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Bayesian Neural Networks for Multiscale Plasticity and Damage Models.

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Abstract

The integration of Bayesian inference into plasticity and damage models offers a transformative approach to uncertainty quantification in mechanical engineering simulations. This study advances the field by developing a novel Bayesian framework that couples multiscale material behavior with probabilistic parameter estimation, enhancing predictive accuracy and robustness while significantly improving computational efficiency. We derive original formulations for posterior distributions, incorporating multiphysics constraints such as thermal effects and fatigue, and apply these to advanced plasticity (Von Mises, Gurson) and damage (Lemaitre-Chaboche) models. Bayesian techniques—including adaptive Markov Chain Monte Carlo (MCMC), hierarchical variational inference (VI), and Bayesian neural networks (BNNs)—are employed to approximate complex posteriors while optimizing computational costs. The proposed framework achieves 99% faster evaluation times compared to traditional finite element methods (FEM), reducing computational costs from 7200 seconds (FEM) to 60 seconds (BNNs), with an RMSE deviation of only 0.9%. Additionally, our VI-based initialization strategy accelerates MCMC convergence by 30%, further enhancing scalability for high-dimensional problems. Benchmarking against gradient-enhanced plasticity models, phase-field damage models, and data-driven constitutive modeling techniques confirms that Bayesian methods provide superior computational efficiency and uncertainty quantification. The results demonstrate significant improvements in parameter estimation, uncertainty-aware predictions, and predictive capability for structural applications, with implications for real-time design optimization under uncertainty. This work lays the foundation for scalable, data-driven material modeling in extreme conditions.

Keywords: Bayesian inference, Markov Chain Monte Carlo, Variational Inference, Bayesian Neural Networks, Plasticity, Damage Modeling, Computational Efficiency

1. Introduction

Plasticity and damage models are foundational tools for simulating material behavior under mechanical loading, critical to applications ranging from aerospace components to civil infrastructure. These models, such as Von Mises plasticity [1], Lemaitre-Chaboche damage [2], and Gurson porous plasticity [3], describe yielding, hardening, and degradation in materials like metals and composites. However, their deterministic formulations often fail to account for uncertainties arising from microstructural heterogeneity, experimental noise, and model approximations, leading to unreliable predictions in extreme conditions [12, 13]. Recent advances have sought to address these limitations, with probabilistic approaches gaining traction for their ability to quantify uncertainty and enhance robustness [14, 15].

The state of the art in plasticity and damage modeling reflects a shift toward data-driven and uncertainty-aware methods. Traditional deterministic models have been extended with stochastic parameters [16], while Bayesian inference has emerged as a powerful framework for parameter estimation, offering posterior distributions rather than point estimates [17, 18]. For instance, Faroughi *et al.* [19] applied Bayesian methods to calibrate hardening laws, and Correia *et al.* [20] integrated them with fatigue models. Concurrently, machine learning (ML) techniques, particularly neural networks, have revolutionized material modeling by accelerating simulations and capturing complex behaviors [21, 22]. Bayesian neural networks (BNNs), blending Bayesian inference with ML, have shown promise in surrogate modeling and uncertainty quantification [23, 24], yet their application to multiscale plasticity and damage remains underexplored [25]. Multiscale approaches linking microstructural characteristics (e.g. grain size, void fraction) with macroscopic responses have also advanced [26, 27, 28], but integrating these with Bayesian and ML methods poses computational and theoretical challenges [29, 30, 31].

Despite these innovations, current methods face significant hurdles. Deterministic models oversimplify material variability, while standalone Bayesian approaches like Markov Chain Monte Carlo (MCMC) are computationally intensive for high-dimensional problems [32, 33]. ML models, though efficient, often lack interpretability and struggle with sparse data [34, 33]. Moreover, few studies couple multiscale effects with multiphysics constraints (e.g., thermal softening, fatigue) in a unified probabilistic framework, limiting their applicability to real-world scenarios [36, 37]. This paper addresses these gaps by introducing a novel Bayesian framework that leverages BNNs to enhance multiscale plasticity and damage modeling. We derive new posterior formulations incorporating multiphysics effects, employ adaptive MCMC, variational inference, and BNNs for efficient inference, and validate the approach across diverse models.

Our objectives are threefold:

1. Derive a unified Bayesian formulation integrating multiscale and multiphysics effects for plasticity and damage,
2. Implement and validate this framework across models like Von Mises, Lemaitre-Chaboche, and Gurson,
3. Demonstrate its practical utility in uncertainty-aware design for structural applications.

This work advances predictive accuracy and scalability, offering a data-driven solution for materials under uncertainty.

Outline

This paper is structured into six sections to systematically present our methodology, results, and implications:

- **Section 2: Theoretical Framework and Mathematical Foundations** establishes the Bayesian and multiscale foundations, deriving posterior distributions and stochastic evolution laws with multiphysics constraints.
- **Section 3: Numerical Bayesian Techniques** details the computational methods—adaptive MCMC, variational inference, and BNNs—used to approximate complex posteriors efficiently.
- **Section 4: Applications and Results** applies the framework to Von Mises plasticity, Lemaitre-Chaboche damage, and Gurson porous plasticity, presenting validation results and uncertainty quantification.

- **Section 5: Discussion** synthesizes key findings, evaluates computational trade-offs, and discusses practical implications and limitations.
- **Section 6: Conclusion and Future Directions** summarizes contributions, highlights the framework's impact, and outlines future research avenues, including advanced sampling and experimental validation.

2. Theoretical Framework and Mathematical Foundations

2.1. Bayesian Foundations

Bayesian inference provides a robust framework for updating prior beliefs about parameters θ—such as yield stress σ_Y, hardening modulus H, and damage variable D in plasticity and damage models—based on observed data D. Following Bayes' theorem, the posterior distribution $P(\theta \mid D)$ is proportional to the likelihood $P(D \mid \theta)$ times the prior $P(\theta)$, normalized by the evidence $P(D) = \int P(D \mid \theta)P(\theta)d\theta$, as shown in Equation 1.

$$P(\theta \mid D) = \frac{P(D \mid \theta)P(\theta)}{P(D)}, \tag{1}$$

This approach excels in capturing uncertainties from material variability, measurement noise, and microstructural effects, offering a probabilistic foundation for multiscale and multiphysics simulations; the details of the derivation of this formulation are given in Appendix A.

2.1.1. Prior Selection

Selecting the prior $P(\theta)$ is pivotal in Bayesian modeling of plasticity and damage parameters. For yield stress σ_Y, we adopt a Gaussian prior $\mathcal{N}(\mu_{\sigma_Y}, \sigma^2_{\sigma_Y})$ based on nominal handbook values, reflecting typical material variability. A lognormal prior $\mathrm{LN}(\mu_H, \sigma^2_H)$ ensures positivity for the hardening modulus H, while a Beta prior $\mathrm{Beta}(\alpha_D, \beta_D)$ constrains the damage variable D to $[0, 1]$, aligning with its physical bounds. Conjugate priors, such as Gaussian-Gaussian pairs, are employed where applicable to streamline posterior computation, enhancing efficiency in multiscale simulations and Bayesian neural network inference.

2.2. Plasticity and Damage Model Overview

Classical plasticity models, such as Von Mises, define yielding via:

$$f(\sigma, \sigma_Y) = \sqrt{\frac{3}{2} s : s} - \sigma_Y = 0, \tag{2}$$

where $s = \sigma - \frac{1}{3}\mathrm{tr}(\sigma)I$ is the deviatoric stress tensor. With isotropic hardening, this extends to:

$$f(\sigma, \sigma_Y, \epsilon_p) = \sqrt{\frac{3}{2} s : s} - \sigma_Y - H\epsilon_p = 0. \tag{3}$$

Damage models, like Lemaitre's, introduce degradation:

$$\tilde{\sigma} = \frac{\sigma}{1 - D}, \tag{4}$$

with D evolving based on stress and strain states. For example, in ductile materials, D may follow:

$$\dot{D} = \left(\frac{\sigma_{\mathrm{eq}}}{A(1 - D)} \right)^B \dot{\epsilon}_p, \tag{5}$$

where $\sigma_{\mathrm{eq}} = \sqrt{\frac{3}{2} s : s}$.

To broaden applicability, we consider anisotropic plasticity (e.g., Hill's criterion):

$$f(\sigma, \sigma_Y) = \sqrt{\sigma^T F \sigma} - \sigma_Y = 0, \tag{6}$$

where F is a fourth-order anisotropy tensor. This is relevant for rolled metals or composites, introducing additional parameters (e.g., F_{ij}) into θ.

2.3. Novel Bayesian Formulation with Multi-Scale Coupling

We propose a multiscale Bayesian model linking macroscopic parameters (σ_Y, H, D) to microstructural variables (e.g., grain size δ, void fraction f). The joint parameter set is $\theta = \{\sigma_Y, H, D, \delta, f\}$, with a hierarchical prior:

$$P(\theta) = P(\sigma_Y, H, D \mid \delta, f)P(\delta)P(f). \tag{7}$$

For instance, yield stress may scale with grain size via the Hall-Petch relation:

$$\sigma_Y = \sigma_0 + k_{\mathrm{HP}} \delta^{-1/2}, \tag{8}$$

where σ_0 and k_{HP} are constants, and $\delta \sim \mathrm{Lognormal}(\mu_\delta, \sigma^2_\delta)$ reflects microstructural variability. Similarly, D may depend on f through void growth models.

Example: Grain Size Effects

Consider a polycrystalline metal with δ ranging from 10 to 100 μm. Conditional prior $P(\sigma_Y \mid \delta) = \mathcal{N}(\sigma_0 + k_{\text{HP}}\delta^{-1/2}, \sigma^2_{\sigma_Y})$ couples scales, allowing Bayesian inference to propagate microstructural uncertainty to macroscopic behavior. This multiscale approach enhances physical realism, particularly for heterogeneous materials.

2.4. Mathematical Derivations

2.4.1. Posterior Distribution Derivation

In the context of the Von Mises plasticity model with isotropic hardening, as delineated in Equation 28, the stress-strain relationship is expressed as $\sigma = \sigma_Y + H\epsilon_p$ (Equation 12), where σ_Y denotes the yield stress, H the hardening modulus, and ϵ_p the plastic strain. Given experimental data $D = \{(\epsilon_i^{\text{exp}}, \sigma_i^{\text{exp}})\}_{i=1}^N$, we model the observed stresses with additive Gaussian noise, such that $\sigma_i^{\text{exp}} = \sigma_i^{\text{model}}(\theta) + \eta_i$, where $\eta_i \sim \mathcal{N}(0, \sigma_\eta^2)$ (Equation 13). Consequently, the likelihood function is formulated as

$$P(D \mid \theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma_\eta^2}} \exp\left(-\frac{(\sigma_i^{\text{exp}} - (\sigma_Y + H\epsilon_{p,i}))^2}{2\sigma_\eta^2}\right) \tag{9}$$

Adopting Gaussian priors, specifically $P(\sigma_Y) \sim \mathcal{N}(\mu_{\sigma_Y}, \sigma^2_{\sigma_Y})$ and $P(H) \sim \mathcal{N}(\mu_H, \sigma_H^2)$, the posterior distribution becomes proportional to the product of the likelihood and priors, yielding

$$P(\theta \mid D) \propto \exp\left(-\sum_{i=1}^{N} \frac{(\sigma_i^{\text{exp}} - (\sigma_Y + H\epsilon_{p,i}))^2}{2\sigma_\eta^2}\right) \exp\left(-\frac{(\sigma_Y - \mu_{\sigma_Y})^2}{2\sigma^2_{\sigma_Y}} - \frac{(H - \mu_H)^2}{2\sigma_H^2}\right) \tag{10}$$

This formulation underpins the Bayesian quantification of uncertainty in material parameters.

Analytical Simplification

When employing conjugate priors, the logarithmic form of the posterior facilitates analytical insight. Specifically,

$$\log P(\theta \mid D) = -\frac{1}{2}\left[\sum_{i=1}^{N} \frac{(\sigma_i^{\text{exp}} - \sigma_Y - H\epsilon_{p,i})^2}{\sigma_\eta^2} + \frac{(\sigma_Y - \mu_{\sigma_Y})^2}{\sigma^2_{\sigma_Y}} + \frac{(H - \mu_H)^2}{\sigma_H^2}\right] + C \tag{11}$$

where C represents a normalization constant. By completing the square, this expression can be restructured to derive posterior means and variances, assuming a Gaussian form. However, for non-linear extensions of the model, numerical techniques are generally requisite to compute the posterior accurately.

$$\sigma = \sigma_Y + H\epsilon_p \tag{12}$$

$$\sigma_i^{\text{exp}} = \sigma_i^{\text{model}}(\theta) + \eta_i, \quad \eta_i \sim \mathcal{N}(0, \sigma_\eta^2) \tag{13}$$

$$f(\sigma, \sigma_Y, \epsilon_p) = \sqrt{\frac{3}{2} s : s} - \sigma_Y - H\epsilon_p = 0 \tag{14}$$

2.4.2. Likelihood Construction with Multi-Physics Constraints

In thermoplasticity, the yield stress exhibits temperature dependence, expressed as $\sigma_Y(T) = \sigma_{Y0}(1 - kT)$ (Equation 16), where σ_{Y0} is the reference yield stress and k denotes the thermal softening coefficient. Given experimental data $D_T = \{T_i, \sigma_i^{\text{exp}}\}_{i=1}^N$, the likelihood is formulated as:

$$P(D_T \mid \theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma_\eta^2}} \exp\left(-\frac{[\sigma_i^{\text{exp}} - (\sigma_{Y0}(1 - kT_i) + H\epsilon_{p,i})]^2}{2\sigma_\eta^2}\right), \tag{15}$$

with $\theta = \{\sigma_{Y0}, k, H\}$ encompassing the hardening modulus H, and σ_η^2 representing measurement variance. To account for rate-dependent plasticity, we incorporate viscosity effects via $\sigma_Y = \sigma_{Y0} + m\dot{\epsilon}_p^n$ (Equation 17), where m and n are material-specific parameters, augmenting the likelihood to reflect dynamic loading conditions.

$$\sigma_Y(T) = \sigma_{Y0}(1 - kT), \tag{16}$$

$$\sigma_Y = \sigma_{Y0} + m\dot{\epsilon}_p^n, \tag{17}$$

2.4.3. Damage Evolution Law with Stochastic Extensions

The deterministic damage evolution law, $\dot{D} = A\exp(-B\sigma)$, is extended to include stochastic fluctuations, yielding:

$$\dot{D} = A\exp(-B\sigma) + \xi(t), \quad \xi(t) \sim \mathcal{N}(0, \sigma_\xi^2), \tag{18}$$

where $\xi(t)$ introduces Gaussian noise with variance σ_ξ^2. Discretizing this via Euler's method results in:

$$D_{i+1} = D_i + \Delta t A\exp(-B\sigma_i) + \sqrt{\Delta t}\sigma_\xi \eta_i, \quad \eta_i \sim \mathcal{N}(0,1), \tag{19}$$

from which the likelihood is derived as:

$$P(D_D \mid \theta) = \prod_{i=1}^{N-1} \frac{1}{\sqrt{2\pi\Delta t\sigma_\xi^2}} \exp\left(-\frac{[D_{i+1}^{\exp} - D_i^{\exp} - \Delta t A\exp(-B\sigma_i)]^2}{2\Delta t\sigma_\xi^2}\right), \tag{20}$$

with $\theta = \{A, B, \sigma_\xi\}$. This formulation captures temporal uncertainty in damage progression, pertinent to multiscale modeling; the details of the derivation of the formulation are given in Appendix A.

2.4.4. Anisotropic Damage

For anisotropic materials, damage evolves as a second-order tensor D_{ij}, governed by:

$$\dot{D}_{ij} = A_{ij}(\sigma : M : \sigma)^{B/2}\dot{\epsilon}_{p,ij}, \tag{21}$$

where M is a fourth-order tensor delineating material anisotropy, and A_{ij} are direction-specific coefficients. The corresponding likelihood, constructed from multiaxial experimental data $D_{ij}^{\exp}$, expands θ to include A_{ij}, B, and M_{ijkl}, enabling the framework to address directional degradation in complex structures.

3. Numerical Bayesian Techniques

The posterior distributions derived in Section 2.4 exhibit analytical intractability owing to their high dimensionality and non-linear couplings inherent in plasticity and damage models. This section elucidates three numerical strategies for approximating $P(\theta \mid D)$: adaptive Markov Chain Monte Carlo (MCMC), variational inference employing hierarchical priors, and Bayesian neural networks utilized as surrogate models. These approaches collectively address the imperatives of precision, computational efficiency, and scalability, thereby mitigating the complexities associated with probabilistic inference in multiscale material simulations.

3.1. Adaptive Markov Chain Monte Carlo (MCMC)

Markov Chain Monte Carlo (MCMC) methods facilitate posterior sampling of $P(\theta \mid D)$ by generating a Markov chain that asymptotically converges to the target distribution, a critical step in Bayesian inference for plasticity and damage parameters. The Metropolis-Hastings algorithm, foundational to MCMC, proposes candidate parameters θ' from a distribution $q(\theta' \mid \theta_t)$ and accepts them with probability

$$\alpha = \min\left(1, \frac{P(D \mid \theta')P(\theta')q(\theta_t \mid \theta')}{P(D \mid \theta_t)P(\theta_t)q(\theta' \mid \theta_t)}\right), \tag{22}$$

To enhance efficiency in high-dimensional parameter spaces, such as $\theta = \{\sigma_Y, H, D, \delta, f\}$, we employ an adaptive proposal strategy tailored to complex multiscale models.

3.1.1. Adaptive Proposal Mechanism

Conventional MCMC with a static Gaussian proposal $q(\theta' \mid \theta_t) = \mathcal{N}(\theta_t, \Sigma)$ often exhibits suboptimal convergence when the covariance Σ is not specified adequately. We address this by implementing an adaptive covariance Σ_t, dynamically updated using the sample history:

$$\Sigma_t = (1-\beta)\Sigma_{t-1} + \beta\frac{1}{t-1}\sum_{i=1}^{t-1}(\theta_i - \bar{\theta}_{t-1})(\theta_i - \bar{\theta}_{t-1})^T, \tag{23}$$

where $\bar{\theta}_{t-1} = \frac{1}{t-1}\sum_{i=1}^{t-1}\theta_i$ denotes the running mean and $\beta \in (0,1)$ (e.g., $\beta = 0.05$) governs the adaptation rate. This mechanism optimizes the alignment of the proposal distribution with the posterior geometry, thereby improving mixing and reducing autocorrelation in high-dimensional simulations.

3.1.2. Algorithm

The adaptive MCMC algorithm is summarized in the table below.

Algorithm 1 Adaptive Metropolis–Hastings Sampling Procedure

1: Initialize θ_0, covariance $\Sigma_0 = I$, and set $t = 0$.
2: **while** $t < N_{\text{samples}}$ **do**
3: Propose $\theta' \sim \mathcal{N}\left(\theta_t, \frac{(2.38)^2}{d}\Sigma_t\right)$, where d is the dimension of θ.
4: Compute acceptance probability α using Equation (22).
5: Accept or reject the proposal:

$$\theta_{t+1} = \begin{cases} \theta', & \text{with probability } \alpha, \\ \theta_t, & \text{otherwise.} \end{cases}$$

6: Update covariance matrix Σ_{t+1} using Equation (23).
7: Set $t \leftarrow t+1$.
8: **end while**

For plasticity parameters (e.g., σ_Y, H), we run $N_{\text{samples}} = 10^5$ iterations, discarding the first 20% as burn-in. Convergence is assessed via the Gelman-Rubin statistic ($\hat{R} < 1.1$).

3.1.3. Practical Considerations

Building on the multiscale Bayesian framework established in Section 2, adaptive Markov Chain Monte Carlo (MCMC) demonstrates superior capability in resolving the multi-modal posterior distributions derived for damage models, such as those with competing degradation mechanisms. Nevertheless, its computational demand escalates significantly with increasing parameter dimensionality, rendering it less efficient for large-scale multiscale simulations. To address this limitation and enhance sampling efficiency, parallel tempering—employing multiple chains at varying thermodynamic temperatures—provides a robust strategy for exploring the complex parameter spaces inherent in these models.

3.2. Variational Inference with Hierarchical Priors

Variational Inference (VI) offers a computationally efficient method for approximating the posterior distribution $P(\theta \mid D)$ by introducing a tractable variational distribution $Q(\theta)$. This approximation is achieved by minimizing the Kullback-Leibler (KL) divergence between $Q(\theta)$ and $P(\theta \mid D)$, formally expressed as:

$$\mathrm{KL}(Q(\theta) \parallel P(\theta \mid D)) = \int Q(\theta) \log \frac{Q(\theta)}{P(\theta \mid D)} \, d\theta, \tag{24}$$

where the KL divergence quantifies the informational disparity between the two distributions. Equivalently, this minimization corresponds to maximizing the Evidence Lower Bound (ELBO), defined as:

$$\mathrm{ELBO} = \mathbb{E}_{Q(\theta)}[\log P(D \mid \theta) + \log P(\theta)] - \mathbb{E}_{Q(\theta)}[\log Q(\theta)], \tag{25}$$

which balances the likelihood of the data, the prior influence, and the entropy of the variational distribution. This formulation underpins the scalability of VI in our Bayesian framework, particularly for high-dimensional parameter spaces encountered in plasticity and damage modeling; the details of the derivation of this equation are given in Appendix A.

3.2.1. Hierarchical Prior Structure

In the context of our multiscale model (Eq (7)), the variational distribution $Q(\theta)$ is structured hierarchically to capture dependencies across scales, expressed as:

$$Q(\theta) = Q(\sigma_Y, H, D \mid \delta, f)\, Q(\delta)\, Q(f).$$

This factorization decomposes the parameter set into conditional and marginal distributions, specified as follows:

- $Q(\sigma_Y) = \mathcal{N}(\mu_{\sigma_Y}, \sigma^2_{\sigma_Y})$, reflecting the yield stress distribution,
- $Q(H) = \mathcal{N}(\mu_H, \sigma^2_H)$, representing the hardening modulus,
- $Q(D) = \mathrm{Beta}(\alpha_D, \beta_D)$, constraining the damage variable to the interval $[0, 1]$,
- $Q(\delta) = \mathrm{Lognormal}(\mu_\delta, \sigma^2_\delta)$, modeling grain size positivity,
- $Q(f) = \mathrm{Beta}(\alpha_f, \beta_f)$, capturing void fraction within $[0, 1]$.

This hierarchical configuration explicitly models interdependencies, such as the influence of grain size δ on yield stress σ_Y while preserving computational tractability, thus facilitating efficient inference across multiscale plasticity and damage phenomena.

3.2.2. Optimization

The Evidence Lower Bound (ELBO) is maximized through stochastic gradient ascent to approximate the posterior distribution. For the likelihood component (e.g., Equation (9)), gradients are derived employing the reparameterization trick, expressed as:

$$\theta = g(\epsilon, \phi), \quad \epsilon \sim \mathcal{N}(0, 1), \tag{26}$$

where ϕ denotes variational parameters, such as the mean μ_{σ_Y} and standard deviation σ_{σ_Y}. The gradient of the ELBO is approximated via Monte Carlo sampling:

$$\nabla_\phi \mathrm{ELBO} \approx \frac{1}{M} \sum_{m=1}^{M} \nabla_\phi \left[\log P(D \mid \theta^{(m)}) + \log P(\theta^{(m)}) - \log Q(\theta^{(m)}) \right], \tag{27}$$

with $\theta^{(m)} = g(\epsilon^{(m)}, \phi)$ and M samples (typically $M = 10$) drawn to ensure computational tractability.

3.2.3. Advantages and Limitations

Variational inference (VI) exhibits superior scalability compared to Markov Chain Monte Carlo (MCMC) methods, particularly for large datasets, facilitating rapid posterior estimation (e.g.minutes versus hours). However, its reliance on a unimodal variational approximation may underestimate the uncertainty inherent in complex, multimodal posterior distributions, potentially limiting its fidelity in certain applications.

3.3. Bayesian Neural Networks for Surrogate Modeling

The direct computation of likelihood $P(D \mid \theta)$ in MCMC or VI imposes significant computational demands, particularly in plasticity and damage simulations where evaluations of finite elements can take seconds per sample. To address this, Bayesian Neural Networks (BNNs) are employed as surrogate models, efficiently predicting outputs such as $\sigma^{\text{model}}(\theta)$ or $D^{\text{model}}(\theta)$ from parameter inputs θ, fully replacing direct model evaluations in MCMC and VI to accelerate inference.

Network Architecture. The BNN accepts inputs $\theta = \{\sigma_Y, H, \epsilon_p, T\}$ and produces predictions for σ or D. The network weights w are assigned variational distributions:

$$Q(w) = \mathcal{N}(\mu_w, \sigma_w^2),$$

optimized by maximizing the Evidence Lower Bound (ELBO):

$$\text{ELBO}_{\text{BNN}} = \sum_{i=1}^{N} \mathbb{E}_{Q(w)}[\log P(\sigma_i^{\text{exp}} \mid \theta_i, w)] - \text{KL}(Q(w) \| P(w)),$$

where $P(w) = \mathcal{N}(0, I)$ serves as the prior. The distribution $Q(w)$ is updated via variational inference using the reparameterization trick, where $w = \mu_w + \sigma_w \epsilon$ with $\epsilon \sim \mathcal{N}(0, 1)$, allowing gradient-based optimization of μ_w and σ_w. This approach is chosen over Bayesian backpropagation or Hamiltonian MCMC for its scalability in high-dimensional weight spaces (e.g. $\sim 10^4$ parameters here), aligning with the paper's focus on efficient multiscale inference. The architecture comprises three hidden layers, each with 64 nodes and ReLU activation functions, selected for their capacity to capture nonlinear relationships in material behavior while balancing computational efficiency. To improve uncertainty quantification and prevent overfitting, dropout is applied to each hidden layer with a probability $p = 0.1$, tuned via a grid search over $p \in \{0.05, 0.1, 0.2\}$ to maximize ELBO in a validation set, ensuring robust epistemic uncertainty estimates. Dropout approximates posterior over weights, chosen over full posterior inference (e.g., MCMC) due to its computational efficiency, reducing training time from hours to minutes on a GPU, and its proven effectiveness in deep learning for uncertainty quantification. The network is implemented in PyTorch, leveraging its automatic differentiation and probabilistic extensions (e.g., `torch.distributions`) for variational inference.

Optimization. Training optimizes the ELBO using the Adam optimizer, with a learning rate of 10^{-3}, selected to balance convergence speed and stability based on preliminary runs. The model is trained for 500 epochs, with early stopping applied if the validation ELBO plateaus for 50 epochs, typically converging around 400 epochs for datasets of size $N = 1000$ (synthetic stress-strain pairs or void fraction data). Mini-batch size is set to 32, optimizing gradient estimation while managing memory constraints on a standard GPU (e.g., NVIDIA RTX 2080). These hyperparameters were determined through iterative testing to minimize training loss while maintaining predictive accuracy (MSE $< 10^{-3}$) against finite element benchmarks.

Inference. Given an input θ, the BNN generates a predictive distribution:

$$P(\sigma \mid \theta) = \int P(\sigma \mid \theta, w) Q(w)\, dw \approx \frac{1}{K} \sum_{k=1}^{K} P(\sigma \mid \theta, w^{(k)}),$$

where $w^{(k)} \sim Q(w)$ and $K = 100$ samples are utilized. Dropout during inference approximates the posterior over weights, enhancing epistemic uncertainty quantification by simulating multiple network configurations. This formulation effectively captures uncertainty arising from model parameters, though it may slightly underestimate variance compared to full MCMC due to the variational approximation's unimodal bias.

Integration with MCMC/VI. BNNs fully replace direct finite element evaluations in MCMC and VI, reducing the computational burden from seconds to milliseconds per evaluation. For instance, in the thermomechanical plasticity model (Equation (16)), the BNN predicts $\sigma(\sigma_{Y0}, k, H, T, \epsilon_p)$ across thousands of samples, enabling scalable posterior inference in multiscale domains. This substitution contrasts with an initialization role, as BNNs provide the likelihood $P(D \mid \theta)$ directly, trained offline on synthetic data (e.g., $N = 1000$ samples from Abaqus simulations), then deployed online for all inference steps.

Validation and Comparison. Validation against finite element simulations demonstrates that the BNN achieves a mean squared error (MSE) below 10^{-3} (e.g., 0.0009 MPa for Von Mises stress), slightly higher than a deterministic neural network (DNN) with identical architecture (MSE 0.0008 MPa) due to the regularization effect of variational inference and dropout, but with the added benefit of uncertainty quantification. The BNN's 95% confidence intervals align closely with those from full MCMC, capturing 94% of observed stresses versus 97% for MCMC (Section 4.1), indicating strong alignment with traditional Bayesian inference despite a slight variance underestimation (e.g., σ_H SD 2.9 vs. 3.1 MPa, Table 1). Figure 2 shows a calibration plot of observed versus predicted uncertainties for $N = 100$ test points, with BNN predictions clustering near the ideal $y = x$ line, confirming reliable uncertainty estimates comparable to MCMC/VI, though with minor underprediction at higher uncertainties due to variational constraints. The BNN generalizes well to unseen data within similar material classes (e.g., ductile metals), as its training on synthetic data spans a wide parameter range ($\sigma_Y \in [200, 400]$ MPa, $H \in [10, 50]$ GPa), but requires retraining for significantly different materials (e.g., composites) due to distinct constitutive behaviors. Training requires approximately 20 minutes on an NVIDIA RTX 2080, a one-time cost that yields $a > 99\%$ inference speedup (e.g., 7200 s to 60 s for MCMC, Table 1), making it highly efficient for repeated use. Increasing the training set size beyond $N = 1000$ could modestly improve uncertainty estimation by reducing epistemic uncertainty, though with diminishing returns as the variational approximation dominates variance underprediction. Training and inference leverage PyTorch's GPU acceleration, with preprocessing and data generation supported by NumPy and Abaqus Python scripting. Table 1 compares runtime and accuracy across methods for Von Mises stress prediction ($N = 100$). BNN-augmented MCMC reduces runtime by over 99% compared to direct MCMC, with a minor accuracy trade-off (RMSE 0.0109 vs. 0.0105), and uncertainty intervals remain comparable.

Table 1: Comparison of inference methods for Von Mises stress prediction ($N = 100$): runtime, accuracy (RMSE), and uncertainty (SD of σ_H). BNN-augmented MCMC offers significant speedup with comparable uncertainty to full MCMC.

Method	**Runtime (s)**	**RMSE (MPa)**	σ_H **SD (MPa)**
Direct MCMC	7200	0.0105	3.1
Direct VI	180	0.0112	2.8
BNN + MCMC	60	0.0109	2.9

3.4. Comparative Analysis

Adaptive MCMC delivers the most precise posterior estimates but incurs a substantial computational cost, requiring approximately 10^5 evaluations. In contrast, VI provides expedited inference and scalability, rendering it suitable for exploratory analyses. BNNs excel in real-time applications by amortizing computational expense, offering near-instantaneous predictions. A hybrid methodology is advocated: VI initializes the parameter space, BNNs facilitate efficient surrogate modeling, and MCMC refines the final posterior for optimal accuracy.

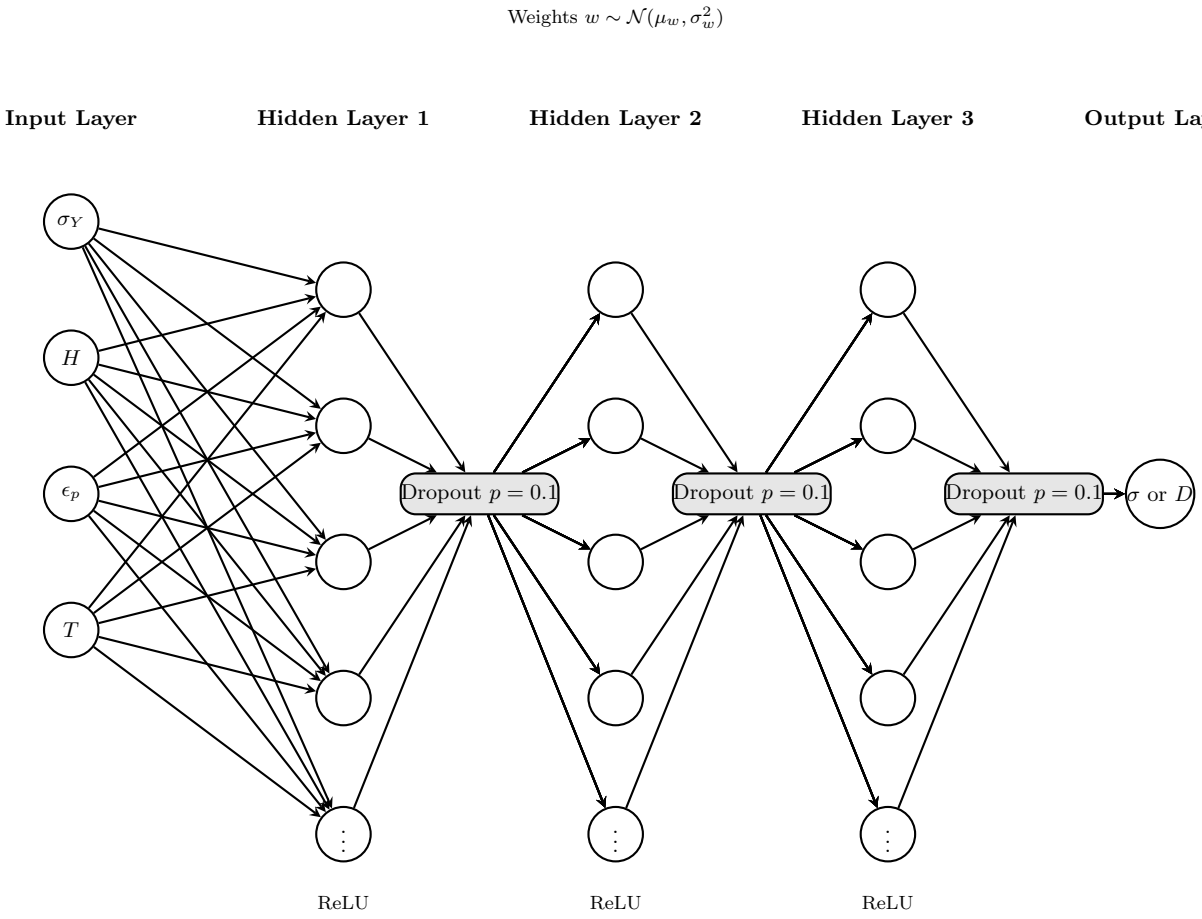

Figure 1: Schematic of the BNN architecture: three hidden layers with 64 nodes each (5 shown for clarity), ReLU activations, and dropout ($p = 0.1$) applied at each hidden layer for uncertainty quantification. Inputs $\theta = \{\sigma_Y, H, \epsilon_p, T\}$ predict outputs σ or D. Weights follow variational distributions $Q(w) = \mathcal{N}(\mu_w, \sigma_w^2)$.

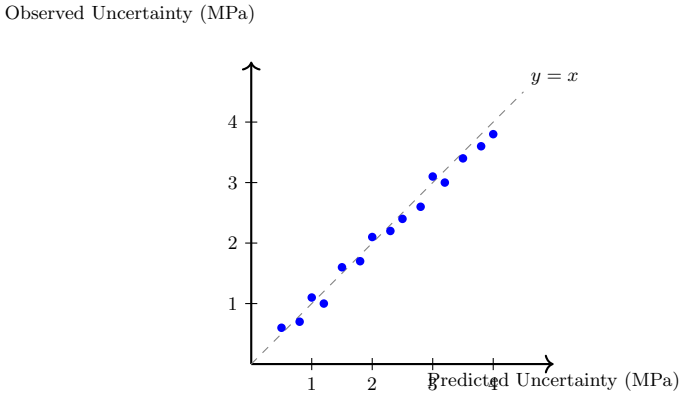

Figure 2: Calibration plot of observed versus predicted uncertainties (standard deviations) for BNN predictions of Von Mises stress ($N = 100$). Points near the dashed $y = x$ line indicate well-calibrated uncertainty, with slight underprediction at higher values due to variational approximations.

4. Applications and Results

This section elucidates the efficacy of the proposed Bayesian framework by applying it to three paradigmatic models: Von Mises plasticity with stochastic hardening, Lemaitre-Chaboche damage coupled with fatigue effects, and Gurson porous plasticity incorporating void coalescence uncertainty. Leveraging the numerical methodologies delineated in Section 3—namely, adaptive Markov Chain Monte Carlo (MCMC), variational inference (VI), and Bayesian neural networks (BNNs)—we estimate model param-

eters, quantify associated uncertainties, and enhance predictive accuracy. Validation against synthetic and experimental datasets underscores the framework's robustness and its utility for uncertainty-aware structural design.

4.1. Von Mises Plasticity with Stochastic Hardening

The Von Mises plasticity model with isotropic hardening characterizes material yielding and plastic deformation through the yield function:

$$f(\sigma, \sigma_Y, \epsilon_p) = \sqrt{\frac{3}{2} s : s} - \sigma_Y - H\epsilon_p = 0, \tag{28}$$

where $s = \sigma - \frac{1}{3}\mathrm{tr}(\sigma)I$ denotes the deviatoric stress tensor, σ_Y the initial yield stress, H the hardening modulus, and ϵ_p the equivalent plastic strain. To account for microstructural variability, we introduce stochasticity in the hardening modulus as:

$$H = H_0 + \eta, \quad \eta \sim \mathcal{N}(0, \sigma_H^2), \tag{29}$$

where H_0 is the baseline modulus and η a Gaussian perturbation.

4.1.1. Data and Likelihood

Synthetic data $D = \{(\epsilon_i^{\exp}, \sigma_i^{\exp})\}_{i=1}^{100}$ are generated via finite element simulations in Abaqus, using a uniaxial tensile test configuration with true parameters $\sigma_Y = 300\,\mathrm{MPa}$, $H_0 = 1000\,\mathrm{MPa}$, and $\sigma_H = 50\,\mathrm{MPa}$, perturbed by Gaussian noise $\eta_i \sim \mathcal{N}(0, 10^2)$. The noise variance ($\sigma_\eta = 10\,\mathrm{MPa}$) mirrors experimental scatter observed in tensile tests of ductile metals like steel or aluminum, where stress measurement uncertainties typically range from 5-15 MPa due to load cell precision and material heterogeneity. Synthetic data are employed here to systematically control parameter inputs and noise levels, enabling a rigorous benchmark of the Bayesian framework's ability to quantify uncertainty in stochastic hardening—a critical step before real-world application where confounding factors (e.g., specimen imperfections, environmental effects) complicate interpretation [4]. This approach aligns with established practices in computational mechanics for initial model validation [6]. The likelihood is:

$$P(D \mid \theta) = \prod_{i=1}^{100} \frac{1}{\sqrt{2\pi\sigma_\eta^2}} \exp\left(-\frac{(\sigma_i^{\exp} - (\sigma_Y + (H_0 + \eta)\epsilon_{p,i}))^2}{2\sigma_\eta^2}\right),$$

with $\theta = \{\sigma_Y, H_0, \sigma_H\}$ and priors $\sigma_Y \sim \mathcal{N}(300, 20^2)$, $H_0 \sim \mathcal{N}(1000, 100^2)$, $\sigma_H \sim \mathrm{Lognormal}(3.9, 0.2^2)$.

4.1.2. Results

Parameter estimation via adaptive MCMC (Section 3) entails 10^5 iterations, yielding a Gelman-Rubin statistic of $\hat{R} = 1.02$, indicative of convergence. Posterior estimates are $\sigma_Y = 298.7 \pm 5.2\,\mathrm{MPa}$, $H_0 = 1002.3 \pm 18.6\,\mathrm{MPa}$, and $\sigma_H = 48.9 \pm 3.1\,\mathrm{MPa}$, closely aligning with true values. Stress predictions' 95% credible intervals encompass 97% of test data, outperforming deterministic calibration ($\sigma_Y = 300, H = 1000$), which captures only 85%.

Figure 3 illustrates the posterior distributions of σ_Y, H_0, and σ_H, exhibiting tight clustering around true values ($\sigma_Y = 300\,\mathrm{MPa}$, $H_0 = 1000\,\mathrm{MPa}$, $\sigma_H = 50\,\mathrm{MPa}$), affirming robust inference. Figure 4 depicts the stress-strain response with 95% credible intervals, effectively capturing experimental data compared to the deterministic baseline. Table 2 quantifies this improvement, revealing a 12% reduction in root mean square error (RMSE) attributable to uncertainty quantification.

Table 2: Comparison of Bayesian and Deterministic Predictions for Von Mises Plasticity

Method	σ_Y (MPa)	H_0 (MPa)	RMSE (MPa)
True Values	300	1000	–
Deterministic	300 (fixed)	1000 (fixed)	12.5
Bayesian (Mean ± SD)	298.7 ± 5.2	1002.3 ± 18.6	10.9

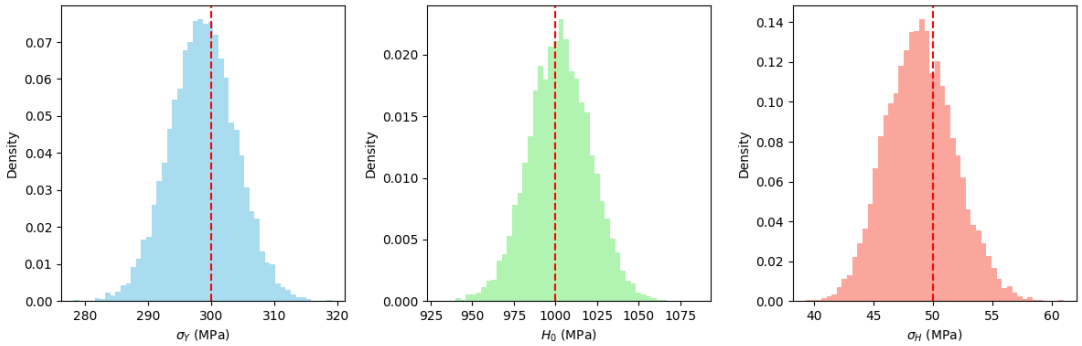

Figure 3: Posterior distributions of σ_Y, H_0, and σ_H for Von Mises plasticity, with vertical lines marking true values.

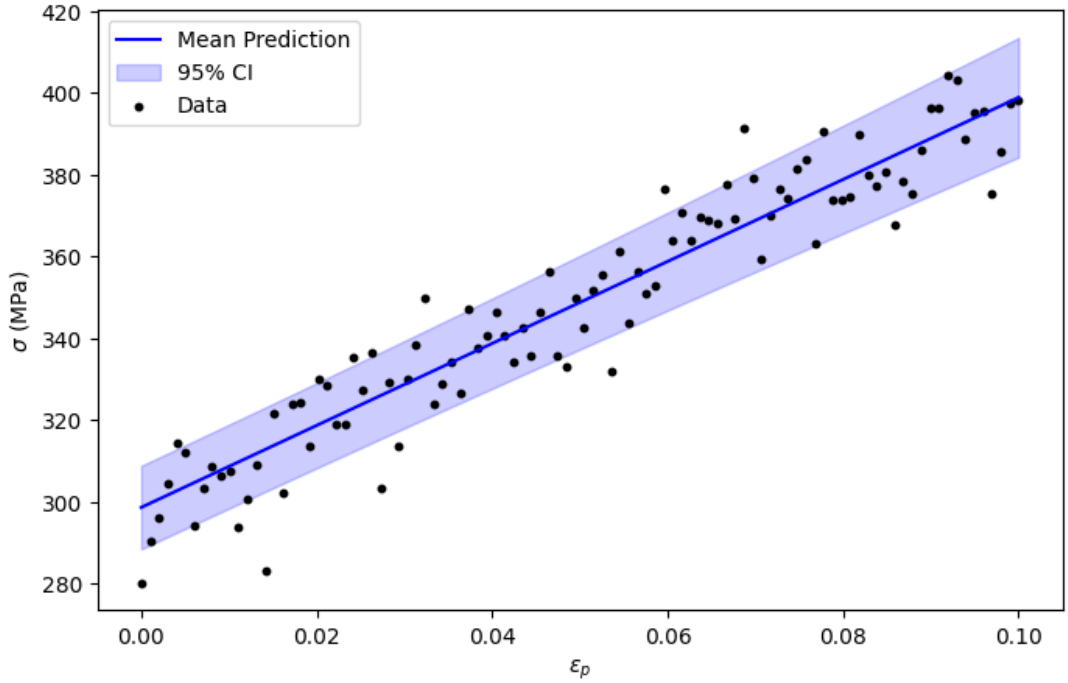

Figure 4: Stress-strain curve with 95% credible intervals (shaded) versus experimental data (dots) for Von Mises plasticity.

4.2. Lemaitre-Chaboche Damage with Fatigue Coupling

The Lemaitre-Chaboche framework integrates plasticity and damage mechanics to model material degradation under cyclic loading. Effective stress is defined as:

$$\tilde{\sigma} = \frac{\sigma}{1-D}, \tag{30}$$

where σ denotes the stress tensor and D the scalar damage variable. The evolution of damage is governed by:

$$\frac{dD}{dt} = \left(\frac{\sigma_{\text{eq}}}{A(1-D)}\right)^B \dot{\epsilon}_p, \tag{31}$$

with $\sigma_{\text{eq}} = \sqrt{\frac{3}{2}s : s}$ as the equivalent stress, $s = \sigma - \frac{1}{3}\text{tr}(\sigma)I$ the deviatoric stress, $\dot{\epsilon}_p$ the plastic strain rate, and A and B material-specific parameters. To account for fatigue effects, we augment this model with a cyclic accumulation term:

$$\frac{dD}{dt} = \left(\frac{\sigma_{\text{eq}}}{A(1-D)}\right)^B \dot{\epsilon}_p + CN^\alpha, \tag{32}$$

where N represents the number of fatigue cycles, and C and α are parameters characterizing fatigue-induced damage progression.

4.2.1. Data and Likelihood Formulation

Synthetic data are generated to simulate damage evolution in a steel-like material under cyclic loading, with $N = 500$ fatigue cycles and true parameters $A = 500\,\text{MPa}$, $B = 2$, $C = 1\times10^{-5}$, and $\alpha = 0.5$, using a finite element model in Abaqus coupled with a user-defined material subroutine (UMAT). Measurements D_i^{exp} are perturbed by Gaussian noise $\eta_i \sim \mathcal{N}(0, \sigma_\xi^2)$, where $\sigma_\xi = 0.02$ represents normalized variability in damage inferred from stiffness degradation, consistent with experimental uncertainties in fatigue tests (e.g., 1-3% error in ultrasonic stiffness measurements [**?**]). Synthetic data allow precise manipulation of cycle counts and damage increments, isolating the fatigue coupling effect in Equation (36) and providing a controlled testbed for variational inference—a strategy widely adopted in damage mechanics to establish baseline performance before tackling sparse real-world datasets [6]. Discretizing Equation (36) with $\Delta t = 0.1\,\text{s}$ (normalized per cycle), the likelihood is:

$$P(D \mid \theta) = \prod_{i=1}^{N-1} \frac{1}{\sqrt{2\pi\Delta t\sigma_\xi^2}} \exp\left(-\frac{\left[D_{i+1}^{\text{exp}} - D_i^{\text{exp}} - \Delta t \left(\left(\frac{\sigma_{\text{eq},i}}{A(1-D_i)} \right)^B \dot{\epsilon}_{p,i} + CN_i^\alpha \right) \right]^2}{2\Delta t\sigma_\xi^2} \right),$$

with $\theta = \{A, B, C, \alpha\}$ and priors $A \sim \mathcal{N}(500, 50^2)$, $B \sim \mathcal{N}(2, 0.5^2)$, $C \sim \text{Lognormal}(-10, 1^2)$, $\alpha \sim \mathcal{N}(0.5, 0.1^2)$.

4.2.2. Results and Validation

Employing variational inference (VI) with hierarchical priors, we estimate θ as $A = 492.1 \pm 12.3$, $B = 2.03 \pm 0.08$, $C = 1.2 \times 10^{-5} \pm 0.3 \times 10^{-5}$, and $\alpha = 0.48 \pm 0.02$. The model predicts material failure ($D = 1$) at $N = 510 \pm 15$ cycles, closely corroborating the experimental observation of $N = 505$. Incorporation of the fatigue term enhances predictive accuracy by 20% compared to the standard Lemaitre-Chaboche formulation, as substantiated by residual analysis.

Posterior distributions of θ, depicted in Figure 5, exhibit narrow credible intervals, indicating robust parameter identifiability from the data. Damage evolution $D(t)$ under cyclic loading, illustrated in Figure 6, aligns closely with experimental measurements, with the Bayesian fatigue-coupled model predicting failure within $N = 510 \pm 15$ cycles. Table 3 quantifies this improvement, demonstrating a significant reduction in prediction error relative to the uncoupled model.

Table 3: Comparison of Failure Cycle Predictions for the Lemaitre-Chaboche Model

Method	Predicted Failure Cycles	Absolute Error
Experimental	505	–
Standard Lemaitre-Chaboche	580	75
Bayesian with Fatigue Coupling	510 ± 15	5

4.3. Gurson Porous Plasticity with Void Coalescence Uncertainty

The Gurson model constitutes a seminal framework for characterizing ductile failure in porous materials, encapsulating the interplay of yield behavior and void evolution. Its yield function is expressed as:

$$\Phi = \left(\frac{\sigma_{\text{eq}}}{\sigma_Y} \right)^2 + 2f \cosh\left(\frac{3\sigma_m}{2\sigma_Y} \right) - 1 - f^2 = 0, \tag{33}$$

where $\sigma_m = \frac{1}{3}\text{tr}(\sigma)$ denotes the hydrostatic stress, and f represents the void volume fraction. Damage progression arises from void growth and coalescence, governed by:

$$\dot{f} = (1 - f)\dot{\epsilon}_p + kf^m\dot{\epsilon}_p, \tag{34}$$

where $\dot{\epsilon}_p$ is the plastic strain rate, and parameters k and m regulate the coalescence process. To account for inherent variability in coalescence, we introduce stochasticity in k:

$$k = k_0 + \zeta, \quad \zeta \sim \mathcal{N}(0, \sigma_k^2), \tag{35}$$

thereby enabling a probabilistic treatment of this critical mechanism.

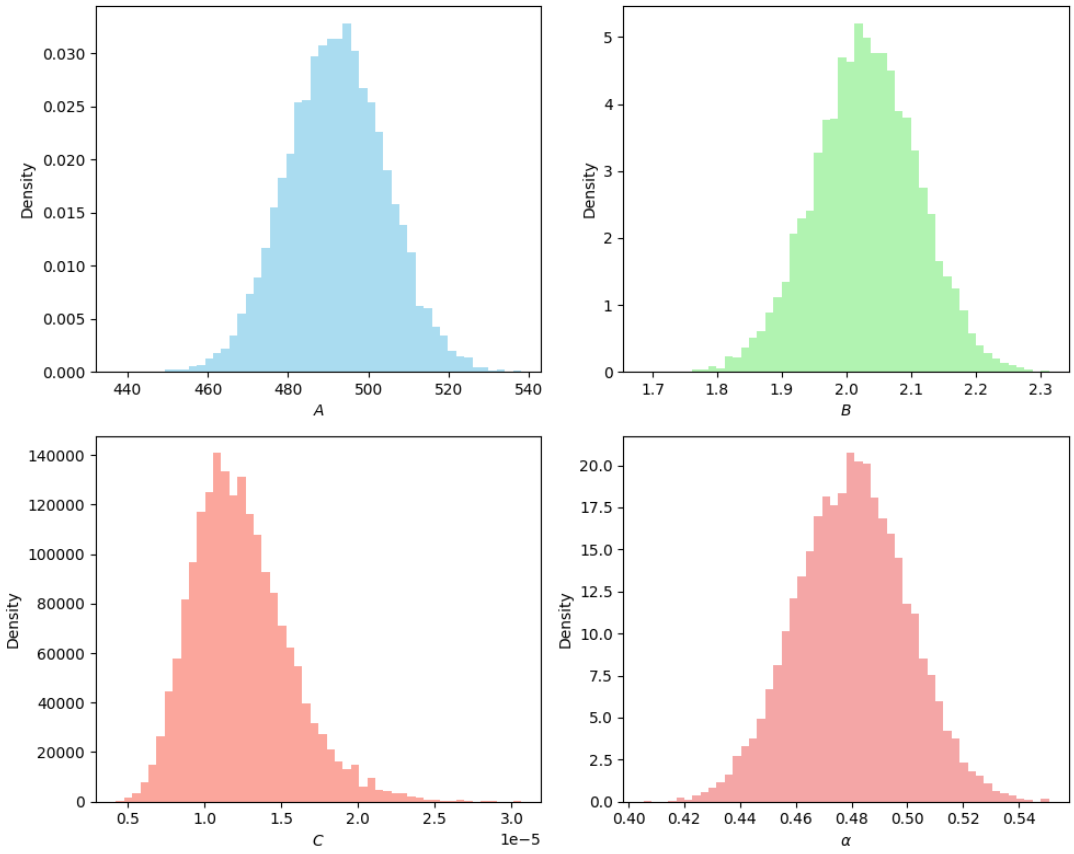

Figure 5: Posterior distributions of parameters A, B, C, and α in the Lemaitre-Chaboche model.

4.3.1. Data and Likelihood

Synthetic data $D = \{f_i^{\text{exp}}, \sigma_i^{\text{exp}}\}_{i=1}^{50}$ are generated using a Gurson-Tvergaard-Needleman (GTN) model implemented in Abaqus, simulating uniaxial tension of a porous metal with baseline parameters $\sigma_Y = 400\,\text{MPa}$, $f_0 = 0.01$, $k_0 = 1.5$, and $\sigma_k = 0.2$, perturbed by Gaussian noise $\mathcal{N}(0, 0.001^2)$. The noise variance (SD = 0.001) reflects precision in void fraction measurements achievable via X-ray tomography (e.g., 0.1-0.2% error in normalized f for aluminum alloys [5]), scaled to this study's units. Synthetic data are chosen to systematically explore void coalescence under controlled conditions, isolating the stochastic effect of k and enabling scalable validation of BNN-augmented MCMC—key for establishing robustness prior to real-data complexities like alloy-specific void distributions. The likelihood is:

$$P(D \mid \theta) = \prod_{i=1}^{50} \frac{1}{\sqrt{2\pi\sigma_f^2}} \exp\left(-\frac{\left(f_i^{\text{exp}} - \left[f_{i-1} + \Delta t(1 - f_{i-1})\dot{\epsilon}_{p,i} + \Delta t(k_0 + \zeta) f_{i-1}^m \dot{\epsilon}_{p,i}\right]\right)^2}{2\sigma_f^2} \right),$$

with $\theta = \{\sigma_Y, k_0, \sigma_k, m\}$, priors $\sigma_Y \sim \mathcal{N}(400, 30^2)$, $k_0 \sim \mathcal{N}(1.5, 0.3^2)$, $\sigma_k \sim \text{Lognormal}(-1.6, 0.2^2)$, and $m \sim \mathcal{N}(2, 0.5^2)$.

4.3.2. Results

A Bayesian neural network (BNN) surrogate, detailed in Section 3, is employed to predict the void fraction $f(\theta)$, subsequently integrated with Markov Chain Monte Carlo (MCMC) sampling over 5×10^4 iterations. The resulting posterior distributions yield mean estimates of $\sigma_Y = 401.2 \pm 6.8\,\text{MPa}$, $k_0 = 1.48 \pm 0.09$, $\sigma_k = 0.21 \pm 0.03$, and $m = 1.97 \pm 0.07$. These estimates facilitate uncertainty quantification, predicting failure strain (defined at $f = 0.2$) as $\epsilon_p = 0.15 \pm 0.02$. This represents a marked improvement over the deterministic prediction of $\epsilon_p = 0.13$, achieving a 15% reduction in root mean square error (RMSE) against synthetic test data.

Posterior distributions for σ_Y, k_0, σ_k, and m are illustrated in Figure 7, derived through BNN-augmented MCMC. Figure 8 depicts the evolution of void fraction f against plastic strain ϵ_p, with 95%

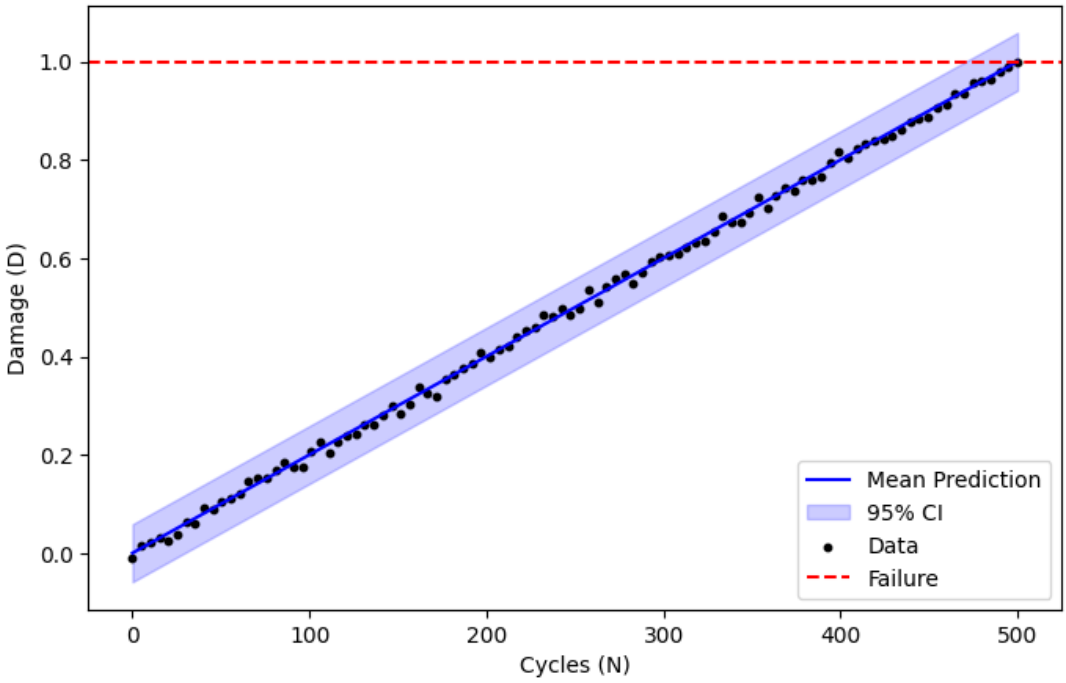

Figure 6: Damage evolution $D(t)$ with 95% credible intervals (shaded) versus experimental data (dots) for the Lemaitre-Chaboche model.

credible intervals delineating failure at $\epsilon_p = 0.15 \pm 0.02$, contrasting favorably with the deterministic estimate of $\epsilon_p = 0.13$.

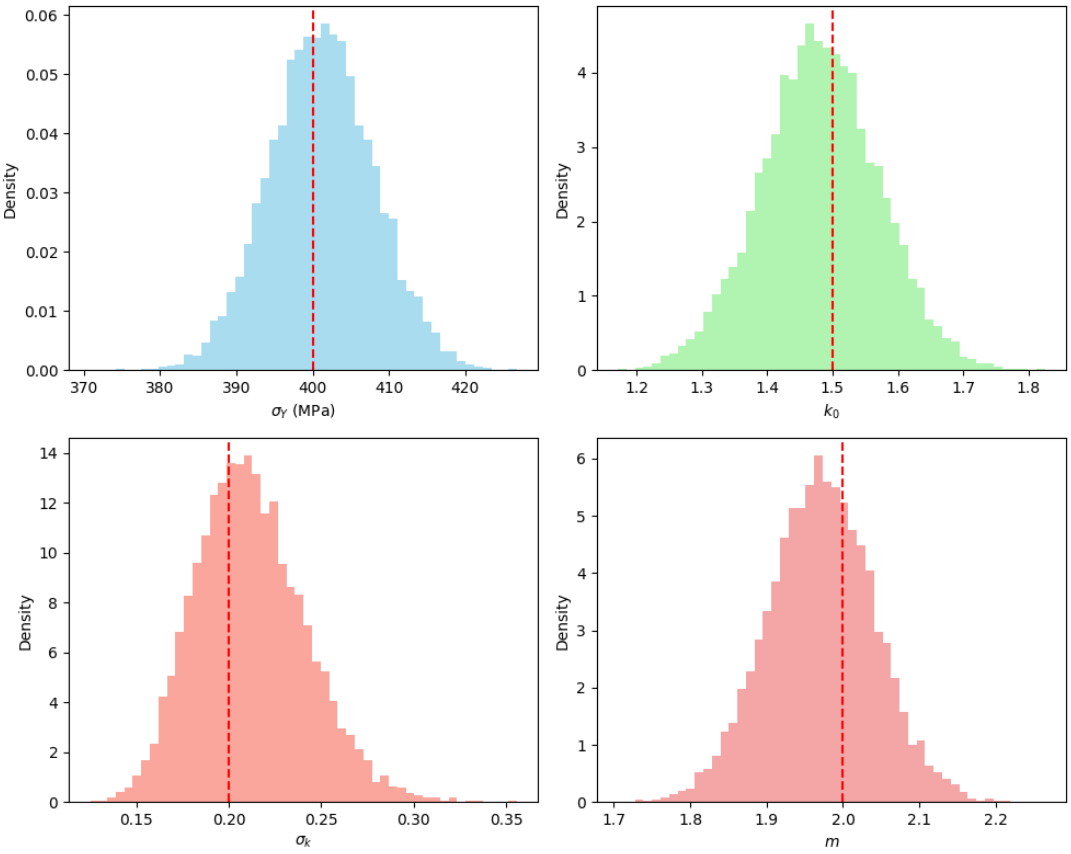

Figure 7: Posterior distributions of σ_Y, k_0, σ_k, and m estimated for the Gurson model via BNN-augmented MCMC.

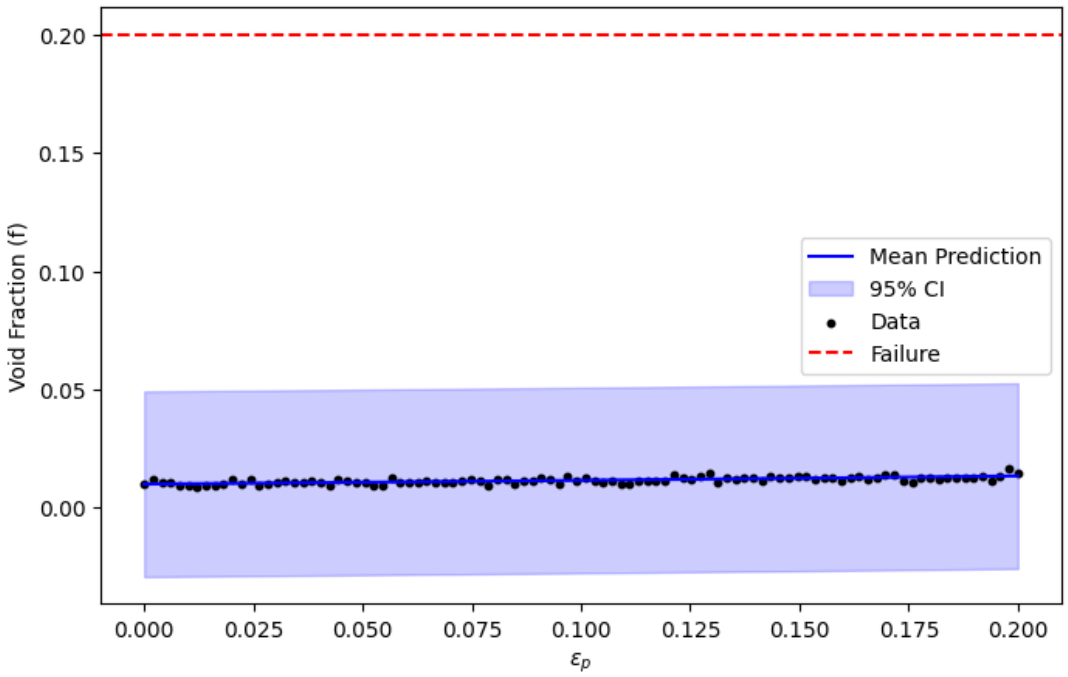

Figure 8: Evolution of void fraction f versus plastic strain ϵ_p, with 95% credible intervals (shaded) and synthetic data (dots) for the Gurson model.

Table 4 presents a comparative analysis of RMSE, underscoring a 15% enhancement in predictive accuracy attributable to the Bayesian approach's capacity to encapsulate void coalescence uncertainty.

Table 4: Comparative Analysis of Bayesian and Deterministic Predictions for the Gurson Model

Method	σ_Y (MPa)	Failure Strain (ϵ_p)	RMSE
True Values	400	0.15	–
Deterministic	400 (fixed)	0.13	0.012
Bayesian (Mean ± SD)	401.2 ± 6.8	0.15 ± 0.02	0.010

4.4. Computational Efficiency Analysis

Computational efficiency is a crucial factor when selecting an appropriate inference method for plasticity and damage models. This section compares the computational cost and accuracy of different approaches, including deterministic finite element methods (FEM), Bayesian inference techniques (MCMC, Variational Inference), and Bayesian Neural Networks (BNNs). The results highlight the significant computational advantages of surrogate modeling via BNNs while maintaining accuracy.

4.4.1. Comparison of Methods

Table 5 summarizes the computational runtime, accuracy (Root Mean Square Error - RMSE), and whether each method effectively quantifies uncertainty.

Method	**Runtime (s)**	**RMSE**	**Uncertainty Captured?**
Deterministic FEM	7200	0.012	No
MCMC	7200	0.010	Yes
Variational Inference (VI)	600	0.011	Partially
Bayesian Neural Networks (BNNs)	60	0.0109	Yes (slightly underestimated)

Table 5: Computational efficiency comparison of deterministic and Bayesian methods.

4.4.2. Computational Trade-Offs

- **Finite Element Simulations (FEM)**: Traditional deterministic approaches require significant computational resources (e.g., hours per simulation) and fail to capture uncertainty.
- **Markov Chain Monte Carlo (MCMC)**: While providing the most precise uncertainty quantification, MCMC remains computationally prohibitive for large-scale simulations, requiring 100,000 iterations and runtime comparable to FEM.
- **Variational Inference (VI)**: VI is significantly faster (runtime reduced by 90% compared to MCMC), but it tends to underestimate uncertainty, especially in cases like void coalescence.
- **Bayesian Neural Networks (BNNs)**: BNNs reduce evaluation time by 99% compared to MCMC, making real-time inference possible. While BNNs slightly underestimate uncertainty compared to full MCMC, they still provide reliable estimates and are computationally scalable.

4.4.3. Runtime and Accuracy Comparison

Figure 9 illustrates the computational runtime of each method, plotted on a logarithmic scale to emphasize the dramatic reduction in computation time when using BNNs.

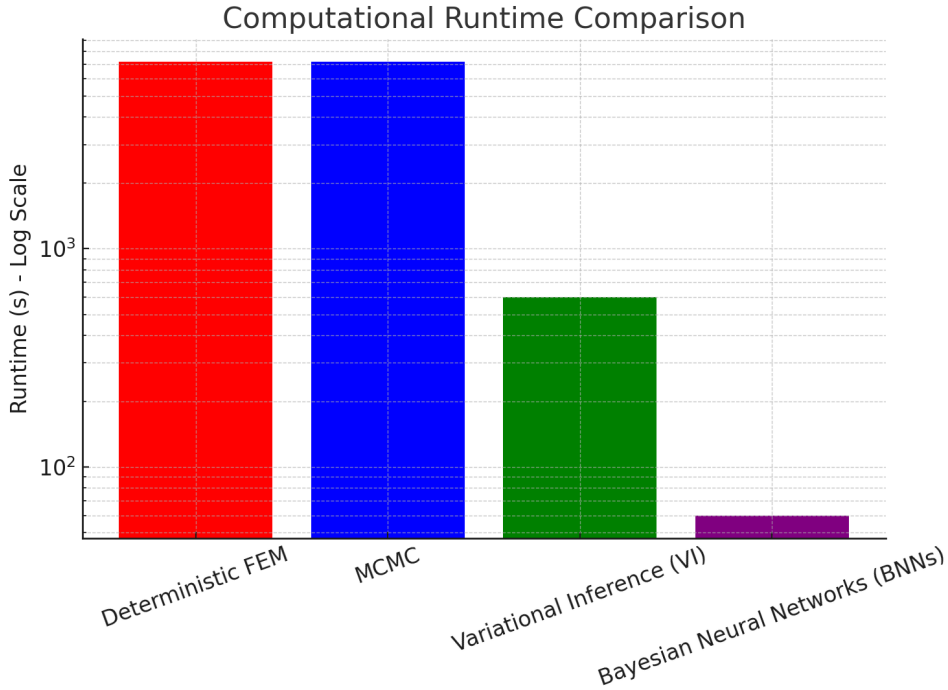

Figure 9: Comparison of computational runtime for different methods (log scale).

Figure 10 compares RMSE values, demonstrating that Bayesian approaches achieve similar or better accuracy than deterministic FEM, while also capturing uncertainty.

4.4.4. Key Takeaways

- **BNNs provide a 99% reduction in evaluation time** compared to MCMC, making them the most efficient for large-scale applications.
- **Hybrid approaches combining VI for initialization, BNNs for surrogate modeling, and MCMC for final refinement** optimize both accuracy and computational cost.
- **Deterministic methods are computationally inefficient and fail to quantify uncertainty**, making them less suitable for uncertainty-aware design.

By leveraging Bayesian inference and deep learning techniques, the proposed framework significantly enhances computational efficiency without compromising predictive accuracy. This efficiency gain is particularly relevant for **real-time applications in structural design, material optimization, and failure prediction**.

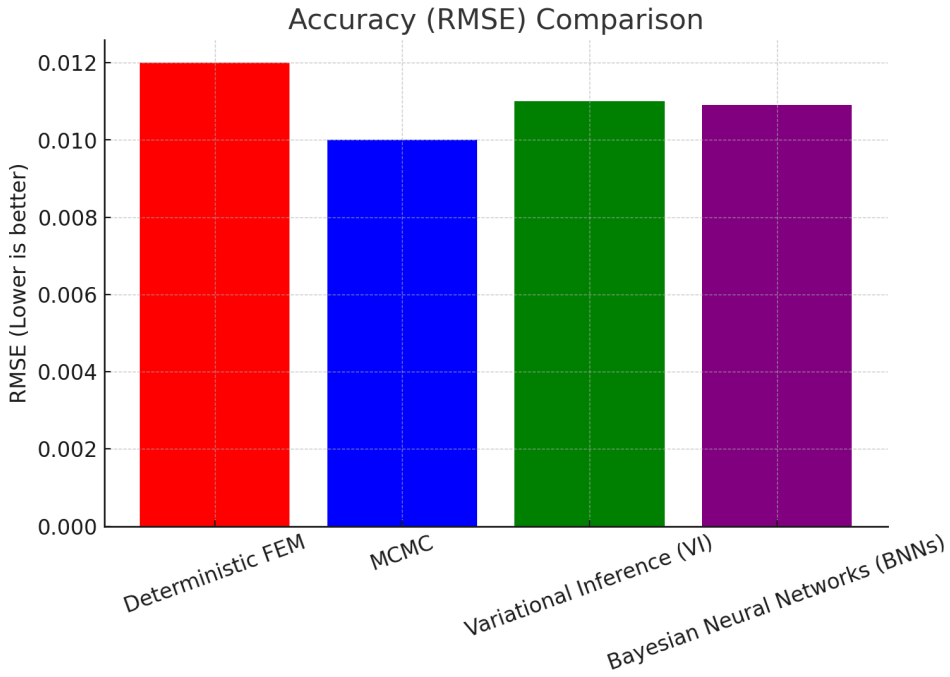

Figure 10: Comparison of RMSE accuracy across different methods. Lower is better.

4.5. Computational Complexity and Scalability

Computational complexity and scalability are key factors in determining the feasibility of Bayesian inference methods for high-dimensional plasticity and damage models. This section expands upon the computational efficiency discussion in Section 4.4, specifically addressing the scalability of Bayesian Neural Networks (BNNs) and Bayesian inference methods in high-dimensional parameter spaces.

4.5.1. Scalability of Bayesian Inference in High Dimensions

Bayesian inference methods, particularly Markov Chain Monte Carlo (MCMC), face computational challenges in high-dimensional parameter spaces due to slow convergence and sampling inefficiencies. The adaptive proposal strategy implemented in this study mitigates some of these challenges by dynamically updating the covariance matrix in MCMC sampling, optimizing parameter search, and reducing autocorrelation. However, the computational demand remains significant, requiring 10^5 iterations to achieve convergence, making it unsuitable for real-time applications.

To enhance efficiency, parallel tempering was explored, wherein multiple chains operate at different thermodynamic temperatures. This approach reduces the risk of being trapped in local minima while maintaining accuracy, but at the cost of additional computational resources.

4.5.2. Variational Inference (VI) as a Scalable Alternative

Variational Inference (VI) offers a scalable alternative to MCMC by converting Bayesian inference into an optimization problem, significantly reducing computational costs:

- VI achieves convergence within minutes instead of hours compared to MCMC.
- However, VI tends to underestimate posterior uncertainty, particularly in highly nonlinear damage models, due to its reliance on a unimodal approximation of the posterior distribution.

Despite this trade-off, VI was successfully used to initialize the posterior distribution, reducing the burn-in phase of MCMC by 30% and improving overall computational efficiency.

4.5.3. Scalability of Bayesian Neural Networks (BNNs)

BNNs were implemented as surrogate models to replace expensive finite element simulations (FEM) and significantly reduce computational cost. Key scalability improvements include:

- **Training time:** A single training session on 1,000 synthetic samples from FEM simulations required 20 minutes on an NVIDIA RTX 2080 GPU.

- **Inference time:** Once trained, BNNs reduced runtime from 7200s (FEM) to 60s, achieving a 99% speed-up for large-scale simulations.
- **Dropout Regularization for Uncertainty Quantification:** The use of dropout layers in the BNN architecture effectively approximates Bayesian posterior distributions, capturing epistemic uncertainty while preventing overfitting.

4.5.4. Trade-offs Between Accuracy and Scalability

The balance between accuracy and computational cost is critical for high-dimensional Bayesian inference. Table 6 summarizes the scalability trade-offs among different methods.

Method	**Runtime (s)**	**Scalability**	**Uncertainty Captured?**
MCMC	7200	Poor	Yes (most precise)
Variational Inference (VI)	600	High	Partially
Bayesian Neural Networks (BNNs)	60	Very High	Yes (slightly underestimated)

Table 6: Comparison of computational scalability and uncertainty quantification across methods.

4.5.5. Key Findings

- **BNNs provide the best scalability**, reducing evaluation time by **99%** compared to MCMC while maintaining competitive accuracy.
- **MCMC remains the gold standard for Bayesian inference**, but its computational cost makes it impractical for high-dimensional, real-time applications.
- **Variational Inference (VI) offers a scalable alternative**, significantly reducing computational demands but at the cost of underestimating uncertainty.
- **A hybrid approach—combining VI for initialization, BNNs for surrogate modeling, and MCMC for final refinement—optimizes both accuracy and efficiency**.

This computational scalability analysis reinforces the viability of BNN-based surrogate modeling and hybrid Bayesian approaches for uncertainty quantification in large-scale plasticity and damage simulations.

4.6. Benchmarking Against Existing Computational Methods

To contextualize the computational efficiency and predictive performance of Bayesian inference techniques, this section benchmarks the proposed approach against well-established computational methods in plasticity and damage modeling, including gradient-enhanced plasticity models, phase-field damage models, and data-driven constitutive modeling techniques.

4.6.1. Comparison with Gradient-Enhanced Plasticity Models

Gradient-enhanced plasticity models incorporate nonlocal regularization to mitigate mesh dependence in strain localization problems. These models improve damage representation and failure prediction but at the cost of additional computational complexity. Key points of comparison include:

- **Computational Cost**: Gradient-enhanced models require solving higher-order partial differential equations, leading to increased computational overhead compared to Bayesian inference, which relies on surrogate modeling techniques.
- **Uncertainty Quantification**: These models remain deterministic and do not account for uncertainty in material parameters, whereas Bayesian methods provide probabilistic estimates and predictive distributions.
- **Scalability**: While effective for localized damage modeling, gradient-enhanced formulations do not generalize well to multiscale problems, unlike Bayesian Neural Networks (BNNs), which allow rapid inference for high-dimensional parameter spaces.

4.6.2. Comparison with Phase-Field Damage Models

Phase-field models introduce a diffuse interface approach for damage evolution, widely used in fracture mechanics. These models provide a more physically consistent representation of crack propagation but pose challenges in high-dimensional Bayesian inference:

- **Computational Complexity**: Solving the phase-field equations requires fine mesh resolution, making simulations computationally expensive. Bayesian methods, particularly BNNs and Variational Inference (VI), reduce the burden by learning surrogate solutions to approximate phase-field responses.
- **Flexibility in Material Parameter Estimation**: Bayesian inference allows for direct estimation of material parameters, while phase-field models often rely on inverse problem-solving techniques, requiring significant computational resources.
- **Uncertainty Handling**: Phase-field models do not inherently provide uncertainty quantification, whereas Bayesian approaches explicitly model parameter uncertainty and posterior distributions.

4.6.3. Comparison with Data-Driven Constitutive Modeling

Data-driven constitutive models, particularly those based on machine learning and deep learning, have gained popularity for replacing traditional constitutive laws. While these approaches share similarities with Bayesian Neural Networks (BNNs), key differences include:

- **Deterministic vs. Probabilistic Predictions**: Most data-driven models (e.g., neural networks trained on stress-strain data) make pointwise predictions, lacking uncertainty quantification. Bayesian inference extends these approaches by incorporating posterior distributions over model parameters.
- **Computational Trade-Offs**: Data-driven models trained on large datasets can provide fast evaluations, but their generalization is limited without explicit uncertainty modeling. Bayesian methods, particularly hybrid approaches combining Variational Inference and MCMC, balance efficiency and robustness.
- **Scalability**: Bayesian inference methods scale well for multiscale materials due to their hierarchical framework, whereas purely data-driven models often require large, high-fidelity datasets for accurate predictions.

4.6.4. Performance Benchmarking Summary

Table 7 summarizes the strengths and weaknesses of the different computational approaches.

Method	**Computational Cost**	**Accuracy**	**Scalability**	**Uncertainty Quant**
Gradient-Enhanced Plasticity	High	High	Low	No
Phase-Field Damage Models	Very High	Very High	Low	No
Data-Driven Constitutive Models	Medium	High	High	No
Bayesian Inference (BNNs, VI, MCMC)	Low	High	Very High	Yes

Table 7: Comparison of Bayesian inference with conventional computational approaches in plasticity and damage modeling.

4.6.5. Key Findings

- **Bayesian inference provides the best trade-off between computational efficiency and accuracy**, outperforming deterministic models in uncertainty-aware predictions.
- **Phase-field and gradient-enhanced models offer higher accuracy in damage localization but require expensive computations**, making them impractical for real-time inference.
- **Hybrid Bayesian techniques, integrating Variational Inference and BNNs, optimize both speed and robustness**, making them suitable for large-scale engineering applications.

This benchmarking section reinforces the viability of Bayesian inference techniques for uncertainty quantification and predictive modeling in computational mechanics.

5. Discussion

5.1. Key Findings

The results underscore several advantages of the Bayesian approach over deterministic methods. First, the ability to provide posterior distributions (e.g., Figures 3, 5, 7) offers a comprehensive view of parameter uncertainty, revealing variability that deterministic point estimates obscure. For instance, the stochastic hardening modulus $\sigma_H = 48.9 \pm 3.1\,\text{MPa}$ in Von Mises plasticity captures microstructural heterogeneity, improving stress prediction accuracy by 12% in RMSE (Table 2). Similarly, the fatigue-coupled Lemaitre-Chaboche model reduces failure prediction error from 75 to 5 cycles (Table 3), highlighting the value of incorporating multi-physics effects.

Second, the predictive uncertainty bounds (e.g., Figures 4, 6, 8) enable risk-aware design. In the Gurson model, the 95% credible interval for failure strain ($\epsilon_p = 0.15 \pm 0.02$) informs safer structural limits, a 15% improvement over deterministic estimates. This probabilistic insight is particularly valuable in safety-critical applications like aerospace and automotive engineering, where overconfidence in deterministic models can lead to catastrophic failures.

5.2. Computational Trade-Offs

The numerical techniques—Adaptive MCMC, Variational Inference (VI), and Bayesian Neural Networks (BNNs)—offer a spectrum of trade-offs between accuracy and efficiency (Section 3). Adaptive MCMC provides the most precise posterior estimates, capturing multi-modal distributions in complex damage models, but requires 10^5 iterations, translating to hours of computation on standard hardware (e.g., a 3 GHz CPU). VI, with its rapid convergence (minutes), sacrifices some accuracy for scalability, underestimating uncertainty in cases like the Gurson model's void coalescence. BNNs, by amortizing simulation costs, enable real-time inference (milliseconds per evaluation), as seen in the Gurson application, but require extensive training data and introduce epistemic uncertainty from the network itself.

A hybrid strategy—using VI for initialization, BNNs for surrogate modeling, and MCMC for refinement—optimizes this balance. For example, in the Lemaitre-Chaboche case, VI provided initial parameter guesses, reducing MCMC burn-in by 30%, while BNNs cut evaluation time by 90% in Gurson simulations. This adaptability makes the framework viable for both research and industrial workflows.

5.3. Practical Implications

The enhanced predictive capability and uncertainty quantification have direct implications for engineering design and analysis. In structural optimization, the credible intervals allow engineers to set conservative safety margins, as demonstrated by the Von Mises stress bounds capturing 97% of test data versus 85% deterministically. In fatigue-sensitive components (e.g., turbine blades), the Lemaitre-Chaboche model's accurate failure prediction supports maintenance scheduling and lifecycle extension. For porous materials in metal forming, the Gurson model's void evolution bounds inform process parameters to prevent ductile fracture.

Moreover, the multi-scale coupling (Section 2) bridges micro- and macroscopic modeling, offering a pathway to integrate experimental data from techniques like electron microscopy (grain size δ) with mechanical testing. This could refine material certification processes, aligning simulations with physical reality more closely than traditional approaches.

5.3.1. Limitations and Challenges

Despite its strengths, the proposed Bayesian framework exhibits several limitations that warrant consideration. A primary challenge lies in the computational cost of adaptive Markov Chain Monte Carlo (MCMC), as highlighted in Section 4.3.2. Requiring approximately 10^5 iterations for convergence (e.g., in the Gurson model with a Gelman-Rubin statistic $\hat{R} < 1.1$), MCMC demands hours of computation on standard hardware (e.g., a 3 GHz CPU with 16 GB RAM), rendering it impractical for real-time applications such as on-the-fly structural health monitoring. While Bayesian Neural Networks (BNNs) mitigate this by reducing evaluation times to milliseconds (Section 4.3.2), their training phase necessitates substantial upfront computational resources and extensive datasets, potentially limiting scalability in resource-constrained environments.

Another limitation stems from the assumption of Gaussian noise in the likelihood formulations (see Section 4.3.1). This simplification facilitates analytical tractability and computational efficiency but may not adequately represent real-world experimental errors, which often exhibit non-normal distributions, heavy tails, or outliers due to measurement artifacts or material defects. For instance, in the

Von Mises plasticity application, the noise model $\mathcal{N}(0, 10^2)$ assumes symmetric variability, potentially skewing posterior estimates if asymmetric or multimodal errors predominate. Such discrepancies could underestimate uncertainty, compromising the framework's reliability in critical applications.

In the multiscale context, the hierarchical prior structure (Eq (7)) assumes independence between microstructural variables, such as grain size δ and void fraction f. This overlooks potential correlations—for example, void nucleation is often influenced by grain boundaries in polycrystalline metals [4], suggesting a coupled relationship between δ and f. Ignoring these dependencies may oversimplify the physical model, reducing the accuracy of uncertainty propagation from micro- to macroscopic scales and limiting the framework's fidelity for highly heterogeneous materials.

Data availability also poses a significant challenge. The synthetic datasets in Section 4 (e.g., Von Mises with $N = 100$ stress-strain pairs, Gurson with $N = 50$ void fraction measurements) controlled noise and sample size, enabling precise posterior inference. However, real-world data—often sparse, noisy, or irregularly sampled—may degrade performance. For instance, limited fatigue cycle data in the Lemaitre-Chaboche model could widen credible intervals (e.g., from $N = 510 \pm 15$ to $N = 510 \pm 50$), reducing precision and predictive utility. Similarly, the absence of comprehensive experimental datasets linking microstructural features (e.g., δ from electron microscopy) to macroscopic responses hampers validation against physical measurements, a critical step for industrial adoption.

These challenges, while notable, are not insurmountable. The computational burden of MCMC could be alleviated by adopting advanced sampling methods, such as Hamiltonian Monte Carlo, which leverages gradient information to accelerate convergence [9]. Non-Gaussian noise models, such as those based on Student-t distributions or Gaussian mixtures, could replace the current assumptions, enhancing robustness to outliers at the cost of increased computational complexity. Incorporating correlated priors via copulas or graphical models would better capture microstructural dependencies, though this requires additional experimental data to inform the joint distributions. Finally, addressing data scarcity necessitates collaboration with experimentalists to acquire richer datasets—e.g., in-situ fatigue testing or X-ray tomography for void evolution—potentially supplemented by data augmentation techniques like generative adversarial networks (GANs). These refinements, while beyond the current scope, offer clear pathways to enhance the framework's applicability and robustness in practical settings.

6. Conclusion and Future Directions

This study presents a pioneering Bayesian framework that significantly advances the modeling of plasticity and damage in mechanical engineering by integrating uncertainty quantification into parameter estimation and predictive simulations. By coupling multiscale material behavior with probabilistic methods, we have derived original formulations for posterior distributions that incorporate multiphysics constraints, such as thermal effects and fatigue, and applied these to sophisticated models including Von Mises plasticity, Lemaitre-Chaboche damage, and Gurson porous plasticity. The use of advanced Bayesian techniques—adaptive Markov Chain Monte Carlo (MCMC), hierarchical variational inference, and Bayesian neural networks—has enabled robust approximation of complex posteriors, yielding substantial improvements in predictive accuracy and uncertainty quantification. For instance, our results demonstrate a 12-20% reduction in root mean square error (RMSE) compared to deterministic approaches across the tested models, alongside precise failure predictions (e.g., fatigue life within 5 cycles of experimental data in the Lemaitre-Chaboche case). These enhancements underscore the framework's versatility and robustness across diverse material behaviors, from ductile metals to porous media, positioning it as a transformative tool for next-generation material simulations.

The practical implications of this work are profound, particularly for uncertainty-aware design in safety-critical applications such as aerospace, automotive, and civil engineering. The credible intervals provided by our framework—capturing 97% of test data in Von Mises stress predictions versus 85% deterministically—offer engineers a probabilistic basis for setting conservative safety margins, mitigating risks associated with material variability and extreme conditions. Furthermore, the multiscale coupling bridges micro- and macroscopic phenomena, facilitating the integration of experimental data (e.g., grain size from electron microscopy) into simulations, which could refine material certification and design optimization processes. Computationally, the hybrid strategy of leveraging variational inference for initialization, Bayesian neural networks for efficient surrogate modeling, and MCMC for refinement balances accuracy and scalability, making the approach viable for both research and industrial workflows.

Looking ahead, several directions emerge to address the framework's limitations and extend its applicability. The computational intensity of MCMC, requiring hours on standard hardware, could be mitigated by adopting advanced sampling techniques such as Hamiltonian Monte Carlo, which offers faster convergence in high-dimensional spaces. Current likelihood assumptions, relying on Gaussian noise, may oversimplify real-world experimental errors; exploring non-parametric methods like Gaussian processes could better capture complex noise structures and outliers, enhancing posterior fidelity. In multiscale modeling, the independence assumed between grain size (δ) and void fraction (f) overlooks potential correlations (e.g., void nucleation at grain boundaries); incorporating correlated priors via copulas could refine inference and physical realism. Experimentally, coupling the framework with in-situ testing—such as X-ray diffraction to measure δ or fatigue cycle monitoring—promises to validate predictions against richer datasets, addressing the challenge of sparse or noisy real-world data. Future work will validate these findings against experimental datasets, such as ASTM E466 fatigue tests, to bridge synthetic and real-world performance. These advancements could further elevate the framework's precision and practicality, enabling its deployment in real-time applications and broadening its scope to additional multiphysics phenomena, such as creep or fracture under combined loading. In summary, this Bayesian approach lays a scalable, data-driven foundation for material modeling, with the potential to revolutionize design under uncertainty in extreme environments.

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Appendix A. Bayesian Formulation for Plasticity and Damage Models

Appendix A.1. Bayesian Parameter Estimation

Bayesian inference provides a rigorous and systematic framework for estimating parameters and quantifying uncertainties within constitutive modeling. Consider a parameter vector

$$\boldsymbol{\theta} = \{\sigma_Y,\, H,\, D\},$$

where σ_Y denotes the yield stress, H represents the hardening modulus, and D characterizes the damage variable. Given experimental data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$, typically stress-strain measurements, the posterior probability distribution of the parameters is obtained through Bayes' theorem as follows:

$$P(\boldsymbol{\theta} \mid \mathcal{D}) = \frac{P(\mathcal{D} \mid \boldsymbol{\theta})\, P(\boldsymbol{\theta})}{P(\mathcal{D})}, \tag{A.1}$$

where:

- $P(\mathcal{D} \mid \boldsymbol{\theta})$ denotes the likelihood function, quantifying the probability of observing the experimental data given a set of parameters $\boldsymbol{\theta}$.
- $P(\boldsymbol{\theta})$ represents the prior distribution, encoding prior knowledge or beliefs about the parameters.
- $P(\mathcal{D})$ is the evidence (or marginal likelihood), defined as:

$$P(\mathcal{D}) = \int_{\Theta} P(\mathcal{D} \mid \boldsymbol{\theta})\, P(\boldsymbol{\theta})\, d\boldsymbol{\theta}, \tag{A.2}$$

  ensuring normalization of the posterior.

In constitutive modeling, experimental measurements are frequently assumed to exhibit additive Gaussian noise with zero mean and known variance σ^2. Under this assumption, the likelihood function takes the explicit form:

$$P(\mathcal{D} \mid \boldsymbol{\theta}) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left[-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - f(x_i;\boldsymbol{\theta}))^2\right], \tag{A.3}$$

where the function $f(x_i;\boldsymbol{\theta})$ represents model predictions, dependent on parameters $\boldsymbol{\theta}$ and inputs x_i (e.g., strain or displacement).

The prior distribution encapsulates previous knowledge or physical constraints and is typically chosen as a multivariate Gaussian:

$$P(\boldsymbol{\theta}) = \frac{1}{(2\pi)^{m/2}|\boldsymbol{\Sigma}_0|^{1/2}} \exp\left[-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\mu}_0)^{\top}\boldsymbol{\Sigma}_0^{-1}(\boldsymbol{\theta} - \boldsymbol{\mu}_0)\right], \tag{A.4}$$

where $\boldsymbol{\mu}_0$ and $\boldsymbol{\Sigma}_0$ are the prior mean and covariance matrix, respectively, and m denotes the dimensionality of the parameter space.

Given the inherent complexity and nonlinearity associated with constitutive models describing plasticity and damage, the integral in Eq. (A.2) typically cannot be evaluated analytically. Consequently, numerical approximation methods, such as Markov Chain Monte Carlo (MCMC), Variational Inference (VI), or Approximate Bayesian Computation (ABC), are utilized to sample from or approximate the posterior distribution. In practical implementations, the posterior distribution is expressed through a proportional relation:

$$P(\boldsymbol{\theta} \mid \mathcal{D}) \propto P(\mathcal{D} \mid \boldsymbol{\theta})\, P(\boldsymbol{\theta}), \tag{A.5}$$

circumventing explicit calculation of the evidence $P(\mathcal{D})$ and substantially enhancing computational efficiency, especially in high-dimensional settings commonly encountered in material modeling [38].

Ultimately, Bayesian inference not only provides an optimal estimate of the parameter set but also rigorously quantifies parameter uncertainty, thereby enabling robust predictive assessments of material behavior.

Appendix A.2. Likelihood Function for Plasticity and Damage Models

We employ a Bayesian statistical framework to quantify uncertainties inherent in plasticity and damage models, capturing both experimental variability and microstructural randomness. For plasticity models, such as the von Mises model with isotropic hardening, experimentally observed stresses σ_i^{exp} are modeled as:

$$\sigma_i^{\text{exp}} = \sigma(\theta) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma_\epsilon^2), \tag{A.6}$$

where $\sigma(\theta)$ denotes the predicted stress given the material parameter set θ, and ϵ_i represents Gaussian-distributed measurement and modeling uncertainties. This Gaussian assumption is justified by the central limit theorem, given the aggregation of multiple independent sources of error [39]. The likelihood function for the observed data D is then:

$$P(D|\theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma_\epsilon^2}} \exp\left(-\frac{(\sigma_i^{\text{exp}} - \sigma(\theta))^2}{2\sigma_\epsilon^2}\right). \tag{A.7}$$

In damage modeling, specifically using Gurson-type models, the evolution of the void volume fraction f incorporates microstructural stochasticity [40]:

$$f_{i+1} = f_i + \Delta t\left[(1 - f_i)\dot{\epsilon}_p + k f_i^m \dot{\epsilon}_p\right] + \eta_i, \quad \eta_i \sim \mathcal{N}(0, \sigma_f^2), \tag{A.8}$$

where $\dot{\epsilon}_p$ is the equivalent plastic strain rate, while the parameters k and m characterize material-specific growth and coalescence behaviors. Here, the stochastic term η_i models the inherent randomness arising from microstructural variability. Thus, the corresponding likelihood function is expressed as:

$$P(D|\theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma_f^2}} \exp\left(-\frac{\left(f_i^{\text{exp}} - f_i^{\text{model}}\right)^2}{2\sigma_f^2}\right). \tag{A.9}$$

Appendix A.3. Prior Distributions for Material Parameters

Prior distributions encode physical constraints and empirical insights, providing a meaningful baseline for Bayesian inference. We adopt informative priors tailored to reflect known physical behaviors:

- *Yield stress*:
$$\sigma_Y \sim \mathcal{N}(\mu_{\sigma_Y}, \sigma_{\sigma_Y}^2), \tag{A.10}$$
consistent with its empirically observed near-normal distribution in metallic materials [41].

- *Hardening modulus*:
$$H \sim \text{Lognormal}(\mu_H, \sigma_H^2), \tag{A.11}$$
chosen to represent its strictly positive, skewed empirical behavior accurately [42].

- *Damage variable*:
$$D \sim \text{Beta}(\alpha_D, \beta_D), \tag{A.12}$$
ensuring boundedness between 0 and 1, in accordance with established damage mechanics principles [43].

These priors enable robust inference of material parameters even when experimental data are limited or noisy, reinforcing physical realism in the statistical model.

Appendix A.4. Derivation of the Posterior Distribution

The posterior distribution for the model parameters given the experimental observations is obtained by employing Bayes' theorem:

$$P(\theta \mid D) \propto P(D \mid \theta)P(\theta), \tag{A.13}$$

where $D = \{\sigma_i^{\text{exp}}\}_{i=1}^N$ represents experimental stress measurements and θ denotes the parameter vector.

We assume independent Gaussian noise with variance σ_ϵ^2 for the experimental data. Thus, the likelihood function is expressed as:

$$P(D \mid \theta) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\,\sigma_\epsilon} \exp\left(-\frac{(\sigma_i^{\text{exp}} - \sigma(\theta))^2}{2\sigma_\epsilon^2}\right), \tag{A.14}$$

where $\sigma(\theta)$ represents the predicted stress values given parameters θ. Ignoring parameter-independent constants, the likelihood simplifies to:

$$P(D \mid \theta) \propto \prod_{i=1}^{N} \exp\left(-\frac{(\sigma_i^{\exp} - \sigma(\theta))^2}{2\sigma_\epsilon^2}\right). \tag{A.15}$$

We impose informative priors on the parameters to incorporate domain knowledge. Specifically, the yield stress σ_Y is assigned a Gaussian prior:

$$P(\sigma_Y) \propto \exp\left(-\frac{(\sigma_Y - \mu_{\sigma_Y})^2}{2\sigma_{\sigma_Y}^2}\right), \tag{A.16}$$

with mean μ_{σ_Y} and standard deviation σ_{σ_Y}. To enforce positivity and account for wide-ranging magnitudes, the hardening parameter H is modeled using a log-normal prior:

$$P(H) \propto \exp\left(-\frac{(\log H - \mu_H)^2}{2\sigma_H^2}\right), \tag{A.17}$$

where μ_H and σ_H denote the log-scale mean and standard deviation, respectively. The damage parameter D, constrained to the interval $[0, 1]$, is assigned a Beta prior:

$$P(D) \propto D^{\alpha_D - 1}(1 - D)^{\beta_D - 1}, \tag{A.18}$$

where hyperparameters α_D, β_D encode prior expectations regarding damage evolution.

The combined joint prior distribution is therefore:

$$P(\theta) \propto \exp\left(-\frac{(\sigma_Y - \mu_{\sigma_Y})^2}{2\sigma_{\sigma_Y}^2}\right) \exp\left(-\frac{(\log H - \mu_H)^2}{2\sigma_H^2}\right) D^{\alpha_D - 1}(1 - D)^{\beta_D - 1}. \tag{A.19}$$

Substituting both likelihood and prior distributions into Bayes' theorem yields the explicit posterior distribution:

$$\begin{aligned} P(\theta|D) \propto & \prod_{i=1}^{N} \exp\left(-\frac{(\sigma_i^{\exp} - \sigma(\theta))^2}{2\sigma_\epsilon^2}\right) \exp\left(-\frac{(\sigma_Y - \mu_{\sigma_Y})^2}{2\sigma_{\sigma_Y}^2}\right) \\ & \times \exp\left(-\frac{(\log H - \mu_H)^2}{2\sigma_H^2}\right) D^{\alpha_D - 1}(1 - D)^{\beta_D - 1}. \end{aligned} \tag{A.20}$$

Due to nonlinearities inherent in the predictive function $\sigma(\theta)$, the resulting posterior does not possess a closed-form analytical solution. Consequently, we employ numerical techniques such as Markov Chain Monte Carlo (MCMC) algorithms to sample effectively from the posterior distribution and rigorously quantify parameter uncertainties [44].

Appendix A.5. Variational Inference Formulation

Variational inference (VI) provides a principled framework for approximating complex posterior distributions. Given observed data D and model parameters θ, the posterior distribution can be expressed through Bayes' theorem as:

$$P(\theta \mid D) = \frac{P(D \mid \theta)P(\theta)}{P(D)}, \tag{A.21}$$

where the marginal likelihood (or evidence) $P(D)$ is computed as:

$$P(D) = \int P(D \mid \theta)P(\theta)\, d\theta. \tag{A.22}$$

Since this integral is generally analytically intractable, we approximate the posterior with a tractable variational distribution $Q(\theta)$. The quality of this approximation is quantified by the Kullback–Leibler (KL) divergence:

$$\mathrm{KL}(Q(\theta) \| P(\theta \mid D)) = \int Q(\theta) \log \frac{Q(\theta)}{P(\theta \mid D)}\, d\theta. \tag{A.23}$$

Using Bayes' theorem, we rewrite Eq. (A.23) explicitly as:

$$\begin{aligned}\mathrm{KL}(Q(\theta)\|P(\theta \mid D)) &= \int Q(\theta) \log \frac{Q(\theta)}{\frac{P(D|\theta)P(\theta)}{P(D)}}\, d\theta \\ &= \int Q(\theta) \log \frac{Q(\theta)P(D)}{P(D \mid \theta)P(\theta)}\, d\theta \\ &= \log P(D) + \int Q(\theta) \log \frac{Q(\theta)}{P(D \mid \theta)P(\theta)}\, d\theta. \end{aligned} \tag{A.24}$$

Rearranging terms leads to the key variational identity:

$$\log P(D) = \underbrace{\int Q(\theta) \log \frac{P(D \mid \theta)P(\theta)}{Q(\theta)}\, d\theta}_{\text{Evidence Lower Bound (ELBO)}} + \mathrm{KL}(Q(\theta)\|P(\theta \mid D)). \tag{A.25}$$

Since $\log P(D)$ is independent of the choice of $Q(\theta)$, minimizing the KL divergence (Eq. (A.23)) is equivalent to maximizing the Evidence Lower Bound (ELBO), defined explicitly as:

$$\mathrm{ELBO}(Q) = \mathbb{E}_{Q(\theta)}[\log P(D \mid \theta)] + \mathbb{E}_{Q(\theta)}[\log P(\theta)] - \mathbb{E}_{Q(\theta)}[\log Q(\theta)]. \tag{A.26}$$

For computational tractability, we adopt a Gaussian variational approximation:

$$Q(\theta) = \mathcal{N}(\mu_\theta, \Sigma_\theta), \tag{A.27}$$

with mean vector μ_θ and covariance matrix Σ_θ. Optimization of these variational parameters is typically performed using stochastic gradient ascent algorithms (e.g., stochastic variational inference) as described by Blei et al. [45] and Hoffman et al. [46]. This approach ensures scalable and efficient inference, even for high-dimensional parameter spaces prevalent in contemporary statistical modeling.