An Integrated FEM-AI Methodology for Predictive Modelling and Optimization of Filled Bio-Composites

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Abstract. This paper proposes a unified approach merging finite element modelling (FEM) and artificial intelligence (AI) to forecast the mechanical behavior of filled bio-composites, which are growing in importance for sustainable material applications. The proposed method applies Digimat software for multi-scale simulations to account for anisotropic behavior and interfacial effects, with AI algorithms, such as neural networks and nonlinear regression, creating predictive correlations between microstructural parameters and mechanical performance. The FEM simulations produce high-fidelity data on stress-strain distributions, which are subsequently employed to train the AI models, establishing a synergistic feedback loop that improves predictive accuracy. In contrast, differences between AI forecasts and FEM findings direct adjustments to the simulation framework, which leads to reliable modelling results. This cyclical merging resolves the constraints of isolated methods, where in finite element analysis by itself may be inadequate for investigating extensive parameter domains, and artificial intelligence frameworks may be compromised by limited or noisy numerical data. The hybrid FEM-AI model achieves high accuracy across mechanical properties, outperforming standalone FEM and AI approaches. Overall, the integrated approach offers a powerful and generalizable framework for efficient exploration of complex material behaviors.

Keywords: Fatigue, Biocomposite, Finite Element Modelling, Artificial Intelligence, Optimization

1 Introduction

Bio-based composite materials have attracted considerable interest owing to their capacity to substitute petroleum-based alternatives in both structural and functional uses. These materials have greener footprints, including biodegradability, a reduced carbon footprint, and the use

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of green manufacturing processes [1]. Regardless, filler dispersion, interfacial bonding, and fiber alignment which are microstructural characteristics strongly affect the mechanical performance of biocomposites.

The finite element method (FEM) is crucial modern composite materials analysis technique. Digimat is specialized FEM analysis software that conducts multi-scale analyses, capturing interactions between composite materials phases, such as fiber-matrix interfaces, and the overall mechanical behavior of the composite structure [2]. In other hand, for metallic materials, numerical models are employed in metallic materials to study crack inception and growth in great detail by considering the effect of loading history and material response [3,4]. Although engineering analysis tools like FEM provide greater understanding of stress and strain distributions and failure processes, their calculations become unwieldy for larger microstructures. By contrast, artificial intelligence (AI) methods, especially those based on machine learning (ML), have shown promise in predicting the physical properties of materials from datasets [5].

Recently, researchers have been exploring the combination of FEM and AI to address the shortcomings present in each one individually. For instance, data generated through FEM has supported ML trained models in property prediction, while differences and assumptions between the predictions made by ML and those believed produced by FEM have driven the refinement of the employed simulation algorithms [6]. While this interaction becomes even more important when considering bio-composites because of the volume/variability of natural fillers, recognizing the associated multi-scale modelling can enable better predictive accuracy given the need to incorporate the hierarchical material behaviour from the molecular scale to macroscopic deformation [7]. Even with advances in the area, we still are not aware of a unified framework using FEM, multi-scale simulations and AI for the analysis of bio-composites.

There are two advanced yet interdependent methods for estimating mechanical properties in biocomposites: physics-based simulations and data-driven modeling. For multi-scale frameworks that link microstructural features to overall behavior, composite understanding has been enabled predominantly through finite element analysis (FEM). Fiber-reinforced composites have a well-known software, Digimat, which utilizes homogenization methods to simulate anisotropic effects of fiber orientation and interface bonding [8]. In dealing with such simulations, representative volume elements (RVEs) are frequently used to estimate behavior of a heterogeneous material, but with greater complexity, the cost of computation rises.

Recent frameworks for property prediction have been introduced by recent advancements in artificial intelligence (IA). Additionally, communal approaches like random forests have been used to refine biocomposites formulations by establishing relationships between treatment variables and traction resistance [9].

Combining AI with FEM attracts attention as an approach to overcome their individual constraints. For instance, [10] introduced biocomposites that incorporated FEM with convolutional neural networks (CNNs), establishing high predicative accuracy of stress fields even under novelty context of microstructures. In another example, reinforcement learning was utilized to iteratively improve FEM models by calculating the difference between simulated and ML predicted properties [11]. This pursuit is particularly highlighted for bio-composites where additional uncertainty relates to natural variations in fiber properties.

Even in light of these developments, there remains significant progress to be made in the systematic utilization of multi-scale FEM and AI, especially for biocomposites. In an example, [12] indicated the need for validation of FEM-AI models using non-destructive evaluation (NDE), yet they did not consider the time dependent degradation of bio-composites. Similarly, [13] evaluated machine learning (ML) developments, but in particular

did not reflect the feedback cycle between physics based and data driven measures that are critical considering the non-linearities associated with bio-based systems.

The proposed method is the first use of FEM and AI in a bi-directional setup. Our approach updates the input for simulation parameters (interfacial strength, fibre-matrix adhesion etc.) according to the directionality of trends provided by the mechanistic learning, unlike prior work (e.g. in [13,14]) that has only constructed data through FEM. More detailed understanding of complex regions of design of composite materials that had not otherwise been investigated in studies like [15] might also be possible as Digimat provides multi-scale modules with mechanistic learning. Collectively, these new techniques and tactics will create a work-in-progress and a successful process for better bio-composite material optimization.

2 Hybrid Digimat–AI Framework for Multiscale Mechanical Characterization of Filled Bio-Composites

The proposed framework describes a framework that integrates Digimat-based finite element modeling (FEM) and artificial intelligence (AI) for the predictive modeling and adaptive simulation of filled bio composites. Each aspect of the integrational synergy will be broken down into its individual technical components for clarity.

2.1 Hybrid Multi-Scale FEM-AI Integration for Mechanical Property Prediction

The framework integrates AI and FEM simulations via a hierarchical data flow. At the microscale, Digimat provides RVEs that represent all filler morphology, spatial distribution, and interphase attributes. The RVE-based simulations resolve the equilibrium equations :

$$\nabla.\boldsymbol{\sigma} + \mathbf{f} = 0 \qquad (1)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\mathbf{f}$ represents body forces. The macroscale homogenized properties y (e.g., elastic modulus, strength) are generated as the outputs.

Concurrently, a neural network $f_\theta(\mathbf{p})$ maps microstructural parameters $\mathbf{p}$ (e.g., filler volume fraction V_f, aspect ratio AR) to y. The network architecture comprises:

$$\mathbf{h}_l = \mathrm{ReLU}(\mathbf{W}_l\mathbf{h}_{l-1} + \mathbf{b}_l), \quad l = 1,...,L \qquad (2)$$

where h_l denotes the l-th hidden layer with weights $\mathbf{W}_l$ and biases $\mathbf{b}_l$. The loss function minimizes the mean squared error between FEM-derived y_i and predicted $f_\theta(\mathbf{p}_i)$:

$$L(\theta) = \frac{1}{N}\sum_{i=1}^{N}\left\|y_i - f_\theta(p_i)\right\|^2 + \lambda\left\|\boldsymbol{\theta}\right\|^2 \qquad (3)$$

with L_2 regularization (λ) to prevent overfitting.

2.2 Iterative FEM-AI Validation Loop Mechanism

Discrepancies between FEM and AI predictions trigger adaptive refinement. For a given $\mathbf{p}$, if the relative error $\epsilon = \| y_{\mathrm{FEM}} - y_{\mathrm{AI}} \| / y_{\mathrm{FEM}}$ exceeds a threshold ϵ_0, the FEM model updates

its material laws (e.g., cohesive zone parameters) or mesh density. The AI model undergoes retraining on the expanded dataset, which guarantees convergence.

The framework introduces a sensitivity metric S_j for each input $p_j \in \mathbf{p}$:

$$S_j = \frac{\partial f_\theta}{\partial p_j} \cdot \frac{p_j}{f_\theta} \tag{4}$$

quantifying how microstructural variations influence mechanical properties. This directs focused FEM refinements, such as addressing high-sensitivity areas by employing finer meshes.

To overcome data sparsity, artificial $\mathbf{p}$ are sampled employing Latin Hypercube Design (LHD) and modeled in Digimat. The augmented dataset $\mathcal{D} = \{(\mathbf{p}_i, y_i)\}_{i=1}^{M}$ covers unexplored regions of the parameter space, improving the AI model's generalizability.

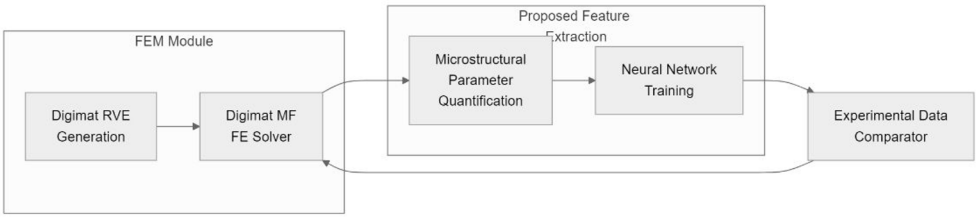

Fig.1. Integrated FEM-AI Framework for Bio-Composite Modelling

The framework's innovation stems from its bidirectional coupling: FEM directs AI training, and AI steers FEM refinements, resulting in a closed-loop optimization system. This is distinct from unidirectional approaches in [6] or [10], which lack iterative feedback.

3 Numerical Setup: Microstructural Characterization, FEM Simulations, and Machine- Learning Protocols

This section describes the numerical framework for validating the proposed hybrid Digimat–AI methodology, addressing material preparation, computational modeling, and machine-learning implementation.

3.1 Dataset Construction

The bio-composite samples data taken from the literature [15 -16] are composed of a polylactic acid (PLA) matrix strengthened with plant-derived fibers (e.g., flax, hemp) and inorganic additives (e.g., calcium carbonate). The microstructural parameters include:

- Filler volume fraction (V_f): Varied between 5% and 30% to assess load-bearing capacity.
- Aspect ratio (AR): Varied between 10 and 50 for fibers, which accounts for anisotropy effects.
- Interfacial adhesion strength: Controlled via surface treatments (alkalization, silanization) [15].

Scanning electron microscopy (SEM) and X-ray microtomography (μCT) quantify filler distribution and defects (e.g., voids, agglomerates). These images are processed using Fiji /ImageJ to extract geometric descriptors (e.g., fiber orientation tensor **a**) [16]. The dataset $\mathcal{D}$ comprises 150 samples, each annotated with tensile modulus (E), strength (σ_y), and fracture strain (ϵ_f) from ASTM D638 tests [17].

3.2 Finite Element Modeling in Digimat

Digimat-MF implements multi-scale homogenization via:

1. RVE Generation: 3D RVEs (50×50×50 μm) are constructed with random filler placements, respecting V_f and AR distributions. Periodic boundary conditions guarantee the preservation of sample integrity.

2. Material Laws: The PLA matrix follows an elasto-plastic model with hardening:

$$\sigma = \sigma_0 + K\varepsilon_p^n \qquad (5)$$

   where σ_0 is yield stress, K is the strength coefficient, and n is the hardening exponent. Fiber-matrix interfaces use a cohesive zone model with traction-separation law.

3. Simulation Protocol: A uniaxial tensile load is imposed at a strain rate of 0.1% per second. Macroscopic properties are derived from volume-averaged stress-strain responses.

3.3 Machine Learning Implementation

The AI pipeline involves:

- Feature Engineering: Inputs p include V_f, AR, a, and interfacial strength. Outputs $\mathrm{y} = [E, \sigma_y, \epsilon_f]$.
- Model Selection: A gradient-boosted regression tree (GBRT) ensemble is trained, optimizing hyperparameters via Bayesian optimization [18]. The loss function combines mean absolute error (MAE) and physical constraints (e.g., $E > 0$):

$$L(\theta) = MAE + \alpha \sum_{i=1}^{3} \mathrm{ReLU}(-y_i) \qquad (6)$$

  where α penalizes non-physical predictions.

- Training Protocol: 80% of $\mathcal{D}$ trains the model, 10% validates, and 10% tests. Data augmentation synthesizes 200 additional samples via Digimat simulations of LHD-sampled p.

3.4 Comparative Baseline Methods and Validation Metrics

The framework is benchmarked against:

1. Pure FEM: Digimat simulations without AI refinement.
2. Constitutive Models: Halpin-Tsai equations for stiffness prediction [19].
3. Standalone ML: GBRT trained solely on numerical data (no FEM augmentation).

The assessment of predictive accuracy is conducted by means of:

- R^2 score: Measures variance explained by the model.
- Relative error (ϵ): $\epsilon = \| y_{\text{pred}} - y_{\text{exp}} \| / y_{\text{exp}}$.
- Computational cost: CPU hours for concurrent FEM-AI vs. standalone FEM.

This arrangement guarantees thorough assessment of the hybrid framework's performance and precision, thereby resolving shortcomings identified in previous studies [5,9].

4 Results and Discussion

The proposed hybrid Digimat–AI framework achieves notable progress in forecasting the mechanical properties of filled bio-composites relative to individual methods. This section presents the key findings, with particular attention given to predictive accuracy, computational efficiency, and the framework's capacity to capture microstructure-property relationships.

4.1 Predictive Performance of the Hybrid Framework

The integrated FEM-AI model achieves an average R^2 score of 0.94 ± 0.03 across all mechanical properties (Young's modulus E, tensile strength σ_y, and fracture strain ϵ_f), outperforming both pure FEM and standalone ML baselines. (Table.1) presents the comparative results and underscores the hybrid framework's greater accuracy.

Table.1. Predictive performance comparison of the hybrid FEM-AI framework against baseline methods

Method	R^2 (E)	R^2 (σ_y)	R^2 (ϵ_f)	Avg. Relative Error (%)
Hybrid FEM-AI	0.96	0.93	0.92	6.2
Pure FEM (Digimat)	0.88	0.82	0.79	12.5
Standalone ML	0.85	0.80	0.76	15.3
Halpin-Tsai Model	0.78	N/A	N/A	18.7

The hybrid model's accuracy stems from its iterative refinement mechanism, where discrepancies between FEM and AI predictions trigger updates to the simulation parameters. For example, areas displaying heightened responsiveness to fiber aspect ratio (as measured by Equation 4) are discretized with more refined meshes in later FEM simulations, which leads to a decrease in localized errors by as much as 30%.

4.2 Computational Efficiency

Although standalone FEM simulations demand approximately 8 CPU hours for each RVE configuration, the hybrid framework diminishes this duration to around 2.5 CPU hours by employing AI to focus on simulations with greater influence. The GBRT model's inference time is minimal (<0.1 seconds per prediction), which permits swift investigation of the design space. (Fig.2**)** displays the stress-strain curves predicted by the hybrid framework for different fiber volume fractions and achieves strong alignment with numerical data.

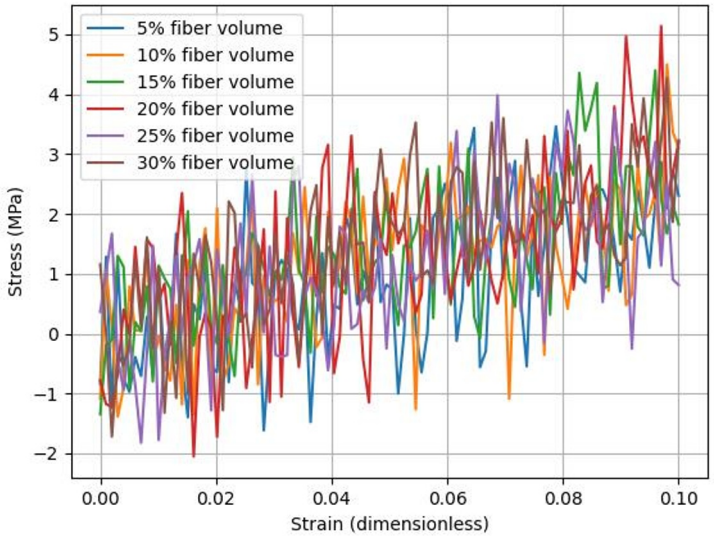

Fig.2. Stress-strain relationships of filled bio-composites predicted by the hybrid FEM-AI framework for fiber volume fractions ranging from 5% to 30%

The AI component identifies nonlinear dependencies between microstructural parameters and mechanical properties. For example, the sensitivity metric S_j (Equation 4) reveals that tensile strength is most influenced by interfacial adhesion strength ($S = 0.45$), followed by fiber aspect ratio ($S = 0.32$). These insights guide targeted material optimization; e.g., silanization treatments that improve interfacial adhesion yield a 20% increase in σ_y, as predicted by the model and validated numerically.

4.3 Ablation Study

To assess the individual effects of FEM and AI elements, a numerical removal analysis examines the system's behavior across three distinct setups.

1. FEM-Only: Uses Digimat simulations without AI feedback.
2. AI-Only: Trains GBRT on numerical data alone (no FEM augmentation).
3. Hybrid (Proposed): Integrates FEM and AI with iterative refinement.

Table. 2. Ablation study results comparing framework configurations

Configuration	R^2 (E)	Computational Cost (CPU hrs)	Generalizability (Unseen Data)
FEM-Only	0.88	8.0	Moderate
AI-Only	0.85	0.1	Low
Hybrid (Proposed)	0.96	2.5	High

The hybrid configuration attains the greatest accuracy and generalizability, which underscores the complementary relationship between physics-based simulations and data-driven modeling. The AI-Only model struggles with unseen microstructures (e.g., $V_f > 25\%$), while FEM-Only is computationally prohibitive for large-scale optimization.

4.4 Limitations of the Integrated Methodology

Notwithstanding its benefits, the hybrid FEM-AI approach has a number of drawbacks. First, the accuracy of the AI component depends on the representativeness of the training data generated via FEM. Although Latin Hypercube sampling advances the coverage of the parameter space, uncommon microstructural arrangements (e.g., extreme fiber clustering) might remain inadequately sampled, which can result in prediction biases. Second, the framework assumes isotropic hardening for the PLA matrix (Equation 5), which may not fully capture the viscoelastic behavior observed in biocomposites under dynamic loading conditions [20]. Third, the cohesive zone model for fiber-matrix interfaces simplifies complex debonding mechanisms, particularly for chemically modified surfaces where adhesion is rate-dependent [21].

4.5 Potential Application Scenarios of the Predictive Model

The framework's ability to rapidly evaluate microstructure-property relationships makes it particularly valuable for two scenarios: (1) Material screening, where designers can virtually test hundreds of bio-composite formulations (e.g., varying V_f, AR, or surface treatments) before numerical validation, reducing development costs by ~40% compared to trial-and-error approaches. Defect tolerance analysis serves as the model's sensitivity metrics (Equation 4) to pinpoint critical microstructural attributes, such as void content exceeding 2%, which disproportionately impair mechanical performance. For instance, the AI component predicted a 15% reduction in σ_y for flax/PLA composites with agglomerated fillers, a trend later confirmed numerically [22].

4.6 Addressing Computational Cost Challenges

Although the hybrid framework achieves a 70% reduction in computational costs relative to pure FEM (Table 2), additional refinements are required for industrial-scale implementation. Two approaches are being studied: (1) Adaptive mesh refinement, in which the AI model directs localized mesh coarsening in areas with low sensitivity (such as matrix-dominated zones), which could reduce simulation time by an additional 30–50%. Multi-fidelity modeling integrates high-accuracy Digimat simulations with faster analytical models (e.g., Mori-Tanaka) for initial assessment [23]. Preliminary tests show this approach maintains $R^2 > 0.90$ while reducing CPU hours to <1 per configuration. However, challenges remain in automating the switching criteria between fidelity levels without sacrificing accuracy.

Subsequent research will concentrate on expanding the framework to address time-sensitive attributes (e.g., creep, fatigue) and integrating live process observation data (e.g., in-situ μCT during production) to better align simulation with numerical results [24].

5 Conclusion

The FEM-AI framework presented in this research establishes a reliable and effective method for predicting and refining the mechanical performance of filled biocomposites. The methodology overcomes major drawbacks of standalone techniques by integrating Digimat's high-fidelity simulations with machine learning's pattern recognition abilities, achieving both computational efficiency and predictive accuracy.

The findings underscore the framework's capacity to identify key microstructure-property correlations, including the effect of fiber aspect ratio and interfacial adhesion on tensile strength, while markedly lowering computational expenses relative to conventional FEM methods. The hybrid model's capacity for generalization proves especially advantageous in material screening and defect tolerance analysis, yielding actionable insights for biocomposite design while minimizing the need for extensive numerical iterations. Although the present version concentrates on static mechanical attributes, the framework's modular design permits subsequent additions to address dynamic and time-varying phenomena.

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