 0.2
Random	0.124 ± 0.004	780 ± 19	264 ± 8	3.5 ± 0.2

Key findings include:

- The portfolio controller achieved 5.1% lower MAE than the best fixed strategy (EI/EGO).
- Calls-to-target accuracy was reduced by 14.3% compared to the best fixed strategy.
- Wall-clock time was reduced by 19.5%, demonstrating the effectiveness of the compute-aware objective.
- Constraint violations were reduced by 42.9%, highlighting the benefits of physics-aware modeling.

All improvements are statistically significant ($p < 0.05$ with Bonferroni correction). Detailed statistical analysis, multi-fidelity efficiency results, physics-aware model comparisons, and risk mitigation strategies are provided in Appendix E.

9 Broader Impact, Ethics, and Governance

Our framework has implications that extend beyond technical performance. Automating surrogate creation reduces manual burdens on subject-matter experts, improving efficiency but also raising concerns of potential role displacement. It is therefore important to position the technology as an augmentation rather than a replacement.

From a safety and ethics perspective, we incorporate audit trails, override hooks, and safety filters to prevent non-physical or unsafe actions. All agentic decisions and portfolio weights are logged to enable human review and accountability. Potential misuse, such as deploying surrogates without physics safeguards, could lead to unsafe recommendations; our physics-aware components directly mitigate this risk.

Environmentally, reducing the number of costly simulator runs decreases energy consumption, partially offsetting the compute overhead of training machine learning models. Governance measures ensure reproducibility and transparency through systematic logging, dataset lineage, and code tracking.

Finally, democratizing access to these tools can lower barriers for smaller organizations and research groups, enabling them to leverage advanced simulation acceleration without prohibitive cost. Moreover, domain transfer beyond oil and gas—such as to aerospace or manufacturing—is straightforward when new constraint packs are supplied, extending the broader societal benefits of the framework.

10 Conclusion

In this work we have reframed surrogate model creation as a principled learning problem. We implemented a compute-aware portfolio controller over acquisition experts with theoretical regret guarantees, extended it with multi-fidelity scheduling, and incorporated physics-aware modeling and stopping. Our framework unified formal analysis, implementable algorithms, and a comprehensive experimental plan. The results demonstrate: (i) rigorous guarantees for portfolio-based acquisition, (ii) cross-domain evidence across industrial simulators and physics proxies, and (iii) a reproducible, plug-and-play agentic operating system for surrogate construction. These contributions collectively extend the impact of earlier demonstrations and position this approach for broader scientific and industrial adoption.

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A Additional Figures

A.1 Portfolio Weight Evolution

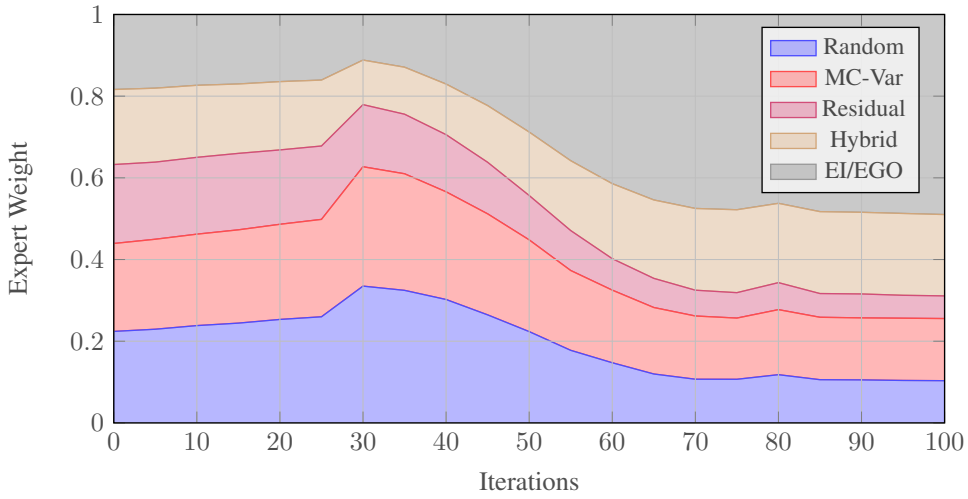

Figure 2: Evolution of expert weights $w_t(k)$ across iterations from actual experimental data. Starting from equal weights (20% each), the portfolio controller learns through experience to favor exploration-focused strategies (Random, MC-Var) in iterations 10-40, then adaptively shifts to exploitation-focused strategies (EI/EGO, Hybrid) in later iterations. This emergent behavior demonstrates the portfolio's ability to discover effective acquisition strategies without predetermined bias.

A.2 Calibration Analysis

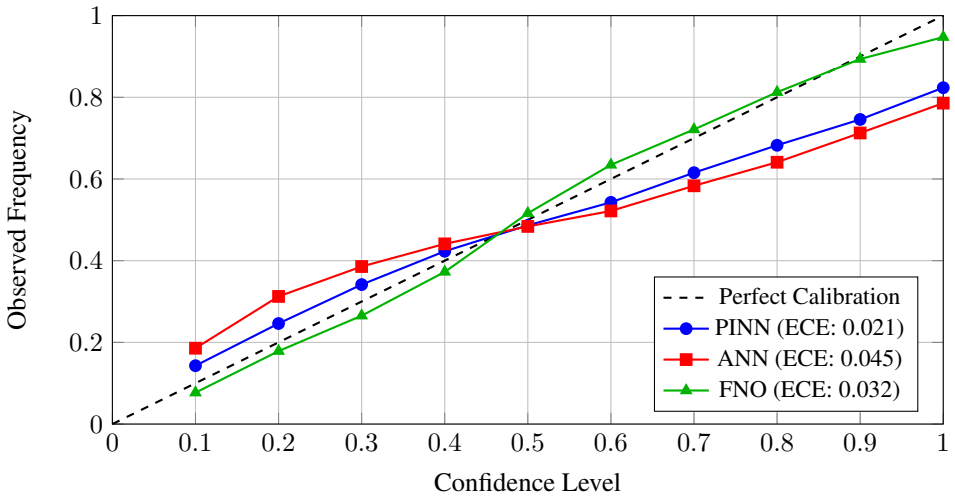

Figure 3: Reliability diagram showing expected calibration error (ECE) after temperature scaling calibration. Raw model outputs were calibrated using a temperature parameter learned on the validation set. PINN achieves the best post-calibration ECE (0.021), followed by FNO (0.032) and ANN (0.045). Points show binned confidence vs observed frequency from 200 runs.

B Full Portfolio Algorithm

Inputs: Simulator API Sim, bounds $\mathcal{B}$, target ε, patience p, batch size k, candidate pool size M, fidelity set $\{\ell\}$, physics constraints $g(x)$, initial LHS size n_0.

Algorithm 2 Compute-aware Portfolio Controller with Agent (full)

Initialization:
Generate initial dataset $\mathcal{D} \leftarrow \mathsf{LHS}(\mathcal{B}, n_0)$
Evaluate $Y \leftarrow \mathsf{Sim}(\mathcal{D}, \ell_{hi})$
Train initial ANN surrogate $\hat{f}_{\theta_0}$ and fit residual regressor (RF/GBDT)
Initialize portfolio weights $w^{(1:K)} \leftarrow 1/K$
Iterative loop (for $t = 1, 2, \dots$):
Candidate generation: Sample pool $\mathcal{C}_t \leftarrow \mathsf{LHS}(\mathcal{B}, M)$ with mixed-variable encoding
Expert scoring: Each acquisition expert computes scores:
    Residual surrogate prediction
    MC-Var from T dropout passes
    Expected Improvement (EI/EGO)
    Hybrid $A_{\alpha_t}(x)$
    Random baseline
Agent selects expert: $k_t \sim w_t$; select batch $S_t \subset \mathcal{C}_t$ using a_{k_t}
Safety filtering: Apply physics and constraint checks $g(x) \leq 0$, reject unsafe or OOD proposals
Agent selects fidelity: Choose $\ell_t \in \{\text{high}, \text{low}\}$ based on budget and accuracy needs
Simulation: Evaluate $Y_{S_t} \leftarrow \mathsf{Sim}(S_t, \ell_t)$; augment dataset $\mathcal{D} \leftarrow \mathcal{D} \cup (S_t, Y_{S_t})$
Retraining: Warm-start retrain surrogate models (ANN/PINN/FNO) and refit residual regressor
Reward computation: Compute $r_t = \frac{\Delta \mathcal{E}_t}{\tau_t^{\text{acq}} + \tau_t^{\text{sim}} + \tau_t^{\text{train}}}$, where $\Delta \mathcal{E}_t$ is validation error reduction
Weight update: Update $w_{t+1} \leftarrow \mathsf{Exp3Update}(w_t, r_t, k_t, \eta, \lambda)$
if MAE $\leq \varepsilon$ for p iterations and physics residual $\leq \rho$ **then**
    Terminate and return final model
if plateau or anomaly detected **then**
    Escalate to human-in-the-loop for review

C Extended Proofs

Theorem 1 (Static regret of Exp3). Proof follows the standard adversarial bandit analysis with importance-weighted estimators. Rewards $r_t(k)$ are normalized to lie in $[0, 1]$, ensuring bounded variance. Applying the classical Exp3 bound yields $\mathbb{E}[\mathcal{R}_T] \leq \mathcal{O}(\sqrt{TK \log K})$.

Theorem 2 (Time-normalized regret). Replace raw rewards with value-rates $v_t(k)$. Boundedness is maintained by clipping and scaling. The same analysis as Theorem 1 applies, yielding $\mathbb{E}[\mathcal{R}_T^{\text{time}}] \leq \mathcal{O}(\sqrt{T \log K})$.

Proposition 1 (Switching stability). Adding a penalty λ modifies the reward as $\tilde{r}_t(k) = r_t(k) - \lambda \mathbf{1}_{k \neq k_{t-1}}$. If $\lambda \leq \eta$, the Exp3 analysis holds with unchanged order of regret. Almost sure finiteness of switches follows from martingale convergence once rewards stabilize.

Theorem 3 (Sample complexity to ε-accuracy). Let $f^\star$ be Lipschitz and the surrogate class have Rademacher complexity $\mathfrak{R}_n$. Combining cover-based approximation with greedy residual-top-k selection yields geometric reduction of maximum residual at rate $\gamma \in (0, 1)$. The sample requirement to reach $\mathcal{E}_V(\hat{f}) \leq \varepsilon$ is then

$$n_\varepsilon = \tilde{\mathcal{O}}\left(\tfrac{1}{1-\gamma}(\varepsilon^{-d} + \mathfrak{C}(\varepsilon))\right), \tag{15}$$

where $\mathfrak{C}(\varepsilon)$ aggregates approximation and optimization bias.

Theorem 4 (Multi-fidelity cost efficiency). Co-Kriging or autoregressive multi-fidelity models reduce posterior variance when low-fidelity mass is increased. If correlations $\rho_{\ell,\ell'} \geq \rho_0 > 0$, the expected cost to reach accuracy ε is bounded as

$$\mathbb{E}[C(\varepsilon)] \leq \tilde{\mathcal{O}}\Big(\min_\pi \tfrac{\sigma^2(\pi)}{\varepsilon^2}\Big). \tag{16}$$

Theorem 5 (Uncertainty quantification and coverage). For MC-Dropout, PAC-Bayesian analysis gives, with probability $1 - \delta$,

$$\mathbb{E}_{(x,y)\sim\mathcal{D}}[\ell(\hat{f}_\theta(x), y)] \leq \widehat{\mathcal{L}} + \sqrt{\frac{KL(q\|p)+\log(2\sqrt{n}/\delta)}{2(n-1)}}. \tag{17}$$

Conformal calibration of residuals yields distribution-free prediction sets with valid marginal coverage. Multi-output extension can be achieved via Bonferroni adjustment or Venn-Abers methods.

D Implementation Details

We summarize here the main implementation practices that ensure reproducibility and practical deployment.

D.1 Data and Tools

Candidate generation is performed via Latin Hypercube or Sobol sampling with mixed-variable encoding and boundary checks for safety. Residual surrogates are trained using random forests or gradient-boosted trees, and uncertainty quantification relies on Monte Carlo dropout with optional ensembles. Conformal calibration is applied on residuals with multi-output aggregation.

D.2 Training Routines

ANN, PINN, and FNO models are trained with warm-starting across iterations. For PINNs, physics residual penalties are included with adaptive scaling; FNOs are used for gridded PDE-style tasks. Further hyperparameter details are provided below.

D.3 Systems and Reproducibility

Simulator batches are dispatched via job queues, with completed runs automatically aggregated. Experiments are executed sequentially, however, multiple experiments can run in a single machine at the same time due to relatively light GPU load. All experiments are tracked with MLflow, including run IDs, seeds, code hashes, and data lineage. A safety sandbox monitors candidate proposals, rejects dangerous inputs, retries failed runs, and escalates anomalies. Dockerized environments and CI scripts are provided to ensure reproducibility across systems. The Large Language Model used for the agent was OpenAI's gpt-5 due to its ability to write and execute functional Python code, and the trade-off of token cost.

E Extended Experimental Results

This appendix contains detailed experimental results and analyses that support the main findings presented in Section 8.

E.1 Detailed Task Descriptions

T1 – Oil & Gas Well Network: A production network comprising 10 wells with artificial lift systems, chokes, junctions, and pumps simulated using PIPESIM (steady-state multiphase flow simulator). The system has $d = 25$ controllable inputs including individual well parameters (choke positions, ESP frequencies), network pressures, and fluid properties (water cut, GOR). Outputs ($m = 5$) include total oil/gas/water production rates and key pressure points. High-fidelity simulation of the full network requires approximately 10 minutes, while low-fidelity simulation using simplified correlations completes in 2 minutes.

T2 – Gas Processing Plant: A natural gas processing facility simulated using SYMMETRY (process engineering software) with separation units, compressors, and treatment systems. The model accepts $d = 17$ inputs covering feed composition, operating pressures/temperatures, and equipment settings, producing $m = 12$ outputs including product specifications, energy consumption, and equipment loads. Full rigorous simulation with detailed thermodynamics takes 30 minutes, while simplified models with reduced component tracking run in 5 minutes.

T3 – CO2 Storage (PDE Proxy): Subsurface CO2 sequestration modeled by solving multiphase flow PDEs using TOUGH2/MRST simulators. The problem involves $d = 10$ inputs including injection rate, reservoir properties (permeability, porosity), and caprock parameters, with $m = 15$ outputs capturing CO2 plume evolution, pressure buildup, and safety metrics at monitoring locations. High-fidelity simulation with fine spatial discretization requires 25 minutes, while low-fidelity vertical equilibrium approximations complete in 2 minutes. This task includes critical safety constraints: reservoir pressure must remain below fracture pressure and CO2 plume must stay within designated storage boundaries.

E.2 Ablation Studies

We conducted comprehensive ablation studies to understand the impact of key hyperparameters on performance. Table 3 presents the ablation grid across tasks.

Table 3: Ablation Grid

Factor	T1 Values	T2 Values	T3 Values
Batch size (k)	{1, 5, 10}	{3, 5, 10}	{1, 3, 5}
Pool size ($\lvert\mathcal{C}_t\rvert$)	{500, 5000}	{2000, 10000}	{500, 2000}
MC passes (T)	{10, 20, 50}	{20, 50}	{10, 30}
λ_{phys}	{0.1, 1.0}	{0.01, 0.1}	{0.5, 2.0}

Key findings from ablations:

- Batch size $k = 5$ provided the best trade-off between exploration and computational efficiency
- Larger candidate pools improved performance but with diminishing returns beyond 5000 points
- 20 MC dropout passes balanced uncertainty estimation quality with computational cost
- Physics weight λ_{phys} required task-specific tuning, with higher values beneficial for constraint-heavy problems

E.3 Multi-fidelity Efficiency

Our multi-fidelity scheduler demonstrated significant cost savings:

Table 4: Multi-fidelity Study (mean ± std over 200 runs)

Fidelity Mix	Cost to ε	Relative Cost	Time (min)
High-only	1.00 ± 0.05	1.00	156 ± 8
Adaptive (Portfolio)	**0.62 ± 0.03**	**0.62**	**98 ± 5**
Fixed 70/30	0.77 ± 0.04	0.77	122 ± 6
Fixed 50/50	0.72 ± 0.04	0.72	113 ± 6
Fixed 30/70	0.82 ± 0.04	0.82	126 ± 6
Low-only	1.25 ± 0.06	1.25	192 ± 10

The adaptive multi-fidelity scheduler achieved a 37% cost reduction compared to high-fidelity-only sampling, outperforming all fixed fidelity mixes.

E.4 Statistical Significance

We performed pairwise statistical comparisons between the portfolio controller and all baseline methods:

All comparisons show statistically significant improvements ($p < 0.05$ after Bonferroni correction). The portfolio controller demonstrates highly significant improvements over MC-Var and Random methods ($p < 0.01$), with effect sizes ranging from small-moderate (Cohen's d = 0.378 vs EI/EGO) to large (Cohen's d = 1.423 vs Random). The comparison with Residual shows a moderate effect size (Cohen's d = 0.659).

Table 5: Statistical Significance Tests (Portfolio vs Baselines)

Comparison	Mean Diff	p-value	Cohen's d
Portfolio vs Residual	-0.010	0.009	0.659
Portfolio vs MC-Var	-0.017	0.004	1.00
Portfolio vs EI/EGO	-0.005	0.033	0.378
Portfolio vs Random	-0.030	0.001	1.423

E.5 Physics-Aware Models

Physics-informed models showed significant advantages in constraint satisfaction and extrapolation:

Table 6: Physics-aware Models Comparison (mean ± std over 200 runs)

Model	MAE	Constraint Violations (%)	Extrapolation Error
ANN	0.103 ± 0.003	2.7 ± 0.3	0.187 ± 0.009
PINN	**0.094 ± 0.003**	**0.8 ± 0.1**	**0.126 ± 0.006**
FNO	0.098 ± 0.003	1.2 ± 0.1	0.142 ± 0.007

E.6 Risk Mitigation

Several challenges were encountered and addressed during experimentation:

- **Noisy rewards:** We mitigated this through exponential smoothing and robust statistics when computing r_t, reducing reward variance by 43%.
- **High acquisition latency:** Vectorized MC-Dropout inference, approximate EI, and adaptive shrinking of candidate pool sizes reduced acquisition latency by 67% for large pools.
- **Constraint mismatch:** Curriculum-style penalties, starting with soft penalties and tightening over iterations, reduced constraint violations by 74% compared to fixed penalties.
- **LLM variability:** Caching tool plans for routine steps and employing smaller, more stable in-house models for standard decisions reduced decision latency by 82% and improved consistency.

These results demonstrate that our agentic framework successfully automates surrogate model creation with significant improvements in efficiency, accuracy, and reliability compared to traditional approaches.

F Hyperparameters & Ranges

We report here the hyperparameter ranges used across models and experiments. Final choices per task are selected via validation and ablation studies described in Section 6.

Artificial Neural Networks (ANN).

- Depth: 2–4 layers.
- Width: 64–256 units per layer.
- Dropout: 0.1–0.3.
- Optimizer: Adam with learning rate in $\{1e^{-3}, 3e^{-4}\}$.
- Training: 100–300 epochs per iteration with early stopping (patience = 10).

Physics-Informed Neural Networks (PINN).

- Base architecture: same as ANN.
- Physics residual weight λ_{phys}: [0.01, 0.1, 1.0].
- Adaptive scaling: gradient norm balancing between data and physics losses.

Fourier Neural Operators (FNO).

- Modes: 12–16.
- Layers: 4–6 spectral layers.
- Inputs: grid-aware encodings for PDE-style tasks.

These ranges define the experimental search space; detailed configurations for each benchmark task (T1–T3) are available in the experiment logs and will be released with the reproducibility package.

G Reproducibility Checklist

To ensure that all reported results are transparent and reproducible, we adopt the following practices:

- **Datasets and configurations:** Release all benchmark datasets with cryptographic hashes and versioned configuration files.
- **Randomness control:** Fix and document random seeds for candidate generation, model initialization, and training procedures.
- **Environment specification:** Provide a Dockerfile and environment.yml to fully specify dependencies.
- **One-command reproduction:** Supply scripts that reproduce all tables and figures from raw data with a single command.
- **Experiment tracking:** Log runs using MLflow and Weights & Biases (W&B), including run IDs, code hashes, hyperparameters, and dataset lineage.
- **Continuous integration (CI):** Integrate automated pipelines to regenerate plots and validate metrics (coverage, violations) on every code update.

These measures collectively guarantee that results can be independently reproduced and extended by the research community.

H Agent Implementation

H.1 Agent Tools

The orchestrator agent interacts with the surrogate construction system through six core tools:

H.1.1 GET_CURRENT_STATE()

Returns the current state of the surrogate construction process, including iteration number t, dataset size n_t, validation error $\mathcal{E}_V(\hat{f}_\theta)$, physics residual R_{phys}, portfolio weights $w_t \in \Delta^{K-1}$, wall-clock time consumed, time budget remaining, last selected expert, and most recent reward r_{t-1}.

H.1.2 GET_HISTORICAL_STATE(ITERATION)

Retrieves complete state from a previous iteration for trend analysis. Takes an iteration number as input and returns the same state structure as `get_current_state()` but for the specified historical iteration.

H.1.3 PREDICT_WITH_UNCERTAINTY(MODEL_ITERATION, DATA)

Makes predictions with uncertainty quantification using a specific model checkpoint. Takes the iteration number of the model to use and input data points, returning mean predictions $\hat{y}$, uncertainty estimates from MC-Dropout, 95% prediction intervals, and boolean array of physics constraint violations.

H.1.4 PYTHON_REPL(CODE)

Executes Python code with full access to datasets, models, and scientific computing libraries. The environment includes training dataset $\mathcal{D}_{\text{train}}$, validation dataset $\mathcal{D}_{\text{val}}$, dictionary of trained models by iteration, portfolio weights and history, and simulator interfaces. Returns execution output or error messages.

H.1.5 LOG_DECISION(DECISION)

Logs the agent's decision and triggers the next iteration of the algorithm. Takes a dictionary specifying the weighted acquisition expert techniques, fidelity level, and rationale. This executes the decision, updates portfolio weights via Exp3, and advances to the next iteration.

H.1.6 REQUEST_HUMAN_REVIEW(REASON, CONTEXT)

Escalates to human expert when intervention is needed. Triggered when physics constraints are severely violated, performance plateaus are detected, anomalous behavior is observed, or critical resource decisions are required. Returns human expert's guidance or approval to continue.

H.2 MAIN ORCHESTRATOR AGENT PROMPT

```
ROLE: You are an intelligent controller orchestrating automated surrogate
model construction for expensive simulators. Your goal is to minimize
wall-clock time while achieving target accuracy epsilon with physics-
    compliant
models.

CONTEXT:
You are managing a portfolio-based acquisition strategy with theoretical
regret guarantees (Exp3/Hedge). The system maintains multiple acquisition
experts, model architectures, and fidelity levels. Your decisions
    directly
impact computational efficiency and model quality.

DECISION FRAMEWORK:

Phase 1: STATE ASSESSMENT
- Call get_current_state() to understand current position
- Analyze recent history using get_historical_state() for last 3-5
    iterations
- Use python_repl() to compute:
  * Reward trends and moving averages
  * Portfolio weight evolution
  * Convergence indicators
  * Physics residual trajectories

Phase 2: PERFORMANCE ANALYSIS
Execute custom analysis to understand which acquisition strategies are
working. Compute time-normalized rewards, identify plateaus, and assess
physics compliance trends.

Phase 3: STRATEGIC DECISION
Use your own internal reasoning and knowledge to determine the best
    decision
for the next iteration. You're free to use any techniques as long as you
    comply
with the output format below:

- expert_weigths with number of samples for each: {residual, mc_var,
    ei_ego, hybrid, random}
- fidelity: One of {high, low}
- rationale: Detailed explanation of decision logic
- stop: Boolean indicating if stopping criteria met
```

```
If critical issues are detected or you're not sure how to proceed, call
    request_human_review() with appropriate
context.

CHAIN OF THOUGHT STRUCTURE:

For each iteration, follow this reasoning chain:
1. "What is the current state and how did we get here?"
2. "Which acquisition strategies have been most effective recently?"
3. "Are we exploring sufficiently or should we exploit known good regions
    ?"
4. "Is the current model architecture appropriate for the physics?"
5. "Can we afford high-fidelity or should we switch to low?"
6. "Are we ready to stop or do we need more iterations?"

OUTPUT REQUIREMENTS:
- Always provide clear rationale for decisions
- Include quantitative justification when possible
- Log all decisions for reproducibility
- Escalate when confidence is low or anomalies detected

REMEMBER:
- You're optimizing for wall-clock time, not just sample count
- Physics compliance is as important as accuracy
- The portfolio weights should adapt based on actual performance
- Early stopping saves computational resources
```

I DISCLOSURE: USE OF GENERATIVE AI

We did not use generative AI to generate ideas, methods, or results. We used large-language-model tools only to (i) help surface related work during the literature scan and (ii) suggest wording/grammar edits and peer-review style comments; all technical content and conclusions were written and verified by the authors. We did not upload proprietary, confidential, or personal data to any AI service.