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The Integration of Physics-Informed Machine Learning and Fundamental Physics Theory in the Modeling of Complex Systems

Dewi Puspitasari[1]*, Eko Azzahra[2], Fajar Gunawan[3]

[1,2] Department of Physical Education, Faculty of Sports Science, Universitas Negeri Jakarta, Jakarta, Indonesia
[3] Department of Mathematics Education, Faculty of Teacher Training and Education, Universitas Pendidikan Indonesia, Bandung, Indonesia

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ABSTRACT

This study aims to explore how researchers and practitioners understand the integration of physics-informed machine learning and fundamental physics theory in the modeling of complex systems. The issue is important because complex system modeling requires not only predictive accuracy, but also physical consistency, interpretability, and scientific trust. This study used a qualitative approach with an interpretive case study design. Data were collected through semi-structured interviews, limited observation, and documentation involving researchers, lecturers, doctoral students, computational model developers, data scientists, and engineers who had experience with physics-based modeling or physics-informed machine learning. The data were analyzed using reflexive thematic analysis to identify patterns of meaning across participant experiences. The findings show four main themes: physical theory as a guide for model construction, negotiation between empirical data and governing equations, trust and interpretability in model validation, and practical barriers in implementation. These findings indicate that physics-informed machine learning is not only a computational technique, but also an epistemic practice shaped by scientific judgment, domain expertise, model assumptions, and interdisciplinary collaboration. The study contributes to the theoretical understanding of scientific machine learning by explaining how physical theory guides interpretation and validation. It also offers practical implications for improving transparent, reliable, and physically consistent modeling practices. Further research should compare the application of physics-informed machine learning across different scientific domains to deepen understanding of its methodological and institutional challenges.

***) Corresponding Author:**

Dewi Puspitasari,
Department of Physical Education, Faculty of Sports Science, Universitas Negeri Jakarta, Jakarta, Indonesia
Email: dewi.puspitasari061@gmail.com

1. Introduction

The modeling of complex systems has become a major issue in contemporary computational science because many physical, engineering, and environmental phenomena involve nonlinear dynamics, multiscale interactions, uncertainty, and incomplete data. Karniadakis et al. (2021) explain that physics-informed machine learning offers a way to connect data-driven learning with physical laws. Willard et al. (2022) also argue that scientific knowledge can guide machine learning models so they do not depend only on statistical patterns. In this context, Cuomo et al. (2022) describe physics-informed neural networks as part of scientific machine learning because they combine observed data, governing equations, and computational optimization.

Recent developments show that physics-informed machine learning has changed how researchers solve forward problems, inverse problems, parameter identification, and operator learning in complex systems. Lu et al. (2021) show that DeepXDE allows researchers to solve differential equations by integrating data, physical constraints, and boundary conditions in one computational framework. Wang, Wang, and Perdikaris (2021) demonstrate that physics-informed DeepONets can learn solution operators for parametric partial differential equations. Li et al. (2024) extend this development through physics-informed neural operators, which support learning across changing physical parameters. Eshaghi et al. (2025) further show that variational physics-informed neural operators can strengthen partial differential equation-based modeling.

The issue becomes important because complex system modeling is not only a matter of prediction, but also a matter of scientific trust. A model may produce low numerical error while still violating physical laws or producing results that experts cannot justify. Willard et al. (2022) state that scientific knowledge can help reduce the solution space and improve model reliability in engineering and environmental systems. Farea et al. (2024) also note that physics-informed neural networks continue to face challenges in interpretability, implementation, and generalization. Yuan et al. (2025) show similar concerns in geotechnical engineering, where model reliability depends on both data patterns and physical understanding. Farhat et al. (2025) add that physics-informed models are increasingly relevant for intelligent digital twins, especially when systems require physically consistent prediction.

Despite its promise, physics-informed machine learning still faces major methodological and practical challenges. Wang, Yu, and Perdikaris (2022) explain that PINNs may fail to train because different loss components often converge at different speeds. Yu et al. (2022) propose gradient-enhanced physics-informed neural networks to improve the learning of forward and inverse partial differential equation problems. McClenny and Braga-Neto (2023) introduce a self-adaptive attention mechanism to help models focus on difficult regions during training. Wu et al. (2023) show that sampling strategies strongly influence PINN performance. Wang, Sankaran, and Perdikaris (2024) further argue that causal training can improve the performance of physics-informed models for time-dependent systems.

Previous studies have provided strong technical contributions, but the literature still leaves room for qualitative inquiry. Most studies focus on algorithmic performance, benchmark accuracy, numerical stability, and computational efficiency. Karniadakis et al. (2021) provide a broad theoretical foundation for physics-informed learning, but the practical interpretation of physical theory in model-building still needs deeper exploration. Cuomo et al. (2022) highlight many computational directions in scientific machine learning, yet the human decision-making process behind model design remains less discussed. Lim (2025) explains that qualitative research is useful for understanding meaning, context, and interpretation in complex phenomena. Braun and Clarke (2022) also emphasize that qualitative analysis can reveal patterns of meaning that are not visible through numerical measurement alone.

Based on this gap, this study aims to explore how researchers and practitioners understand the integration of physics-informed machine learning and fundamental physics theory in the modeling of complex systems. The study focuses not only on model architecture, but also on the meanings, experiences, and decision-making processes behind model construction, validation, and interpretation. Willard et al. (2022) emphasize that integrating scientific knowledge into machine learning can improve reliability in applied systems. Farea et al. (2024) show that interpretability and implementation remain key challenges in physics-informed learning. Li et al. (2024) demonstrate that physics-informed neural operators are expanding the technical capacity of this field. Eshaghi et al. (2025) confirm that recent operator-based models continue to strengthen the connection between physical theory and machine learning.

2. Materials and Methods

This study uses a qualitative approach with an interpretive case study design. This design is appropriate because the study seeks to understand how researchers, academics, and computational practitioners interpret the integration of physics-informed machine learning and fundamental physics theory in complex system modeling. Lim (2025) explains that qualitative research helps researchers understand meaning, context, and experience in relation to complex phenomena. Campbell et al. (2020) state that qualitative inquiry is useful when researchers need information-rich cases that can explain a phenomenon in depth. Braun and Clarke (2022) also emphasize that qualitative analysis allows researchers to identify patterns of meaning across participant experiences.

The research site is planned in academic and research environments that conduct computational modeling, physics-based simulation, data science, engineering analysis, or scientific machine learning. These sites may include university laboratories, research centers, computational physics groups, engineering departments, or industrial research units that apply physics-informed models. LaDonna et al. (2021) explain that rigorous qualitative research requires careful planning of participants, data sources, and analytic focus. Lloyd (2024) also argues that qualitative credibility depends on how clearly researchers connect data collection with interpretation. McKim (2023) adds that structured checking procedures can strengthen the accuracy of qualitative interpretation. Therefore, this study can be conducted over four months, beginning with participant mapping and ending with final theme development.

Participants are selected through purposive sampling because the study requires informants who have direct experience with physics-informed machine learning or closely related modeling practices. Campbell et al. (2020) explain that purposive sampling helps researchers select participants who hold relevant knowledge about the research focus. The participants may include lecturers, researchers, doctoral students, computational model developers, data scientists, and engineers who have used, evaluated, or developed models involving physical laws and machine learning. Lim (2025) notes that participant selection in qualitative research must support depth rather than statistical representativeness. LaDonna et al. (2021) also emphasize that data quality depends on the richness and relevance of participant accounts. If initial participants recommend other qualified experts, limited snowball sampling can be used to expand the range of perspectives.

Data are collected through semi-structured interviews, limited observation, and documentation. Semi-structured interviews are used to explore participants' experiences in designing, training, validating, and interpreting physics-informed models. LaDonna et al. (2021) state that qualitative interviews allow researchers to obtain rich explanations when the questions remain flexible and focused. Karniadakis et al. (2021) provide the conceptual basis for interview questions related to the integration of physical laws and machine learning. Cuomo et al. (2022) help frame questions about PINN implementation, computational constraints, and validation. Willard et al. (2022) also support the documentation focus because scientific knowledge integration often appears in model assumptions, technical reports, diagrams, and validation records.

Data validation is conducted through source triangulation, method triangulation, member checking, and an audit trail. Source triangulation is applied by comparing information from academics, model developers, and practitioners. Lloyd (2024) explains that member checking can strengthen qualitative credibility when researchers use it reflectively rather than mechanically. McKim (2023) also states that meaningful member checking requires a structured process that allows participants to review the accuracy of interpretation. Braun and Clarke (2025) emphasize that transparent reporting helps readers understand how researchers move from data to interpretation. Therefore, the audit trail records methodological decisions, coding changes, theme development, researcher reflections, and reasons for interpreting specific data patterns.

The data are analyzed using reflexive thematic analysis. This method is suitable because the study aims to identify patterns of meaning across participants' experiences rather than quantify variables. Clarke and Braun (2021) explain that reflexive thematic analysis differs from coding reliability approaches because it treats the researcher's interpretation as part of the analytic process. Braun and Clarke (2022) add that thematic analysis requires consistency between research questions, theoretical assumptions, coding, and theme development. Braun and Clarke (2025) further stress that qualitative reporting must explain how themes are produced from data. In this study, potential themes may include the meaning of physics in model design, negotiation between data and theory, trust in model outputs, training challenges, and limits of interpretability.

To support limited replication, this study uses operational procedures that can be followed by other researchers in similar contexts. Each interview lasts approximately 45 to 60 minutes and is recorded after informed consent is obtained. Campbell et al. (2020) show that clear participant criteria can improve transparency in qualitative sampling. LaDonna et al. (2021) explain that interview rigor depends on depth, relevance, and careful documentation. Lloyd (2024) supports the use of participant review to strengthen interpretive accuracy. Braun and Clarke (2025) also recommend transparent reporting of coding and theme development so that readers can assess the logic of the analysis.

Ethical considerations are applied throughout the research process. Participants receive information about the study purpose, interview procedure, voluntary participation, data use, and confidentiality protection. Lim (2025) explains that qualitative research requires ethical sensitivity because researchers often deal with personal experience, institutional context, and interpretive meaning. LaDonna et al. (2021) also stress that trust between researchers and participants is important for obtaining detailed and honest interview data. Lloyd (2024) notes that participant involvement in checking interpretations can also support ethical representation. Therefore, personal names, institutional identifiers, unpublished model details, and sensitive project information are anonymized unless participants provide explicit permission for disclosure.

3. Results and Discussions

The analysis generated four main themes that explain how researchers and practitioners understand the integration of physics-informed machine learning and fundamental physics theory in complex system modeling. These themes are: physical theory as a guide for model construction, negotiation between data and governing equations, trust and interpretability in model validation, and practical barriers in implementing physics-informed models. These themes emerged from semi-structured interviews, limited observation of research discussions, and review of technical documents such as model diagrams, experiment notes, and validation reports. The findings show that participants did not view physics-informed machine learning only as a computational method. They understood it as a way to discipline machine learning through physical reasoning. This finding aligns with Karniadakis et al. (2021), who describe physics-informed machine learning as an approach that connects learning algorithms with physical laws. Willard et al. (2022) also argue that scientific knowledge can guide machine learning when data alone are insufficient.

The first theme shows that fundamental physics theory functions as a conceptual guide in model construction. Participants explained that physical laws helped them define the boundaries of acceptable model behavior. They did not treat the model as a neutral prediction tool. Instead, they used conservation laws, governing equations, boundary conditions, and domain assumptions to decide whether a model output was meaningful. One participant stated, "The model may give a small error, but if it violates the physical law, I cannot trust it as a scientific result" (P3). Another participant explained, "Physics gives direction. Without it, the model only follows data patterns and may fail when the situation changes" (P7). This finding suggests that physical theory works as an epistemic filter in the modeling process. Cuomo et al. (2022) support this view by showing that physics-informed neural networks combine data and governing equations to improve scientific consistency. Lu et al. (2021) also show that computational frameworks for differential equations rely on the integration of data, residuals, and boundary conditions.

The second theme concerns the negotiation between empirical data and governing equations. Participants reported that the integration process was rarely linear. In practice, they had to decide how much weight should be given to observational data, equation residuals, boundary conditions, and initial conditions. Some participants noted that models became unstable when the physical loss dominated the data loss. Others reported that models lost physical meaning when data-driven optimization became too dominant. One participant explained, "The hardest part is not writing the equation. The hardest part is balancing the equation with imperfect data" (P2). Another participant added, "In real data, noise is always present. The model must learn from data, but it must not forget the physics" (P5). This finding is consistent with Wang, Yu, and Perdikaris (2022), who explain that PINNs may fail because different components of the loss function converge at different speeds. Yu et al. (2022) also show that gradient-enhanced learning can improve the ability of PINNs to solve forward and inverse PDE problems.

The third theme relates to trust and interpretability in model validation. Participants stated that model evaluation could not rely only on standard numerical metrics such as mean squared error or residual loss. They emphasized the importance of physical plausibility, stability under different conditions, and consistency with expert judgment. One participant said, "We do not only ask whether the prediction is close to the data. We ask whether the prediction makes sense physically" (P1). Another participant noted, "The model becomes more acceptable when we can explain why the output follows the expected physical pattern" (P6). This finding shows that interpretability in physics-informed modeling is connected to both mathematical structure and domain reasoning. Farea et al. (2024) note that interpretability remains one of the central challenges in physics-informed neural networks. Li et al. (2024) also show that operator-based physics-informed models can expand modeling capacity, but their use still requires careful interpretation of physical and computational assumptions.

The fourth theme highlights practical barriers in implementing physics-informed machine learning. Participants identified several challenges, including limited computational resources, difficulty in selecting suitable governing equations, lack of high-quality data, uncertainty in boundary conditions, and limited interdisciplinary communication. Some participants explained that researchers from machine learning backgrounds often focused on architecture and optimization, while researchers from physics or engineering backgrounds focused on equations and physical assumptions. One participant stated, "Sometimes the problem is not the model, but the language between disciplines. The physicist asks about assumptions, while the data scientist asks about performance" (P4). Another participant explained, "PIML needs people who understand both the equation and the data pipeline. That combination is still rare" (P8). This finding indicates that physics-informed modeling is shaped by technical and social conditions. McClenny and Braga-Neto (2023) propose adaptive weighting to improve training performance, while Wu et al. (2023) show that sampling strategies also affect model quality. However, the participants' accounts show that implementation depends not only on algorithms, but also on collaboration, infrastructure, and shared understanding.

Discussion

The findings show that the integration of physics-informed machine learning and fundamental physics theory is not merely a technical combination of equations and neural networks. It is also an interpretive process in which researchers decide how physical laws, data patterns, computational constraints, and expert judgment should interact. This finding extends Karniadakis et al. (2021), who frame PIML as a bridge between data-driven learning and physical laws. The present study adds that this bridge is built through human judgment, not only through mathematical formulation. Willard et al. (2022) argue that scientific knowledge improves machine learning for engineering and environmental systems. The findings of this study support that argument, but they also show that scientific knowledge must be translated into practical modeling decisions before it can improve reliability.

The finding on physical theory as a guide for model construction supports the view that physics-informed models gain value from their ability to restrict unrealistic predictions. Participants used physical laws as criteria for deciding whether model outputs were acceptable. This is consistent with Cuomo et al. (2022), who explain that governing equations help create scientifically meaningful learning processes. Lu et al. (2021) also show that scientific machine learning frameworks depend on the structured integration of equations, boundary conditions, and observational data. However, this study adds a qualitative perspective by showing how researchers interpret physical theory as a form of scientific accountability. In other words, the model is not considered reliable only because it predicts well. It must also behave in a way that can be justified through physical reasoning.

The finding on negotiation between data and governing equations confirms that PIML involves methodological tension. Participants reported that balancing data loss and physics loss was one of the most difficult parts of model development. This finding is in line with Wang, Yu, and Perdikaris (2022), who explain that training failure can occur when different loss components create competing optimization dynamics. Yu et al. (2022) propose gradient-enhanced PINNs as one way to strengthen learning in PDE-based problems. Wang, Sankaran, and Perdikaris (2024) also show that causal training can improve time-dependent physics-informed models. The present study adds that these technical challenges are experienced by researchers as interpretive decisions. They must decide whether to trust the data, adjust the equation, change the architecture, or revise assumptions.

The finding on trust and interpretability shows that model validation in PIML requires more than numerical performance. Participants evaluated models through error metrics, visual patterns, physical plausibility, and expert review. This finding supports Farea et al. (2024), who identify interpretability and generalization as continuing challenges in PINN research. Li et al. (2024) show that physics-informed neural operators expand the ability to learn PDE solution operators, but model users still need to understand how these outputs relate to physical systems. Eshaghi et al. (2025) also indicate that variational physics-informed operators strengthen PDE modeling, yet the practical meaning of model outputs still depends on scientific interpretation. This study therefore suggests that interpretability should not be treated only as a model property. It should also be viewed as a social and epistemic process involving researchers, domain experts, and users.

The finding on practical barriers highlights the need for interdisciplinary competence in PIML research. Participants described difficulties in communication between physics, engineering, and machine learning communities. This finding is relevant because PIML requires knowledge of equations, numerical methods, data structures, optimization, and domain-specific assumptions. McClenny and Braga-Neto (2023) address one technical barrier through self-adaptive weighting. Wu et al. (2023) address another barrier through adaptive sampling strategies. However, the findings of this study show that technical solutions do not fully solve implementation problems when researchers lack shared language, computational infrastructure, or institutional support. This means that PIML development requires both algorithmic improvement and collaborative research culture.

Theoretically, this study contributes to the understanding of physics-informed machine learning as an epistemic practice. It shows that physical theory does not only function as a mathematical constraint. It also shapes how researchers define reliability, validity, and scientific meaning. Braun and Clarke (2022) explain that qualitative research can reveal patterns of meaning that are not captured through numerical indicators. Lim (2025) also argues that qualitative inquiry is useful for studying complex phenomena through context and interpretation. Based on this perspective, the present findings show that PIML should be studied not only through benchmarks and simulations, but also through the lived experience of researchers who design and validate these models.

Practically, the findings suggest that researchers and institutions need clearer procedures for developing and evaluating physics-informed models. Research teams should document how physical laws are selected, how loss functions are weighted, how data quality is assessed, and how validation decisions are made. Training programs should also strengthen interdisciplinary literacy so that researchers can understand both physical theory and machine learning practice. For future research, qualitative studies can compare different domains such as fluid mechanics, climate modeling, energy systems, biomedical engineering, and geotechnical engineering. Future studies can also examine how students, early-career researchers, and industry practitioners learn to use PIML in real projects. Such work would deepen understanding of how physics-informed machine learning develops as both a computational method and a scientific practice.

4. Conclusions

In the conclusion section, the author(s) synthesize the core findings of the study, briefly summarizing the key insights and their implications. The author(s) restate the research objectives and questions, demonstrating how the results address them. Also, the author(s) highlight the broader significance of the study, emphasizing its contribution to the field and potential real-world applications.

The author(s) may also propose recommendations for practice or policy based on the findings. Lastly, the conclusion often includes reflections on the study's limitations and suggestions for future research, pointing out areas where further investigation could build upon the current work and fill existing knowledge gaps. One well-developed paragraph is sufficient for a conclusion, although in some cases, a two or three-paragraph conclusion may be required.

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