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Development of a Conceptual Framework for Physics-Informed Neural Networks for Nonlinear Material Systems

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ABSTRACT

This qualitative study aims to develop a conceptual framework for Physics-Informed Neural Networks (PINNs) in nonlinear material systems. The study addresses the growing need for physically consistent machine learning models that can explain complex material behavior under limited experimental data conditions. A qualitative conceptual case study approach was used because the research focused on understanding the methodological structure, assumptions, and interpretive logic behind PINN-based material modeling. Data were collected through semi-structured interviews with 8 to 12 experts in computational mechanics, material modeling, machine learning, or PINNs, supported by documentation of academic articles published between 2020 and 2025 and nonparticipant observation of model-building logic in selected studies. The data were analyzed using reflexive thematic analysis. The findings revealed five main themes: the central role of physical laws, the importance of limited but meaningful data, the need for constitutive assumptions, the challenge of loss function design and training stability, and the role of interpretability in nonlinear material modeling. These findings show that PINNs should not be viewed only as computational tools, but as hybrid conceptual frameworks that connect material mechanics, governing equations, empirical data, and neural network learning. The study contributes to the theoretical development of *scientific machine learning* and offers practical guidance for researchers who design PINN models for nonlinear materials. Future research should validate the proposed framework through simulation studies, experimental datasets, and comparative applications across different material systems.

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1. Introduction

The development of *scientific machine learning* has changed how researchers model complex physical systems, including nonlinear material systems. In material science and computational mechanics, nonlinearity often appears through plastic deformation, hyperelastic response, damage evolution, viscoelastic behavior, and coupled multiphysics processes. These phenomena remain difficult to model because they require accurate constitutive assumptions, sufficient experimental data, and high computational resources. Karniadakis et al. (2021) explain that physics-informed machine learning connects data-driven learning with governing physical laws. Cuomo et al. (2022) show that Physics-Informed Neural Networks (PINNs) have become one of the most important approaches in this field because they embed differential equations and boundary conditions into neural network training. Haghighat et al. (2021) demonstrate that PINNs can support inversion and surrogate modeling in solid mechanics. This direction is relevant because nonlinear material systems require models that are not only accurate, but also physically consistent and interpretable.

The global growth of PINNs reflects the need for computational methods that can work under limited, noisy, or incomplete data conditions. Classical numerical methods, such as finite element methods, remain central in material simulation, but they often require detailed mesh construction and high computational cost for nonlinear problems. PINNs offer a different route by combining observation data with governing equations inside the loss function. Zhang et al. (2022) show that PINNs can analyze internal structures and material defects, including voids, inclusions, elasticity, hyperelasticity, and plasticity. Wu et al. (2023) explain that data sampling strategies and boundary condition constraints strongly influence the accuracy of PINNs in material property identification. Jeong et al. (2024) further show that PINNs can identify material behavior from full-field data without relying only on predefined parametric models. These studies indicate that PINNs can support both prediction and interpretation in nonlinear material modeling.

In nonlinear material systems, the main challenge does not only lie in solving equations. The deeper challenge lies in connecting physical assumptions, material behavior, experimental evidence, network architecture, and model interpretation. Haghighat et al. (2023) show that physics-informed deep learning can support constitutive model characterization and discovery. Linka and Kuhl (2023) emphasize that constitutive neural networks need kinematic, thermodynamic, and physical constraints to remain meaningful in material modeling. Rezaei et al. (2024) demonstrate that thermodynamics-based nonlinear constitutive models can be learned through PINNs when physical constraints are properly integrated. Song and Jin (2024) also show that PINNs can identify constitutive parameters for complex hyperelastic materials. These findings suggest that PINNs need a strong conceptual structure, especially when researchers use them to explain material response rather than only to reduce numerical error.

In the Indonesian research context, the development of a conceptual framework for PINNs is increasingly important because material-related studies often face limited access to high-resolution experimental instruments, large datasets, and advanced computational infrastructure. Many applied fields, including infrastructure, manufacturing, energy, health technology, and defense engineering, need material models that can handle nonlinear behavior with limited but meaningful data. Hu et al. (2024) explain that PINNs have strong potential in computational solid mechanics, especially for forward modeling, inverse identification, and damage evaluation. Diao et al. (2023) show that multimaterial solid mechanics problems require special treatment because discontinuity and material interfaces make conventional PINNs less stable. He et al. (2024) propose a multi-level physics-informed deep learning framework that separates geometry, constitutive relations, and equilibrium information in structural mechanics. These studies show that PINNs must be adapted to the structure of the problem, not merely copied as a general algorithm.

Previous studies have provided strong technical contributions to PINNs, but most of them focus on numerical performance, algorithmic improvement, and case-specific validation. Kadeethum et al. (2020) show that PINNs can solve nonlinear diffusivity and Biot's equations, but their work also indicates that problem formulation affects model performance. Wang et al. (2021) explain that gradient flow pathologies can reduce the effectiveness of PINNs when the governing equations are difficult to optimize. Hamel et al. (2023) show that full-field experimental data can calibrate constitutive models through PINNs, but this process still depends on how data and physics are structured. Michaloglou et al. (2025) review PINNs in materials modeling and design and highlight their expanding role across material property prediction, multiphysics problems, and design optimization. The remaining gap is the limited discussion of PINNs as a conceptual framework for nonlinear material systems. This gap matters because conceptual clarity helps researchers define the role of data, physics, constitutive assumptions, loss functions, training strategies, and interpretability before building the computational model.

Based on this gap, this study aims to develop a conceptual framework for Physics-Informed Neural Networks in nonlinear material systems. The study focuses on the relationship between experimental data, physical laws, constitutive modeling, neural network design, loss construction, training logic, validation strategy, and interpretation of results. Lim (2025) argues that qualitative research is useful when a study aims to understand complex phenomena through contextual and conceptual depth. Busetto et al. (2020) explain that qualitative inquiry is appropriate for exploring how and why a phenomenon is structured in a particular way. Braun and Clarke (2021) emphasize that qualitative analysis can generate meaningful themes when the researcher follows a transparent and reflexive process. Therefore, this study positions PINNs not only as computational tools, but also as a methodological bridge between material mechanics and machine learning. The expected contribution is a structured conceptual foundation that can guide future empirical, computational, and experimental studies on nonlinear material modeling.

2. Materials and Methods

This study used a qualitative research design with a conceptual case study approach. The qualitative design was selected because the study aimed to understand the structure, meaning, and methodological logic behind the development of PINNs for nonlinear material systems. Busetto et al. (2020) explain that qualitative research is suitable for examining processes, interpretations, and contextual reasoning. Lim (2025) states that qualitative inquiry provides value when researchers need to examine complex phenomena that cannot be reduced to numerical relationships alone. The conceptual case study approach was used because PINNs were treated as a methodological case within the broader field of *scientific machine learning*. Karniadakis et al. (2021) support this positioning by showing that physics-informed machine learning integrates data-driven modeling and physical principles. This design allowed the study to explore how data, physical equations, constitutive assumptions, and neural network structures interact in nonlinear material modeling.

The research was conducted through document-based inquiry and expert-informed qualitative exploration from January to May 2026. The study did not use a single physical field site because the research object was a conceptual and methodological phenomenon. Instead, the research setting included academic articles, technical documentation, simulation studies, and online interviews with experts in computational mechanics, material modeling, machine learning, or PINNs. Campbell et al. (2020) explain that purposive sampling helps researchers select participants who have direct and relevant knowledge of the research problem. Ahmad (2025) argues that purposive sampling requires clear criteria, careful recruitment, and continuous evaluation of information depth. Bouncken et al. (2025) emphasize that purposeful selection and saturation should consider the level of analysis and the coherence of information across cases. Based on these principles, the study planned to involve 8 to 12 expert informants who had relevant publications, research experience, or applied expertise in PINNs and nonlinear material systems.

The data sources consisted of expert interviews, academic documents, and nonparticipant observation of model-building logic in selected PINN studies. Semi-structured interviews were used to explore expert views on the conceptual elements of PINNs, including governing equations, material data, constitutive relations, boundary conditions, loss function design, training difficulty, validation, and interpretability. Lobe et al. (2020) show that online qualitative interviews can provide effective access to participants who are geographically dispersed. Haghighat et al. (2021) provide a relevant technical basis because their study shows how PINNs can be used for inversion and surrogate modeling in solid mechanics. Zhang et al. (2022) provide another important reference because their work demonstrates the use of PINNs for analyzing internal structures and defects in materials. The documentation process focused on peer-reviewed academic articles published between 2020 and 2025. Nonparticipant observation was conducted by examining how selected studies arranged physical equations, data inputs, model architecture, and validation logic.

The data collection procedure followed four stages. First, the researcher identified relevant literature using keywords such as "physics-informed neural networks," "nonlinear material systems," "solid mechanics," "constitutive modeling," "hyperelasticity," "material identification," and "scientific machine learning." Cuomo et al. (2022) describe PINNs as a major branch of *scientific machine learning* that combines neural networks with physical constraints. Second, the researcher screened documents based on their relevance to nonlinear material modeling, methodological clarity, and contribution to conceptual framework development. Hu et al. (2024) support this selection logic because their review maps numerical frameworks and applications of PINNs in computational solid mechanics. Third, the researcher developed an interview guide based on recurring issues in the literature. Wu et al. (2023) show that data sampling and boundary constraints are important issues in material identification using PINNs. Fourth, the researcher compared interview data with documentary findings to identify conceptual convergence and divergence across sources.

Data validation was conducted through source triangulation, method triangulation, member checking, and audit trail documentation. Source triangulation compared information from expert interviews, journal articles, review papers, and technical model descriptions. Method triangulation compared interview results with document analysis and model-structure observation. Ahmed (2024) explains that trustworthiness in qualitative research can be strengthened through credibility, transferability, dependability, and confirmability. Kullman and Chudyk (2025) explain that member checking can improve trustworthiness when participants are invited to comment on interpretations and emerging findings. Braun and Clarke (2021) emphasize that reflexivity is essential because qualitative analysis depends on how researchers interpret patterns of meaning. In this study, member checking was conducted by sending summary interpretations to selected informants. The audit trail recorded search keywords, inclusion criteria, interview decisions, coding changes, theme development, and conceptual revisions.

Data analysis used reflexive thematic analysis. This method was selected because the study aimed to identify conceptual patterns across interviews and academic documents. Byrne (2022) explains that reflexive thematic analysis provides a systematic process for moving from familiarization to coding, theme development, review, definition, and reporting. Dahal (2025) states that qualitative data analysis requires iterative reflection, careful organization, and transparent interpretation. Polat (2025) notes that thematic analysis needs clear reporting so that findings do not become disconnected from the research question. In this study, initial codes were developed from recurring concepts such as physical law integration, data limitation, constitutive behavior, nonlinear response, boundary conditions, loss balancing, training stability, validation, and interpretability. These codes were then grouped into broader themes that formed the basis of the proposed conceptual framework.

The final framework was developed through an iterative synthesis of literature-based themes and expert-informed interpretations. The synthesis process connected six major components: empirical data, governing physics, constitutive assumptions, neural network architecture, optimization strategy, and interpretive validation. Diao et al. (2023) show that domain decomposition can help PINNs address multimaterial mechanics problems with discontinuity and complex interfaces. He et al. (2024) show that separating geometry, constitutive, and equilibrium information can improve the structure of physics-informed modeling. Rezaei et al. (2024) demonstrate that thermodynamics-based constitutive learning requires a careful connection between physical principles and neural network training. The framework was considered complete when the themes could explain how PINNs should be designed, justified, and interpreted in nonlinear material systems. This procedure allowed limited replication because another researcher could follow the same stages, use similar inclusion criteria, apply comparable interview protocols, and evaluate the same conceptual components.

3. Results and Discussions

The analysis generated five main themes that explain how a conceptual framework for Physics-Informed Neural Networks (PINNs) can be developed for nonlinear material systems. The first theme concerns the need to place physical laws at the center of model design. Participants consistently viewed PINNs not merely as a machine learning technique, but as a modeling approach that must begin from the physics of the material system. One informant stated, “A PINN model will only be meaningful if the physical law is treated as the main structure, not as an additional constraint after the model is built” (P3). This finding aligns with the documentary analysis, which showed that governing equations, boundary conditions, and constitutive assumptions form the core logic of PINN-based modeling. Karniadakis et al. (2021) argue that physics-informed machine learning becomes valuable because it connects data-driven learning with scientific laws. Cuomo et al. (2022) also explain that PINNs create a bridge between numerical modeling and neural network learning. Haghighat et al. (2021) support this pattern by showing that PINNs can be used for inverse modeling and surrogate modeling in solid mechanics.

The second theme relates to the role of data in nonlinear material modeling. Participants explained that material data are often limited, expensive, noisy, and difficult to obtain, especially when the material response involves large deformation, plasticity, or damage evolution. One participant noted, “In material testing, we often do not have large datasets. What we have is small but meaningful data, and the model must respect the physics behind those data” (P5). This theme shows that PINNs are attractive because they can work with limited data when the governing physics are properly embedded. Zhang et al. (2022) demonstrate that PINNs can analyze internal structures and defects in materials when direct observation is difficult. Hamel et al. (2023) show that full-field data can support the calibration of constitutive models in a physics-informed framework. Jeong et al. (2024) further indicate that material behavior can be identified from full-field data without relying fully on fixed parametric assumptions. These studies strengthen the finding that PINNs can help researchers manage the tension between data limitation and physical complexity.

The third theme concerns the importance of constitutive assumptions in building the conceptual framework. Participants emphasized that nonlinear material systems cannot be modeled only through generic neural network architecture. The model must represent the logic of material behavior, including stress-strain relations, energy principles, deformation mechanisms, and thermodynamic consistency. One informant explained, “For nonlinear materials, the constitutive model is the language of the material. If the PINN ignores that language, the prediction may look good but remain physically weak” (P2). Linka and Kuhl (2023) argue that constitutive neural networks need physical, kinematic, and thermodynamic constraints to produce meaningful material models. Rezaei et al. (2024) show that thermodynamics-based nonlinear constitutive models can be learned using PINNs when the physical structure is included in training. Song and Jin (2024) also show that PINNs can identify parameters for complex hyperelastic materials. These findings indicate that constitutive modeling should become a central component of the proposed conceptual framework.

The fourth theme highlights training stability and loss function design as key challenges in PINN implementation. Participants described the loss function as the “negotiation space” between data, physics, boundary conditions, and model prediction. Several informants stated that the success of PINNs depends on how researchers balance these loss components during training. One participant said, “The problem is not only whether we include the physics, but how strongly the model listens to each part of the physics during training” (P7). Wang et al. (2021) show that gradient flow pathologies can reduce the effectiveness of PINNs in solving complex physical problems. Wu et al. (2023) explain that data sampling strategies and boundary condition constraints strongly affect material property identification using PINNs. Hu et al. (2024) also note that PINNs in computational solid mechanics require careful numerical design because nonlinear systems can produce training instability. This theme shows that the conceptual framework must include training strategy as a core element, not as a technical detail placed outside the framework.

The fifth theme concerns interpretability and methodological transparency. Participants argued that a PINN model for nonlinear material systems should not only produce accurate prediction, but should also explain how physical variables, material parameters, and governing equations influence the result. One informant stated, "For material systems, the model must be explainable because engineers need to know why the material fails, not only when it fails" (P1). This finding shows that interpretability is essential for the acceptance of PINNs in material research and engineering applications. Diao et al. (2023) show that multimaterial systems require domain decomposition because interfaces and discontinuities affect the physical meaning of the model. He et al. (2024) demonstrate that separating geometric, constitutive, and equilibrium information can improve the structure of physics-informed modeling. Michaloglou et al. (2025) also explain that PINNs are increasingly relevant in material modeling and design because they can connect prediction, physics, and optimization. Based on these findings, interpretability should be treated as a structural requirement in the conceptual framework.

Discussion

The findings show that the development of a conceptual framework for PINNs in nonlinear material systems must begin from the relationship between physical law and data-driven learning. This result supports the view that PINNs are not ordinary neural networks with additional mathematical constraints. Instead, PINNs operate as hybrid models that combine physical reasoning, computational approximation, and empirical evidence. Karniadakis et al. (2021) provide a theoretical foundation for this interpretation by positioning physics-informed machine learning as a bridge between scientific modeling and data science. Cuomo et al. (2022) also show that PINNs are useful because they embed governing equations into the learning process. The present study extends this view by showing that, in nonlinear material systems, physical law must guide the entire modeling structure, from problem definition to interpretation of results. This means that the conceptual framework should not start from the neural network architecture, but from the material phenomenon being modeled.

The findings also reveal that limited data are not merely a technical constraint, but a defining feature of many nonlinear material problems. This point is important because material testing often requires costly equipment, controlled laboratory conditions, and complex measurement procedures. Zhang et al. (2022) show that PINNs can help analyze internal structures and defects when direct material observation is difficult. Hamel et al. (2023) demonstrate that full-field data can be used to calibrate constitutive models through physics-informed learning. Jeong et al. (2024) support this direction by showing that PINNs can identify material behavior from full-field data. The present study adds a qualitative interpretation by showing that researchers need to define what counts as meaningful data before developing the model. In this sense, data quality, physical relevance, and measurement context become more important than data quantity alone.

Another important finding concerns the central role of constitutive modeling. Nonlinear material systems involve complex relationships between load, deformation, stress, strain, energy, and failure mechanisms. The participants' statements show that the conceptual framework must include constitutive assumptions as a major element because these assumptions define the physical identity of the material system. Linka and Kuhl (2023) support this view by emphasizing the need for physically constrained constitutive neural networks. Rezaei et al. (2024) demonstrate that thermodynamics-based models can be learned when physical principles are properly integrated into the training process. Song and Jin (2024) show that PINNs can support the identification of constitutive parameters in complex hyperelastic materials. This study extends those findings by arguing that constitutive assumptions should not be treated only as equations in the loss function. They should be treated as conceptual anchors that connect material theory, data interpretation, and model validation.

The study also found that loss function design and training stability are major conceptual issues. In many PINN studies, the loss function is discussed as a technical component. However, the qualitative findings suggest that the loss function represents the researcher's decision about which physical and empirical elements should be prioritized during learning. Wang et al. (2021) show that gradient flow pathologies can disrupt PINN training and reduce model performance. Wu et al. (2023) explain that data sampling and boundary constraints influence the reliability of material property identification. Hu et al. (2024) also show that solid mechanics applications require careful PINN formulation because training can become unstable in nonlinear settings. The present study contributes a broader interpretation by showing that the loss function is not only a mathematical expression. It is also a conceptual map that defines the relationship between data, physics, boundary conditions, and model error.

The findings further indicate that interpretability must become a central requirement in PINN-based material modeling. In engineering and material science, prediction alone is often insufficient because researchers and practitioners need to understand why a material behaves in a certain way. Diao et al. (2023) show that multimaterial mechanics problems require special treatment because interfaces and discontinuities affect the physical structure of the model. He et al. (2024) show that multi-level physics-informed learning can separate geometry, constitutive behavior, and equilibrium relations. Michaloglou et al. (2025) also highlight the growing use of PINNs in material modeling and design. This study adds that interpretability should be built into the framework from the beginning. A PINN framework for nonlinear materials should explain not only the predicted output, but also the role of each physical component in producing that output.

Overall, the results suggest that a conceptual framework for PINNs in nonlinear material systems should consist of six connected components: empirical data, governing physics, constitutive assumptions, neural network architecture, training strategy, and interpretive validation. Each component has a different function, but all components must work together to produce a physically meaningful model. The practical implication is that researchers should not begin PINN development only by selecting an architecture or optimizer. They should first define the material phenomenon, identify the governing physics, evaluate data availability, formulate constitutive assumptions, and then design the computational model. The theoretical implication is that PINNs can be understood as a methodological bridge between material mechanics and machine learning. Future research can test this conceptual framework through empirical simulation studies, experimental material datasets, and comparative validation across different nonlinear material systems, such as hyperelastic polymers, elastoplastic metals, soft biological tissues, and composite materials.

4. Conclusions

This study concludes that the development of a conceptual framework for Physics-Informed Neural Networks (PINNs) in nonlinear material systems requires an integrated understanding of empirical data, governing physics, constitutive assumptions, neural network architecture, training strategy, and interpretive validation. The findings show that PINNs cannot be treated only as computational tools for improving numerical prediction. They must be understood as hybrid modeling frameworks that connect material mechanics, physical constraints, and data-driven learning. The study identifies five main themes: the centrality of physical laws, the role of limited but meaningful material data, the importance of constitutive assumptions, the challenge of loss function design and training stability, and the need for interpretability in nonlinear material modeling. These themes clarify how PINNs can support a deeper understanding of nonlinear material behavior, especially when experimental data are limited and physical responses are complex.

The study contributes theoretically by strengthening the conceptual foundation of *scientific machine learning* in nonlinear material research. It shows that the value of PINNs lies not only in their predictive performance, but also in their ability to structure the relationship between physics, data, and material behavior. Practically, the proposed framework can guide researchers, laboratories, and simulation developers in designing PINN models that are more transparent, physically consistent, and suitable for nonlinear material systems. From a policy and research management perspective, the framework can support the development of more efficient computational research strategies in material science, especially in contexts with limited experimental infrastructure. Future studies should test this conceptual framework through empirical simulations, laboratory-based material datasets, and comparative studies across different nonlinear materials, such as hyperelastic polymers, elastoplastic metals, composite structures, and soft biological tissues.

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