Machine Learning Approaches to Natural Fiber Composites: A Review of Methodologies and Applications

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In recent years, the process of optimizing the design of natural fiber reinforcement in natural fiber composites (NFCs) with distinct properties has been redefined through the application of machine learning (ML). This work elucidates the functions of the types and applications of the ML algorithms and evolutionary computing techniques, with a particular focus on their applicability within the domain of NFCs. Moreover, the solution methodologies and associated databases were employed throughout various stages of the product development journey, from the raw material selection through the final end-use application for the NFCs. The strengths and limitations of the ML in the NFCs industry, together with relevant challenges, such as interpretability of ML models, in materials science was detailed. Finally, future directions and emerging trends in the ML are discussed.

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INTRODUCTION

Overview of Natural Fiber Composites (NFCs) and their Significance in Materials Science

Natural fiber composites (NFCs) are advanced materials that combine a polymer matrix—thermoset or thermoplastic—with reinforcing materials of lignocellulosic or biogenic ceramic nature, in geometries that include fibers or less elongated fillers, normally defined as "particles", in a micrometric or nanometric size to achieve enhanced properties tailored to specific applications (Palanisamy *et al.* 2022a; Seydibeyoğlu *et al.* 2023; Palaniappan *et al.* 2024c). These materials have the potential to be pivotal in modern materials science due to their versatility, by ultimately offering a unique blend of characteristics, which surpass those of their individual components (Jagadeesh *et al.* 2022; Ayrilmis *et al.* 2024). The selection of polymer matrix and reinforcement type allows engineers to optimize properties, such as strength, stiffness, durability, thermal and

electrical conductivity, and resistance to aging over time, or to more instantaneous damage phenomena, such as abrasion or impact. Other factors, which would be essential to tailor performance, together with reducing scattering of properties, are the application of compatibilizers (Hubbe and Grigsby 2020) and fiber treatment (Latif *et al.* 2019). This versatility, though obtainable through the control of a number of parameters, has led to widespread adoption across various industries, including aerospace, automotive, renewable energy, construction, and biomedical sectors. In aerospace, for example, NFCs are starting to be used extensively in aircraft structures, mainly in interiors, to reduce weight while maintaining structural integrity and fuel efficiency (Asim *et al.* 2018; Kar *et al.* 2023; Palaniappan *et al.* 2024b). In automotive applications, they contribute to weight reduction efforts, improving fuel economy and performance (Naik and Kumar 2021). In renewable energy, composite materials form critical components of wind turbine blades, where they enhance efficiency and durability (Hussain and Immanuel 2021; Gebrehiwet *et al.* 2023). In the construction industry, natural fiber composites offer alternatives to traditional materials, providing high strength-to-weight ratios and resistance to abrasion, plus effectively replacing fiberglass (Silva *et al.* 2020). Additionally, NFCs are employed in biomedical fields for developing implants and prosthetics that mimic natural tissues' mechanical properties (Kim and Chalivendra 2020; Sumesh *et al.* 2023, 2024). The integration of machine learning (ML) with science of NFCs further enhances their significance by enabling predictive modeling, optimization of material formulations, and automation of design processes (Malalli and Ramji 2022). The ML algorithms analyze complex datasets to predict material behaviors based on composition, processing parameters, and environmental conditions, thereby accelerating innovation and reducing development costs. These methods also have brought potential advantages in particularly computationally complex fields, *e.g.*, whenever the effect of vibrations on materials is involved (Guo *et al.* 2024; Mahariq *et al.* 2020). There still are challenges, such as data scarcity, interpretability of models, and computational complexity. However, ongoing research and interdisciplinary collaborations promise to overcome these hurdles, unlocking new possibilities for composite materials in diverse applications (Karuppiah *et al.* 2020; Mulenga *et al.* 2021).

Importance of Predictive Modeling and Optimization in Composite Materials Design

Predictive modeling and optimization play crucial roles in advancing composite materials design, particularly when integrated with ML techniques tailored for NFCs (Shahzad *et al.* 2024). These methodologies are essential for efficiently and effectively tailoring material properties to meet specific performance requirements across various industrial applications. Predictive modeling leverages computational algorithms to simulate and predict the behavior of composite materials based on input variables such as material composition, processing conditions, and environmental factors. Through harnessing ML algorithms—which build on regression models, decision trees, neural networks, and more sophisticated deep learning architectures, not dismissing the importance of the former, yet hopefully improving their performance namely for easier interpretation of the results (Levy and O' Malley 2020) —engineers can analyze vast datasets and extract meaningful insights that inform design decisions (Karuppiah *et al.* 2022; Feng *et al.* 2024). This capability not only accelerates the materials development process, but it also enhances the accuracy of predictions regarding mechanical strength, thermal stability, electrical conductivity, and other critical properties. Optimization

techniques further refine composite formulations by identifying optimal combinations of matrix materials, reinforcements, and additives to achieve desired performance metrics while minimizing costs and at the same time reducing environmental impact (Husain 2023). ML-driven optimization frameworks enable rapid iteration and exploration of design spaces that may not be feasible through traditional empirical methods alone, thereby fostering innovation and competitiveness in industries such as aerospace, automotive, renewable energy, and the biomedical sector. Through integrating predictive modeling and optimization with ML, researchers and engineers can navigate complex material interactions, overcome design challenges, and deliver composite materials with enhanced functionality, durability, and sustainability, thereby shaping the future of materials science and engineering (Sadeghi *et al.* 2024).

When analyzing polymeric composites, the many existing parameters and different combinations that need to be evaluated to boost applications with multi-functional requirements is motivating researchers to carry out more systematic and data-intensive research. The combination of experiments and computer simulations has produced a huge amount of data that has enabled the integration of machine learning algorithms with materials science, which has been a key driver in the development of new materials (Sharma *et al.* 2022; Goutham *et al.* 2023). The mining of large-scale data is the work of accessing hidden information (Wu *et al.* 2013; Jaseena and David 2014; Westermayr *et al.* 2021). In data analysis, statistics plays a crucial role in addressing a variety of problems and is extensively employed in finding solutions.

However, it is difficult to use in some problems. Especially, very large statistical methods may appear inadequate when working with large amounts and variety of data. In these circumstances, data mining addresses the need for solutions to complex problems. Machine learning has started to be used in the last few years to tailor and optimize the properties of composite materials (Terzi *et al.* 2014). This acts more generally also on the production process to accelerate evaluation and increase the level of accuracy as regards the relation between structure and properties, which is reflected in a combination of phenomena during fabrication, namely tension, flexure, inter and intra-ply shear, and compaction (Guo *et al.* 2021; Govindarajan *et al.* 2024; Padmanabhan *et al.* 2024). Achieving successful results in future predictions with artificial neural networks depends also on the degree of independence of the variables and is influenced by the degree of accuracy in the measurement of their values. Results can be enhanced by using different network structures and determining which of these is more suitable for the problem type (Tkáč and Verner 2016; Abdolrasol *et al.* 2021). Data mining algorithms are available and continuously improved in many fields, including marketing, social, education, communication, and engineering (Terzi 2007; Küçüksille *et al.* 2011; Özel and Topsakal 2014). Many different methods are used in data mining, among which the most diffuse are classification, Gaussian regression analysis, clustering, association analysis, ordered sequence analysis, and time series analysis (Fu 2011; Romero and Ventura 2013; Hokeš *et al.* 2016; Aye and Heyns 2017; Gong *et al.* 2024).

Introduction to ML and its Applications in Materials Science

Since ML has emerged as a transformative paradigm in materials science, it is also able to offer powerful tools to revolutionize the design, characterization, and optimization of the composites, starting from the simplest models of unidirectional fibers-matrix interaction (Zhang *et al.* 2018). At its core, ML involves the development of algorithms and statistical models that enable computers to learn from and make predictions or

decisions based on data. In this sense, the question of ML transparency is essential, as it is recognized *e.g*., in the medical field, and it can be somehow enhanced by exploring the variance statistics and the model accuracy (Huang and Huang 2023).

In the context of NFCs, ML techniques are employed to analyze complex datasets derived from material characterization, processing parameters, and performance testing. These algorithms range from classical regression and decision trees to more advanced approaches, such as neural networks and deep learning architectures, each of these tailored to extract meaningful insights and patterns from large volumes of heterogeneous data (Yao *et al.* 2020). The ML facilitates predictive modeling of material properties, enabling researchers to simulate and predict behaviors, such as mechanical strength, thermal conductivity, and chemical stability, under varying conditions. This predictive capability accelerates materials discovery and optimization, reducing time-to-market and costs associated with empirical testing. Moreover, ML-driven approaches enable automated design workflows, where algorithms iteratively refine composite formulations and manufacturing processes based on performance criteria and constraints, thereby pushing the boundaries of materials science innovation in fields ranging from aerospace and automotive to renewable energy and biomedical applications (Alli *et al.* 2024). As ML continues to evolve, its integration with materials science promises to unlock new frontiers in composite materials design, offering unprecedented opportunities for customization, efficiency, and sustainability in manufacturing and product development.

TRADITIONAL METHODS IN THE FORMULATION OF NFCs

Description of Traditional Empirical Methods for Characterizing and Designing NFCs

Traditional empirical methods have long been foundational in characterizing and designing NFCs, relying on direct observation, experimentation, and physical testing to understand material behaviors and optimize performance. These methods encompass a range of techniques tailored to assess various aspects of composite materials, starting with material formulation and continuing through processing, testing, and evaluation phases (Sapuan and Mansor 2014). At the formulation stage, empirical methods involve manual selection and blending of polymer matrices with reinforcing agents, fillers, and additives based on prior knowledge, experience, and heuristics. Experimental techniques, such as differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and Fourier-transform infrared spectroscopy (FTIR), are employed to analyze thermal properties, chemical composition, and molecular structure, providing insights into material stability and compatibility (Lin 2021; Mylsamy *et al.* 2024; Ramasubbu *et al.* 2024). Mechanical testing methods, including tensile, flexural, impact, and hardness testing, offer the assessment of properties, such as strength, stiffness, toughness, and resistance to deformation or fracture, under different loading conditions. Microscopic techniques, such as scanning electron microscopy (SEM) and transmission electron microscopy (TEM), offer detailed visual analysis of composite microstructures, revealing information about phase distribution, interfacial bonding, and defect morphology (Palanisamy *et al.* 2022b; Liu *et al.* 2023). Despite their effectiveness in providing detailed insights into material characteristics, traditional empirical methods are labor-intensive, time-consuming, and limited in their ability to comprehensively explore complex material interactions across diverse environmental and operational conditions. As such, there is a growing interest in

complementing these methods with ML techniques, which can leverage large datasets to enhance predictive modeling, optimize composite formulations, and accelerate materials development processes in a more efficient and cost-effective manner (Nguyen *et al.* 2022; Krzywanski *et al.* 2024).

Machine learning (ML) could offer a new pathway for data-driven design and development of reinforced composites. Figure 1 illustrates a framework for the data-driven composite design, highlighting manufacturing processes, data collection sources, and simulation tools. This approach utilizes forecasting models and decision-making strategies for designing reinforced composites, utilizing data from the manufacturing process, micromechanics, finite element analysis, academic literature, and digital databases, among others. In the specific case of NFCs, the inherent limitations of any applied method, which of course impact also on ML, is the difficulty to add to the evaluation data about local interface strength, particularly variable in the case of NFCs for the conflicting geometries of matrix and reinforcement and the large effect of unavoidable porosities. This could be possibly in the future addressed by inserting in modelling large databases of microscopical images and features, yet this is unpractical so far, though it has been proposed on traditional composites (Romanov *et al.* 2013).

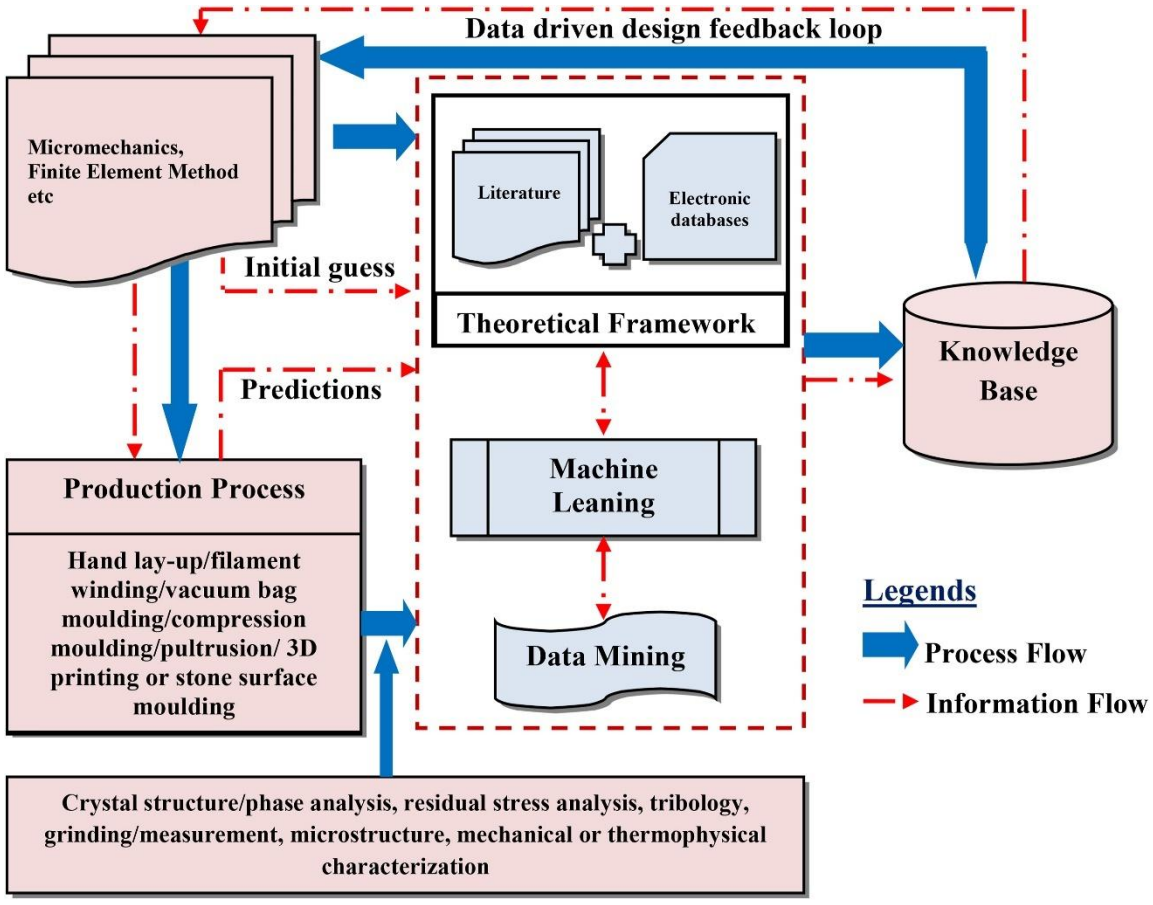

Fig. 1. Data-driven design of composite materials, illustrating production pathways, data acquisition sources, and simulation tools (Okafor *et al.* 2023; CC BY 4.0)

Strengths: Detailed Physical Insights, Established Methodologies

The strengths of traditional methods in NFCs lie in their ability to provide detailed physical insights and their reliance on well-established methodologies that have been refined over decades of materials research and development (Song *et al.* 2020; Palaniappan *et al.* 2024a). One key advantage offered is the depth of understanding these methods into the physical and chemical properties of composite materials. Techniques, such as differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and Fourier-transform infrared spectroscopy (FTIR) enable precise characterization of thermal stability, chemical composition, and molecular structure, which are essential for assessing material performance and stability (Al-Quraishi *et al.* 2020). Mechanical testing methods—such as tensile, flexural, impact, and hardness testing—offer quantitative data on mechanical properties such as strength, stiffness, toughness, and resilience under varying conditions, providing critical insights into material behavior under stress (Falsafi *et al.* 2020). Microscopic analyses, including SEM and TEM, allow for detailed visualization of composite microstructures, revealing information about phase distribution, interfacial bonding, and defect morphology at microscopic scales (Foster *et al.* 2018). Furthermore, traditional methodologies benefit from well-established protocols and standards, ensuring consistency and comparability across different studies and laboratories. This historical foundation has built a robust framework for characterizing, designing, and evaluating NFCs, offering a solid baseline against which new advancements, such as ML techniques, can be compared and integrated to further enhance materials science and engineering practices.

Limitations: Time Consumption, Cost, Difficult Scale-up for Complex Material Interactions

Despite their strengths, traditional methods in NFCs suffer from significant limitations that impact their applicability and efficiency in modern materials science. One prominent drawback is their inherent time-consuming nature, stemming from the sequential and labor-intensive processes involved in empirical testing and physical characterization. Techniques, such as DSC, TGA, FTIR, and mechanical testing, require meticulous sample preparation, experimental setup, and data collection, extending the timeframe from material formulation to final evaluation (Gomes Souza, Jr. *et al.* 2024). Moreover, the need for skilled personnel to operate specialized equipment and interpret results adds to the time investment and operational costs. These methods are also costly, primarily due to the expenses associated with acquiring and maintaining sophisticated instrumentation, conducting experiments, and analyzing data. The procurement of high-quality raw materials and the stringent environmental conditions required for accurate testing further contribute to the financial burden (Salgueiro *et al.* 2010). Additionally, traditional methods may not scale well to handle the complexities of modern composite materials, which often involve intricate combinations of polymers, reinforcements, additives, and processing techniques. The interactions between these components can lead to nonlinear and multidimensional effects that traditional empirical methods may struggle to capture comprehensively. As a result, there is a growing recognition of the need for complementary approaches, such as ML, which can leverage large datasets and computational power to overcome these limitations, accelerate materials development, and optimize composite formulations in a more cost-effective and scalable manner (Suwardi *et al.* 2022).

Once these difficulties have been recognized, another open question is whether NFCs deserve more accurate analyses such as those performed using ML, which can be costly and not easy to implement. However, the perspective has gradually changed over the last few years, due to the increasingly extensive use of NFCs in challenging fields such as automotive and even aviation and nautical sectors. As a result of this, more modelling works are coming out, which have recognized the distinctly different characteristics of these materials with respect to the more ordered and repeatable structures of traditional composites, so that models used for them fall short of effectively explaining the behavior of NFCs (Xiong *et al.* 2018).

ROLE OF MACHINE LEARNING IN NFC

Explanation of How ML Algorithms Analyze Complex Datasets to Predict Material Properties and Behavior

The ML algorithms have revolutionized the study and prediction of material properties and behaviors within NFCs by harnessing the power of data-driven analysis and computational modeling. At the core of ML's application in this domain lies its ability to handle large, complex datasets derived from diverse sources such as experimental measurements, simulations, and historical records (Zhong *et al.* 2021). The process begins with data preprocessing, where raw data are cleaned, normalized, and transformed into a suitable format for analysis. Feature engineering follows, where relevant input variables (features) are selected or generated from the data, capturing essential aspects of material composition, processing conditions, and environmental factors. These features serve as the basis for building predictive models that aim to establish correlations between input parameters and desired output variables, such as mechanical strength, thermal conductivity, or durability (Stergiou *et al.* 2023). The ML algorithms employ various techniques to analyze these datasets and develop predictive models. Supervised learning methods, such as regression and classification algorithms, learn from labeled datasets where the relationships between inputs and outputs are explicitly provided (Singh *et al.* 2016). For instance, regression models can predict continuous properties such as tensile strength based on factors such as polymer type, reinforcement material, and curing temperature. Classification algorithms, on the other hand, categorize materials into classes based on predefined criteria, such as identifying composite formulations that meet specific performance standards (Diniță *et al.* 2023). Furthermore, ML algorithms excel in capturing nonlinear relationships and patterns that may not be apparent through traditional analytical methods. Complex algorithms including decision trees, random forests, support vector machines (SVMs), and neural networks are adept at identifying intricate interactions among multiple variables within the dataset. Neural networks, particularly deep learning architectures, are capable of learning hierarchical representations of data, enabling them to model highly complex relationships and make accurate predictions in materials science applications (Taye 2023).

Once trained, ML models undergo validation and evaluation processes to assess their performance and generalizability. Techniques such as cross-validation ensure that models can effectively predict outcomes on new, unseen data, thereby confirming their reliability in practical applications (Nicora *et al.* 2022). Moreover, ML facilitates continuous model refinement through techniques, such as ensemble learning and hyperparameter tuning, which optimize model performance and enhance predictive

accuracy (Abnoosian *et al.* 2023). The integration of ML with NFC science not only accelerates the materials discovery and optimization processes but also enables more informed decision-making in design and manufacturing. Through leveraging predictive models developed through ML, researchers and engineers can explore a broader design space, identify optimal material combinations, and predict material behaviors under varying conditions with greater efficiency and cost-effectiveness (Herbol *et al.* 2020). This capability not only reduces reliance on costly and time-consuming empirical testing but also opens avenues for innovation in composite materials tailored to meet specific performance criteria across industries such as aerospace, automotive, renewable energy, and beyond. As ML techniques continue to evolve and datasets grow in complexity and size, their application in NFC science promises to drive significant advancements in materials design, sustainability, and technological innovation (Obaideen *et al.* 2024).

Types of ML Techniques Commonly Used Available for NFCs

In the realm of NFCs, ML techniques encompass a diverse array of methodologies tailored to analyze complex datasets and predict material properties and behaviors. One of the fundamental ML techniques employed is regression analysis, which encompasses linear regression for modeling relationships between input variables (*e.g.*, composition of NFCs and processing parameters) and continuous output variables (*e.g.*, mechanical strength or thermal conductivity) (Özkan *et al.* 2019). Decision trees, another prevalent technique, offer a hierarchical approach to decision-making, where composite properties are predicted based on a series of binary decisions at each node of the tree. Ensemble methods, such as random forests, combine multiple decision trees to enhance prediction accuracy and robustness. Moreover, neural networks represent a cornerstone of ML applications in NFCs, particularly deep learning architectures, which are capable of learning intricate patterns and nonlinear relationships within datasets (Hussain *et al.* 2020). Convolutional neural networks (CNNs) and recurrent neural networks (RNNs) are adapted for tasks, such as image analysis of composite microstructures or time-series prediction of material degradation under varying environmental conditions. SVMs are utilized for classification tasks, distinguishing between different composite material classes based on specified features. Bayesian methods provide probabilistic frameworks for uncertainty quantification in predictions, offering insights into the reliability and variability of estimated material properties (Liu *et al.* 2024). Reinforcement learning, although less commonly applied in materials science, explores optimal strategies for composite manufacturing processes and material design through iterative learning and decision-making. Each of these ML techniques brings unique strengths to the field, enabling researchers and engineers to extract valuable insights from data, optimize composite formulations, and advance the understanding and application of NFCs across diverse industrial sectors.

Advantages: Speed, Scalability, Ability to Handle Large Datasets, Potential for Automation

The ML techniques offer significant advantages in the context of the NFCs, revolutionizing the traditional approaches to design, optimization, and characterization. One of the primary advantages is speed, as ML algorithms can rapidly analyze and process large volumes of complex data, significantly accelerating materials discovery and development timelines. This capability is particularly valuable in industries such as aerospace, automotive, and renewable energy, where fast-paced innovation is crucial for

maintaining competitiveness. Scalability is another key benefit, as ML models can efficiently scale to handle vast datasets encompassing diverse parameters, from material composition and processing conditions to performance metrics and environmental factors (Ninduwezuor-Ehiobu *et al.* 2023). This scalability allows for comprehensive exploration of design spaces and optimization of composite formulations without the limitations of traditional empirical methods. Additionally, ML's ability to handle large datasets facilitates more robust and accurate predictive modeling of material properties and behaviors, leveraging patterns and correlations that may not be apparent through conventional analytical techniques alone. Furthermore, ML techniques enable automation of repetitive tasks in materials science, such as data preprocessing, feature selection, and model training. Automated workflows streamline processes, reduce human error, and enhance reproducibility in experimental design and data analysis (Klenam *et al.* 2023). This automation not only improves efficiency but also frees up researchers' time to focus on more strategic aspects of materials research, fostering innovation and interdisciplinary collaboration. As ML continues to advance and integrate with experimental techniques and computational simulations, its potential for automation in NFCs promises to reshape how materials are designed, tested, and optimized, paving the way for enhanced performance, sustainability, and technological innovation in diverse industrial applications (Ma *et al.* 2023).

Examples of Successful Applications in Aerospace, Automotive, Renewable Energy, and Biomedical Fields

Machine learning has catalyzed significant advancements in NFCs across various industries, showcasing successful applications in aerospace, automotive, renewable energy, and biomedical fields. In aerospace, ML-driven approaches have revolutionized the design and optimization of lightweight composite structures, essential for reducing aircraft weight and improving fuel efficiency. For instance, Airbus employs ML to predict the mechanical properties of composite materials used in aircraft components, optimizing their performance while ensuring safety and durability. Similarly, in the automotive sector, ML techniques are leveraged to enhance the development of composite materials for vehicle lightweighting, improving fuel economy and reducing emissions (Ye *et al.* 2005). Companies including BMW use ML algorithms to simulate and predict the behavior of composite materials under different driving conditions, optimizing vehicle performance and structural integrity. In renewable energy, particularly in wind energy applications, ML plays a crucial role in predicting and optimizing the performance of composite materials used in wind turbine blades. The ML models analyze data from sensors embedded in blades to monitor structural health, predict maintenance needs, and optimize operational efficiency, thereby increasing energy production and reducing downtime (Nachtane *et al.* 2023). Moreover, in biomedical fields, NFCs reinforced with biocompatible materials are transforming the development of medical implants and prosthetics. The ML algorithms analyze patient-specific data to customize implant designs, predict material biocompatibility, and optimize mechanical properties to enhance patient outcomes and longevity. These examples illustrate how ML is not only enhancing the performance and efficiency of NFCs across industries but also driving innovation and sustainability in materials science and engineering (Feng *et al.* 2024). As ML techniques continue to evolve and integrate with traditional empirical methods, their potential to further advance composite materials' capabilities and applications remain promising regarding continued progress in efficiency, safety, and performance across global industries (Zadpoor 2017).

CHALLENGES AND CONSIDERATIONS

Data Scarcity and Quality Issues Specific to NFCs

Data scarcity and quality issues pose significant challenges in the application of ML to the NFCs. The NFCs exhibit inherent variability due to factors such as material composition, processing conditions, and environmental influences, making it challenging to collect comprehensive and standardized datasets. Unlike conventional materials with well-documented properties, NFCs often lack extensive datasets that encompass diverse variations and scenarios (Ge *et al.* 2023). This scarcity limits the scope and accuracy of ML models trained on insufficient or biased data, potentially leading to unreliable predictions and suboptimal material designs. In addition, ensuring data quality is paramount, as inconsistencies, errors, or incomplete datasets can skew model outcomes and hinder the generalizability of findings. The variability in experimental techniques and measurement protocols across different laboratories further complicates data integration and comparison, undermining the reliability of composite material databases (Gibert *et al.* 2016). Addressing these challenges requires collaborative efforts to establish standardized testing protocols, improve data collection methodologies, and enhance data sharing practices within the materials science community. Advances in sensor technology, computational simulations, and materials informatics offer promising avenues to augment existing datasets and mitigate data scarcity issues. Once this is achieved, researchers can enhance the robustness and applicability of ML models in NFCs, unlocking new opportunities for innovation and optimization in materials design and engineering (Xu *et al.* 2023).

The choice of a machine learning technique for a particular design problem is difficult because of the large number of algorithms readily available. The limited computer skills of most materials designers have been a major issue that has limited the large-scale use of machine learning in reinforced composite technology (Gu *et al.* 2018). Although there are many databases on natural fiber composites' properties, drawbacks include the lack of easily accessible data sources, inconsistencies between data produced by different groups, and inadequacies of the current database. Other limitations of the machine learning approach are shown in Fig. 2.

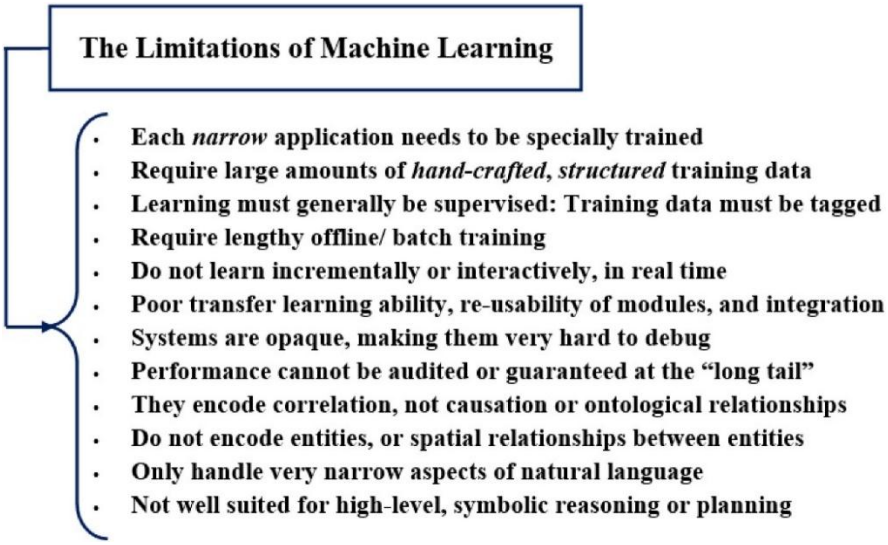

Fig. 2. The limitations of machine learning (Okafor *et al.* 2023; CC BY 4.0)

Despite the challenges inherent to the application of machine learning in this context, there are significant opportunities for future research. These include the development of more sophisticated algorithms, the enlargement of the dataset used for training, the combination of machine learning with simulation tools, and an investigation of the limitations and challenges associated with this approach.

There are several difficulties and limitations associated with the application of machine learning to NFCs, despite its great potential. The difficulties in using machine learning techniques to optimize NFCs are illustrated in Fig. 3. Verification of the accuracy of machine learning models is the third challenge. This can be a lengthy and costly process, as the accuracy of machine learning algorithms needs to be tested against experimental data.

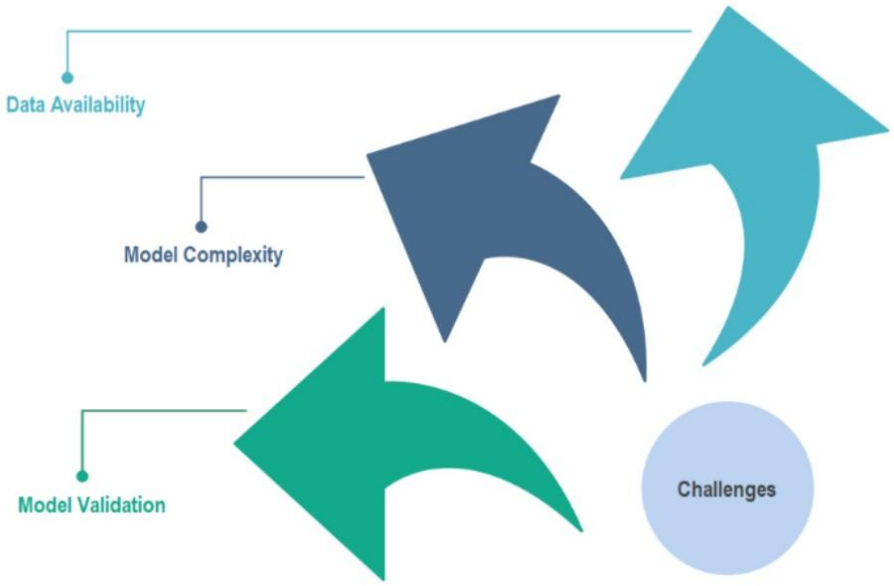

Fig. 3. Machine learning challenges in designing and optimizing NFCs (Maniraj *et al.* 2023; CC BY 4.0)

The lack of high-quality, relevant data is a major barrier to the use of machine learning in this context. Large datasets of NFCs test results are required for accurate predictions by machine learning algorithms. Moreover, the data must be varied and be an accurate reflection of the materials and microstructures of interest. A further problem is that NFCs are complex materials, constituted by a minimum of two phases, normally geometrically complex and irregular, yet often including further fillers, and it is a difficult task to predict their properties based on their microstructures.

Interpretability of ML Models in Materials Science

Interpretability of ML models in materials science presents a critical challenge due to the complexity and multidimensional nature of data-driven predictions. In the context of NFCs, more risks for over-simplification, hence inaccuracy in the relation between data and models exist, due to the hierarchical structure of natural fillers and the complex relation with environment this might involve, which might impact crucial sectors, such as assessment of properties following artificial aging tests (Mejri *et al*. 2018). The ML models, such as neural networks and ensemble methods, are adapted at extracting intricate

patterns and correlations from large datasets, enabling accurate predictions of material properties and behaviors (Stoll and Benner 2021). However, the trade-off for this predictive power often lies in the opacity of these models, making it difficult to decipher how inputs translate into outputs. In traditional empirical methods, engineers and researchers can directly interpret results based on well-established principles and physical laws. In contrast, ML models operate as "black boxes," where the internal workings are obscured, raising concerns about the reliability and trustworthiness of their predictions, particularly in safety-critical applications. This lack of interpretability impedes the validation of model outcomes and the identification of causal relationships between composite characteristics and performance metrics. Moreover, stakeholders, such as regulatory bodies and industry professionals, require transparent and interpretable models to ensure compliance with standards and regulations (Bongomin *et al.* 2024). Addressing these challenges necessitates the development of explainable AI techniques tailored to materials science, enabling researchers to gain insights into how ML models arrive at their predictions. Techniques, such as feature importance analysis, sensitivity analysis, and model-agnostic approaches, like SHAP (SHapley Additive exPlanations) are emerging as promising methods to enhance interpretability. Furthermore, integrating physics-based models with data-driven (Papadimitriou *et al.* 2024). ML approaches can provide hybrid models that combine predictive accuracy with explanatory capabilities, leveraging domain knowledge to validate and interpret predictions effectively. Through enhancing the interpretability of ML models in materials science, researchers can improve confidence in model outcomes, foster interdisciplinary collaboration, and accelerate the adoption of advanced technologies in the design, optimization, and deployment of the NFCs (Azevedo *et al.* 2024).

Computational Complexity and Scalability Challenges

In the realm of ML applied to the NFCs, computational complexity and scalability present significant challenges that impact the efficiency and applicability of predictive models. The NFCs are inherently complex materials with diverse compositions and processing parameters that influence their properties and behaviors. The ML algorithms, such as neural networks and ensemble methods, excel at extracting patterns and relationships from large datasets to predict material properties like mechanical strength, thermal conductivity, and durability (Stergiou *et al.* 2023). However, the computational demands of training and deploying these models increase with dataset size and complexity. Training deep neural networks, for instance, requires substantial computational resources and time, often involving high-performance computing clusters or cloud infrastructure. This computational complexity limits the scalability of ML approaches, especially when scaling up to handle massive datasets or when conducting simulations at multiple scales (*e.g.*, microscale to macroscale). Furthermore, the integration of ML with physics-based models to capture multiscale interactions in the NFCs introduces additional computational challenges. However, it is possible also to predict that, together with the application of other damage monitoring techniques on NFCs (Natesan and Krishnasamy 2024), which are gradually diffusing, as illustrated further in the following Section, ML might also assist a possible etiology of fracture on NFCs. Balancing the need for accuracy and efficiency in model training and deployment remains a critical consideration, particularly in industries like aerospace and automotive, where real-time decision-making and optimization of composite materials are essential (Yassin *et al.* 2023). Addressing these challenges requires advancements in algorithmic efficiency, parallel computing techniques, and hardware acceleration, alongside the development of scalable ML frameworks tailored to the specific

characteristics of NFCs. Collaborative efforts between materials scientists, data scientists, and computational experts are crucial to overcoming these computational hurdles and harnessing the full potential of ML for advancing materials design, optimization, and manufacturing processes.

FUTURE DIRECTIONS AND EMERGING TRENDS

Potential for Automated Composite Design and Manufacturing

The potential for automated composite design and manufacturing using ML represents a transformative frontier in NFCs, promising to revolutionize how materials are developed, optimized, and manufactured across various industries. Automation in composite design begins with the ability of ML algorithms to analyze vast datasets, encompassing material properties, processing parameters, environmental conditions, and performance metrics. Through leveraging this data, ML can automate the selection and optimization of composite formulations tailored to meet specific performance requirements (Chinchanikar and Shaikh 2022). For instance, ML algorithms can identify optimal combinations of polymer matrices, reinforcement materials, and additives to achieve desired mechanical, thermal, or electrical properties, while minimizing weight and cost. Moreover, automated design workflows can simulate and predict the behavior of composite materials under different loading conditions, environmental exposures, and manufacturing processes. This predictive capability accelerates the iterative design process, reducing the reliance on time-consuming empirical testing and enabling rapid prototyping and iteration of composite structures (Yuan *et al.* 2021). In the manufacturing sector, ML-driven automation enhances process control and optimization, ensuring consistency in material properties and product quality while reducing waste and energy consumption. Technologies such as robotic process automation (RPA) and adaptive manufacturing systems integrate ML models with real-time sensor data to adjust manufacturing parameters dynamically, optimizing production efficiency and reducing downtime (Bhadra *et al.* 2023). Furthermore, the integration of digital twins—virtual replicas of physical composite materials and manufacturing processes—facilitates predictive maintenance, fault detection, and optimization of production schedules. As advancements in ML algorithms, computational power, and sensor technologies continue, the vision of fully automated composite design and manufacturing becomes increasingly feasible, promising unprecedented levels of customization, efficiency, and sustainability in materials science and engineering. Collaborative efforts between academia, industry, and government stakeholders will be crucial in realizing this vision, driving innovation and competitiveness in sectors such as aerospace, automotive, renewable energy, and beyond (Ninduwezuor-Ehiobu *et al.* 2023).

Integration of ML with Experimental Techniques for Enhanced Predictive Capabilities

The integration of ML with experimental techniques represents a promising frontier in advancing predictive capabilities and accelerating innovation in NFCs. The ML algorithms offer powerful tools to analyze complex datasets derived from experimental measurements, simulations, and historical data, enabling researchers to extract actionable insights and predict material behaviors with unprecedented accuracy (Morgan *et al.* 2022). Through integrating ML with experimental techniques, such as spectroscopy, microscopy,

and mechanical testing, researchers can enhance the understanding of composite material properties and their underlying mechanisms. For example, ML models can analyze spectroscopic data to identify molecular structures and chemical interactions within polymer matrices and reinforcements, offering insights into material composition and stability. A combination of microscopic techniques, such as SEM and atomic force microscopy (AFM), provide detailed images of composite microstructures in the three directions down to the micron and below, which ML algorithms can analyze to predict mechanical properties, such as strength and stiffness, based on features such as fiber orientation or interfacial bonding (Ge *et al.* 2020). Furthermore, ML enhances the predictive capabilities of mechanical testing by correlating experimental data with material composition and processing parameters, facilitating the optimization of composite formulations for specific applications. Through integrating real-time sensor data with ML algorithms, researchers can monitor and predict material degradation, fatigue behavior, and environmental resilience, enabling proactive maintenance and lifecycle management strategies. Collaborative efforts between materials scientists, data scientists, and experimentalists are essential to developing robust ML frameworks that leverage the complementary strengths of experimental techniques and computational modeling, advancing the reliability, efficiency, and sustainability of NFCs in diverse industrial applications.

Advances in Hybrid Models Combining Mechanical Properties-based Simulations with ML Algorithms

Advances in hybrid models that combine mechanical properties (MP)-based simulations with ML algorithms represent a cutting-edge approach in the future of the NFCs. These hybrid models integrate the strengths of MP-based models that rely on fundamental principles and equations to simulate material behavior at various scales, with the predictive capabilities of ML, which excels in learning complex patterns from data (Rocha *et al.* 2023; Rudolph *et al.* 2024). Through merging these two approaches, researchers aim to overcome the limitations of purely empirical or theoretical methods, offering a more holistic understanding and predictive power for composite materials. MP-based simulations provide a foundational understanding of material properties and processes, such as polymer matrix behavior, reinforcement mechanics, and interfacial interactions, based on first principles and experimental data. These simulations can capture intricate details of composite structures and their responses to external stimuli, offering insights into performance under specific conditions (Bishara *et al.* 2023). The ML algorithms complement these simulations by learning from large datasets, including experimental measurements and simulations outputs, to optimize model parameters, predict material behaviors with greater accuracy, and explore complex design spaces beyond the capabilities of traditional MP-based approaches alone. For example, hybrid models can enhance the prediction of composite material properties under varying environmental conditions, simulate manufacturing processes with improved efficiency and precision, and optimize material formulations for specific performance criteria. Furthermore, integrating MP-based simulations with ML facilitates real-time adaptation and learning, enabling adaptive modeling approaches that adjust predictions based on new data and evolving conditions (Struzziero *et al.* 2019; Krzywanski *et al.* 2024). Collaborative research efforts across disciplines—such as materials science, computer science, and applied mathematics—are essential to advancing hybrid modeling techniques, developing standardized methodologies, and validating model accuracy to accelerate

innovation and application in sectors, such as aerospace, automotive, renewable energy, and biomedical.

Opportunities for Interdisciplinary Collaboration and Industry Adoption

The future of ML in the NFCs presents abundant opportunities for interdisciplinary collaboration and widespread industry adoption, fostering innovation across diverse sectors. Interdisciplinary collaboration is essential as ML intersects with materials science, computational modeling, data science, and engineering disciplines. By bringing together experts from these fields, researchers can leverage complementary expertise to address complex challenges in materials design, optimization, and manufacturing. For instance, materials scientists provide domain knowledge on composite materials' chemical composition, mechanical properties, and environmental interactions, guiding the development of ML models that accurately predict material behaviors (Sparks *et al.* 2020; Pilania 2021). Computational modelers contribute expertise in developing physics-based simulations and numerical methods, integrating them with ML algorithms to enhance predictive capabilities across multiple scales—from molecular dynamics to macroscopic material properties. Data scientists play a crucial role in processing and analyzing vast datasets, implementing advanced ML algorithms, and developing interpretable models that align with industry standards and regulatory requirements (Carvalho *et al.* 2019; Shah 2021). Engineers and industry practitioners bring practical insights into manufacturing processes, performance requirements, and market demands, ensuring that ML-driven solutions are not only innovative but also feasible and scalable for industrial applications. Furthermore, interdisciplinary collaboration accelerates knowledge transfer and skill development, nurturing a new generation of researchers and practitioners skilled in both materials' science and advanced data analytics. Industry adoption of ML in the NFCs holds transformative potential by optimizing product development cycles, reducing costs, and enhancing product performance and sustainability. Companies in aerospace, automotive, renewable energy, and biomedical sectors are increasingly integrating ML-driven approaches to innovate new materials, improve manufacturing efficiency, and address environmental challenges (Popescu *et al.* 2024). For example, ML models can streamline composite material selection, predict material degradation, and optimize manufacturing processes, leading to lighter, stronger, and more durable products. Collaborations between academia, government agencies, and industry partners are critical in fostering technology transfer, validating ML models in real-world applications, and establishing best practices for integrating ML into existing workflows (Terranova *et al.* 2024). Through embracing interdisciplinary collaboration and industry adoption, the future of ML in the development and analysis of NFCs promises to unlock unprecedented opportunities for innovation, competitiveness, and sustainable development across global markets.

CONCLUDING STATEMENTS

The quality of the test facilities, the research climate, and the experience of the designer determine the success of experimental measurement. Experimental research can therefore be expensive and time-intensive, particularly if numerous tests are needed to analyze each material variable. This is the case of multiphase and irregular natural fiber composites (NFCs). The three key data sources recognized for machine learning-based

design of reinforced composites include finite element analysis/high-throughput simulations, experimental data, and material databases/literature.

A variety of options are now available to data scientists and materials engineers for the development of models for a wide range of ML needs in the areas of reinforced composite design. Thus, the review evaluated popular digital tools and platforms, such as MATLAB, TensorFlow, Scikit-learn, and Weka, used by various researchers for implementing ML algorithms over the last years.

To make a more significant impact on the field of machine learning in fiber composite research, experts in reinforced composites should be encouraged to provide the data most suitable for further processing to tailor and examine the material structure. Importance of continued research, development, and collaboration for advancing materials science through ML.

The use of machine learning algorithms to automate the forecasting of natural fiber composite properties based on microstructural data can lead to enhanced efficiency, precision, and cost savings.

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Data Availability Statement

Data is available on request from the authors.

Declaration of Conflicting Interests

The authors declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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