Exploring Physics-Informed Machine Learning for System Matrix Formulation in X-Ray Imaging Forward Models

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ABSTRACT

This study presents an innovative approach to constructing a representative system matrix in X-ray imaging forward models. The approach leverages the combination of machine learning algorithms and fundamental physical principles through the use of physics-informed machine learning (PIML). The main goal is to seamlessly integrate machine learning algorithms with core physical principles to provide a nuanced perspective on the development of an interpretable and adaptive system matrix. In contrast to traditional data-intensive methods, this research intentionally prioritizes the incorporation of physics-based constraints into the machine learning framework. The methodology involves carefully extracting relevant features from X-ray imaging data to capture essential object characteristics, which are then integrated into a machine learning model. By including physics-based constraints, the model aligns with the underlying principles that govern X-ray interactions. Through rigorous mathematical validation and preliminary experimentation, the approach demonstrates its feasibility, particularly in situations where acquiring extensive datasets is challenging. From a technical standpoint, the strength of this methodology lies in the inherent adaptability and interpretability of the system matrix, which are crucial for accurate image reconstruction and measurement prediction. The implications of this research span diverse domains and highlight the potential transformative effects on X-ray imaging applications in electronics, medical imaging, and material inspection. In the realm of electronics, the adaptable system matrix improves non-destructive testing by aiding in defect detection and ensuring the reliability of electronic components. In medical imaging, enhanced interpretability leads to improved diagnostic accuracy while reducing radiation exposure. In material inspection, this approach facilitates the identification of structural anomalies and material composition, thereby advancing quality control practices. While recognizing the preliminary nature of the framework, this study lays the groundwork for future research at the intersection of machine learning and physics in X-ray imaging, representing a progressive step towards unlocking transformative possibilities for enhanced accuracy and adaptability across various domains.

Keywords: X-ray imaging, Physics-informed Machine Learning, System Matrix, Forward Models

1. INTRODUCTION

1.1 Motivation

The rationale behind this study originates from the constraints of conventional machine learning methodologies, which frequently necessitate extensive datasets and lack of explainability when utilized in complex systems like X-ray imaging.[1] Physics-Informed Machine Learning (PIML) presents an innovative resolution by integrating fundamental physical principles into machine learning algorithms,[2] ensuring that the models not only derive insights from data but also comply with the established laws governing X-ray interactions. The incorporation of PIML into X-ray imaging forward models results in a more precise and adaptable system matrix, thereby enhancing image reconstruction and measurement prediction. This methodology proves particularly advantageous in fields such as electronics, medical imaging, and material inspection, where it holds the potential to transform practices by enhancing defect identification, diagnostic precision, and quality assurance through a more comprehensible and dependable framework.

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Developments in X-Ray Tomography XV, edited by Bert Müller, Ge Wang,
Proc. of SPIE Vol. 13152, 131521W · © 2024 SPIE
0277-786X · doi: 10.1117/12.3027381

1.2 Problem Statement

The issue explored in this research concerns the challenge of accurately constructing a system matrix for X-ray imaging forward models. Conventional methods encounter obstacles such as restricted datasets, absence of interpretability, and inadequate integration of the fundamental physical principles that govern X-ray interactions.

1.3 Proposed Solution

The suggested solution entails the utilization of Physics-Informed Neural Networks (PINNs) for formulating the system matrix in X-ray imaging forward models. This strategy seamlessly incorporates fundamental physical principles, such as X-ray attenuation and scattering regulated by the Beer-Lambert law,[3] directly within the machine learning framework. Through the creation of a network that minimizes a combined loss function, balancing data fidelity with compliance to these physical laws, the technique guarantees precise and understandable system matrix construction, even with limited training data. This amplifies the predictive capabilities and resilience of the model in X-ray imaging applications.

2. RELATED WORKS

2.1 Physics-Informed Machine Learning (PIML) in Computational Imaging

Physics-Informed Machine Learning (PIML) has garnered considerable attention in the field of computational imaging, presenting a new approach in which the fusion of physical principles into machine learning frameworks enhances interpretability and precision. In contrast to conventional data-driven methodologies that often necessitate extensive datasets and may encounter challenges in generalization, PIML integrates fundamental equations—such as those governing wave propagation, heat diffusion, or X-ray attenuation—directly into the structure of the model. This integration guarantees that the acquired models are not only physically accurate but also resilient, particularly in scenarios with limited data availability. For instance, in the domain of X-ray imaging, the incorporation of the Beer-Lambert law into the model ensures adherence to established physical laws, resulting in more dependable image reconstructions and improved handling of noisy data. Research indicates that PIML not only diminishes the reliance on large training datasets but also enhances the model's capacity to extrapolate beyond the observed data, a feature especially beneficial in fields like medical imaging, non-destructive testing, and remote sensing applications.[4–8] This burgeoning field holds the potential to transform computational imaging by furnishing models that are not solely data-centric but also deeply rooted in the physics underlying the problem, thereby paving the way for more precise, effective, and comprehensible imaging solutions. Figure 1 illustrates an example process of how PIML can be integrated in computational imaging.

2.2 Underlying Physics Principles in X-ray Imaging

X-ray imaging operates based on the fundamental principles of X-ray attenuation and scattering, primarily elucidated by the Beer-Lambert law. This law delineates the exponential reduction in X-ray intensity as they traverse a substance, where attenuation is contingent upon the density and thickness of the material, characterized by its linear attenuation coefficient.[10,11] Moreover, scattering phenomena, such as Compton and Rayleigh scattering, play a role in shaping the propagation of X-rays, contributing intricacy to the process of image formation. These foundational physical principles are essential for precise establishment of the system matrix in X-ray imaging, ensuring that algorithms for image reconstruction faithfully depict the interactions between X-rays and the substances under examination.[12,13]

3. METHODOLOGY

3.1 Components of X-ray Imaging Forward Models

The main elements of X-ray imaging forward models consist of the system matrix, the measurement vector, and the object's attenuation coefficients. The system matrix $\mathbf{A}$ illustrates the X-ray attenuation process, linking the object's internal structure to the measurements detected by the sensor. The measurement vector $\mathbf{y}$ is derived from projecting X-rays through the object and capturing the attenuated beams, expressed as $\mathbf{y} = \mathbf{Ax} + \mathbf{n}$, where $\mathbf{x}$ represents the object's attenuation coefficients and $\mathbf{n}$ denotes noise. The attenuation of X-rays follows the Beer-Lambert law, which mathematically explains the exponential reduction in X-ray intensity based on

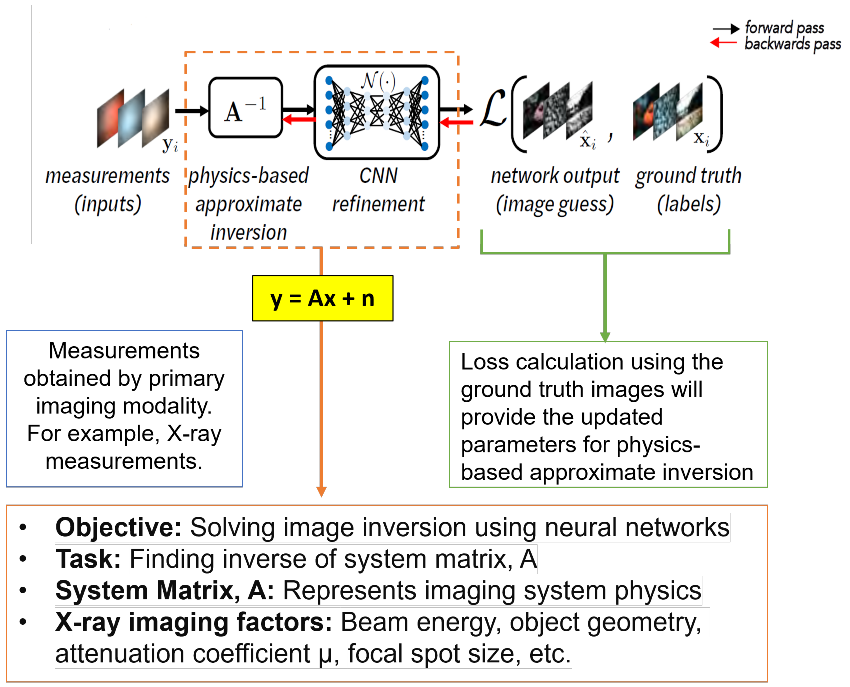

Figure 1: Applications of Physics-Informed Neural Networks in Computational Imaging.[9]

material thickness and attenuation coefficient μ. The system matrix $\mathbf{A}$ encompasses these physical interactions, incorporating the X-ray system's geometry and the object's material properties.[3,14]

3.2 Mathematical Formulation of System Matrix for X-ray Imaging Forward Models

The system matrix $\mathbf{A}$ in X-ray imaging forward models encapsulates the relationship between the attenuation properties of an object and the detected X-ray measurements. This matrix plays a pivotal role in translating the internal structure of the object into measurable projection data at the detector.[12,13,15,16] The measurement at the i-th detector element, denoted as b_i, is given by:

$$b_i = \sum_{j=1}^{N} A_{ij} x_j, \tag{1}$$

where:

- b_i is the measured projection data at the i-th detector element, representing the total X-ray signal detected after passing through the object.
- A_{ij} is the i, j-th element of the system matrix, quantifying the contribution of the j-th voxel to the i-th detector element.
- x_j is the attenuation coefficient of voxel j, indicating how much the X-ray is attenuated as it passes through that voxel.
- N is the total number of discretized voxels in the object, each contributing to the overall projection measured by the detector.

The updated formulation of the system matrix element A_{ij} incorporates several key factors that influence the detection process. It is mathematically expressed as:

$$A_{ij} = G_j \cdot S_j \cdot E_j \cdot e^{-\mu_j l_{ij}} \cdot (1 + \sigma_j) \cdot H_j \cdot N_j, \tag{2}$$

where each term is defined as follows:

- **Geometric Efficiency G_j:** This term represents the fraction of X-ray photons that successfully reach the detector after interacting with the object. It accounts for the geometrical configuration of the X-ray source, the object, and the detector. The geometric efficiency is crucial because it ensures that the system matrix reflects the physical reality of how X-rays traverse through the object, considering factors like the divergence of the X-ray beam and the distance from the source to the detector.

- **Detector Sensitivity S_j:** Detector sensitivity reflects the detector's capability to convert the incident X-ray photons into measurable electrical signals. This term accounts for the detector's intrinsic properties, including its material composition and design, which influence its responsiveness to the incoming X-ray flux. High detector sensitivity is essential for accurate measurement, as it maximizes the conversion of X-ray energy into a detectable signal.

- **Electronic Efficiency E_j:** The electronic efficiency term accounts for the effectiveness of the detector's electronic components in converting the analog signals generated by the incident X-rays into digital data. This includes the efficiency of analog-to-digital conversion processes, signal amplification, and noise reduction mechanisms within the detector's electronics. Higher electronic efficiency ensures that the detected signals are accurately digitized with minimal loss of information.

- **Attenuation Term $e^{-\mu_j l_{ij}}$:** This exponential term represents the attenuation of X-ray intensity as it passes through the j-th voxel of the object. According to the Beer-Lambert law, the X-ray intensity decreases exponentially with the product of the attenuation coefficient μ_j and the path length l_{ij} through the voxel. This term is fundamental to the system matrix as it directly relates the material properties of the object to the X-ray measurements, ensuring that denser or thicker materials contribute more to the attenuation.

- **Scatter Correction Factor σ_j:** The scatter correction factor accounts for the contribution of scattered radiation from the j-th voxel to the measured data. Scattered X-rays, which deviate from their original path after interacting with the object, can introduce errors in the measurement. The correction factor σ_j adjusts for these errors, improving the accuracy of the system matrix by mitigating the impact of scatter on the detected signal.

- **Beam Hardening Correction Factor H_j:** Beam hardening occurs when X-rays of different energies are attenuated at different rates, leading to a shift in the effective energy spectrum of the X-ray beam as it passes through the object. The beam hardening correction factor H_j compensates for this effect, ensuring that the attenuation term accurately reflects the energy-dependent attenuation characteristics of the material. This correction is particularly important for imaging materials with high atomic numbers, where beam hardening effects are more pronounced.

- **Detector Noise Factor N_j:** This term models the impact of noise on the measured data, encompassing various sources of uncertainty, such as electronic noise in the detector, quantum noise from the X-ray source, and environmental noise. The detector noise factor N_j contributes to the overall uncertainty in the reconstructed images and is essential for accurately representing the stochastic nature of the measurement process.

Incorporating these factors into the system matrix **A** allows for a more accurate and realistic representation of the X-ray imaging process, capturing the complex interplay between the X-ray source, the object, and the detector. This comprehensive formulation is critical for improving the accuracy of image reconstruction, particularly in applications where high precision is required.

3.3 Key Assumptions in Defining Prior System Matrix

The fundamental assumptions incorporated in the prior system matrix for X-ray imaging forward models involve the assumptions of homogeneity and isotropy of material properties within individual voxels, together with the assumption of linearity in X-ray interactions with the object. Typically, Gaussian priors are employed to initialize the system matrix due to their capacity to offer mathematical tractability and effectively capture the anticipated smooth variations in attenuation coefficients throughout the object. The rationale behind this selection lies in the Gaussian distribution's capability to portray uncertainty and establish a statistically sound framework, which is crucial for incorporating physical constraints and noise characteristics into the model.[17] This methodology guarantees that the initial system matrix is both practical and computationally effective, thereby laying a strong groundwork for further enhancement through iterative techniques or Physics-Informed Neural Networks (PINNs).

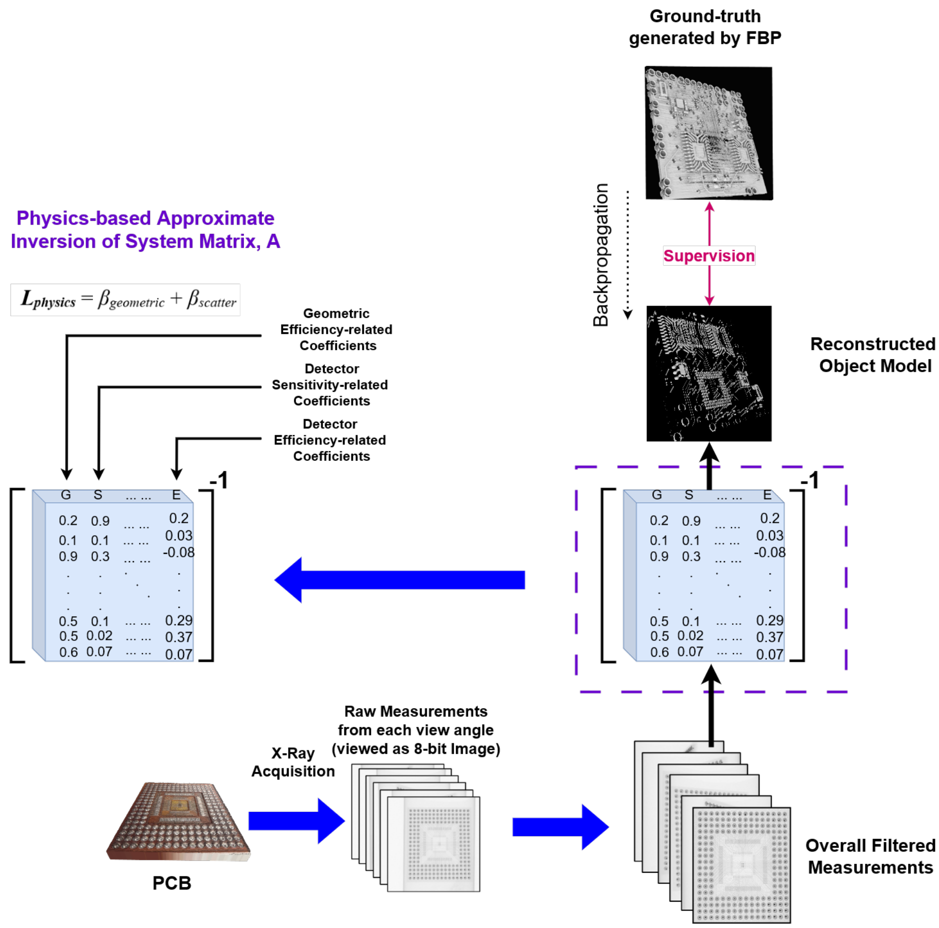

Figure 2: Physics-Informed Machine Learning for System Matrix Formulation in X-Ray Imaging Forward Models: A PCB inspection case study

3.4 Integration of PIML

The incorporation of Physics-Informed Machine Learning (PIML) within the matrix formulation of the X-ray imaging system serves to improve the precision and resilience of image reconstruction by directly embedding physical constraints into the model. The process involves a physics-based approximate inversion of the system matrix **A**, as depicted in the figure (Figure 2), where coefficients linked to geometric efficiency G, detector sensitivity S, and detector efficiency E are initially included. These coefficients undergo refinement via the minimization of a loss function L_{physics} defined as:

$$L_{\text{physics}} = \beta_{\text{geometric}} + \beta_{\text{scatter}}, \tag{3}$$

with $\beta_{\text{geometric}}$ addressing geometric efficiency-related adjustments and β_{scatter} accommodating the scatter correction element.

Subsequently, the refined system matrix $\mathbf{A}$ is employed for object model reconstruction based on the overall filtered measurements. This reconstruction procedure is guided by a reference model created using conventional methods like Filtered Back Projection (FBP).[3,10,18] The guidance from this reference model enables the PIML system to undergo iterative enhancements to the system matrix. This iterative process is carried out for all projections to maintain the consistency of the system matrix with the fundamental principles governing X-ray interactions, thereby significantly enhancing the faithfulness of the reconstructed images.

3.5 Influential Factors

The formulation of the initial system matrix and the integration of Physics-Informed Machine Learning (PIML) are influenced by multiple crucial factors that necessitate meticulous consideration to ensure precision and dependability in X-ray imaging forward models:

- **Material Properties:** The assumptions of homogeneity and isotropy concerning the material properties of the object can significantly impact the accuracy of the system matrix. Variations in density and composition necessitate the adaptability of the system matrix to reflect these heterogeneities, thus averting reconstruction errors.
- **Geometric Configuration:** The relative positions of the X-ray source, object, and detector exert influence on the geometric efficiency term. Precise modeling of these configurations is imperative to guarantee that the system matrix accurately depicts the X-ray paths through the object.
- **Energy Spectrum and Detector Response:** The energy spectrum of the X-ray source and the response function of the detector must be meticulously considered in the system matrix. These aspects directly impact the attenuation and detector sensitivity terms, underscoring the significance of their accurate representation for realistic imaging.
- **Scattering Effects:** Materials with high density can introduce substantial scattering, potentially distorting the measured signals. The inclusion of scatter correction factors within the system matrix is crucial to alleviate these effects and uphold the fidelity of the reconstruction.
- **Noise Modeling:** Environmental noise as well as electronic noise within the detector system can influence the assumptions of the initial system matrix. Robust noise modeling and correction mechanisms are imperative to ensure that the integration of PIML adeptly manages these uncertainties, thereby preserving the accuracy of the reconstructed images.

4. DISCUSSIONS

4.1 Existing Challenges

The development of forward models for X-ray imaging presents several significant obstacles that hinder the accuracy and dependability of image reconstruction. A principal obstacle is the precise characterization of X-ray interactions with heterogeneous and anisotropic materials. Simplified assumptions regarding material characteristics can result in considerable inaccuracies, particularly when confronted with varied material compositions and densities. Specifically, physical phenomena such as beam hardening introduce nonlinearities in attenuation, which can distort the acquired signals and lead to erroneous reconstructions if not adequately addressed.

Another substantial challenge arises from scattering effects, particularly within high-density materials, where Compton and Rayleigh scattering contribute to noise and signal distortion. The mitigation of these effects is computationally demanding, necessitating sophisticated scatter correction methodologies that accurately simulate these interactions. Furthermore, the geometric configuration of the X-ray apparatus, encompassing the alignment of the X-ray source, object, and detector, complicates the formulation of the system matrix. Even slight misalignments can yield considerable errors in image reconstruction, necessitating precise calibration and geometric correction strategies.

Moreover, achieving computational efficiency presents considerable challenges, especially in high-dimensional and real-time imaging contexts. The incorporation of physical constraints within the Physics-informed Machine Learning (PIML) framework, while augmenting accuracy and interpretability, also escalates computational requirements. The optimization of computational performance within the PIML framework without compromising accuracy remains a pertinent challenge, particularly in the context of large-scale imaging endeavors.

Lastly, validating the robustness and generalizability of the system matrix formulation is of paramount importance. The prevailing framework is predicated on a restricted set of experimental data, which may not adequately encompass the full spectrum of variations encountered in real-world imaging conditions. Consequently, a more exhaustive validation procedure is requisite to ensure that the model operates reliably across diverse conditions, thereby enhancing its generalizability in various imaging scenarios.

4.2 Future Research Directions

Future investigations should concentrate on overcoming the previously mentioned obstacles by refining and advancing the forward models used in X-ray imaging. A vital area for enhancement lies in the precise depiction of material heterogeneity and anisotropy within the system matrix. This will require the creation of more advanced models that effectively address nonlinear attenuation effects, such as beam hardening, particularly in materials with high density. The integration of beam-hardening correction algorithms within the PIML framework will be essential to ensure that attenuation is accurately modeled across various material properties and X-ray energy spectra.

Simultaneously, it is essential to improve the computational efficiency of the PIML framework. Approaches such as multi-GPU parallelization, sparse matrix representations, and reduced-order modeling should be investigated to lessen the computational expenses linked to extensive imaging operations. These enhancements will facilitate the effective management of high-dimensional data and support real-time processing, thereby broadening the practical uses of PIML-based models.

Advancing scatter correction techniques represents another significant research avenue, as effective modeling of scatter is crucial. Future studies should concentrate on improving X-ray imaging forward models by enhancing the representation of material heterogeneity and anisotropy. This entails the development of sophisticated models that tackle nonlinear attenuation effects, such as beam hardening, particularly in high-density materials. Incorporating beam-hardening correction algorithms within the PIML framework will ensure more precise attenuation modeling.

Maximizing the computational efficiency of PIML is vital for managing extensive imaging tasks. Methods like multi-GPU parallelization, sparse matrix representations, and reduced-order modeling can greatly diminish computational costs, allowing for real-time processing without compromising precision.

Enhancing scatter correction techniques, particularly for Compton and Rayleigh scattering, will improve image quality in dense materials. It is crucial to develop efficient algorithms that can effectively handle these scattering effects while still being computationally feasible.

Refining geometric calibration methods to minimize errors resulting from system misalignment will further improve accuracy. Real-time correction algorithms will guarantee dependable system matrix formulations even in dynamic configurations.

Finally, broadening the validation framework with a wider array of datasets and utilizing advanced cross-validation methods will ensure the models' robustness and generalizability. Incorporating thorough noise modeling, potentially through machine learning, will also enhance the system's reliability in dealing with uncertainties.

5. CONCLUSION

In summary, this study delves into the incorporation of Physics-Informed Machine Learning (PIML) in the development of the system matrix for X-ray imaging forward models, introducing an innovative strategy that merges machine learning with foundational physical principles. Through the incorporation of physical constraints such as X-ray attenuation and scattering directly within the machine learning framework, it was illustrated that PIML has the ability to enhance the precision, resilience, and interpretability of the system matrix, even in scenarios with limited data. The approach outlined in this paper not only tackles current obstacles in modeling intricate material interactions and reducing noise but also establishes the foundation for future progress in X-ray imaging across diverse domains. The outcomes underscore the capacity of PIML to transform imaging procedures, offering a more dependable and flexible framework that can substantially elevate image reconstruction and diagnostic accuracy in fields spanning from medical imaging to materials examination. Subsequent research endeavors should concentrate on broadening this integration, perfecting the physical models, and delving into new applications to fully exploit the transformative potential of PIML in computational imaging.

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