REAL-TIME X-RAY BEAMLINE SURROGATE MODELING VIA A PHYSICS-INFORMED LOG-MANIFOLD LEARNING FRAMEWORK *

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Abstract

Wave-optical simulation of undulator radiation through X-ray beamlines is computationally prohibitive, limiting real-time optimization. The high-frequency diffraction structures and extreme dynamic range of focal spot distributions pose significant challenges to conventional surrogate models. We propose a log-manifold surrogate modeling framework that represents intensity distributions in logarithmic space, converting highly nonlinear diffraction structures into low-rank learnable manifolds. With physics-informed OOD-aware Residual method, the model attains less than 1% relative error over the full dynamic range, faithfully reconstructs fine diffraction fringes, and generalizes robustly across beamline configurations. Single prediction takes only milliseconds, yielding thousands of speedup over SRW simulation and enabling real-time surrogate-based beamline optimization. This work demonstrates an efficient path toward real-time digital-twin beamline modeling for fourth-generation light sources, enabling online optimization, rapid parameter scans, and virtual diagnostics.

INTRODUCTION

High-coherence synchrotron radiation sources are essential for advanced imaging and nanoscale characterization. Steady-State Microbunching (SSMB) [1] is a promising scheme for next-generation coherent light sources capable of generating nearly fully coherent radiation in storage rings. In this context, accurate modeling of wavefront propagation in synchrotron radiation beamlines is important for beamline design and parameter optimization.

High-fidelity wave optics simulations such as Synchrotron Radiation Workshop (SRW) [2] can accurately describe diffraction and coherence effects but are computationally expensive for large-scale parameter scans or real-time optimization. Machine learning–based [3] surrogate models provide a promising approach to accelerate beamline simulations. However, synchrotron radiation intensity distributions typically exhibit high dynamic range and fine diffraction fringes with high spatial frequencies, while purely data-driven models often suffer from limited extrapolation capability.

In this work, we propose a surrogate modeling framework combining log-manifold representation with physics-informed residual learning. The log-manifold mapping compresses the dynamic range and reveals a low-rank structure for efficient reduced-order modeling. A residual learning strategy further integrates prior physical models with data-driven corrections to improve robustness and extrapolation capability.

Numerical experiments based on SRW simulations demonstrate that the proposed approach accurately predicts complex diffraction patterns while significantly reducing computational cost.

LOG-MANIFOLD REPRESENTATION

Log-Manifold Mapping

In Steady-State Microbunching (SSMB) light sources, electrons in a microbunch radiate coherently in the radiation element, producing radiation spots with complex diffraction patterns and fine high-frequency interference fringes. In addition, the radiation intensity scales approximately as $I \propto N^2$ with respect to the electron number, resulting in an extremely large dynamic range.

Such characteristics lead to numerical imbalance in the original linear intensity space. High-intensity regions tend to dominate error metrics, while fine diffraction structures in low-intensity regions become difficult to capture for data-driven surrogate models. Therefore, an appropriate representation is required to balance the dynamic range and improve the learnability of diffraction patterns.

To alleviate this problem, a log-manifold mapping is introduced to map the radiation intensity into a more balanced representation space. Let $I(x)$ denote the radiation intensity distribution at spatial coordinate x in linear space. The log-manifold mapping [4] is defined as

$$T : I(x) \to L(x) = \log(I(x) + \epsilon), \quad \epsilon \ll 1 . \qquad (1)$$

This mapping significantly compresses the dynamic range of the radiation intensity. Intensity variations spanning several orders of magnitude are mapped into a more balanced numerical scale. Meanwhile, the log-manifold mapping partially equalizes intensity variations across spatial regions, making high-frequency diffraction structures more uniformly represented.

Log-Domain Proper Orthogonal Decomposition

In the log-manifold, the dynamic range of synchrotron radiation intensity is significantly reduced, leading to more balanced numerical representation across spatial regions. As a result, radiation patterns typically exhibit low-dimensional structures. In this work, Proper Orthogonal Decomposition (POD) [5] is applied to the log-domain radiation snapshots to extract the dominant modes.

Let $\phi_j(x)$ denote the j-th log-domain radiation snapshot. POD seeks a set of orthogonal basis functions $\{\psi_k(x)\}_{k=1}^{r}$

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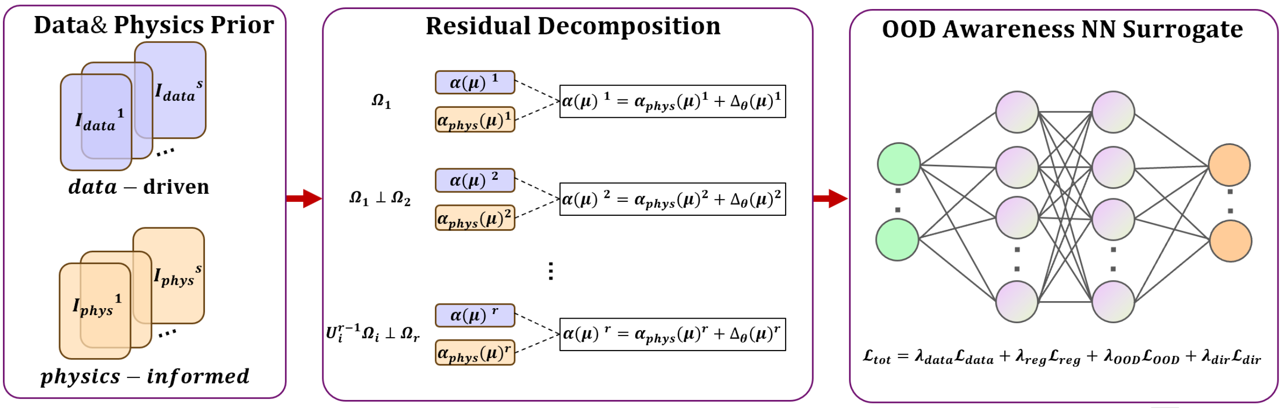

Figure 1: Physics-informed residual surrogate.

such that the radiation field can be optimally approximated in the least-squares sense using r modes,

$$\min_{\{\psi_k\}_{k=1}^{r}} \frac{1}{M}\sum_{j=1}^{M}\left\|\phi_j - \sum_{k=1}^{r} a_{jk}\psi_k\right\|^2_{L^2(\Omega)} \tag{2}$$

where a_{jk} denotes the corresponding modal coefficients.

Numerical results show that synchrotron radiation patterns in the logarithmic manifold exhibit strong low-rank characteristics. Only a small number of POD modes are required to preserve more than 99.99% of the energy of the dataset. Based on this reduced representation, the original high-dimensional radiation prediction problem can be transformed into the prediction of a small set of POD coefficients, which provides the foundation for constructing efficient surrogate models.

PHYSICS-INFORMED RESIDUAL SURROGATE

In surrogate modeling, the target physical quantity can often be partially described by simplified physical models. However, due to model approximations and parameter uncertainties, such models are generally unable to accurately reproduce high-fidelity simulation results.

To address this limitation, a physics-informed residual learning framework is adopted in this work. The physical model provides a prior prediction, while a neural network learns the systematic discrepancy between the physical model and the high-fidelity simulation data. This strategy enables accurate surrogate modeling while preserving physical consistency.

Residual Learning Framework

Let $I_{\text{phys}}(x)$ denote the radiation intensity distribution predicted by a simplified physical model. After applying the same log-manifold mapping and POD procedure, the corresponding physical prior POD coefficients can be obtained as $\alpha_{\text{phys}}(\mu)$, where μ represents the system input parameters.

A neural network is then introduced to learn the residual correction between the physical prior and the true data,

$$\alpha(\mu) = \alpha_{\text{phys}}(\mu) + \Delta_\theta(\mu) \tag{3}$$

where $\alpha(\mu)$ denotes the final predicted POD coefficients, $\Delta_\theta(\mu)$ represents the residual correction predicted by the neural network, and θ denotes the network parameters.

The neural network therefore learns only the residual not captured by the physical model, reducing the learning complexity and improving model stability.

As shown in Fig.1, the network parameters are optimized by minimizing the weighted mean squared error between the predicted POD coefficients and the reference coefficients obtained from SRW simulations during the training. A weak residual regularization term is introduced to constrain large non-physical corrections, and a cosine similarity constraint is applied to maintain directional consistency with the physical prior in the POD coefficient space.

OOD-Aware Residual Correction

To further improve the stability and generalization capability of the residual surrogate model under parameter extrapolation (Out-of-Domain, OOD), a distance-aware extrapolation constraint is introduced.

During training, additional sampling points are randomly generated in the parameter space, and their distance to the boundary of the training data distribution is evaluated. When the input parameters move away from the training domain, stronger penalties are imposed on the residual correction predicted by the neural network,

$$\mathscr{L}_{OOD} = \lambda(d)|\Delta_\theta(\mu)| \tag{4}$$

where d denotes the distance between the sample and the boundary of the training domain, and $\lambda(d)$ is a distance-dependent weighting function.

In the present implementation, $\lambda(d)$ increases quadratically with the distance. As a result, when the input parameters move further away from the training region, the residual correction gradually diminishes, preventing unstable extrapolation behavior.

With this mechanism, the surrogate model can perform accurate residual corrections within the training domain, while gradually reverting to the calibrated physical model in the extrapolation region. This design improves the robustness and stability of the surrogate model while maintaining high prediction accuracy.

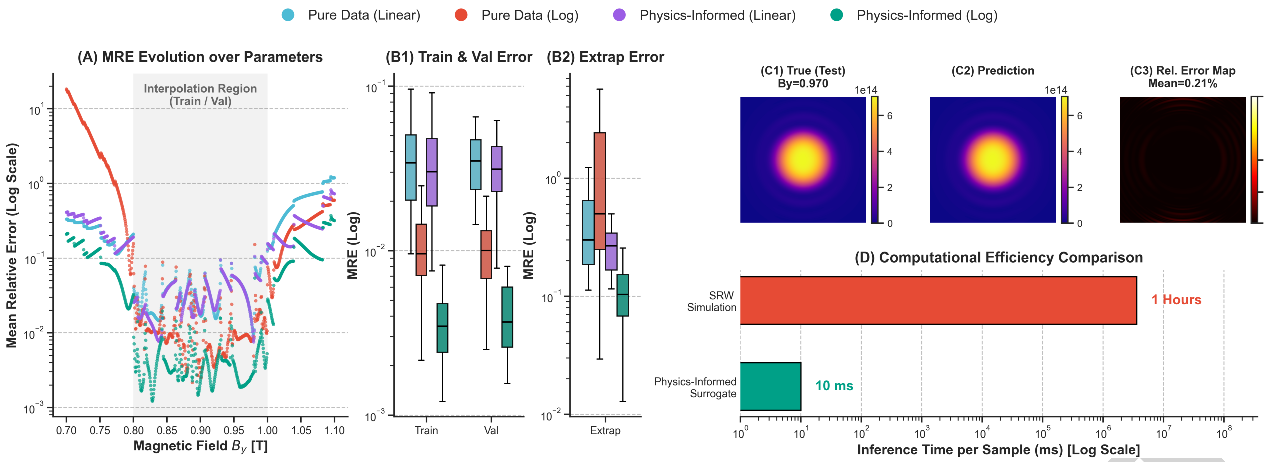

Figure 2: Performance and efficiency of surrogate models. (A) MRE vs. magnetic field B_y(shaded: interpolation). (B1-B2) Error boxplots confirming the superior extrapolation robustness of the Physics-Informed model. (C1-C3) 2D intensity prediction and spatial error for a representative test sample. (D) Inference time comparison showing massive acceleration.

NUMERICAL RESULTS

To validate the proposed physics-informed residual surrogate model, a representative undulator radiation case corresponding to the fundamental harmonic is constructed using SRW. The undulator consists of 70 periods with a period length of 33 mm. The electron beam energy is 6 GeV with an energy spread of 1.1×10^{-3}, and the beam parameters correspond to a fourth-generation diffraction-limited storage ring.

Radiation intensity distributions are generated by scanning the undulator magnetic field B_y from 0.7 T to 1.1 T (corresponding to variations of the undulator parameter K). These high-fidelity SRW simulations serve as reference solutions, while a simplified physical model provides prior predictions.

The approximate radiation intensity given by the simplified physical model is expressed as

$$I_1 = I_0 \,\mathrm{sinc}^2\left(\frac{N_u \pi \gamma^2}{1+\frac{K^2}{2}} \frac{x^2+y^2}{z^2}\right) \tag{5}$$

$$I_{\mathrm{phys}} = I_1 \otimes \mathcal{N}\left(0, \sigma^2_{\mathrm{eff},x}, \sigma^2_{\mathrm{eff},y}, \sigma^2_{\mathrm{eff},\delta}\right).$$

Based on the generated dataset, a physics-informed residual surrogate model is constructed using the radiation intensity distributions and compared with a purely data-driven surrogate model.

As shown in Fig.2, numerical results show that the proposed model can more accurately capture the spatial structure of the radiation intensity distribution for both interpolation tests within the training domain and extrapolation tests outside the training domain. Compared with the purely data-driven surrogate model, the physics-guided residual learning framework significantly reduces the relative prediction error. In particular, with the introduction of the OOD distance-aware constraint, the model exhibits improved stability and generalization performance in the extrapolation region.

Furthermore, compared with the computationally expensive SRW simulations, the proposed surrogate model achieves significant computational acceleration while maintaining high prediction accuracy.

CONCLUSION

A surrogate modeling framework for synchrotron radiation prediction based on log-manifold representation and physics-guided residual learning has been proposed. By incorporating physical model priors and learning residual corrections with a neural network, efficient prediction of radiation intensity distributions can be achieved.

In the future, the proposed framework will be applied to SSMB radiation dynamics analysis and beamline optimization problems. It also provides a promising approach for digital twin modeling of beamline systems in fourth-generation synchrotron light sources, supporting applications such as online parameter optimization, fast parameter scanning, and virtual diagnostics.

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