Physics-Informed Machine Learning and Dynamic Graph Neural Networks: A Survey

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Abstract

Physics-Informed Machine Learning (PIML) and dynamic graph models represent a paradigm shift in the modeling and prediction of complex systems across diverse domains. By embedding physical laws into machine learning frameworks, PIML enhances model interpretability and prediction accuracy, particularly in scenarios with limited data availability. This survey explores the interdisciplinary integration of physics principles with advanced machine learning techniques such as Graph Neural Networks (GNNs), illustrating their potential to efficiently predict and interpret complex system behaviors. The synthesis of these methodologies is crucial for advancing the modeling and understanding of complex systems in fields ranging from materials science to neuroscience and environmental modeling. The survey also highlights significant applications of PIML, including improved simulations in fluid dynamics, enhanced structural health monitoring, and optimized energy systems. However, challenges such as scalability, data availability, and model interpretability remain. Future research directions include refining PIML models for broader applicability, enhancing robustness, and integrating multimodal information to improve model performance and explainability. Overall, the integration of PIML with dynamic graph models promises to unlock new possibilities for innovation and discovery, offering transformative improvements in predictive accuracy and computational efficiency across various scientific and engineering domains.

1 Introduction

1.1 Interdisciplinary Approach

The integration of physics principles with machine learning and graph neural networks (GNNs) represents a transformative interdisciplinary strategy for modeling and predicting complex systems. This fusion capitalizes on the empirical rigor of physics and the computational power of machine learning, enhancing the understanding of multiscale networked systems. Notably, STONet exemplifies this approach by learning the dynamics of spatially continuous physical quantities, illustrating the potential of merging physics with machine learning [1]. Additionally, combining classical reduced-order modeling with GNNs offers a flexible method for predicting reduced-order bases across various geometries, further demonstrating the innovative nature of this interdisciplinary approach [2].

Dynamic representation optimization in machine learning tasks is underscored by exploring dynamic relationships within data, as shown in recent studies [3]. The application of GNNs for modeling structure-property relationships in Metallic Glasses (MGs) highlights the interdisciplinary integration, showcasing the efficiency in predicting and interpreting energy barriers [4]. This synthesis is crucial for advancing the modeling and understanding of complex systems across diverse fields.

The interdisciplinary nature of combining physics with machine learning is further emphasized in condition monitoring and anomaly detection, as highlighted in recent surveys [5]. By embedding physical laws within machine learning frameworks, models achieve enhanced accuracy and efficiency,

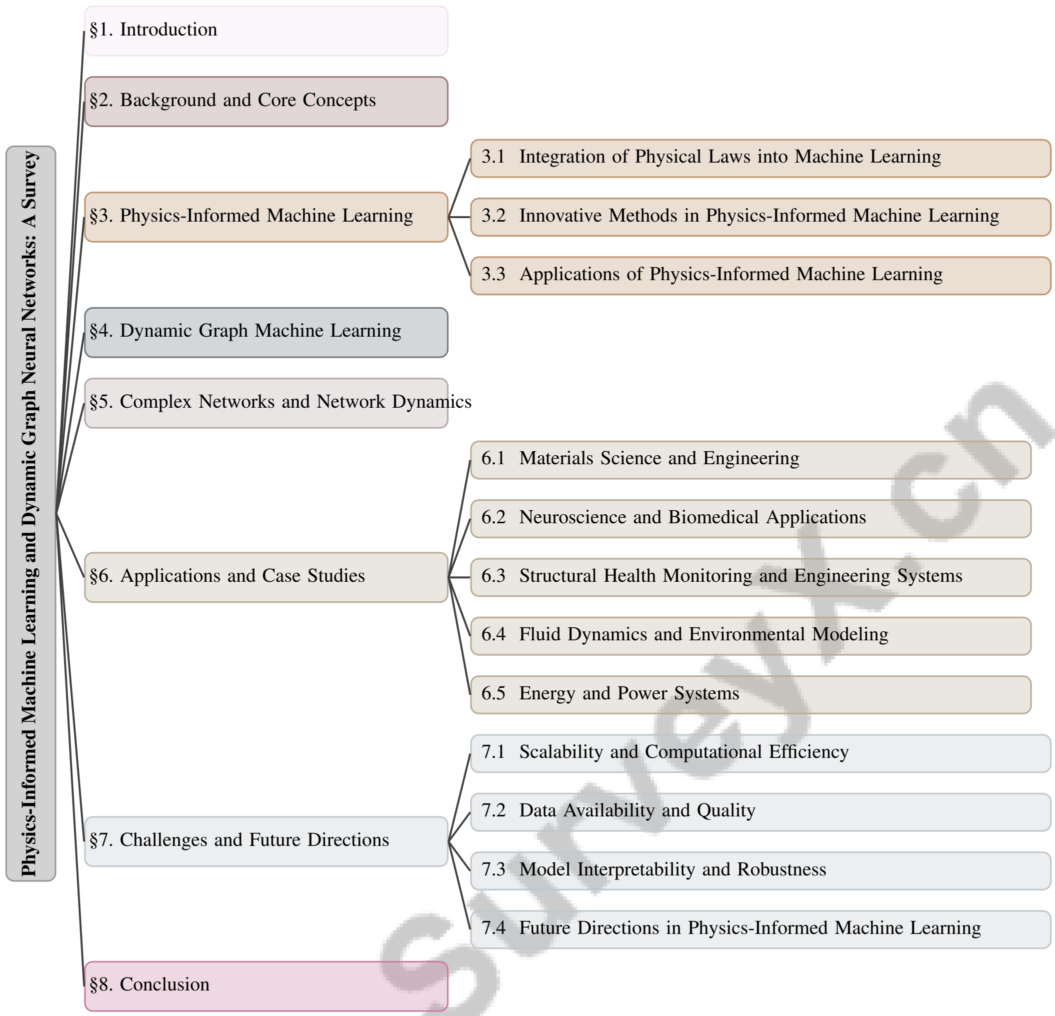

Figure 1: chapter structure

addressing challenges across engineering and environmental science. This integration promises novel solutions, advancing complex system modeling and prediction.

1.2 Significance and Applications

The convergence of physics-informed machine learning (PIML) with dynamic graph models signifies a paradigm shift in modeling and predicting complex systems across various domains. By embedding physical laws into machine learning frameworks, PIML enhances interpretability and prediction accuracy, particularly in data-scarce scenarios [6]. This approach effectively addresses challenges related to data scarcity, generalizability, and physical plausibility, significantly improving performance in tasks governed by physical mechanisms.

In engineering, especially in safety-critical areas, PIML enhances reliability by incorporating physical constraints, ensuring safety and efficiency. For example, in turbulence modeling for core-collapse supernovae simulations, PIML improves simulation fidelity by overcoming limitations of existing subgrid models [7]. In environmental modeling, PIML is pivotal in accurately predicting oceanic variables in data-scarce environments, which is crucial for climate science and oceanography [8].

The integration of PIML with dynamic graph models is essential for estimating inaccessible parameters in complex systems, enhancing understanding and prediction of system behaviors [9]. In public safety management, frameworks combining PIML with dynamic graph models show promise in simulating realistic crowd behaviors, contributing to improved safety strategies [10]. Moreover, the incorporation of causal learning with GNNs enhances applications in fraud detection and recommendation systems, bolstering their reliability and effectiveness [11].

PIML's applications extend to traffic modeling, where contextual information like curb configuration and driver behavior enhances flow predictions [12]. In particle physics, GNNs show potential in data reconstruction, classification, and simulation tasks, underscoring the importance of integrating physics-informed machine learning with dynamic graph models [13]. Furthermore, embedding thermodynamic principles into neural networks significantly enhances predictive capabilities, crucial for forecasting physical phenomena governed by complex dynamics [14].

In optical composites, PIML improves model efficiency and generalizability, optimizing design processes [15]. Its integration with statistical mechanics has significant implications for predicting the structure of oxide glasses, vital for high-tech applications [16]. Additionally, PIML's role in subsurface energy systems, including seismic applications and reservoir simulations, highlights its potential for intelligent decision-making [17].

The transformative impact of merging PIML with dynamic graph models is evident across numerous scientific and engineering domains. These interdisciplinary approaches address longstanding challenges and expand predictive modeling capabilities in complex systems, paving the way for innovative solutions [18].

1.3 Structure of the Survey

This survey is systematically organized to provide a comprehensive understanding of the integration of physics-informed machine learning with dynamic graph models, focusing on their applications in modeling complex systems. It begins with an **Introduction** that outlines the interdisciplinary approach merging physics principles with machine learning and GNNs, emphasizing the novelty and potential of this synthesis. The subsequent **Background and Core Concepts** section delves into foundational theories underlying physics-informed machine learning, dynamic graph machine learning, and complex networks, providing essential definitions and frameworks.

The third section, **Physics-Informed Machine Learning**, explores the integration of physical laws into machine learning models, highlighting the role of physics-informed neural networks (PINNs) and their applications across various domains. Following this, **Dynamic Graph Machine Learning** examines methods and models used to capture temporal and structural changes in networks, emphasizing recent advancements and their impact on dynamic systems modeling.

In the **Complex Networks and Network Dynamics** section, the focus shifts to analyzing the dynamic behaviors of complex networks, discussing the significance of understanding network dynamics for predicting and controlling interconnected systems. The survey then presents **Applications and Case Studies**, showcasing real-world applications where the integration of physics-informed machine learning and dynamic graph models has been successfully applied across fields such as materials science, neuroscience, structural health monitoring, fluid dynamics, and energy systems.

The penultimate section, **Challenges and Future Directions**, identifies current challenges in the field, such as scalability, data availability, and computational complexity, while discussing potential future research directions and technological advancements. Finally, the **Conclusion** summarizes the key points discussed in the survey, reinforcing the importance of combining physics-informed machine learning with dynamic graph techniques to advance the modeling and understanding of complex systems.The following sections are organized as shown in Figure 1.

2 Background and Core Concepts

2.1 Graph Neural Networks: Foundations and Applications

Graph Neural Networks (GNNs) provide a powerful framework for modeling graph-structured data, adeptly addressing applications across diverse fields [19]. Central to GNNs is the message-passing architecture, which facilitates information propagation through nodes and edges, effectively capturing complex dependencies [5]. This is particularly advantageous for dynamic systems modeling, where accurate prediction of system behaviors is essential [20].

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A critical challenge for GNNs involves generalizing across varied instances of complex dynamical systems. Integrating belief propagation (BP) algorithms within probabilistic graphical models (PGMs) enhances GNN generalization, thereby improving complex system modeling [21]. Additionally, attention mechanisms in GNNs have proven effective in identifying intricate patterns, extending their applicability to a wide range of datasets [19].

GNNs also facilitate the generation of reduced-order bases for complex physical systems, particularly in structural dynamics. Coupling classical reduced-order modeling with GNNs offers a flexible and efficient approach to predict reduced-order bases across varied geometries [2]. In high-energy particle physics, GNNs are utilized for tasks like image classification and energy estimation, highlighting their foundational role in modeling complex data representations [3].

In the realm of metallic glasses, the Symmetrized Graph Neural Network (SymGNN) exemplifies GNNs' utility in predicting energy barriers, thereby enhancing understanding of structure-property relationships [4]. Moreover, GNNs have been applied to model brain graphs derived from neuroimaging data, demonstrating their efficacy in representing biological networks [22].

Recent advancements in Temporal Graph Neural Networks (TGNs) underscore the need for comprehensive evaluation frameworks that consider various model configurations and performance metrics. Such advancements enhance understanding of how different TGN configurations affect prediction accuracy, thus advancing dynamic graph analysis [20]. As GNNs continue to evolve, their applications in dynamic systems modeling are expected to expand, offering novel insights across scientific and engineering domains.

2.2 Physics-Based Modeling

Physics-based modeling is pivotal for integrating empirical data with governing physical laws within machine learning frameworks for complex systems, enhancing model interpretability and predictive accuracy. This approach addresses the limitations of purely data-driven methods. Integrating thermodynamic principles from statistical mechanics into machine learning significantly improves predictions of behaviors such as the structure of oxide glasses, critical for high-tech applications [16].

The challenge of predicting formation energies of high-entropy alloys (HEMs) highlights the necessity of modeling varying chemical orders and compositions using machine learning [23]. This emphasizes the importance of incorporating physics-based insights to enhance predictive capabilities. Additionally, applying physics-informed machine learning to polar ice dynamics addresses critical modeling of mass loss from polar ice sheets, with significant implications for global sea levels [24].

GNNs excel in modeling graph-structured data, capturing complex interactions that traditional deep learning methods might overlook [22]. In physics-based modeling, the challenge is to learn effective low-dimensional representations while preserving essential structural information [22]. Furthermore, physics-based modeling extends to optimizing simulation parameters through techniques like automatic differentiation, refining machine learning models to align with physical principles [22].

Incorporating physics-based constraints, such as time-reversibility and symplecticity, into machine learning models ensures accurate representation of physical system dynamics. This is crucial in scenarios where conventional machine learning techniques may falter, necessitating the integration of physics-based constraints to effectively address complex system dynamics [22]. Thus, physics-based modeling is vital for advancing machine learning applications in complex systems, ensuring alignment with the physical realities they aim to represent.

3 Physics-Informed Machine Learning

The convergence of physics and machine learning has led to methodologies that significantly elevate traditional models by embedding physical laws, thus enhancing their predictive power and interpretability within complex systems. This section explores these methodologies, emphasizing their integration into machine learning frameworks to improve model accuracy and understanding. Table 1 offers a detailed summary of various methods employed in Physics-Informed Machine Learning, showcasing the integration of physical laws, innovative approaches, and their applications in improving model accuracy and interpretability. Figure 2 illustrates the structured approach of

Category	Feature	Method
Integration of Physical Laws into Machine Learning	Physics Integration	DRN[3], GNN-BP[21]
Innovative Methods in Physics-Informed Machine Learning	Activation Management Invariant Properties	MADM[19] SymGNN[4]
Applications of Physics-Informed Machine Learning	Hybrid and Multi-Fidelity Models Integration Techniques Simulation and Analysis Training and Convergence Strategies	FAMF-NN[25], IC[26] DIEP[27], PINN[28], GNN[29] AN[30], PFDON[31] PIML-KR[32], ST-COT[33]

Table 1: This table provides a comprehensive summary of methods in Physics-Informed Machine Learning (PIML), categorized into the integration of physical laws, innovative methods, and applications. It highlights specific features and methodologies, including Dynamic Reduction Networks, Symmetrized Graph Neural Networks, and Physics-Informed Neural Networks, illustrating their roles in enhancing model performance and applicability across diverse scientific domains.

Physics-Informed Machine Learning (PIML), detailing its integration of physical laws into machine learning, innovative methodologies, and various applications. The hierarchical structure depicted in the figure highlights the benefits and examples of integrating physical laws, innovative methods enhancing model performance, and the diverse scientific domains where PIML is applied, showcasing its transformative impact on predictive accuracy and computational efficiency.

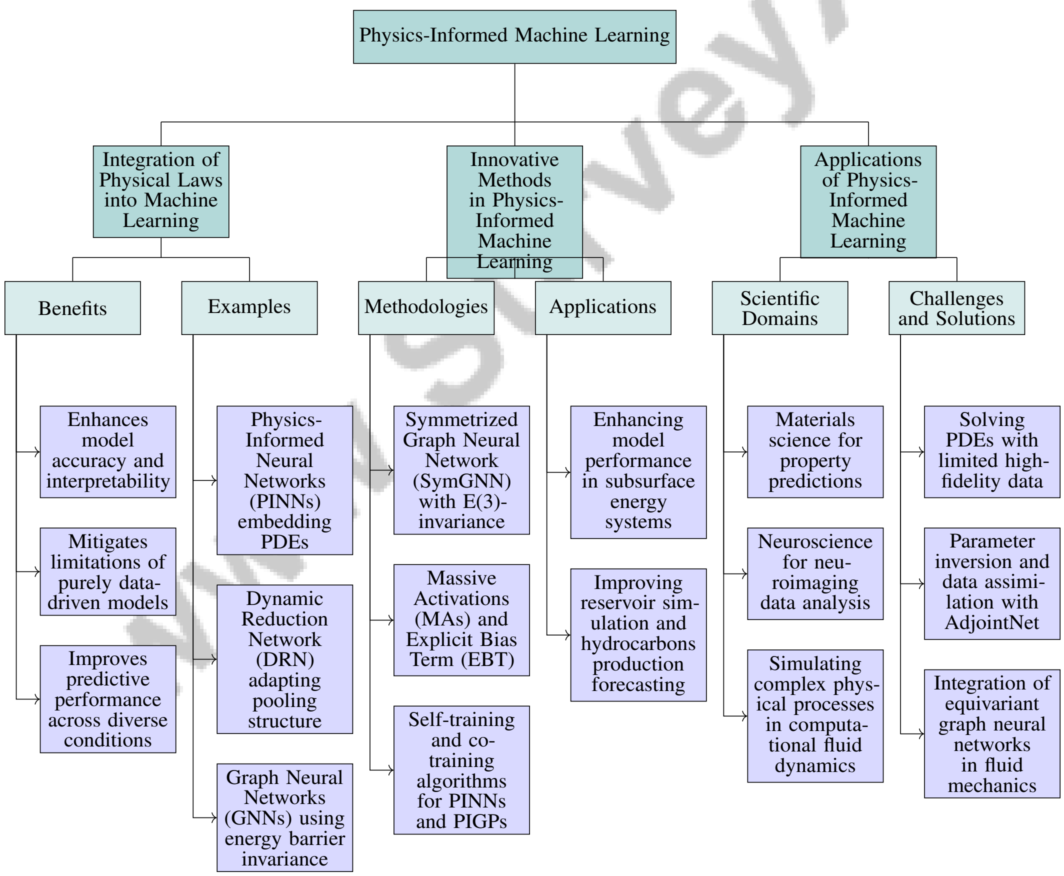

Figure 2: This figure illustrates the structured approach of Physics-Informed Machine Learning (PIML), detailing its integration of physical laws into machine learning, innovative methodologies, and various applications. The hierarchical structure highlights the benefits and examples of integrating physical laws, innovative methods enhancing model performance, and the diverse scientific domains where PIML is applied, showcasing its transformative impact on predictive accuracy and computational efficiency.

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3.1 Integration of Physical Laws into Machine Learning

Integrating physical laws into machine learning frameworks enhances model accuracy and interpretability, particularly in complex dynamical systems. This approach mitigates the limitations of purely data-driven models, which struggle with generalization and robustness in the presence of limited or noisy data [5]. By incorporating domain-specific physics, models achieve better predictive performance across diverse conditions [34].

Physics-Informed Neural Networks (PINNs) exemplify this integration by embedding partial differential equations (PDEs) into the training process, surpassing traditional numerical methods in solving complex PDEs with improved accuracy and efficiency [34]. The Dynamic Reduction Network (DRN) further demonstrates this by adapting its pooling structure based on data topology, enhancing model adaptability and precision [3].

Graph Neural Networks (GNNs) also integrate physical laws effectively, as seen in metallic glasses where the Symmetrized Graph Neural Network (SymGNN) uses energy barrier invariance to predict material properties with higher accuracy [4]. This is further applied in learning universal dynamics across complex systems by capturing specific structures while understanding overarching dynamics [21].

A key challenge in physics-informed machine learning is propagating information from data points to enable accurate extrapolations, especially with stiff PDEs [33]. Effective training schemes are essential to ensure predictions are accurate and physically consistent.

The integration of physical laws into machine learning models not only enhances predictive performance but also ensures models align with the physical realities they represent. This is crucial for overcoming challenges related to high-dimensionality, computational costs, and reliable data acquisition, paving the way for innovative solutions across various domains [5].

3.2 Innovative Methods in Physics-Informed Machine Learning

Advancements in physics-informed machine learning (PIML) have introduced methodologies that enhance model performance by integrating physical principles. The Symmetrized Graph Neural Network (SymGNN) incorporates E(3)-invariance, improving predictions of energy barriers and offering new perspectives in PIML [4]. Physics-Informed Neural Networks (PINNs) leverage physical laws to improve learning, enabling accurate predictions with limited data and providing differentiable solutions for optimization [34].

The development of methodologies for Massive Activations (MAs) and Explicit Bias Term (EBT) significantly advances the characterization and mitigation of massive activations in neural networks, crucial for improving model robustness and accuracy [19]. This underscores the importance of addressing biases in neural network architectures for optimal performance.

Self-training and co-training algorithms for PINNs and physics-informed Gaussian processes (PIGPs) enhance prediction accuracy and uncertainty quantification, enabling independent or joint model training to improve generalization and accuracy in complex systems [33]. The survey on PIML categorizes methods such as Physics Embedded in Feature Space and Physics-Informed Regularization, providing a comprehensive overview of innovative approaches integrating physical laws into machine learning models [5].

As illustrated in Figure 3, the innovative methodologies in PIML highlight advancements in model enhancements, training improvements, and application domains. Key methods such as SymGNN, PINNs, and Massive Activations are categorized under model enhancements, while self-training and co-training are noted for training improvements. Application domains include subsurface energy systems and condition monitoring, showcasing the diverse applicability of PIML techniques.

Innovative methods in PIML significantly enhance model accuracy, interpretability, and robustness by systematically integrating machine learning algorithms with physical laws and mathematical models. This integration develops effective solutions to complex challenges in scientific and engineering fields, such as subsurface energy systems, where PIML techniques improve reservoir simulation and hydrocarbons production forecasting. By leveraging domain-specific knowledge, PIML not only enhances model generalization but also ensures compliance with governing physical principles, revolutionizing predictive capabilities and operational efficiencies across applications [35, 36, 5, 37, 17].

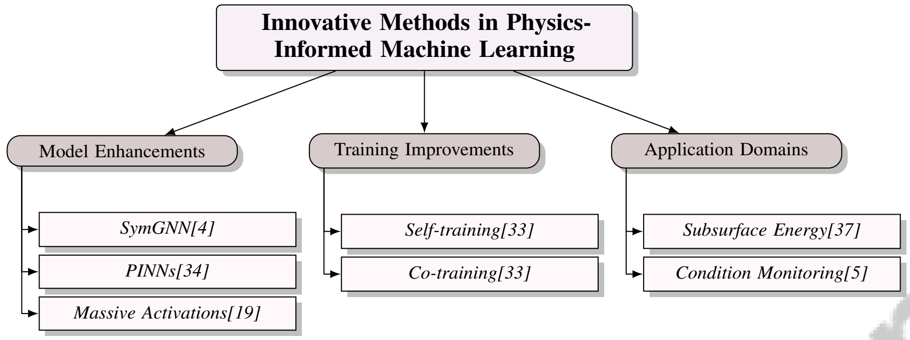

Figure 3: This figure illustrates the innovative methodologies in Physics-Informed Machine Learning (PIML), highlighting advancements in model enhancements, training improvements, and application domains. It categorizes key methods such as SymGNN, PINNs, and Massive Activations under model enhancements, while self-training and co-training are noted for training improvements. Application domains include subsurface energy systems and condition monitoring, showcasing the diverse applicability of PIML techniques.

3.3 Applications of Physics-Informed Machine Learning

Physics-Informed Machine Learning (PIML) has advanced numerous scientific and engineering domains by embedding physical principles within machine learning frameworks, enhancing predictive accuracy and model interpretability. In materials science, PIML has transformed material property predictions, with models like the Deep Integration of Energy Prediction (DIEP) improving predictions of total energy and fracture onset, facilitating high-throughput material discovery [27]. This is crucial for high-entropy alloys (HEMs), where machine learning models generalize from simpler to more complex compositions, highlighting the importance of dataset size and structural relaxation [23].

In neuroscience, PIML advances neuroimaging data analysis through spatio-temporal graph neural networks (STGNNs), leveraging network structures to provide insights into brain dynamics and improving diagnostic accuracy for neurological disorders through enhanced brain graph representation [22].

PIML is also vital in simulating complex physical processes. The Phase-Field DeepONet framework efficiently simulates pattern formation dynamics governed by gradient flows, reducing computational costs while maintaining accuracy [31]. In computational fluid dynamics, PIML approaches accurately predict melt pool dynamics, optimizing metal additive manufacturing processes [28].

PIML addresses challenges in solving partial differential equations (PDEs) with limited high-fidelity data. Multi-fidelity architectures leverage lower-fidelity data to enhance accuracy, offering cost-effective solutions for complex simulations [25]. Physics-Informed Neural Networks (PINNs) provide a mesh-free solution approach, adapting to complex geometries and allowing simultaneous resolution of forward and inverse problems with minimal adjustments [34].

In parameter inversion and data assimilation, methods like AdjointNet estimate process model parameters while adhering to physical constraints, proving valuable for climate modeling and environmental science [30]. Structural constraints in physics-augmented learning ensure models maintain physical accuracy while fitting data [26].

The integration of equivariant graph neural networks in fluid mechanics benchmarks their performance against non-equivariant models, highlighting their effectiveness in predicting dynamic interactions [38]. In high-energy physics, GNNs in the IceCube experiment improve signal classification, showcasing PIML's potential [29].

The application of PIML across these domains emphasizes its transformative impact, offering enhanced predictive accuracy, reduced computational costs, and robust modeling of complex systems. As PIML advances, its integration into diverse domains is set to enhance innovation and discovery by combining machine learning algorithms with physical constraints and mathematical models. This

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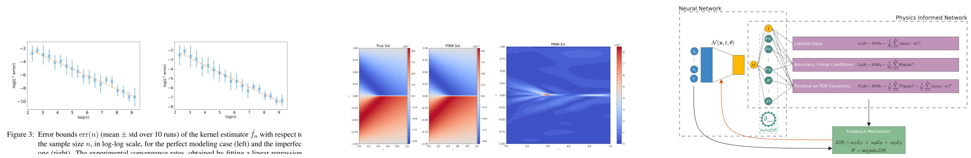
approach not only improves model generalizability and interpretability but also ensures adherence to fundamental physical laws, unlocking new opportunities for applications in system identification, control, and digital twin development [35, 36, 37].



(a) Error bounds err(n) (mean ± std over 10 runs) of the kernel estimator fn with respect to the sample size n, in log-log scale, for the perfect modeling case (left) and the imperfect one (right). The experimental convergence rates, obtained by fitting a linear regression, are shown as dashed lines.[32]

(b) Comparison of True Solution, PINN Solution, and PINN Error for a Specific Problem[33]

(c) Physics-Informed Neural Networks for Solving Partial Differential Equations[34]

Figure 4: Examples of Applications of Physics-Informed Machine Learning

As shown in Figure 4, Physics-Informed Machine Learning (PIML) is an innovative approach that integrates the principles of physics with machine learning algorithms to enhance the predictive capabilities and accuracy of models, particularly in complex systems. The figure presented showcases three distinct applications of PIML, emphasizing its versatility and effectiveness. The first subfigure illustrates the error bounds of a kernel estimator, demonstrating the convergence rates in both perfect and imperfect modeling scenarios through a log-log scale analysis. This highlights the robustness of PIML in handling varying sample sizes and modeling conditions. The second subfigure provides a comparative analysis of a true solution and a solution obtained via a Proximal Isometric Neural Network (PINN), alongside the error margin, offering insights into the precision of PINNs in approximating complex solutions. The final subfigure presents a flowchart for training a PINN specifically designed to solve partial differential equations (PDEs), underscoring the structured approach of integrating labeled data, boundary conditions, and PDE residuals. Collectively, these examples demonstrate the profound potential of PIML in improving model accuracy and solving sophisticated mathematical problems by leveraging the inherent laws of physics [32, 33, 34].

4 Dynamic Graph Machine Learning

4.1 Advancements in Dynamic Graph Machine Learning

Dynamic graph machine learning has seen significant advancements, enhancing the modeling of complex systems through innovative graph neural network (GNN) techniques. The integration of physics knowledge with machine learning addresses data scarcity and model complexity while balancing physical principles and adaptability [39]. The STONet framework exemplifies this by using neural operators to learn mappings between infinite-dimensional function spaces, marking a notable progression in dynamic graph techniques [1].

The GNN-PGD generator advances the field through a hybrid numerical approach that combines reduced-order modeling with GNNs, improving the modeling of complex systems [2]. This hybrid strategy efficiently predicts reduced-order bases across various geometries, illustrating dynamic graph machine learning's versatility. Additionally, simultaneous training of multiple GNNs on different probabilistic graphical models (PGMs) to learn universal dynamics alongside specific structures propels the field forward [21].

Innovations such as classifying neutrino events in KM3NeT detectors demonstrate the impact of dynamic graph machine learning on classification accuracy and reconstruction capabilities [40]. Benchmark analyses of spatial-temporal dependence structure learning on dynamic graphs provide insights into the effectiveness of various temporal graph networks (TGNs) in node and edge prediction tasks [20].

Addressing Massive Activations (MAs) in GNN attention layers has led to methodologies that stabilize and enhance model performance [19]. These advancements improve dynamic system modeling, yielding more accurate, interpretable, and robust models that leverage data-driven insights and physical principles. As the field progresses, these innovations are poised to unlock new possibilities for understanding and predicting complex network behaviors across scientific and engineering domains.

4.2 Graph Neural Networks in Analyzing Complex Networks

Graph Neural Networks (GNNs) have become essential tools for analyzing complex networks, overcoming challenges like graph irregularity, node connectivity variability, and the difficulty of applying traditional neural network operations to graph domains [41]. GNNs employ a message-passing framework crucial for learning graph-structured data representations, vital for applications such as material property prediction [41].

The GRADE method advances GNN methodologies by using aggregation-diffusion equations to balance node feature clustering and prevent over-smoothing, preserving node feature integrity and enhancing the model's ability to capture complex network behaviors [42]. The LSPE approach emphasizes separating positional from structural information, enabling nuanced learning that reflects nodes' unique roles within a network [43].

In dynamic graph analysis, methods like DySAT excel in link prediction tasks by leveraging joint structural and temporal attention mechanisms, effectively capturing evolving network structures [44]. Filtration surfaces extend previous work on filtration curves to dynamic contexts, providing a comprehensive classification framework for dynamic graphs [45].

GNNs are also critical in brain networks, capturing complex connectivity patterns that enhance diagnostic tools and insights into neurological conditions [22]. Methodologies that convert node centrality approximation problems into machine learning tasks offer novel approaches for node ranking in large-scale networks [46].

GNNs enable a deeper understanding of complex network structures by providing robust tools for analyzing multifaceted interactions within these systems. As these methodologies evolve, they are expected to yield new insights into the dynamics of complex networks across scientific and engineering domains, harnessing both reversible and irreversible dynamics to capture intricate behaviors in data-driven tasks [47].

5 Complex Networks and Network Dynamics

5.1 Understanding Network Dynamics in Various Domains

Understanding the dynamics of complex networks is vital for predicting and controlling system behaviors, due to their intricate temporal and structural characteristics. In neuroscience, combining structural and functional imaging data enhances the understanding of directed relationships between brain regions, offering insights into cognitive functions and disorders [48]. This integration is critical for unraveling interactions among brain regions over time, illuminating mechanisms underlying neurological conditions.

In sensor networks, modeling heterogeneous temporal dynamics is challenging, especially as sensor signals are influenced by external variables. Advanced graph neural network (GNN) models are needed to effectively disentangle dynamic interactions where traditional data-driven methods fail [9]. By addressing these complexities, GNNs improve predictive and control capabilities in environments where sensor data varies due to external influences.

Dynamic GNNs also provide significant insights into molecular dynamics, crucial for predicting and controlling molecular behavior. Analyzing the conformational dynamics of molecular structures enhances understanding of their implications for chemical reactions and material properties [49]. This approach underscores the importance of GNNs in capturing complex interactions within molecular systems, essential for advancements in drug discovery and materials science.

The graph translator represents a notable advancement by generalizing GNN models to new instances of the same system, enhancing the modeling of complex systems by disentangling dynamics from structure [21]. This capability is crucial for developing predictive models that adapt to new conditions, thereby improving the reliability of network-based solutions across diverse domains.

Examining network dynamics across various fields highlights the importance of advanced modeling techniques in understanding and predicting complex system behaviors. Leveraging GNN capabilities allows researchers to create models that enhance accuracy and interpretability while capturing intricate temporal and structural dynamics in networks. This progress paves the way for innovative solutions in drug design, social network analysis, traffic management, and medical diagnostics, where understanding intricate relationships is key [43, 50, 51].

5.2 Challenges in Modeling Complex Network Dynamics

Modeling complex network dynamics involves significant challenges due to the intricate nature of network structures and their dynamic behaviors. A primary challenge is the computational cost associated with training models that capture these intricacies, particularly when using equivariant models, which maintain symmetry and invariance properties but require substantial computational resources, limiting their practicality in large-scale networks [38].

Accurate node ranking based on centrality metrics poses another challenge, as existing methods demand considerable processing time and are sensitive to minor network structure perturbations, making them impractical for large networks where rapid and reliable node ranking is essential [46]. Furthermore, the lack of effective distance measures between graphs of varying sizes complicates clustering and testing, hindering the development of universally applicable methodologies [52].

The modeling of network dynamics is further complicated by the vast number of distinct configurations networks can adopt, rendering exact solutions computationally expensive [53]. This complexity is heightened in multivariate time series data, where high computational and memory costs pose significant challenges [54].

Moreover, the extensive time required for estimation in models focused on deterministic motion equations and pairwise interactions limits their scalability and applicability to broader network dynamics [55]. Accurately representing speed-flow relationships in dynamic networks is further complicated by existing models' failure to account for contextual factors crucial for understanding dynamics [12].

The potential increase in prediction error with longer temporal sequences underscores the need for improved recurrent training strategies capable of handling extended temporal dependencies [56]. Additionally, challenges arise in managing non-periodic functions or excessively complex graph structures, which can hinder the training efficiency of models designed to capture dynamic behaviors [57].

These challenges highlight the urgent need for innovative methodologies that integrate temporal and structural patterns, leveraging advancements from fields such as GNNs and network neuroscience. Such methodologies must address computational and methodological limitations while facilitating efficient representation, processing, and analysis of large-scale dynamic datasets across domains, including social networks, biological systems, and machine learning applications. Interdisciplinary collaboration will be essential in unlocking new frontiers for understanding and manipulating complex networks [58, 59, 60, 51, 61]. Developing scalable, adaptive, and context-aware models is crucial for advancing the understanding and prediction of complex network behaviors across various domains.

6 Applications and Case Studies

The integration of advanced methodologies such as Graph Neural Networks (GNNs) and physics-informed machine learning has profoundly influenced various domains, with significant implications for materials science and engineering. This section examines their application in these fields, highlighting their role in advancing material understanding and design.

6.1 Materials Science and Engineering

In materials science and engineering, the synergy of GNNs and physics-informed machine learning has catalyzed progress in material analysis and design. The PI-GNN framework exemplifies this by improving predictions of dislocation mobility in crystalline materials, essential for modeling deformation processes [62]. This demonstrates GNNs' capacity to handle complex graph-structured data, crucial for predicting material properties and optimizing designs.

Symmetrized Graph Neural Networks (SymGNN) have surpassed traditional molecular dynamics methods in predicting energy barriers for metallic glasses, emphasizing GNNs' efficacy in modeling structure-property relationships [4]. A dataset of approximately 84,000 structures, including ordered and disordered alloys, supports principles-based modeling of high-entropy alloys (HEAs), underscoring the significance of dataset size and structural relaxation in enhancing predictive performance [23].

Physics-informed machine learning has also advanced turbulence modeling, improving Reynolds stress predictions essential for fluid dynamics simulations [63]. Its efficacy in condition monitoring across engineering systems is demonstrated through various case studies [5].

The fusion of GNNs and physics-informed machine learning in materials science enables precise predictions of complex material properties, including those of high-entropy alloys and oxide glasses, through advanced graph representations and the incorporation of physical laws into machine learning models. This fosters exploration of disordered materials and enhances property extrapolation beyond existing datasets, facilitating tailored material design for specific applications [34, 64, 41, 65, 16]. These methodologies pave the way for next-generation materials with optimized properties and performance.

6.2 Neuroscience and Biomedical Applications

GNNs have become vital tools in neuroscience and biomedical applications, enhancing neural network and brain dynamics modeling. The GL-GNN framework exemplifies this by improving node classification performance and providing interpretable predictions [66]. This is crucial for understanding complex neural interactions and improving diagnostic accuracy in neurological disorders.

Physics-informed machine learning has also advanced neuroscience by enhancing signal detection sensitivity, crucial for modeling neural networks and brain dynamics [67]. The Foundation Model Informed Message Passing (FIMP) highlights GNNs' applicability to biological data, including single-cell RNA sequencing and fMRI recordings, offering insights into cellular and neural dynamics [68]. GNNs have also been applied to classify and reconstruct neutrino events detected by KM3NeT, showcasing their versatility in handling intricate network data [40].

Frameworks designed for learning dynamics and structure in complex systems, applicable in celestial mechanics and epidemiology, hold promise for neuroscience by modeling neural dynamics and capturing overarching patterns [21].

Recent advancements in GNNs and physics-informed machine learning underscore their transformative influence on neuroscience and biomedical applications. Innovations such as attention mechanisms and learnable structural representations enhance GNNs' ability to model complex patterns, improving predictive accuracy and reliability in drug design, disease classification, and medical diagnosis [19, 43, 50, 51].

6.3 Structural Health Monitoring and Engineering Systems

The integration of physics-informed machine learning (PIML) and GNNs in structural health monitoring (SHM) and engineering systems has led to significant advancements in maintaining structural integrity. These approaches provide interpretable models that incorporate physical insights, enhancing trust and reliability in SHM applications, essential for the safety and longevity of critical infrastructure [69].

In distributed control applications, stability conditions for Gated Graph Neural Networks (GGNNs) enhance robustness and performance, demonstrating their potential for real-world applications [70]. The GNN-PGD methodology exemplifies advancements in computational efficiency and accuracy for structural dynamics, proving effective for rapid design iterations in engineering applications [2].

PIML models have been employed to predict seismic responses of nonlinear steel moment-resisting frame structures, enhancing predictive accuracy and generalization across varying operational conditions, critical for assessing structural resilience during seismic events [71, 72]. Additionally, PIML's application in reconstructing dynamic forces is vital for maintaining structural integrity, further supported by frameworks suitable for digital twins, which improve accuracy in high-dimensional structural dynamics modeling [73, 74].

The PIML model's ability to predict temperature fields in the Laser Metal Deposition (LMD) process without labeled training data highlights its potential for smart manufacturing, achieving a maximum absolute error of 61.2 K [75]. This capability is crucial for optimizing manufacturing processes and ensuring the structural integrity of components.

Collectively, advancements in PIML and GNNs underscore their transformative impact on SHM and engineering systems, offering enhanced predictive accuracy, robustness, and efficiency in maintaining structural integrity. As methodologies like PIML advance, they unlock unprecedented opportunities for innovation in engineering, particularly by enhancing model interpretability and integrating domain-specific knowledge. This evolution promises improved resource management and operational efficiency in subsurface energy systems, such as oil and gas, and breakthroughs in areas like carbon and hydrogen storage and geothermal systems [35, 36, 51**?** , 17].

6.4 Fluid Dynamics and Environmental Modeling

The integration of physics-informed machine learning (PIML) and advanced graph-based models has significantly advanced fluid dynamics and environmental modeling by enhancing prediction accuracy and reducing computational costs. Dynamic Physics-Informed Neural Networks (DPINN) exemplify this by outperforming traditional methods in solving advection-dominant problems, achieving high accuracy with reduced computational expenses, crucial for efficient fluid dynamics simulations [76].

PIML's utility in fluid dynamics has been validated through benchmark problems, such as the Michaelis-Menten enzyme reaction and the 3D Sel'kov model of glycolytic oscillations, highlighting its ability to capture complex dynamic interactions [77]. The STONet framework emphasizes neural operators' potential for forecasting spatially continuous physical quantities on irregularly distributed points, relevant in fluid dynamics and environmental modeling [1].

Graph-based models, including dynamic GNNs, show promise in molecular dynamics by improving the prediction accuracy of time-dependent molecular structure changes, which is critical for advancing drug discovery and materials science [49].

PIML's application in environmental modeling integrates machine learning with physical laws to accurately predict climate-related factors and ecological dynamics. This approach enhances prediction reliability by incorporating fundamental physical principles, addressing challenges posed by limited data, and improving model generalizability and interpretability in complex environmental systems [35, 36, 78**?**]. Adapting PIML to ecological systems, such as mosquito population dynamics modeling, demonstrates improved accuracy and stability compared to traditional methods, crucial for ecological forecasting and management.

The integration of PIML and graph-based models in fluid dynamics and environmental modeling offers transformative improvements in predictive accuracy and computational efficiency. This synergy represents a significant advancement, combining deep learning with established physical principles to enhance model interpretability and adherence to governing laws, facilitating innovative solutions. Successful applications of PIML in subsurface energy systems, including oil and gas exploration, reservoir simulation, and resource management, promise to improve operational efficiency and open new avenues for understanding and managing complex environmental systems, including carbon and hydrogen storage and geothermal energy [17, 37].

6.5 Energy and Power Systems

Advanced machine learning techniques, such as GNNs and PIML, have significantly enhanced the optimization and prediction of power grid behaviors, transforming energy and power systems. Symplectic Neural Networks (SympNets) utilize Hamiltonian dynamics to optimize and predict energy system behaviors, providing a robust framework for improving system stability and efficiency [79].

GNNs, particularly Graph Convolutional Networks (GCNs), demonstrate superior performance in fault diagnosis and power flow calculations compared to traditional methods, highlighting their

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potential to enhance power system operation accuracy and reliability [80]. The GAT model has shown significant improvements in forecast accuracy and calibration for weather predictions, crucial for optimizing power grid operations by accurately predicting energy demands and supply fluctuations [81].

Physics-informed machine learning methods contribute to energy systems by optimizing simulation parameters, enhancing stability and security, which are vital for maintaining reliable power supplies and preventing disruptions in energy distribution networks [82]. The Dynamic Reduction Network (DRN) showcases its potential in handling complex and irregular data, essential for modeling intricate power system dynamics [3].

Future research may focus on improving the scalability of these methods for larger systems and exploring additional applications in various nonlinear processes, thereby expanding the applicability of these advanced techniques in energy systems [83]. The integration of GNNs and PIML in energy and power systems promises to unlock new possibilities for optimizing and predicting power grid behaviors, paving the way for innovative solutions in energy management and sustainability.

7 Challenges and Future Directions

Recent advancements in machine learning, particularly Graph Neural Networks (GNNs) and Physics-Informed Machine Learning (PIML), have significantly impacted various fields. However, integrating these methodologies into practical applications presents several challenges. This section examines critical issues related to scalability and computational efficiency, essential for deploying GNNs and PIML frameworks in complex systems. Addressing these challenges is vital for developing robust methodologies capable of handling large-scale applications.

7.1 Scalability and Computational Efficiency

Scalability and computational efficiency are crucial for applying GNNs and PIML frameworks to large-scale complex systems. A primary concern is the exponential growth of parameters needing estimation as the number of interacting nodes increases, leading to high computational costs and potential instabilities [14]. Despite the accuracy of physics-informed approaches in defect prediction, their noise sensitivity during partial differential equation (PDE) discovery challenges scalability and efficiency [84].

GNN scalability is also hindered by the reliance on high-quality, diverse training data, especially in complex materials modeling [62]. Clustering algorithm choices further complicate performance, highlighting scalability and efficiency issues [3]. Moreover, many studies overlook the reproducibility of results across different datasets and the interpretability of GNN models, limiting broader applicability [22].

Model performance, such as that of STONet, can degrade with high missing data ratios in the temporal domain, indicating further scalability challenges [1]. Additionally, neural network architecture and hyperparameter dependencies affect solution accuracy and convergence, posing further scalability issues [85].

The SymGNN model's computational efficiency addresses scalability in modeling complex systems like metallic glasses [4], yet the computational expense of physics-based modeling and data scarcity for training remain significant barriers [5]. To overcome these challenges, future research should focus on developing robust methodologies that effectively manage network dynamics, reduce computational costs, and enhance model generalization. Prioritizing the optimization of computational resources, exploring self-supervised learning techniques, and managing uncertainty and noise in complex environments are essential for enhancing GNN and PIML frameworks' applicability. Integrating physical constraints with machine learning can lead to more robust, data-efficient models that maintain physical plausibility, expanding potential use cases in scientific and engineering domains [35, 36, 86].

7.2 Data Availability and Quality

Data availability and quality are crucial for the performance and reliability of models, particularly in complex systems characterized by high-dimensional data and intricate dynamics. A significant challenge in developing accurate machine learning models is the need for large training datasets, often impractical in complex composite scenarios like optical composites [15]. Existing datasets, such as those from Density Functional Theory (DFT), may introduce biases due to the underrepresentation of non-equimolar compositions, affecting model generalizability [23].

In polar regions, the lack of high-quality observational data presents challenges for physics-informed machine learning models, which require comprehensive datasets for physically consistent predictions [24]. The computational intensity of physical models, combined with the black-box nature of data-driven models, complicates the production of reliable outcomes in data-scarce environments.

The quality of training data significantly influences models' generalization capabilities, particularly in fluid dynamics. Poor representation of flow characteristics in training sets can hinder models' ability to generalize to new flow scenarios, negatively impacting predictive performance [63]. Ensuring high-quality, representative datasets is essential for enhancing model applicability across various domains.

To improve model performance and reliability, addressing data availability and quality challenges is critical, as these factors significantly influence the representation, processing, and analysis of complex structured data. Integrating advanced techniques from graph signal processing and physics-informed machine learning can optimize data structures, improve computational efficiency, and ensure adherence to physical constraints, leading to more robust and interpretable outcomes across applications [35, 87, 36, 88, 59]. Access to comprehensive, high-quality datasets will enhance model effectiveness, facilitating accurate and robust predictions across diverse scientific and engineering fields.

7.3 Model Interpretability and Robustness

Model interpretability and robustness are critical for developing reliable systems, particularly in PIML and GNN contexts. Interpretability ensures transparency in decision-making processes within machine learning frameworks, fostering trust and facilitating practical deployment [89]. Robustness pertains to a model's ability to maintain performance across varied conditions, including those not represented in training data, which is vital for edge cases where models may encounter scenarios outside their training distribution [89].

The development of GDyNets emphasizes local dynamics, which are crucial for material performance and contribute to model interpretability and robustness [90]. By focusing on local interactions, GDyNets enhance models' ability to capture relevant features impacting material behavior, improving prediction reliability in complex systems.

Challenges remain in ensuring robust model performance, particularly in optimization problems. For example, combinatorial optimization using physics-inspired graph models may face limitations due to GNNs potentially becoming trapped in local optima from random initialization, affecting solution quality [91]. Addressing these limitations is vital for enhancing GNN-based models' robustness and reliability, ensuring consistent delivery of accurate outcomes across diverse applications.

Improving model interpretability and robustness is essential for enhancing the reliability of PIML and GNN frameworks, particularly in out-of-distribution (OOD) forecasting tasks. Integrating physical constraints and employing meta-learning techniques for causal structure discovery can yield more accurate predictions under varying initial conditions and unknown parameters, advancing effectiveness in dynamical system modeling and control [92, 36]. By focusing on transparent decision-making and consistent performance, these models can be effectively integrated into practical applications, paving the way for innovative solutions in scientific and engineering domains.

7.4 Future Directions in Physics-Informed Machine Learning

The future of PIML research lies in developing robust, scalable, and interpretable models capable of addressing complex scientific and engineering challenges. Key areas of focus include refining Physics-Informed Neural Networks (PINNs) to accommodate a broader spectrum of material behaviors and enhance robustness and computational efficiency for inverse design problems [85]. Additionally, improving models like STONet to handle substantial missing data through alternative architectures or additional physical knowledge represents a promising avenue [1].

Expanding training datasets to encompass a wider range of flow conditions and geometries is crucial for enhancing PIML models' generalizability and robustness, particularly in fluid dynamics [63]. Moreover, extending GNN-PGD methods to include non-linear problems and integrating more physical insights into GNN architectures will enhance model versatility and precision [2].

Refining clustering algorithms within the Dynamic Reduction Network (DRN) and exploring its applications beyond high-energy physics can broaden its utility across diverse machine learning tasks [3]. Investigating Temporal Graph Networks (TGNs) through varied configurations and evaluation metrics will provide deeper insights into their applicability and effectiveness [20].

Developing customized adversarial techniques for handling Massive Activations (MAs) and extending analyses to additional models and datasets will contribute to more robust and accurate machine learning frameworks [19]. Furthermore, refining PINN architectures, exploring novel optimization techniques, and addressing theoretical challenges in diverse scientific domains remain critical for advancing PIML [34].

Incorporating multimodal information and enhancing GNN interpretability, particularly in analyzing brain graphs, is another vital research direction promising improved neural connectivity analysis [22]. Additionally, enhancing model robustness across materials and refining integration techniques for better performance and explainability are essential for broader adoption and trust in critical applications.

Collectively, these research directions aim to push PIML boundaries, offering innovative solutions and expanding model applicability across various scientific and engineering domains. As methodologies in graph theory, machine learning, and physics-informed models continue to advance, they hold the potential to significantly enhance our ability to analyze, visualize, and manage complex systems across diverse fields, from subsurface energy systems to graph-represented data structures [17, 88, 51, 59].

8 Conclusion

The integration of physics-informed machine learning (PIML) with dynamic graph methodologies represents a significant advancement in the modeling and understanding of complex systems. By merging empirical data with foundational physical laws, this interdisciplinary strategy enhances both the accuracy and robustness of models across various fields. The exploration of Universal Differential Equations (UDEs) within this context highlights the ongoing need for research aimed at optimizing PIML's capabilities. Embedding physics knowledge into machine learning frameworks not only improves predictive performance but also addresses the limitations inherent in data-driven approaches, fostering innovation and interdisciplinary collaboration. This synthesis of methodologies holds the promise of advancing predictive modeling, offering more accurate and interpretable solutions across a broad spectrum of scientific and engineering applications.

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