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Uncertainty Quantification in Machine Learning Models for Additive Manufacturing: A Bayesian Approach to Enhancing Model Robustness and Trustworthiness

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Abstract: Machine learning approaches have become increasingly prevalent in the optimization and control of additive manufacturing processes over the past decade. Despite their widespread adoption, quantifying uncertainty in these models remains a significant challenge for ensuring reliable predictions in critical manufacturing applications. This paper presents a comprehensive Bayesian framework for quantifying uncertainty in machine learning models specifically tailored for additive manufacturing processes. We develop a hierarchical probabilistic approach that captures both aleatoric uncertainty arising from inherent process variability and epistemic uncertainty stemming from model limitations and data scarcity. Our methodology integrates Gaussian process regression with Markov Chain Monte Carlo methods to provide robust uncertainty estimates across diverse additive manufacturing scenarios. Experimental validation on laser powder bed fusion processes demonstrates that our approach reduces prediction error by 37% compared to deterministic methods while providing well-calibrated uncertainty bounds. Furthermore, the proposed framework enables adaptive sampling strategies that optimize material property predictions with 42% fewer experiments. This work establishes a foundation for uncertainty-aware decision-making in additive manufacturing, enhancing process reliability and accelerating qualification procedures for critical components.

1. Introduction

The widespread adoption of AM in high-consequence applications remains hindered by challenges in ensuring consistent part quality and reliable performance prediction. The complex, multi-scale physical phenomena governing AM processes create significant variability in material properties and geometric accuracy, making deterministic prediction models insufficient for critical applications.

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Machine learning (ML) approaches have demonstrated considerable promise in addressing these challenges by capturing complex process-structure-property relationships without requiring complete physical models. Recent advances in deep learning, reinforcement learning, and Bayesian optimization have accelerated process parameter optimization and real-time control in various AM processes. Nevertheless, a critical limitation remains: most ML implementations in AM fail to adequately quantify prediction uncertainty, which is essential for risk assessment and certification in high-consequence applications.

Uncertainty in AM manifests through multiple mechanisms, including inherent process stochasticity, measurement noise, model form errors, and limited training data. Traditional ML approaches typically provide point estimates without confidence intervals, leading to potentially dangerous overconfidence in regions of sparse data or novel process conditions. This limitation becomes particularly problematic when ML models are deployed for quality prediction in safety-critical components, where understanding prediction reliability is as important as the prediction itself.

The field of uncertainty quantification (UQ) provides formal mathematical frameworks for characterizing, propagating, and reducing uncertainties in computational models. Bayesian approaches to UQ have gained traction in various scientific domains for their ability to coherently update beliefs in light of new evidence while maintaining principled representations of uncertainty. However, the application of rigorous UQ methodologies to ML-based AM models remains nascent, with significant gaps in methodology and practical implementation.

This paper addresses these gaps by developing a comprehensive Bayesian framework for uncertainty quantification in ML models for additive manufacturing [1]. We focus specifically on melt pool modeling in laser powder bed fusion (L-PBF) processes, where accurate prediction of thermal history directly impacts microstructure formation and resultant mechanical properties. Our approach distinguishes between aleatoric uncertainty (irreducible randomness in the physical process) and epistemic uncertainty (reducible uncertainty due to limited knowledge or data), providing targeted strategies for uncertainty reduction and experimental design.

The primary contributions of this work include: (1) a hierarchical Bayesian framework that integrates physical constraints with data-driven learning; (2) a novel method for calibrating model uncertainty through multi-fidelity experimental data fusion; (3) adaptive experimental design strategies that efficiently reduce uncertainty in regions of interest; and (4) comprehensive validation against experimental datasets across multiple materials and process conditions. The proposed framework not only improves prediction accuracy but also enables risk-informed decision-making through well-calibrated uncertainty estimates. [2]

The remainder of this paper is structured as follows: Section 2 reviews relevant literature on uncertainty quantification and machine learning in additive manufacturing. Section 3 presents our Bayesian framework for uncertainty quantification. Section 4 details the mathematical formulation of our approach, including Gaussian process models and computational implementation. Section 5 describes the experimental methodology used for model validation [3]. Section 6 presents results and discussion, followed by conclusions and future directions in Section 7.

2. Background and Related Work

The intersection of machine learning and additive manufacturing has evolved rapidly in recent years, with applications spanning process monitoring, defect detection, parameter optimization, and microstructure prediction. Early applications of ML in AM focused primarily on supervised learning approaches, where models were trained to predict process outcomes from input parameters. These approaches typically employed neural networks, support vector machines, or random forests trained on experimental datasets. [4] [5]

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Process modeling in AM presents unique challenges due to the complex physical phenomena involved, including powder spreading dynamics, laser-material interactions, rapid solidification, and thermal cycling. These processes span multiple length and time scales, from nanoscale nucleation events to part-level residual stress development. Traditional physics-based models, while mechanistically sound, often become computationally intractable when attempting to capture these multi-scale interactions. This computational challenge has motivated the development of surrogate models using machine learning techniques, which aim to approximate the input-output relationships of physics-based models at reduced computational cost. [6]

However, the use of purely data-driven approaches in AM modeling introduces significant epistemic uncertainty, particularly when extrapolating beyond the training data domain. Several researchers have attempted to address this limitation through physics-informed machine learning, where known physical constraints are incorporated into model architectures or loss functions. Physics-informed neural networks have shown particular promise by enforcing conservation laws and boundary conditions within model training, thereby improving model accuracy and generalizability with limited data.

The quantification of uncertainty in AM models remains relatively underexplored compared to point prediction methods [7]. Early work in this area focused primarily on parametric uncertainty analysis, where uncertainties in input parameters were propagated through deterministic models to estimate output variability. While valuable, these approaches fail to capture model form uncertainty, which often dominates in complex AM processes where perfect physical models are unavailable.

Bayesian approaches to uncertainty quantification have emerged as a promising alternative for AM modeling. Bayesian neural networks, which place probability distributions over model weights, have been applied to melt pool prediction and porosity detection, providing prediction intervals alongside point estimates. Similarly, Gaussian process regression has found application in AM for its natural uncertainty quantification capabilities and ability to incorporate prior physical knowledge through kernel design. [8]

Multi-fidelity modeling approaches have also gained traction in AM, where high-fidelity experimental data is supplemented with lower-fidelity simulation data to improve prediction accuracy while maintaining uncertainty awareness. These approaches typically employ hierarchical models that capture correlations between fidelity levels, enabling efficient knowledge transfer. Kennedy and O'Hagan's pioneering work on Bayesian calibration has inspired several AM-specific adaptations, where model parameters are calibrated against experimental data while accounting for model inadequacy.

Active learning and Bayesian optimization have demonstrated particular promise for efficient experimental design in AM, where the high cost of experiments necessitates intelligent sampling strategies [9]. These approaches leverage uncertainty estimates to identify high-information experiments that efficiently reduce prediction uncertainty. Recent work has demonstrated substantial reductions in required experimental iterations for process optimization through uncertainty-guided sampling.

Despite these advances, several key challenges remain in uncertainty quantification for AM modeling. First, most existing approaches focus on either aleatoric or epistemic uncertainty, rarely addressing both simultaneously within a unified framework [10]. Second, the validation of uncertainty estimates in AM models remains limited, with few studies assessing calibration quality or decision-making utility. Third, the computational expense of rigorous UQ methods has limited their application to realistic AM problems with high-dimensional input spaces and complex output responses.

This paper addresses these limitations by developing a comprehensive Bayesian framework that simultaneously accounts for multiple uncertainty sources while maintaining computational tractability for practical AM applications.

By integrating physical constraints with data-driven learning and employing multi-fidelity data fusion, our approach provides well-calibrated uncertainty estimates that support risk-informed decision-making in AM process design. [11]

3. Bayesian Framework for Uncertainty Quantification

Our uncertainty quantification framework adopts a Bayesian perspective, treating all unknown parameters as random variables with associated probability distributions. This approach provides a natural mechanism for updating knowledge as new data becomes available while maintaining a comprehensive representation of uncertainty throughout the modeling process. The framework consists of four primary components: (1) hierarchical model structure, (2) uncertainty decomposition, (3) prior specification, and (4) posterior computation.

The hierarchical model structure captures relationships between process parameters, melt pool characteristics, microstructure formation, and resultant material properties [12]. Each level of the hierarchy represents a distinct physical process with associated uncertainties. At the lowest level, process parameters such as laser power, scan speed, and layer thickness serve as controlled inputs. These parameters influence melt pool dynamics, characterized by dimensions, temperature gradients, and cooling rates. Melt pool characteristics, in turn, determine microstructure formation, including grain size, texture, and phase composition [13]. Finally, microstructure determines material properties such as strength, ductility, and fatigue performance.

By structuring the model hierarchically, we can incorporate domain knowledge at each level while allowing uncertainty to propagate through the system. This approach enables the identification of uncertainty sources and targeted data collection for uncertainty reduction. Furthermore, the hierarchical structure facilitates transfer learning between different materials and machine configurations by separating material-specific parameters from process-specific parameters. [14]

Uncertainty in AM processes can be decomposed into aleatoric and epistemic components, each requiring different treatment within the Bayesian framework. Aleatoric uncertainty represents inherent process randomness that cannot be reduced through additional data collection. In AM, sources of aleatoric uncertainty include powder size distribution variability, random fluctuations in laser power delivery, and stochastic nature of solidification nucleation. We model aleatoric uncertainty using heteroscedastic noise terms with input-dependent variance. [15]

Epistemic uncertainty represents knowledge gaps that can be reduced through additional data or improved modeling. Sources of epistemic uncertainty in AM modeling include limited training data, simplified model forms, and measurement errors. We capture epistemic uncertainty through prior distributions over model parameters, with variance reflecting confidence in prior knowledge. As additional data becomes available, these priors are updated to posterior distributions with reduced variance, reflecting increased knowledge [16].

Prior specification represents a critical component of our Bayesian framework, encoding physical constraints and domain knowledge [17]. For Gaussian process models, priors are specified through kernel selection and hyperparameter distributions. We employ composite kernels that combine multiple basis functions to capture relevant physical behaviors. For instance, periodic kernels capture thermal cycling effects, while Matérn kernels represent spatial correlation in microstructure formation. Hyperpriors on length scales and output scales are selected based on physical considerations, such as characteristic thermal diffusion lengths and expected property ranges. [18]

For neural network components, we employ functional priors rather than parameter priors, specifying distributions over function outputs rather than weights. This approach enables more intuitive prior specification based on physical

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constraints, such as monotonicity relationships between process parameters and outputs. We implement these functional priors through virtual observables—synthetic data points generated from physical models or theoretical bounds.

Posterior computation presents significant challenges in complex AM models with high-dimensional parameter spaces [19]. We employ a combination of sampling-based and variational inference methods, selected based on model complexity and computational constraints. For moderate-dimensional problems, we use Hamiltonian Monte Carlo (HMC) with adaptive step sizes to efficiently explore posterior distributions while maintaining detailed uncertainty representation. For higher-dimensional problems, we employ stochastic variational inference with normalizing flows to approximate complex posterior geometries while maintaining computational tractability.

To address computational challenges in posterior predictive distribution computation, we employ ensemble methods that combine multiple model instances sampled from the posterior [20]. This approach provides computationally efficient uncertainty estimates that account for both parameter uncertainty and model inadequacy. For real-time applications requiring rapid uncertainty estimation, we implement amortized inference techniques that learn mappings from data to approximate posterior distributions, enabling fast uncertainty quantification during process monitoring.

The proposed Bayesian framework provides several advantages over traditional deterministic approaches. First, it naturally accommodates multi-fidelity data fusion, allowing integration of sparse experimental measurements with abundant simulation results [21]. Second, it provides well-calibrated uncertainty estimates that support risk-informed decision-making in process design. Third, it enables adaptive experimental design through acquisition functions that balance exploration and exploitation based on prediction uncertainty. Fourth, it accommodates non-stationary behavior common in AM processes through input-dependent noise models and locally adaptive kernel parameters.

This comprehensive treatment of uncertainty in AM modeling lays the foundation for subsequent mathematical development and computational implementation described in the following section. [22]

4. Advanced Uncertainty Quantification Models

This section presents the mathematical formulation of our Bayesian uncertainty quantification approach, with particular emphasis on Gaussian process models and their application to additive manufacturing processes. We develop the theoretical underpinnings necessary for rigorous uncertainty propagation through complex process-structure-property relationships while maintaining computational tractability.

Let $\mathbf{x} \in \mathbb{R}^d$ represent the vector of process parameters, including laser power P, scan speed v, hatch spacing h, and layer thickness t. The process output of interest $y \in \mathbb{R}$ may represent a melt pool characteristic, microstructural feature, or mechanical property. The true process response function $f : \mathbb{R}^d \to \mathbb{R}$ maps process parameters to outputs but is unknown and can only be observed through noisy measurements.

We model the relationship between inputs and outputs as:

$$y = f(\mathbf{x}) + \epsilon(\mathbf{x})$$

where $\epsilon(\mathbf{x})$ represents heteroscedastic noise with variance $\sigma^2(\mathbf{x})$ that may depend on the input location. This formulation captures both the deterministic process response and stochastic variability inherent to AM processes. [23]

In the Bayesian paradigm, we place a prior distribution over the unknown function f. Specifically, we model f as a realization of a Gaussian process:

$f \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$

where $m(\mathbf{x})$ represents the mean function encoding prior knowledge about the expected response, and $k(\mathbf{x}, \mathbf{x}')$ is the covariance kernel function that determines the smoothness and correlation structure of the process.

For AM applications, we construct physically-informed mean functions that incorporate theoretical relationships when available. For instance, when modeling melt pool depth d as a function of laser power P and scan speed v, we use the Rosenthal solution for a moving point heat source as a mean function: [24]

$m(\mathbf{x}) = \frac{\alpha P}{\pi k v} \exp\left(-\frac{v}{2\kappa} r\right)$

where α is absorptivity, k is thermal conductivity, κ is thermal diffusivity, and r is the radial distance from the heat source. This physics-based mean function provides a reasonable first approximation, while the Gaussian process captures deviations due to physical effects not included in the simplified model.

The covariance kernel function determines the correlation structure of the process response across the parameter space. We employ a composite kernel structure that combines multiple basis kernels to capture relevant physical behaviors: [25]

$k(\mathbf{x}, \mathbf{x}') = k_{\text{se}}(\mathbf{x}, \mathbf{x}') + k_{\text{per}}(\mathbf{x}, \mathbf{x}') + k_{\text{lin}}(\mathbf{x}, \mathbf{x}')$

The squared exponential kernel k_{se} captures smooth variations in the response:

$k_{\text{se}}(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\frac{1}{2} \sum_{i=1}^{d} \frac{(x_i - x_i')^2}{l_i^2}\right)$

where σ_f^2 is the signal variance and l_i are length scales corresponding to each input dimension. These length scales control the rate at which the response varies with each parameter and are learned during model training.

The periodic kernel k_{per} captures cyclic variations often observed in layer-by-layer building processes:

$k_{\text{per}}(\mathbf{x}, \mathbf{x}') = \sigma_p^2 \exp\left(-\frac{2 \sin^2(\pi |x_t - x_t'|/p)}{l_p^2}\right)$

where x_t represents the layer thickness dimension, p is the period corresponding to thermal cycling frequency, and l_p is the length scale controlling smoothness of periodic variations.

The linear kernel k_{lin} captures global trends in the response:

$k_{\text{lin}}(\mathbf{x}, \mathbf{x}') = \sigma_l^2 (\mathbf{x}^T \Sigma \mathbf{x}')$

where Σ is a positive semi-definite matrix determining the correlation between input dimensions in their linear contribution to the output.

To capture heteroscedastic noise, we model the noise variance function $\sigma^2(\mathbf{x})$ using a separate Gaussian process:

$\log \sigma^2 \sim \mathcal{GP}(m_\sigma(\mathbf{x}), k_\sigma(\mathbf{x}, \mathbf{x}'))$

This formulation ensures positive noise variance while allowing flexible modeling of input-dependent noise characteristics [26]. For AM processes, this captures increased variability in regions of parameter space associated with mode transitions, such as conduction to keyhole mode welding.

Given a dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ of process parameters and corresponding measurements, the posterior distribution over the function f is also a Gaussian process:

$f|\mathcal{D} \sim \mathcal{GP}(\mu_{\text{post}}(\mathbf{x}), \Sigma_{\text{post}}(\mathbf{x}, \mathbf{x}'))$

with posterior mean and covariance functions:

$\mu_{\text{post}}(\mathbf{x}) = m(\mathbf{x}) + \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \Sigma_n)^{-1}(\mathbf{y} - \mathbf{m})$

$\Sigma_{\text{post}}(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}, \mathbf{x}') - \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \Sigma_n)^{-1}\mathbf{k}(\mathbf{x}')$

where $\mathbf{k}(\mathbf{x}) = [k(\mathbf{x}, \mathbf{x}_1), \ldots, k(\mathbf{x}, \mathbf{x}_n)]^T$, $\mathbf{K}$ is the $n \times n$ matrix with elements $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$, Σ_n is a diagonal matrix with elements $\sigma^2(\mathbf{x}_i)$, $\mathbf{y} = [y_1, \ldots, y_n]^T$, and $\mathbf{m} = [m(\mathbf{x}_1), \ldots, m(\mathbf{x}_n)]^T$.

The posterior predictive distribution for a new input $\mathbf{x}_*$ is Gaussian:

$p(y_*|\mathbf{x}_*, \mathcal{D}) = \mathcal{N}(\mu_{\text{post}}(\mathbf{x}_*), \Sigma_{\text{post}}(\mathbf{x}_*, \mathbf{x}_*) + \sigma^2(\mathbf{x}_*))$

This distribution provides both the expected prediction and associated uncertainty, decomposed into epistemic uncertainty (captured by $\Sigma_{\text{post}}(\mathbf{x}_*, \mathbf{x}_*)$) and aleatoric uncertainty (captured by $\sigma^2(\mathbf{x}_*)$).

For multi-fidelity modeling, we extend this formulation to accommodate data sources of varying fidelity. Let f_l represent the process response function at fidelity level $l \in \{1, \ldots, L\}$, where $l = L$ corresponds to the highest fidelity (typically experimental measurements) and $l = 1$ to the lowest (typically coarse simulations). We model the relationship between fidelity levels using an autoregressive structure: [27]

$f_l(\mathbf{x}) = \rho_{l-1}(\mathbf{x})f_{l-1}(\mathbf{x}) + \delta_l(\mathbf{x})$

where $\rho_{l-1}(\mathbf{x})$ is a scaling function and $\delta_l(\mathbf{x})$ is a discrepancy function capturing fidelity level differences. Both ρ_{l-1} and δ_l are modeled as Gaussian processes:

$\rho_{l-1} \sim \mathcal{GP}(m_\rho(\mathbf{x}), k_\rho(\mathbf{x}, \mathbf{x}'))$ $\delta_l \sim \mathcal{GP}(m_\delta(\mathbf{x}), k_\delta(\mathbf{x}, \mathbf{x}'))$

This formulation enables efficient knowledge transfer between fidelity levels while maintaining uncertainty awareness.

To address computational challenges with large datasets, we employ sparse Gaussian process approximations based on inducing points. Let $\mathbf{Z} = \{\mathbf{z}_j\}_{j=1}^m$ represent a set of $m \ll n$ inducing inputs with corresponding function values $\mathbf{u} = [f(\mathbf{z}_1), \ldots, f(\mathbf{z}_m)]^T$. The joint distribution of function values at observed and inducing points is:

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{u} \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mathbf{m} \\ \mathbf{m}_Z \end{bmatrix}, \begin{bmatrix} \mathbf{K}_{nn} & \mathbf{K}_{nm} \\ \mathbf{K}_{mn} & \mathbf{K}_{mm} \end{bmatrix} \right)$$

where $\mathbf{K}_{nm}$ is the cross-covariance matrix between observed and inducing points. Under the inducing point approximation, the predictive distribution becomes: [28]

$p(f_*|\mathbf{x}_*, \mathcal{D}) \approx \mathcal{N}(m(\mathbf{x}_*) + \mathbf{k}_{*m}\mathbf{K}_{mm}^{-1}(\mathbf{u} - \mathbf{m}_Z), k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_{*m}\mathbf{K}_{mm}^{-1}\mathbf{k}_{m*} + \mathbf{k}_{*m}\mathbf{K}_{mm}^{-1}\mathbf{\Sigma}_u\mathbf{K}_{mm}^{-1}\mathbf{k}_{m*})$

where $\mathbf{k}_{*m} = [k(\mathbf{x}_*, \mathbf{z}_1), \ldots, k(\mathbf{x}_*, \mathbf{z}_m)]$ and $\mathbf{\Sigma}_u$ is the posterior covariance of inducing point values. This approximation reduces computational complexity from $\mathcal{O}(n^3)$ to $\mathcal{O}(nm^2)$, enabling scalable inference with large datasets.

For uncertainty propagation through the process-structure-property chain, we employ nested Gaussian processes where the output of one model serves as input to the next. Let f_1 map process parameters to melt pool characteristics, f_2 map melt pool characteristics to microstructure features, and f_3 map microstructure to properties:

$\mathbf{z} = f_1(\mathbf{x}) + \epsilon_1(\mathbf{x})$ $\mathbf{w} = f_2(\mathbf{z}) + \epsilon_2(\mathbf{z})$ $y = f_3(\mathbf{w}) + \epsilon_3(\mathbf{w})$

Each function f_i is modeled as a Gaussian process with appropriate mean and covariance functions. The posterior

predictive distribution for property y given process parameters $\mathbf{x}$ requires propagating uncertainty through this chain. We employ moment matching techniques to approximate the predictive distribution: [29]

$$p(y|\mathbf{x}, \mathcal{D}) \approx \mathcal{N}(\mathbb{E}[y|\mathbf{x}], \mathbb{V}[y|\mathbf{x}])$$

where moments are computed through nested expectations:

$$\mathbb{E}[y|\mathbf{x}] = \mathbb{E}_{z|x}[\mathbb{E}_{w|z}[\mathbb{E}_{y|w}[y|\mathbf{w}, \mathcal{D}_3]|\mathbf{z}, \mathcal{D}_2]]|\mathbf{x}, \mathcal{D}_1]$$

$$\mathbb{V}[y|\mathbf{x}] = \mathbb{E}_{z|x}[\mathbb{E}_{w|z}[\mathbb{V}_{y|w}[y|\mathbf{w}, \mathcal{D}_3]|\mathbf{z}, \mathcal{D}_2]]|\mathbf{x}, \mathcal{D}_1] + \ldots$$

These nested expectations are computed using either analytic approximations or Monte Carlo integration, depending on kernel complexity and computational constraints.

For model calibration and validation, we employ Bayesian model averaging across multiple model forms, each with different kernel structures and hyperparameters. The posterior predictive distribution becomes a mixture: [30]

$$p(y_*|\mathbf{x}_*, \mathcal{D}) = \sum_{i=1}^{M} w_i p(y_*|\mathbf{x}_*, \mathcal{D}, \mathcal{M}_i)$$

where $\mathcal{M}_i$ represents model form i, and weights w_i are computed based on model evidence:

$$w_i = \frac{p(\mathcal{D}|\mathcal{M}_i)p(\mathcal{M}_i)}{\sum_{j=1}^{M} p(\mathcal{D}|\mathcal{M}_j)p(\mathcal{M}_j)}$$

This Bayesian model averaging approach accounts for model form uncertainty, providing more robust predictions in regions where different models diverge.

The mathematical framework described above provides a rigorous foundation for uncertainty quantification in AM modeling, capturing both aleatoric and epistemic uncertainty while maintaining computational tractability for practical applications. In the following sections, we demonstrate the application of this framework to experimental data and evaluate its performance in predicting AM process outcomes with quantified uncertainty.

5. Experimental Methodology

To validate the uncertainty quantification framework, we conducted a comprehensive experimental campaign using laser powder bed fusion (L-PBF) systems with varying configurations and materials [31]. This section details the experimental setup, measurement protocols, and data collection procedures used to generate validation datasets for model development and evaluation.

The experimental work utilized two commercial L-PBF systems: an EOS M290 and a Concept Laser M2. The EOS M290 features a 400W Yb-fiber laser with 100m spot size, while the Concept Laser M2 employs a 400W Yb-fiber laser with 150m spot size. Both systems operate in an inert argon atmosphere with oxygen concentration maintained below 0.1% [32]. These two machine configurations enabled exploration of machine-to-machine variability and testing of model transferability across different systems.

Three metal alloy powders were investigated: Ti-6Al-4V (Grade 5), Inconel 718, and AlSi10Mg. These materials were selected to represent a range of thermal properties and solidification behaviors commonly encountered in industrial applications. The Ti-6Al-4V powder had particle size distribution of 15-45m (D50 = 32m), the Inconel 718 powder had particle size distribution of 15-53m (D50 = 35m), and the AlSi10Mg powder had particle size distribution of 20-63m (D50 = 43m) [33]. All powders were characterized for flowability, apparent density, and particle morphology prior to processing.

A design of experiments (DOE) approach was employed to systematically explore the process parameter

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space while enabling uncertainty quantification. We utilized a central composite design with four primary process parameters: laser power (P), scan speed (v), hatch spacing (h), and layer thickness (t). The parameter ranges were selected based on preliminary experiments to span both stable processing regions and boundary conditions where process instabilities emerge. For Ti-6Al-4V, power ranged from 150-350W, scan speed from 600-1400mm/s, hatch spacing from 0.08-0.14mm, and layer thickness from 30-60m. [34] [35]

Beyond the structured DOE, additional experiments were conducted at randomly selected parameter combinations to provide validation data for assessing model extrapolation capabilities. These random validation points were concentrated in regions of high predicted uncertainty to challenge the uncertainty quantification framework. In total, 87 parameter combinations were tested for Ti-6Al-4V, 62 for Inconel 718, and 54 for AlSi10Mg.

For each parameter combination, we fabricated standardized test specimens including 10mm cubes for microstructural analysis, 15mm cylinders for density measurements, and ASTM E8 tensile specimens for mechanical property evaluation [36]. Each parameter combination was repeated three times with specimens distributed across the build platform to capture spatial variability within the build chamber. This replication enabled direct measurement of aleatoric uncertainty associated with inherent process variability.

In-situ monitoring was employed to capture process dynamics during fabrication. A high-speed thermal camera (FLIR A6750sc) operating at 1000Hz with 640×512 resolution monitored the melt pool thermal profile [37]. Concurrent optical monitoring using a 5MP machine vision camera captured layer-wise information at 30Hz. Additionally, photodiode sensors measured reflected laser radiation to detect process anomalies. This multi-modal monitoring approach generated rich datasets for correlating process signatures with resultant material states.

Post-process characterization followed standardized protocols to ensure measurement consistency [38]. Density measurements utilized Archimedes' principle with ethanol immersion medium and were verified using optical microscopy of polished cross-sections with image analysis. Microstructural characterization employed a combination of optical microscopy and scanning electron microscopy (SEM) with electron backscatter diffraction (EBSD) to quantify grain size, orientation, and phase composition. Mechanical testing followed ASTM standards, with tensile testing conducted at a strain rate of $10^{-}3s^{-}1$.

Measurement uncertainty was rigorously quantified for each characterization method [39]. For density measurements, the expanded uncertainty (k=2) was 0.15%. For grain size measurements, the expanded uncertainty was 12% based on multiple measurements across different sample locations. For tensile properties, expanded uncertainties were 3% for elastic modulus, 2% for yield strength, and 4% for ultimate tensile strength. These measurement uncertainties were incorporated into the Bayesian framework as components of the observation noise model. [40]

To support multi-fidelity modeling, we generated companion simulation datasets using both high-fidelity and low-fidelity computational models. High-fidelity simulations employed a coupled computational fluid dynamics (CFD) and discrete element method (DEM) approach implemented in Flow-3D to capture melt pool dynamics with phase change and Marangoni effects. Low-fidelity simulations utilized a simplified thermal conduction model based on the Rosenthal solution, implemented in MATLAB. These simulation results were calibrated against experimental measurements to quantify model bias and uncertainty. [41]

Data preprocessing included outlier detection using the modified Z-score method with threshold value 3.5, followed by robust scaling to normalize different output quantities to comparable ranges. Missing data, which constituted less than 3% of the dataset, was handled within the Bayesian framework rather than through imputation, as the Gaussian process formulation naturally accommodates incomplete observations.

The experimental dataset was partitioned into training (60%), validation (20%), and testing (20%) subsets, with stratification based on parameter combinations to ensure representative distribution across the parameter space. The training data was used for model development, validation data for hyperparameter tuning and model selection, and testing data for final performance evaluation [42]. This partitioning strategy ensured unbiased assessment of predictive performance and uncertainty calibration.

The experimental methodology described above generated comprehensive datasets capturing the complex process-structure-property relationships in additive manufacturing across multiple materials and machine configurations. These datasets enabled rigorous validation of the uncertainty quantification framework and assessment of its practical utility in predicting AM process outcomes with quantified confidence.

6. Results and Discussion

This section presents the results of applying our Bayesian uncertainty quantification framework to the experimental datasets described previously [43]. We evaluate the performance of our approach in terms of prediction accuracy, uncertainty calibration, and utility for decision-making in additive manufacturing processes.

The predictive performance of our hierarchical Bayesian framework was assessed using root mean square error (RMSE) and coefficient of determination (R^2) metrics across all three materials and multiple output quantities. Table 1 summarizes these results for the highest fidelity models trained on the complete dataset. For Ti-6Al-4V, our approach achieved RMSE values of 17.3m for melt pool depth, 32.8m for melt pool width, 0.12% for porosity, and 42MPa for ultimate tensile strength. These results represent improvements of 32%, 27%, 44%, and 37% respectively compared to deterministic neural network models trained on the same dataset [44] [45].

The superior performance of our Bayesian approach is particularly evident in regions of sparse data, where epistemic uncertainty becomes significant. For example, when predicting mechanical properties of Inconel 718 parts produced with laser power exceeding 300W and scan speed below 800mm/s, the deterministic models exhibited average prediction errors of 89MPa, while our Bayesian framework reduced this to 51MPa while simultaneously providing uncertainty bounds that contained the true values in 94% of cases.

Uncertainty decomposition into aleatoric and epistemic components provided valuable insights into the dominant sources of prediction variability across the parameter space. Figure 1 illustrates this decomposition for melt pool depth prediction in Ti-6Al-4V as a function of energy density [46]. At low energy densities (<50 J/mm³), epistemic uncertainty dominates due to limited data availability and model form limitations in capturing conduction mode melting. At moderate energy densities (50-100 J/mm³), aleatoric uncertainty becomes more prominent, reflecting inherent process variability in the stable processing region. At high energy densities (>100 J/mm³), both uncertainty components increase significantly, with epistemic uncertainty dominating in the keyhole regime where complex fluid dynamics govern melt pool behavior.

The capability to distinguish between these uncertainty sources enables targeted strategies for uncertainty reduction [47]. In regions dominated by epistemic uncertainty, additional data collection can substantially improve prediction confidence. Conversely, in regions dominated by aleatoric uncertainty, process modifications or control strategies may be necessary to reduce inherent variability. This distinction is particularly valuable for process certification and qualification, where understanding the reducibility of uncertainty directly impacts qualification requirements.

Multi-fidelity modeling demonstrated significant improvements in prediction accuracy and uncertainty quantification compared to single-fidelity approaches [48]. By integrating experimental measurements with

computational simulations of varying fidelity, our framework achieved a 42% reduction in experimental data requirements while maintaining equivalent prediction accuracy. Figure 2 illustrates the posterior predictive distributions for melt pool depth as a function of laser power and scan speed, showing narrower uncertainty bounds when incorporating multi-fidelity data compared to experimental data alone.

The autoregressive structure of our multi-fidelity model effectively captured correlations between fidelity levels, enabling knowledge transfer from abundant low-fidelity simulations to sparse high-fidelity experiments. The estimated scaling functions (x) revealed interesting patterns in model biases across the parameter space [49]. For example, thermal simulations consistently underestimated melt pool dimensions at high energy densities, with the discrepancy increasing nonlinearly with energy input. This pattern was captured by the learned scaling function, which showed values exceeding 1.5 in the keyhole regime, indicating that experimental measurements were substantially larger than predicted by simulations.

Uncertainty calibration analysis confirmed that our framework produces well-calibrated uncertainty estimates across all materials and output quantities. Figure 3 shows calibration curves for melt pool depth prediction, where the fraction of observations falling within predicted confidence intervals closely matches the theoretical fractions [50]. The mean calibration error was 3.2% for Ti-6Al-4V, 4.7% for Inconel 718, and 5.1% for AlSi10Mg, all within acceptable limits for engineering applications. This calibration quality is crucial for risk-informed decision-making, where miscalibrated uncertainty estimates could lead to either overly conservative or dangerously optimistic process boundaries.

Comparative analysis of kernel structures revealed significant performance differences across the parameter space. The composite kernel combining squared exponential, periodic, and linear components outperformed simpler alternatives in terms of both prediction accuracy and uncertainty calibration [51]. This performance advantage was particularly pronounced in capturing non-stationary behavior across processing regimes. For instance, the learned length scales in the squared exponential component showed systematic variation with energy density, with shorter length scales in the keyhole regime reflecting the rapid variation in process outcomes with small parameter changes.

Model selection via Bayesian model averaging demonstrated improvements in robustness compared to single-model approaches. By combining predictions from multiple model forms weighted by their evidence, the framework mitigated the risk of model misspecification while providing more reliable uncertainty estimates [52]. The posterior model weights revealed interesting material-dependent patterns, with more complex kernel structures receiving higher weights for Inconel 718 compared to AlSi10Mg, reflecting the more complex process-structure-property relationships in the nickel-based superalloy.

The sparse approximation methods employed for computational efficiency showed minimal degradation in predictive performance while enabling scalable inference. With 200 inducing points strategically placed within the parameter space, the sparse approximation achieved prediction accuracy within 3% of the full Gaussian process while reducing computation time by a factor of 87. This computational efficiency enables practical application to industrial-scale datasets generated by in-process monitoring systems. [53]

Cross-material and cross-machine transfer learning demonstrated the framework's ability to leverage data across different materials and equipment configurations. When trained on Ti-6Al-4V data with a small supplement of Inconel 718 samples, the model achieved 76% of the prediction accuracy obtained from Inconel-specific training, with appropriately wider uncertainty bounds reflecting the transfer uncertainty. Similarly, models trained on the EOS M290 system could be transferred to the Concept Laser M2 with 68% accuracy retention, requiring only 23% of the original data volume for adaptation.

Adaptive experimental design guided by uncertainty estimates demonstrated significant efficiency improvements compared to traditional design of experiments approaches. By iteratively selecting new experiments that maximize information gain, our framework achieved target prediction confidence with 42% fewer experiments compared to uniform sampling [54]. Figure 4 illustrates this efficiency gain for porosity prediction in AlSi10Mg, showing the rapid reduction in prediction uncertainty with adaptively selected experiments concentrated in high-uncertainty regions.

The practical utility of the uncertainty quantification framework was demonstrated through a case study on process window identification for a complex geometry component. Traditional approaches typically define process windows based on point estimates of acceptable parameter combinations, leading to either overly conservative or risky boundaries. Our approach instead defined process windows probabilistically, with contours corresponding to different risk tolerances [55]. For a safety-critical aerospace component with stringent porosity requirements (<0.01%), the uncertainty-aware process window was 27% smaller than the deterministic window, eliminating parameter combinations with high uncertainty that could not reliably guarantee the required quality.

Conversely, for non-critical components with relaxed requirements, the uncertainty-aware process window was 18% larger than the deterministic window, allowing the use of parameter combinations that would have been unnecessarily excluded by deterministic approaches. This risk-informed process window definition directly translates to practical benefits in manufacturing flexibility and component qualification.

In-process monitoring data integration further enhanced the framework's utility by enabling dynamic uncertainty updating during fabrication [56]. By assimilating thermal signatures from melt pool monitoring, the framework could update property predictions in real-time, reducing prediction uncertainty by up to 48% compared to a priori estimates. This capability supports adaptive process control and early defect detection by continuously refining property predictions as new data becomes available.

The propagation of uncertainty through the process-structure-property chain revealed interesting amplification and attenuation effects. Uncertainty in melt pool dimensions showed amplification when propagated to microstructural features, with relative uncertainty increasing by a factor of approximately 1.5 [57]. However, uncertainty in microstructural features showed attenuation when propagated to mechanical properties, with relative uncertainty decreasing by a factor of approximately 0.8. These effects reflect the complex nonlinear relationships between processing, structure, and properties in additive manufacturing.

Sensitivity analysis within the Bayesian framework identified key parameters driving prediction uncertainty across different materials and properties. For Ti-6Al-4V mechanical properties, scan speed emerged as the dominant contributor to uncertainty, accounting for 47% of the total prediction variance [58]. For Inconel 718 microstructure, the interaction between power and scan speed contributed 53% of the prediction uncertainty. These insights enable targeted parameter control strategies focused on the most influential factors for specific outcomes.

The quantification of measurement uncertainty contributions revealed that for most output quantities, process variability dominated over measurement uncertainty, accounting for 75-85% of the total observed variance. However, for microstructural features such as grain size and texture, measurement uncertainty contributed significantly (30-45%) to the total uncertainty budget [59]. This finding highlights the importance of improved characterization techniques for microstructure quantification in AM process optimization.

Uncertainty propagation through thermal history revealed that transient thermal effects have substantial impacts on prediction uncertainty for multi-layer builds. Temperature gradients and cooling rates showed high sensitivity to small perturbations in process parameters, with uncertainty amplification through subsequent layers. This effect was particularly pronounced for thin-walled structures, where the limited thermal mass led to greater thermal variability and consequently higher uncertainty in mechanical properties. [60]

Analysis of spatial variability within the build volume identified systematic patterns in prediction uncertainty. Regions near the build plate edges showed consistently higher uncertainty due to thermal boundary effects, while central regions exhibited more predictable behavior. This spatial mapping of uncertainty provides valuable guidance for part placement within the build volume to minimize property variability in critical components.

Comparative analysis with other uncertainty quantification approaches demonstrated the advantages of our Bayesian framework [61]. Traditional methods such as Monte Carlo simulation with deterministic models achieved similar mean predictions but significantly underestimated uncertainty in sparse data regions. Meanwhile, frequentist approaches such as bootstrapped neural networks provided reasonable uncertainty estimates but lacked the coherent mechanism for incorporating prior knowledge and multi-fidelity data that our Bayesian framework offers.

The computational implementation of our framework demonstrated scalability to industrial datasets. Using GPU acceleration and sparse approximation methods, the framework processed 10^6 data points in 3.2 hours for model training and generated predictions with uncertainty estimates at a rate of 10^3 predictions per second during inference. This performance enables practical application to large-scale manufacturing data and real-time process monitoring. [62]

In summary, our Bayesian uncertainty quantification framework demonstrates significant advantages over traditional deterministic approaches for additive manufacturing modeling. By providing well-calibrated uncertainty estimates that distinguish between aleatoric and epistemic uncertainty sources, the framework enables risk-informed decision-making, efficient experimental design, and robust process optimization. The multi-fidelity modeling capability efficiently leverages data from different sources, while the hierarchical structure captures complex process-structure-property relationships with quantified confidence.

7. Conclusion

This paper has presented a comprehensive Bayesian framework for uncertainty quantification in machine learning models for additive manufacturing [63]. By integrating physical constraints with data-driven learning and employing multi-fidelity data fusion, our approach provides well-calibrated uncertainty estimates that support risk-informed decision-making in AM process design and qualification. The key contributions and findings from this work are summarized below.

First, we have developed a hierarchical Bayesian modeling approach that captures the complex relationships between process parameters, melt pool characteristics, microstructure formation, and mechanical properties in AM processes. This hierarchical structure enables uncertainty propagation through the process-structure-property chain, providing insights into how uncertainties amplify or attenuate across different process stages [64]. The framework distinguishes between aleatoric uncertainty arising from inherent process variability and epistemic uncertainty stemming from model limitations and data scarcity, enabling targeted strategies for uncertainty reduction.

Second, our multi-fidelity modeling approach efficiently integrates data from different sources, including high-fidelity experiments, medium-fidelity detailed simulations, and low-fidelity analytical models. This approach reduces experimental data requirements by 42% while maintaining prediction accuracy, substantially improving the efficiency of AM process development. The autoregressive structure of our multi-fidelity model effectively captures correlations between fidelity levels, enabling knowledge transfer from abundant low-fidelity simulations to sparse high-fidelity experiments. [65]

Third, the Gaussian process models employed in our framework provide naturally principled uncertainty quantification with flexible kernel structures tailored to AM phenomena. The composite kernel combining squared

exponential, periodic, and linear components captures both smooth variations and cyclical thermal effects characteristic of layer-by-layer building processes. The sparse approximation methods enable scalable inference for large-scale manufacturing datasets without significant degradation in predictive performance.

Fourth, experimental validation across multiple materials and machine configurations demonstrates the generalizability and robustness of our uncertainty quantification approach [66]. The framework achieves improvements of 27-44% in prediction accuracy compared to deterministic methods while providing well-calibrated uncertainty estimates with mean calibration errors below 5%. Cross-material and cross-machine transfer learning capabilities enable efficient adaptation to new materials and equipment with minimal additional data collection.

Fifth, practical applications demonstrate the tangible benefits of uncertainty-aware modeling for AM process development. Adaptive experimental design guided by uncertainty estimates reduces experimental requirements by 42% compared to traditional approaches [67]. Probabilistic process window definition enables risk-informed parameter selection tailored to specific application requirements. Real-time uncertainty updating during fabrication supports adaptive process control and early defect detection by continuously refining property predictions as new data becomes available.

These contributions address critical challenges in AM process modeling and qualification, where understanding prediction reliability is essential for safety-critical applications. By providing well-calibrated uncertainty estimates, our framework enables engineers to make informed decisions about process parameters, part placement, and quality control strategies based on quantified risk assessments rather than deterministic predictions alone. [68]

Several important directions for future research emerge from this work. First, extending the uncertainty quantification framework to capture microstructural heterogeneity and anisotropy could improve predictions for complex geometries with varying thermal histories. Second, incorporating more sophisticated physics-based constraints into the Bayesian prior could further improve model accuracy in sparse data regions while maintaining well-calibrated uncertainty estimates. Third, developing computationally efficient methods for real-time uncertainty quantification during process monitoring could enable closed-loop control strategies that adaptively respond to prediction uncertainty. [69]

From a practical implementation perspective, integrating the uncertainty quantification framework with commercial AM software and hardware systems represents an important step toward industrial adoption. Standardized protocols for uncertainty reporting and risk assessment would facilitate communication between designers, manufacturers, and regulatory authorities, potentially streamlining qualification procedures for critical components.

In conclusion, the Bayesian uncertainty quantification framework presented in this paper provides a powerful toolset for addressing the challenges of variability and reliability in additive manufacturing. By capturing both aleatoric and epistemic uncertainty in a principled manner, the framework enables more informed decision-making throughout the AM process chain, from design and parameter selection to in-process monitoring and quality control. This uncertainty-aware approach represents an important step toward broader adoption of additive manufacturing for safety-critical applications where reliability and consistency are paramount concerns. [70]

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