Transforming Chemical Research with Physics-Informed Neural Networks

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Abstract

Physics-Informed Neural Networks (PINNs) have emerged as a transformative tool in computational chemistry, bridging the gap between traditional numerical methods and data-driven approaches. This survey provides a comprehensive analysis of PINN applications in chemistry, categorizing their use across domains such as reaction kinetics, catalytic processes, diffusion-reaction systems, and non-equilibrium flows. The paper critically evaluates the methodologies and innovations in PINN architectures, highlighting their strengths, limitations, and computational efficiencies compared to conventional methods. By integrating physics-based principles with machine learning, PINNs achieve remarkable accuracy while significantly reducing computational costs, making them invaluable for real-time decision-making in complex chemical systems.

The survey also explores challenges such as computational intensity, hyperparameter tuning, and reliance on well-defined governing equations, offering solutions like transfer learning, multi-fidelity modeling, and hybrid frameworks. Furthermore, it examines future directions, including the integration of experimental data, advancements in multi-scale modeling, uncertainty quantification, and applications in frontier areas like quantum chemistry and nanotechnology. This survey consolidates knowledge in the field and provides a roadmap for researchers, emphasizing

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the transformative potential of PINNs in addressing pressing challenges in chemistry and advancing the understanding of complex chemical phenomena (Almeldein and Van Dam [2023], Zanardi et al. [2023]).

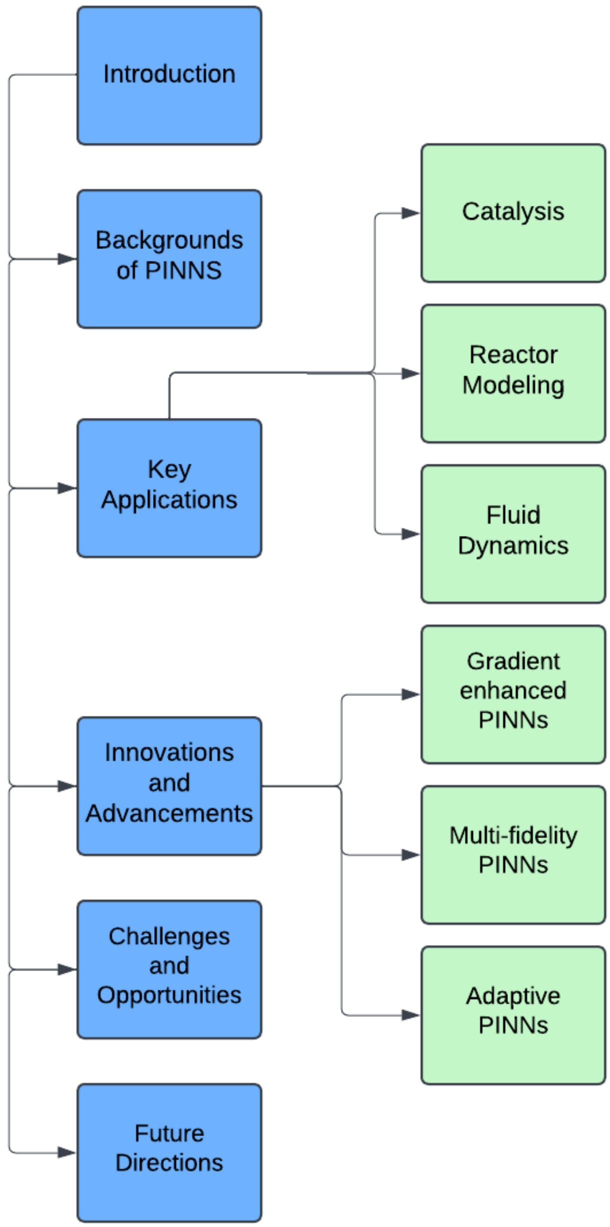

Figure 1: Hierarchical structure of the paper, summarizing the key sections and subsections discussed.

1 Introduction

Advances in the field of chemistry have historically relied on the development and application of sophisticated computational models to enhance our understanding and prediction of complex physical and chemical phenomena. These models are critical for analyzing processes such as reaction kinetics, diffusion mechanisms, catalytic systems, and molecular dynamics, domains in which direct experimental observation is either infeasible or impractical due to the intricacies involved. Accurate mathematical modeling thus serves as a cornerstone for addressing these challenges, enabling scientists to simulate and explore systems that would otherwise remain beyond our grasp. However, traditional numerical techniques, such as the finite element method (FEM) and finite difference method (FDM), often encounter significant limitations. These include computational inefficiencies, instability, and a heavy dependence on extensive datasets for parameter estimation. These challenges become even more pronounced in the context of multiscale or high-dimensional systems, where the computational cost and complexity escalate exponentially, rendering traditional approaches impractical.

In recent years, the advent of machine learning (ML) has heralded a paradigm shift in computational modeling, offering innovative tools to overcome these challenges. With its inherent ability to identify underlying patterns, interpolate between data points, and optimize intricate functions, ML has emerged as a transformative approach for understanding and simulating chemical systems. Among the diverse array of ML methodologies, Physics-Informed Neural Networks (PINNs) have gained prominence as a groundbreaking framework that synergizes data-driven modeling with fundamental physical principles. PINNs leverage established physical laws, such as conservation equations, reaction-diffusion dynamics, and thermodynamic constraints, to enhance the fidelity and interpretability of computational models (Raissi et al. [2019]).

Physics-Informed Neural Networks (PINNs) integrate physical laws, such as PDEs and ODEs, into their loss functions, enabling models to adhere to scientific principles even with limited or noisy data. This fusion of neural network adaptability with physical constraints offers a robust and interpretable framework, making PINNs invaluable for solving complex challenges in chemical research and development (Chen et al. [2024]).

The architecture of a PINN encompasses several key components:

1. **Neural Network Approximation:** A deep neural network serves as the function approximator for the target physical system, such as predicting temperature distributions, concentration profiles, or reaction rates. The network is optimized by minimizing a composite loss function that accounts for both empirical data and governing physical laws.

2. **Loss Function Design:** The loss function in PINNs is meticulously constructed to incorporate:

    - **Data Loss Term:** This component quantifies the discrepancy between model predictions and available empirical data.

- **Physics Loss Term:** Derived from the residuals of governing equations such as $f(u) = 0$, this term ensures that the model adheres to fundamental physical laws, including conservation of mass, momentum, and energy.
- **Boundary and Initial Condition Terms:** These terms impose constraints at the spatial boundaries and initial temporal states of the system, maintaining the model's physical consistency across the domain.

3. **Physics-Driven Regularization:** By embedding the governing equations as a form of regularization, PINNs guide the neural network toward solutions that align with underlying physical principles. This characteristic proves especially advantageous in scenarios with limited or noisy datasets, as it reduces the network's reliance on extensive data while preserving robustness (Chen et al. [2024]).

Through the incorporation of these elements, PINNs deliver generalizable and reliable predictions, making them particularly well suited for applications where data availability is limited, costly, or uncertain. This capability is critical in domains such as modeling reaction pathways under extreme conditions, simulating catalytic processes, and investigating rare chemical events.

The domain of chemistry presents a plethora of challenges necessitating the simultaneous modeling of intertwined physical and chemical phenomena. For instance, in reaction-diffusion systems, PINNs excel at modeling the spatiotemporal evolution of chemical species, capturing both kinetic and diffusion dynamics. Similarly, in catalytic systems, they effectively characterize the interplay between surface reactions and mass transport phenomena (Ngo and Lim [2021]). In molecular simulations, PINNs have demonstrated the ability to approximate quantum mechanical computations with significantly reduced computational overhead (Ji et al. [2021]), offering a viable alternative to traditional quantum chemistry methods. Furthermore, in the field of materials science, PINNs have been utilized to predict the properties of complex materials under various conditions, facilitating advances in materials design and characterization.

Moreover, the versatility of PINNs has been enhanced through their integration with other computational techniques. For example, hybrid models that combine PINNs with molecular dynamics simulations enable the seamless modeling of chemical systems across multiple scales, bridging the gap between atomistic and macroscopic representations. Furthermore, the incorporation of Bayesian inference frameworks within PINNs has facilitated uncertainty quantification, providing a robust mechanism for assessing the reliability of predictions in regions with sparse or absent data (Hao et al. [2023]).

The potential applications of PINNs in the field of chemistry are vast and transformative. They hold promise to accelerate drug discovery by modeling molecular interactions, advance the design of sustainable catalysts for green chemistry initiatives, and optimize chemical processes for industrial applications. As the intersection of machine learning, computational modeling, and experimental chemistry continues to evolve, PINNs are poised to play a central role in driving groundbreaking innovations and discoveries. By uniquely integrating data-driven methodologies with fundamental physical laws, PINNs represent a transformative approach that is reshaping the landscape of computational chemistry and engineering.

Physics-Informed Neural Networks have demonstrated remarkable efficacy in addressing a wide array of computational challenges in chemistry and engineering. By embedding physical principles into the neural network training process, PINNs provide a robust and interpretable framework that overcomes the limitations of traditional numerical methods. Their ability to model complex systems with limited data, coupled with their versatility and scalability, positions them as an indispensable tool for advancing the frontiers of chemical science and technology.

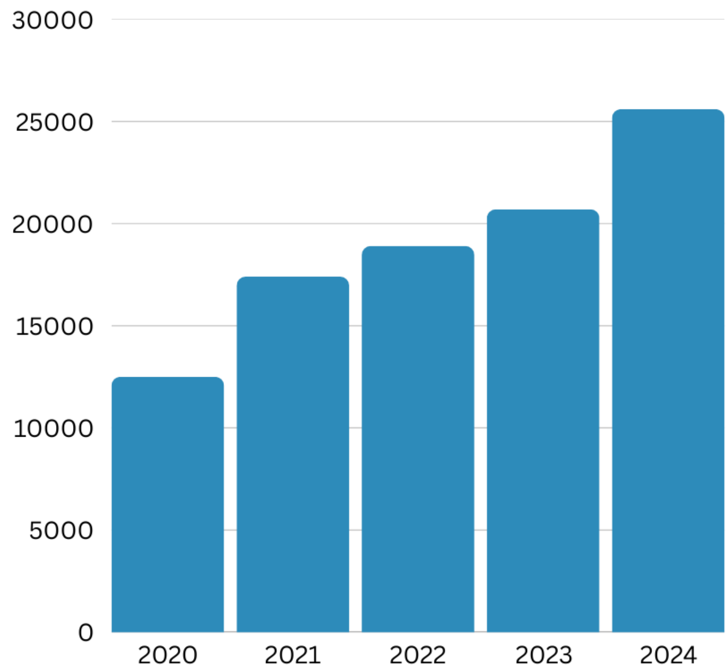

Figure 2: Above figure illustrates the annual growth in the number of PINN-related publications, reflecting the rapid adoption and advancement of this methodology. A sharp increase is evident post-2020, correlating with the broader application of PINNs across domains such as chemistry, environmental modeling, and material sciences. This survey incorporates a representative sample of these works to ensure comprehensive coverage of foundational concepts and innovations.

Data retrieved from Google Scholar using year-wise filters in January 2025 Google Scholar [2025].

2 CONTRIBUTIONS OF THE PAPER

The paper makes several contributions to the field of computational chemistry, with a particular focus on the transformative role of Physics-Informed Neural Networks (PINNs). By drawing from over 20 research papers, it provides an extensive and multifaceted analysis that not only summarizes the current state of research but also critically evaluates the methodologies, results, and future directions in this area.

1. **Comprehensive Analysis and Categorization of PINN Applications:** One of the paper's primary contributions is its thorough analysis and categorization of PINN applications across diverse chemical domains.

It systematically organizes these applications into key areas such as reaction kinetics, diffusion-reaction systems, catalytic processes, and non-equilibrium flows.This categorization serves as a roadmap for researchers and practitioners, helping them navigate the complex and varied ways in which PINNs are being employed in chemical research. The clear and structured presentation of these applications not only aids in better understanding the scope of PINNs in chemistry but also underscores their adaptability and effectiveness in addressing a wide range of chemical challenges, from fundamental theoretical problems to complex real-world scenarios.

2. **Critical Evaluation of Methodologies and Results:** The paper goes beyond simply listing applications; it offers an in-depth analysis of the methodologies used in PINN research, comparing and contrasting the results and innovations embedded within different PINN architectures. This comparative evaluation covers critical aspects such as computational efficiency, the strengths and limitations of various architectures, and their ability to address specific challenges within chemistry. By doing so, the paper provides a benchmark that can guide future research and help researchers identify best practices when implementing PINNs in their own work. The evaluation also highlights potential areas for improvement, contributing to the ongoing refinement of PINN models and their applications.

3. **Identification of Challenges and Proposed Solutions:** Recognizing that no methodology is without its challenges, the paper adopts a critical stance in discussing the obstacles associated with PINN-based approaches. It thoroughly explores the key difficulties researchers face, such as the high computational intensity required for training PINNs, the complexities of hyperparameter tuning, and the dependence on well-defined governing equations. The paper not only identifies these challenges, but also offers actionable solutions. Among the strategies proposed are transfer learning, multifidelity modeling, and hybrid approaches that combine the strengths of PINNs with traditional methods. These recommendations aim to enhance the robustness, efficiency, and versatility of PINNs, addressing the current limitations and making them more accessible and effective for practical applications in computational chemistry.

4. **Forward-Looking Insights and Research Outlook:** The paper concludes with a visionary outlook, identifying key open questions and opportunities at the intersection of physics-informed AI and computational chemistry. It highlights the potential for further innovation through hybrid models that integrate experimental data with PINN-based approaches, offering a more comprehensive understanding of chemical phenomena. Additionally, the paper emphasizes the importance of advancing algorithms that can handle multi-scale systems, which is crucial for tackling complex, real-world chemical problems. It also points to emerging frontier areas

where PINNs could play a pivotal role, such as quantum chemistry and nanotechnology. By outlining these exciting opportunities, the paper not only helps shape the future direction of PINN research but also encourages further exploration into the untapped potential of PINNs in addressing the chemical challenges of the future.

5. **Consolidating Knowledge and Inspiring Future Exploration:** Through its thorough analysis, critical evaluations, and forward-looking insights, this paper contributes to consolidating the existing body of knowledge on PINNs in computational chemistry. It serves as a comprehensive resource for researchers, offering a deep understanding of the current landscape and inspiring future exploration in the field. The paper's careful consideration of both the strengths and challenges of PINNs ensures that the research community is well-equipped to advance the development of these powerful tools, driving innovation and progress in solving some of the most pressing problems in chemistry. As such, the paper is poised to act as a catalyst for continued advancements in the integration of AI with physics-based modeling, positioning PINNs as a leading methodology for the future of computational chemistry.

3 Key Applications Of PINNS

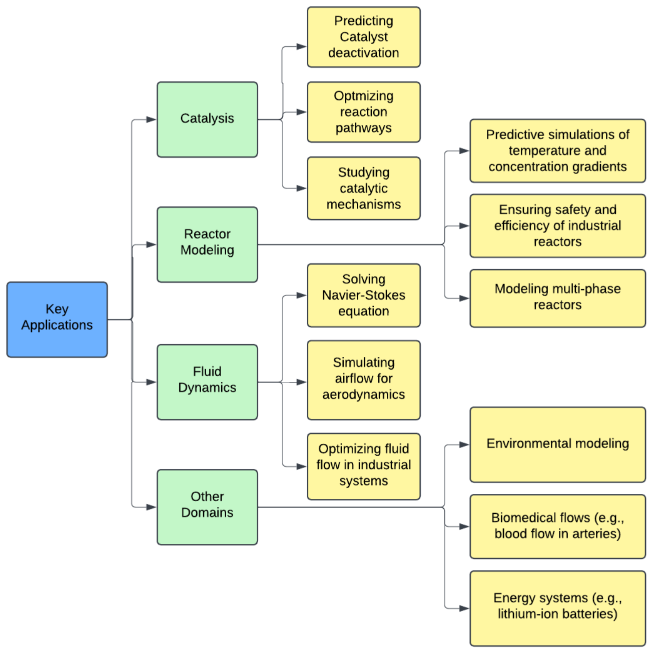

Figure 3: Schematic representation of key applications of PINNs in catalysis, reactor modeling, and fluid dynamics.The figure highlights the diverse areas where PINNs provide predictive accuracy and efficiency.

Physics-Informed Neural Networks(PINNs) have emerged as an exceptional computational framework for addressing intricate problems across various scientific and engineering disciplines. By uniquely combining physical laws with advanced machine learning methodologies, PINNs offer the capability to solve complex mathematical models with unprecedented accuracy and efficiency.

Applications of PINNs in Reaction Kinetics One prominent application of PINNs lies in the domain of reaction kinetics, where chemical reaction networks frequently involve stiff systems of equations. These systems, commonly encountered in fields such as combustion and biochemical pathways, are challenging to resolve using traditional numerical methods due to rapid, multi-scale dynamic behavior. PINNs adeptly address these challenges by efficiently handling such dynamics, enabling faster and more accurate solutions compared to conventional approaches (Zhang et al. [2024]). This advantage is particularly crucial for real-time analysis and scenarios necessitating insights across multiple scales, such as the optimization of reaction conditions in industrial processes (Ji et al. [2021]).

Diffusion-Reaction Systems and Environmental Modeling PINNs have also demonstrated exceptional proficiency in modeling diffusion-reaction systems, which govern the transport and transformation of substances. These processes are integral to diverse fields including environmental science and biomedical engineering. For instance, PINNs can be employed to simulate pollutant dispersion in aquatic systems, providing detailed insights into the interaction between transport and reaction mechanisms (Serebrennikova et al. [2024]). Similarly, in biomedical applications, PINNs have been used to model drug delivery within tissues, capturing spatial and temporal behaviors with exceptional precision (Giampaolo et al. [2022]). This capability enhances our understanding of coupled processes and enables the optimization of systems where transport and reaction phenomena are interdependent.

Catalysis and Reactor Design Optimization The field of catalysis and reactor design is another area where PINNs have shown transformative potential. By enabling detailed analyses of reaction-diffusion phenomena, PINNs facilitate the optimization of catalytic processes, improving both efficiency and selectivity. For example, in CO2 methanation, PINNs offer precise modeling of intricate reaction mechanisms and mass transport, aiding in the design of reactors that maximize performance under varying operational conditions. These contributions are particularly pertinent to advancing sustainable energy solutions and reducing the environmental impact of industrial processes (Ngo and Lim [2021]).

Applications in Non-Equilibrium Flow Systems PINNs have proven invaluable in studying non-equilibrium flow systems, such as those encountered in hypersonic and turbulent environments. These systems involve complex interactions between heat transfer, chemical reactions, and fluid dynamics under extreme conditions. Traditional modeling methods often struggle to capture these phenomena accurately due to their computational intensity and sensitivity to boundary conditions. PINNs overcome these obstacles by providing detailed and reliable insights into critical processes such as shock wave dynamics and energy transfer mechanisms. The implications of this capability are significant, ranging from advancements in aerospace engineering to the optimization of energy production technologies (Zanardi et al. [2023, 2022]).

Broader Impacts and Future Prospects Through their diverse applications, PINNs have established themselves as a versatile and indispensable tool for solving a wide range of scientific and engineering problems. Their ability to integrate physical laws into machine learning frameworks ensures robust, interpretable, and computationally efficient solutions. By bridging gaps between traditional numerical methods and cutting-edge computational approaches, PINNs empower researchers and engineers to tackle challenges in fundamental research and practical applications with greater efficacy and precision (Raissi et al. [2019]).

4 General PINN Methodology and Innovations: A Comprehensive Overview

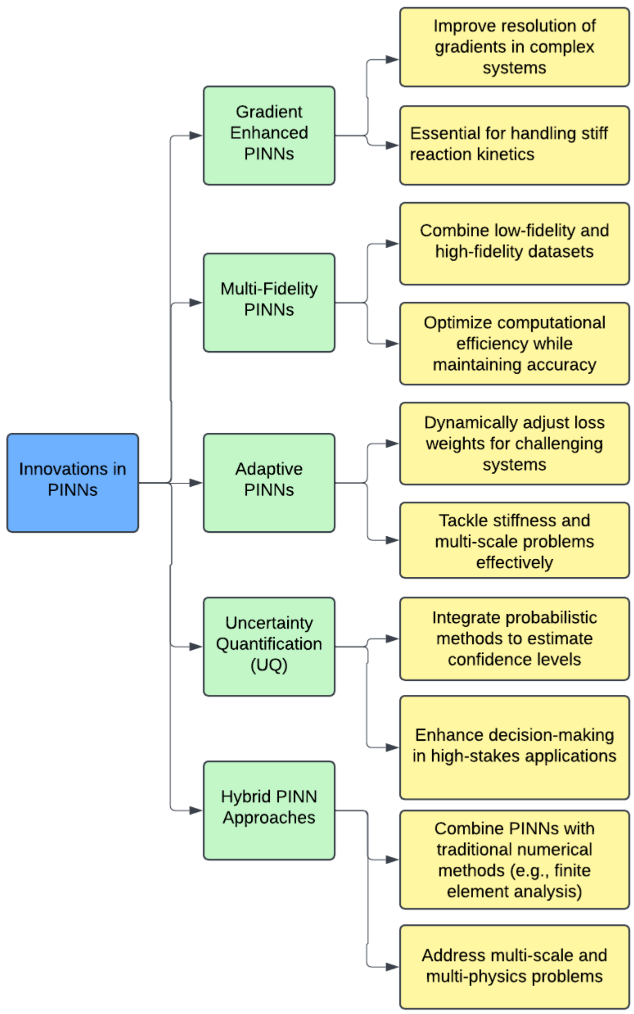

Figure 4: Overview of recent innovations in PINN methodologies, including gradient-enhanced, multi-fidelity, and adaptive frameworks, along with uncertainty quantification and hybrid approaches.

The methodology of Physics-Informed Neural Networks (PINNs) has evolved significantly, introducing cutting-edge approaches that integrate physics-based principles directly into neural network architectures. This evolution has not only refined the accuracy and robustness of PINNs but also enhanced their computational efficiency, making them adaptable and highly versatile across a broad spectrum of applications in chemistry, chemical engineering, and beyond (Raissi et al. [2019]). The ongoing advancements in PINN methodologies promise to revolutionize complex modeling tasks and enable breakthroughs in various scientific domains.

Another significant advancement is the Karush-Kuhn-Tucker Hard-Constrained PINNs (KKT-hPINNs) framework, which addresses the need for strict physical constraint enforcement during training. By utilizing orthogonal projection layers derived from KKT conditions, these PINNs enforce equality constraints with high precision, ensuring that models strictly adhere to physical laws. This approach transforms constraint handling into a quadratic programming problem, bypassing traditional iterative solvers and enhancing computational efficiency. KKT-hPINNs are particularly useful in high-precision applications, such as chemical reactor design, where maintaining conservation principles and other physical laws is essential for producing reliable models (Chen et al. [2024]).

Karush-Kuhn-Tucker Hard-Constrained PINNs (KKT-hPINNs) demonstrate immense utility in solving optimization problems while ensuring strict adherence to physical constraints across various domains. A notable example lies in chemical reactor design, where maintaining conservation laws such as mass and energy balances is crucial for safety and efficiency (Ji et al. [2021]). Traditional PINNs might approximate solutions that slightly violate these principles, leading to suboptimal or unreliable reactor designs. KKT-hPINNs embed equality constraints directly into the training process, ensuring that these physical laws are respected throughout. This leads to highly accurate predictions of key parameters such as reaction rates, heat transfer, and product yields, while simultaneously avoiding the computational inefficiencies associated with iterative solvers.

In **fluid dynamics**, particularly in aerodynamics, KKT-hPINNs shine in simulating airflows around structures like airplane wings. Solving governing equations like the Navier-Stokes equations requires strict compliance with boundary conditions and conservation laws, including maintaining incompressibility (Hao et al. [2023]). By enforcing these constraints during training, KKT-hPINNs provide physically accurate predictions of pressure and velocity distributions, reducing drag and improving aerodynamic designs. Compared to traditional finite-element methods, this approach is not only computationally efficient but also scalable for complex simulations (Frankel et al. [2024]).

Another impactful application of KKT-hPINNs is in **structural mechanics**, such as modeling stress and deformation in bridges under variable loads. Accurate modeling requires adherence to equilibrium equations and material constraints, like Hooke's law. KKT-hPINNs incorporate these constraints into the learning process, ensuring physically consistent predictions. This capability enables engineers to identify potential failure points with high precision and optimize material usage, ultimately enhancing both cost efficiency and safety.

In the field of **energy systems**, KKT-hPINNs have proven effective in modeling lithium-ion batteries by enforcing constraints related to charge and energy conservation (Serebrennikova et al. [2024]). This ensures reliable predictions of capacity fade and heat generation during charging and discharging cycles, which are critical for designing safer and more efficient batteries. Similarly, in renewable energy systems, KKT-hPINNs are employed to optimize wind turbine layouts in wind farms. They simulate wind flows while maintaining conservation principles, enabling efficient turbine placement to maximize energy output and minimize environmental impact (Zanardi et al. [2023]).

In **biomechanics and medical imaging**, KKT-hPINNs facilitate the modeling of blood flow in arteries, aiding in the diagnosis of cardiovascular diseases. By ensuring constraints such as mass conservation and adherence to patient-specific boundary conditions, they produce accurate simulations of blood flow dynamics. These models are invaluable for treatment planning and improving medical outcomes (Frankel et al. [2024]).

The integration of analytical modifications of numerical methods into Physics-Informed Neural Networks (PINNs) enhances their efficiency and precision. Classical numerical techniques, such as modified Runge-Kutta methods, are often used to generate low-fidelity models that serve as efficient starting points for PINN training. For instance, in orbital mechanics, accurately predicting spacecraft trajectories under gravitational forces involves solving complex ordinary differential equations (ODEs). By employing modified Runge-Kutta methods to generate approximate solutions, PINNs can converge faster to high-precision results, ensuring reliable trajectory predictions in mission-critical scenarios (Tarkhov et al. [2023]).

Similarly, in fluid flow simulations, solving the Navier-Stokes equations for industrial pipe systems can be computationally demanding. Enhanced numerical solvers generate low-fidelity velocity and pressure fields as initial approximations, which PINNs refine during training. This hybrid approach allows for faster, resource-efficient predictions without sacrificing accuracy. In climate modeling, low-fidelity models can approximate large-scale phenomena like global temperature and pressure variations, providing a foundation for PINNs to enforce physical constraints like energy conservation while accelerating training (Branca and Pallottini [2022]).

In structural analysis, modified numerical solvers help predict stress and deformation in beams and other load-bearing structures. Low-fidelity approximations generated from traditional methods like the Finite Difference Method (FDM) can be refined using PINNs, ensuring compliance with equilibrium equations and material constraints. This hybrid approach is also effective in biomedical sciences, where solving pharmacokinetics equations for patient-specific models benefits from approximate drug concentration predictions. These predictions, refined through PINNs, enable the creation of efficient and accurate personalized models, paving the way for advances in personalized medicine.

Additionally, analytical modifications of classical numerical methods, such as enhanced Runge-Kutta techniques, have been introduced to bridge traditional numerical approaches with modern machine learning. These methods generate low-fidelity models that serve as efficient starting points for PINN training, accelerating convergence while preserving neural network flexibility. This hybrid approach reduces computational resource requirements and allows PINNs to adapt to complex problems more quickly. Such integration enables more effective solutions to challenging problems, leveraging the strengths of both traditional numerical techniques and neural networks.

The Multi-Fidelity Training Framework optimizes the balance between computational efficiency and predictive accuracy in PINNs by combining low-fidelity predictions with high-fidelity data. This framework is particularly advantageous in applications where acquiring large volumes of high-fidelity data is impractical or cost-prohibitive. For example, in chemical engineering, high-fidelity simulations of complex systems like chemical reactors often require substantial computational resources. By leveraging low-fidelity models or experimental data as starting points, the framework iteratively refines predictions using high-fidelity information, ensuring accurate modeling without excessive computational costs.

This framework is highly effective in hierarchical problems involving multiscale behaviors. In aerospace engineering, predicting the aerodynamic performance of an aircraft necessitates broad approximations of airflow combined with detailed boundary-layer analyses (Hao et al. [2023], Zanardi et al. [2023, 2022]). Multi-fidelity training integrates these disparate sources of data, achieving precise results with reduced computational overhead. Similarly, in climate modeling, satellite-based coarse-grained data can serve as low-fidelity inputs, while high-resolution observational data refine predictions for specific regions.

In biomedical applications such as tumor growth modeling, multi-fidelity approaches combine general low-fidelity models with sparse high-fidelity patient data (Serebrennikova et al. [2024], Frankel et al. [2024]). This results in accurate, patient-specific predictions that are computationally efficient. By integrating low- and high-fidelity data, this framework not only reduces the reliance on expensive datasets but also broadens the applicability of PINNs across diverse fields, making them more accessible for solving complex, real-world problems (Tarkhov et al. [2023], Chen et al. [2024]).

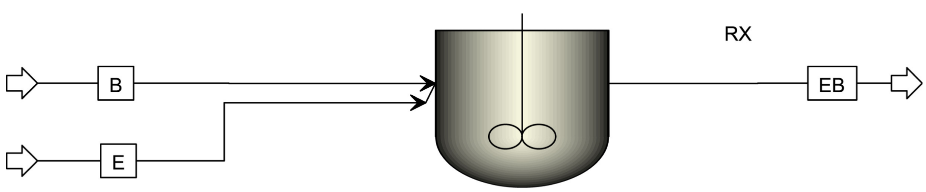

Figure 5: Process flowsheet of the CSTR unit (Chen et al. [2024]).

Innovative PINN methodologies have led to their application in various chemical engineering contexts, such as modeling Continuous Stirred-Tank Reactors (CSTRs). PINNs ensure strict adherence to mass and energy conservation laws, producing accurate and reliable predictions for optimizing reactor designs. Similarly, in extractive distillation systems, PINNs simulate complex mass transfer dynamics and thermodynamic equilibria, providing insights for improving process efficiency (Chen et al. [2024]).

PINNs are also being employed as surrogate models for large-scale chemical plants, integrating unit operations while preserving physical consistency. This capability is particularly valuable in petrochemicals and pharmaceuticals, where optimizing processes can result in significant cost savings and performance improvements.

Despite these advancements, challenges remain.Designing effective low-fidelity models is crucial to avoid compromising the accuracy of final predictions, and selecting optimal neural network architectures remains complex (Tarkhov et al. [2023], Ji et al. [2021]). Integrating highly nonlinear or intricate physical laws into PINNs can introduce computational difficulties, particularly for large-scale or high-dimensional problems. Training PINNs efficiently for systems involving multi-scale dynamics continues to demand significant computational resources. Moreover, generalizing PINNs to handle unseen data and extending their applicability beyond the training domain are ongoing hurdles that require innovative strategies.

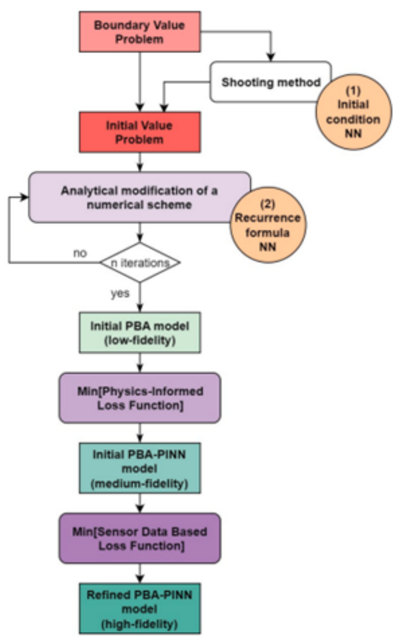

Figure 6: General scheme of constructing and training multi-fidelity physics-informed neural networks with physics-based architecture (PBA-PINN) (Tarkhov et al. [2023]).

Consider an implicit equation

$$y + s\exp(y) = t \tag{1}$$

An approximate solution y(s, t) to is looked for in the form of a neural network with one hidden layer and n neurons per it, which can be expressed as

$$\hat{y}(s,t,\{c_i,a_i\}_{i=1}^{n}) = c_1 + \sum_{i=2}^{n} c_i v(s,t,a_i), \tag{2}$$

Where,

$$v(s,t,\mathbf{a}) = \mathrm{th}(a_1 s + a_2)\,\mathrm{th}(a_3 t + a_4) \tag{3}$$

is an activation function, parameters $c_i, a_i,\ ni = 1$ are learned by minimising the squared error loss

$$J = \sum_{j=1}^{M} \left(\psi(s_j,t_j,\{c_i,a_i\}_{i=1}^{n}) + s_j \exp(\psi(s_j,t_j,\{c_i,a_i\}_{i=1}^{n})) - t_j\right)^2 \tag{4}$$

Throughout this work, in the training process, inputs are resampled after 3–5 steps of nonlinear optimisation of a corresponding loss function in the domain of interest. The resulting solution is:

$$\theta_1(x) = \vartheta(x^2\delta, \delta, \{c_i,a_i\}_{i=1}^{n}) \tag{5}$$

Constructing Physics-Informed Neural Networks with Architecture Based on Analytical Modification of Numerical Methods by Solving the Problem of Modelling Processes in a Chemical Reactor (Tarkhov et al. [2023]).

Emerging terminologies highlight the evolution of PINN methodologies. Physics-Based Architectures embed physical laws directly into neural networks, enhancing accuracy and interpretability. KKT conditions enable the development of KKT-hPINNs by enforcing strict equality constraints during training, ensuring physical validity (Chen et al. [2024]). Orthogonal projection mechanisms ensure model predictions align with feasible solution spaces defined by physical laws. Quadratic programming methods simplify the enforcement of constraints by providing closed-form solutions. Traditional numerical methods like Runge-Kutta serve as the foundation for low-fidelity models, while shooting methods address boundary value problems, aiding stability and convergence. Multi-fidelity models combine low-accuracy approximations with sparse high-fidelity data, optimizing computational efficiency and predictive accuracy (Ji et al. [2021]). Together, these advancements position PINNs as a transformative tool in tackling complex, multi-scale systems across diverse scientific domains.

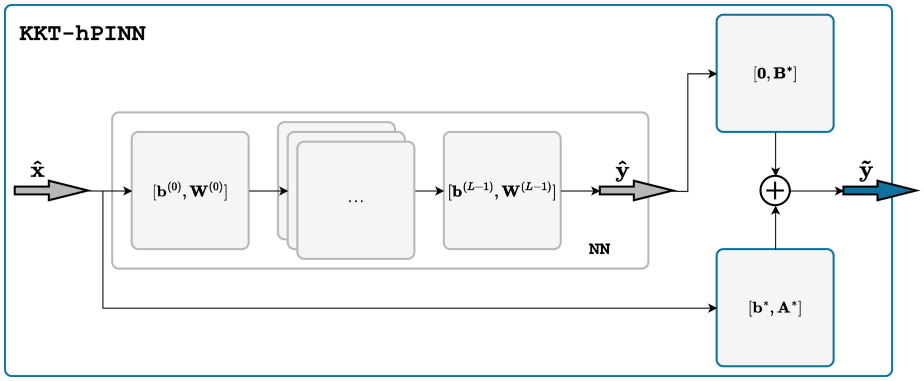

Figure 7: Gray block: illustration of NN architectures; Blue block: illustration of KKT-hPINN architectures consisting of trainable layers and two additional non-trainable projection layers (blue layers) (Chen et al. [2024]).

5 Chemical Kinetics and Reaction Dynamics: Innovations and Applications of PINNs

Physics-Informed Neural Networks (PINNs) are revolutionizing the field of chemical kinetics and reaction dynamics by providing a novel approach to integrating physical laws directly into neural network architectures. This seamless integration of domain-specific knowledge, including conservation laws, rate laws, transport equations, and thermodynamic principles, allows PINNs to overcome the limitations of traditional data-driven models. By embedding these fundamental physical principles directly into the loss functions, PINNs ensure that predictions made by the model are not only data-driven but also adhere strictly to the underlying physical laws governing the system (Chen et al. [2024], Tarkhov et al. [2023] ,Zhang et al. [2024]). This approach offers a powerful tool for simulating complex chemical systems with high accuracy, even when the available data is sparse, noisy, or incomplete. The ability to incorporate these governing equations enables PINNs to model chemical systems more reliably, overcoming many of the challenges that arise in chemical engineering applications, such as in reacting flows, multiscale phenomena, and stiff chemical systems. As a result, PINNs are rapidly gaining traction across several industries, including energy, materials science, and environmental engineering, as they provide a more efficient and robust approach to solving complex problems. Recent innovations have significantly enhanced the capabilities of PINNs in the domain of chemical kinetics, addressing both accuracy and computational efficiency challenges. One of the key developments in 2023 is the introduction of derivative constraints (Sun et al. [2023]), which specifically address non-physical oscillations in convection-dominated systems. By incorporating derivatives of governing equations into the PINN loss function, this method ensures the model captures steep gradients and stabilizes flow simulations, particularly important for modeling flame front dynamics in combustion systems. This innovation has proven especially valuable in simulations where accurate flow modeling and stability are paramount, such as in the optimization of combustion processes and energy systems (Hao et al. [2023]).

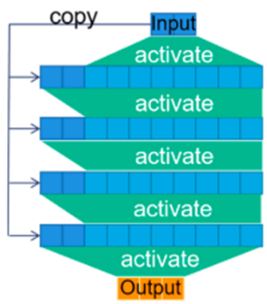

Figure 8: Neural network structure for deep function family construction (Sun et al. [2023]).

In the original PINN, the field function generated using the full connected neural network is expressed by:

$$\mathcal{N}^0 = \mathcal{X}, \tag{6}$$

$$\mathcal{N}^k = \sigma(\mathbf{W}^k \mathcal{N}^{k-1} + \mathbf{b}^k), \text{ for } 1 \leq k \leq L-1 \tag{7}$$

$$\mathbf{u}_\Theta(\mathcal{X}) = \mathcal{N}^L = \sigma(\mathbf{W}^L \mathcal{N}^{L-1} + \mathbf{b}^L), \tag{8}$$

Eqs. (6)-(8) can be simplified to the following form:

$$\mathbf{u}_\Theta(\mathcal{X}) = \sigma \circ \sigma \circ \cdots \circ \sigma(\mathcal{X}; \Theta), \tag{9}$$

where Σ represents the nonlinear functional action. For the k-th layer, the input X is copied and concatenated with the hidden layer neuron N^{k-1}. After that, the weight matrix is applied to the new vectors $N^{k-1} \oplus X$. With added bias, the activation function is then employed and Eq. (7) becomes:

$$N^k = \sigma\left(W^k(N^{k-1} \oplus X) + b^k\right)$$

where $\oplus$ represents the vector concatenation. Differing from Eq. (4) in the original PINN, the $u_\Theta(X)$ is composed by a family of activation functions as:

$$u_\Theta(\mathcal{X}) = \sigma\sigma\cdots\sigma(\mathcal{X};\Theta) + \cdots + \sigma\sigma(\mathcal{X};\Theta) + \sigma(\mathcal{X};\Theta) \tag{10}$$

Since the solution of the CDR system is prone to be u $\ominus$ (X) in Eq. (10), the using of new structure reduces the optimization difficulty of the algorithm and the training time, and hence improves the performance

A physics-informed neural network based simulation tool for reacting flow with multicomponent reactants.

Another milestone in PINN development is the introduction of Deep Function Family Construction, also introduced in 2023. This approach enhances the architecture of neural networks by integrating alternative activation functions and layered structures that optimize training times without sacrificing accuracy. It has been particularly advantageous in computationally expensive simulations of complex reacting flows, where traditional methods are either too slow or fail to capture all the relevant dynamics. These advanced architectures improve both the training efficiency and performance of PINNs, making them a viable solution for industrial applications requiring rapid and accurate simulations of dynamic chemical systems (Sun et al. [2023]).

A particularly exciting development in 2023 is the Mixture-of-Experts (MOE) framework (Almeldein and Van Dam [2023]), which employs multiple specialized subnetworks to model distinct aspects of a chemical system. For example, one subnetwork might be specialized in reaction kinetics, while another could model transport phenomena or turbulence. By simultaneously resolving different coupled dynamics, this framework significantly improves the performance and efficiency of PINNs in complex reaction-transport systems. This innovation enables PINNs to tackle systems with multiple interacting processes, which is particularly useful in applications such as catalytic reactor design, chemical process optimization, and environmental engineering, where multiple phenomena are at play.

To further enhance the applicability of PINNs in chemical kinetics, in August 2024, logarithmic-normalized transformations were introduced (Zhang et al. [2024]). This method stabilizes training in multiscale chemical systems by transforming species concentrations and governing equations into logarithmic scales. This transformation regularizes the data, embedding mass action and conservation laws directly into the model, which leads to more accurate and robust predictions for stiff systems, such as in combustion and reaction-diffusion systems. By improving stability and reducing numerical instabilities, this technique enables the successful application of PINNs to highly complex systems that would otherwise be challenging to model using traditional numerical methods.

$$f_C(t) := \sum_{i=1}^{N_{\text{species}}} N_i^C \frac{\text{MW}_C}{\text{MW}_i}(Y_{i,\text{Pr}} - Y_{i,f}) = 0 \tag{11}$$

$$f_H(t) := \sum_{i=1}^{N_{\text{species}}} N_i^H \frac{\text{MW}_H}{\text{MW}_i}(Y_{i,\text{Pr}} - Y_{i,f}) = 0 \tag{12}$$

$$f_O(t) := \sum_{i=1}^{N_{\text{species}}} N_i^O \frac{\text{MW}_O}{\text{MW}_i}(Y_{i,\text{Pr}} - Y_{i,f}) = 0 \tag{13}$$

$$f_N(t) := \sum_{i=1}^{N_{\text{species}}} N_i^N \frac{\text{MW}_N}{\text{MW}_i}(Y_{i,\text{Pr}} - Y_{i,f}) = 0 \tag{14}$$

The above elemental conservation equations can be integrated with the standard machine learning mean squared error (MSE) loss function as follows:

$$\mathrm{MSE} = (1 - R_{\mathrm{ECE}})\mathrm{MSE}_{\mathrm{Pr}} + R_{\mathrm{ECE}}\mathrm{MSE}_{\mathrm{ECE}} \tag{15}$$

$$\mathrm{MSE}_{\mathrm{Pr}} = \frac{1}{N_{\mathrm{target}}} \sum_{i=1}^{N_{\mathrm{target}}} (Y_{i,\mathrm{Tr}} - Y_{i,\mathrm{Pr}})^2 \tag{16}$$

$$\mathrm{MSE}_{\mathrm{ECE}} = \left(f_C(t)^2 + f_H(t)^2 + f_O(t)^2 + f_N(t)^2\right) \tag{17}$$

Accelerating Chemical Kinetics Calculations With Physics Informed Neural Network (Zhang et al. [2024]).

The introduction of Combustion Reaction Kinetics Physics-Informed Neural Networks (CRK-PINNs) has transformed the modeling and simulation of combustion processes, offering rapid and accurate predictions by incorporating Arrhenius kinetics and enthalpy conservation principles. These capabilities make CRK-PINNs indispensable across various industries. In power generation, they enhance gas turbine efficiency by providing real-time predictions of flame stability, heat release, and pollutant formation, allowing engineers to optimize combustion parameters, improve fuel efficiency, and reduce emissions. Similarly, in aerospace engineering, CRK-PINNs accelerate the simulation of combustion dynamics in rocket engines, enabling rapid design iterations for reusable engines while optimizing thrust and fuel usage under extreme conditions (Zanardi et al. [2023]). In the automotive industry, CRK-PINNs simulate engine combustion cycles, facilitating the design of efficient internal combustion engines, particularly in hybrid vehicles, where precise control of ignition timing and air-fuel ratios is critical.

Industrial applications also benefit significantly from CRK-PINNs. For example, in steel and glass manufacturing, industrial furnaces rely on these networks to monitor temperature distributions and combustion efficiency in real time, ensuring consistent product quality and reduced energy consumption. In aviation, CRK-PINNs simulate jet engine performance under varying conditions, such as altitude and air density changes, enabling optimal engine design while minimizing emissions and development costs (Almeldein and Van Dam [2023]). Environmental applications, such as wildfire modeling, leverage CRK-PINNs to predict fire behavior by simulating vegetation combustion under diverse weather and terrain conditions, improving firefighting strategies. Moreover, as the world transitions to clean energy, CRK-PINNs play a critical role in hydrogen combustion systems, accurately modeling the unique flame characteristics of hydrogen to ensure the safe and efficient design of engines, turbines, and fuel cells (Branca and Pallottini [2022], Zhang et al. [2024]).

CRK-PINNs offer several advantages over traditional computational fluid dynamics (CFD) simulations and experimental approaches. Their computation speed, bolstered by techniques like logarithmic-normalized transformations, enables real-time simulations up to 14.6 times faster than traditional solvers. By incorporating physics-based principles directly into the neural network architecture, CRK-PINNs maintain high accuracy while respecting physical laws, achieving a balance that traditional methods often lack due to resource and time constraints. Additionally, their scalability allows application across a wide range of combustion systems, from small-scale reactors to large industrial furnaces, without the need for recalculations for new geometries or input conditions. Once trained, these networks generalize effectively, offering a significant edge in adaptability and resource efficiency compared to traditional CFD methods, which require computationally expensive iterative processes.

The flexibility of CRK-PINNs further enhances their applicability. They can easily incorporate new constraints or adapt to alternative fuels, such as hydrogen or ammonia, with minimal adjustments to the network architecture. Hybrid modeling approaches that integrate experimental data improve their accuracy even further, bridging the gap between simulation and real-world conditions (Frankel et al. [2024]). Cost efficiency is another key advantage, as CRK-PINNs reduce the reliance on expensive experimental setups and computationally intensive CFD simulations. Their ability to perform real-time optimizations, such as monitoring turbine performance or adjusting fuel injection parameters in engines, drives significant operational savings. By addressing the limitations of traditional methods, CRK-PINNs are transforming combustion modeling, enabling faster, more accurate, and more resource-efficient solutions across industries (Zhang et al. [2024]).

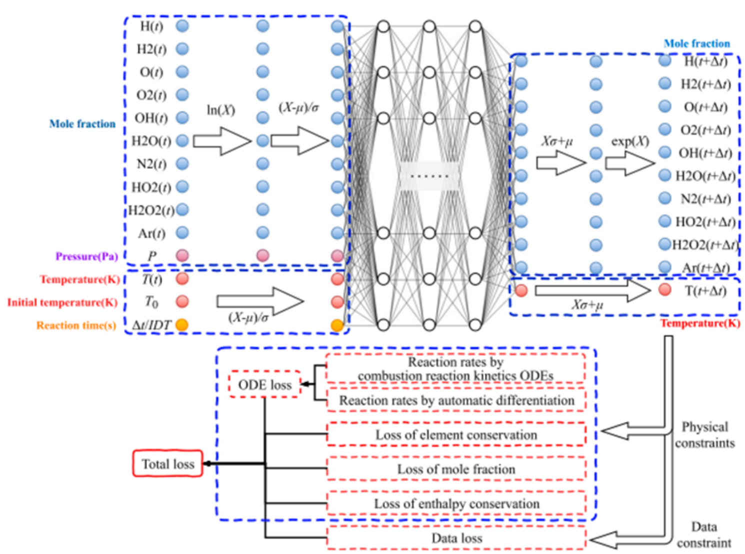

Figure 9: CRK PINN Architecture (Zhang et al. [2024]).

The total loss function of CRK-PINN is given by:

$$L = \lambda_1 L_{\text{ODEs}} + \lambda_2 L_{\text{Enthalpy}} + \lambda_3 L_{\text{Elements}} + \lambda_4 L_{\text{Mole}} + \lambda_5 L_{\text{Data}} \tag{18}$$

The total loss function is composed of five parts: the ODE loss ($\mathcal{L}_{\text{ODEs}}$), the enthalpy conservation loss ($\mathcal{L}_{\text{Enthalpy}}$), the element conservation loss ($\mathcal{L}_{\text{Element}}$), the mole fraction loss ($\mathcal{L}_{\text{Mole}}$), and the data loss ($\mathcal{L}_{\text{Data}}$) Zhang et al. [2024]. The weights for each loss function ($\lambda_1 \sim \lambda_5$) are manually tuned based on their relative magnitudes:

- Magnitudes: $\mathcal{L}_{\text{ODEs}} \approx 10^0$, $\mathcal{L}_{\text{Enthalpy}} \approx 10^1$, $\mathcal{L}_{\text{Element}} \approx 10^{-7}$, $\mathcal{L}_{\text{Mole}} \approx 10^{-7}$, $\mathcal{L}_{\text{Data}} \approx 10^{-3}$
- Coefficients: $\lambda_1 = \frac{10^{-3}}{10^0} = 10^{-3}$, $\lambda_2 = \frac{10^{-3}}{10^{-1}} = 10^{-2}$, $\lambda_3 = \frac{10^{-3}}{10^{-7}} = 10^4$, $\lambda_4 = \frac{10^{-3}}{10^{-7}} = 10^4$, $\lambda_5 = \frac{10^{-3}}{10^{-3}} = 1$

Given that $\mathcal{L}_{\text{Data}}$ provides sufficient training signal, the coefficients for physical constraints are relaxed:

$$\lambda_1 \to 10^{-6}, \quad \lambda_2 \to 10^{-4}, \quad \lambda_3 \to 10^2, \quad \lambda_4 \to 10^2$$

The weights can be dynamically scaled proportionally to:

- Reduce non-physical errors in stiff systems
- Ensure training convergence under varying chemical regimes

$$L_{\text{ODEs}} = \frac{1}{K \cdot N} \sum_{k=1}^{K} \sum_{N} \left(\left.\frac{dX'_{k,l+\Delta t}}{dt'}\right|_{1,\text{ODEs}} - \left.\frac{dX'_{k,l+\Delta t}}{dt'}\right|_{1,\text{AD}} \right)^2 \tag{19}$$

$$L_{\text{Data}} = \frac{1}{(K+1) \cdot N} \sum_{N} \sum_{k=1}^{K+1} (\hat{y}_k - y_k)^2 \tag{20}$$

The introduction of the Extreme Theory of Functional Connections (X-TFC) in 2024 represents a significant leap forward for Physics-Informed Neural Networks (PINNs). X-TFC provides a framework that analytically satisfies initial and boundary conditions, reducing competition between different loss components and improving stability during training (Frankel et al. [2024], Krishnapriyan et al. [2021]). By ensuring the network adheres to these critical conditions at all times, X-TFC is particularly effective for stiff chemical systems where traditional methods struggle to maintain stability and accuracy. This framework guarantees consistent and reliable performance in highly challenging systems, ensuring that PINNs can be used effectively across a wide range of industrial and scientific applications (Raissi et al. [2019]).

X-TFC enhances the stability and accuracy of PINNs by embedding analytical solutions for boundary and initial conditions directly into the network's architecture. This ability ensures that PINNs remain reliable even in challenging environments, such as stiff chemical systems where traditional methods often fail. For example, in industrial chemical plants, stiff reaction systems with rapid changes in reaction rates under extreme temperature and pressure conditions are common. X-TFC stabilizes these models by strictly adhering to critical conditions (Ngo and Lim [2021]), enabling PINNs to optimize chemical yields, energy usage, and reactor designs while enhancing safety measures (Nikolaienko et al. [2024], Frankel et al. [2024]). Similarly, in pharmaceutical manufacturing, X-TFC ensures accurate modeling of complex pharmacokinetics, reducing simulation times and enabling consistent drug formulation with faster development timelines (Ji et al. [2021]).

In environmental modeling, X-TFC plays a crucial role in stabilizing climate simulations, which involve stiff differential equations and highly sensitive parameters. By ensuring adherence to boundary conditions, such as atmospheric pressure and oceanic temperature, X-TFC improves the accuracy of long-term climate predictions (Chen et al. [2024]), aiding in policy decisions for mitigating climate change. Aerospace engineering also benefits significantly from X-TFC, particularly in rocket propulsion systems, where complex and nonlinear combustion dynamics occur under extreme conditions. X-TFC ensures accurate simulations of pressure, temperature, and fuel composition in rocket engines, optimizing fuel efficiency and minimizing risks of instability (Hao et al. [2023], Zhang et al. [2024]). Similarly, in energy storage systems like lithium-ion batteries, X-TFC stabilizes the simulation of electrochemical reactions, ensuring boundary conditions for charge conservation, temperature, and voltage are met (Serebrennikova et al. [2024]). This enables accurate modeling of battery degradation, optimization of charging cycles, and the design of longer-lasting batteries (Chen et al. [2023]).

Nuclear reactors, where interactions between temperature, pressure, and radiation flux are highly complex, also benefit from the stability provided by X-TFC. By maintaining critical safety-related boundary conditions during simulations, X-TFC ensures accurate modeling of neutron transport and fuel depletion, reducing risks and improving energy efficiency (Zhang et al. [2024], Tarkhov et al. [2023]). When compared to traditional numerical methods, such as computational fluid dynamics (CFD) or finite element analysis (FEA), X-TFC offers superior stability and computational efficiency. Traditional methods often require highly refined meshes or iterative solvers that can become computationally expensive and unstable under certain conditions. While implicit techniques in traditional solvers address some challenges, they significantly increase computational costs. In contrast, X-TFC eliminates the need for such methods by analytically embedding physical constraints into the network, reducing computational overhead and enabling faster convergence.

Unlike other machine learning models that may lack physics-informed structures, X-TFC ensures PINNs respect physical laws such as mass and energy conservation, achieving high accuracy even in stiff systems (Frankel et al. [2024]). The framework also excels in computational efficiency by reducing competition between loss components during training, resulting in convergence up to 14.6 times faster than traditional methods. Scalability is another strength, as X-TFC allows PINNs to generalize across different input conditions without requiring recalculations for each new scenario. This capability makes X-TFC ideal for real-time applications in fields like automotive engineering and aerospace, where frequent simulations under varying conditions are necessary (Branca and Pallottini [2022], Zanardi et al. [2023]. Moreover, X-TFC's flexibility allows it to incorporate new constraints or adapt to changing configurations with minimal effort, making it suitable for applications ranging from chemical systems to energy storage and beyond.

The X-TFC framework significantly enhances the capabilities of PINNs by combining stability, accuracy, scalability, computational efficiency, and flexibility. Its ability to enforce physical constraints analytically and efficiently positions it as a transformative tool for tackling complex simulations across diverse domains, including industrial processes, environmental modeling, aerospace engineering, energy systems, and nuclear safety (Chen et al. [2023], Tarkhov et al. [2023]). By addressing limitations in traditional numerical methods and other machine learning approaches, X-TFC ensures that PINNs can deliver reliable and resource-efficient solutions for real-world challenges (Serebrennikova et al. [2024]).

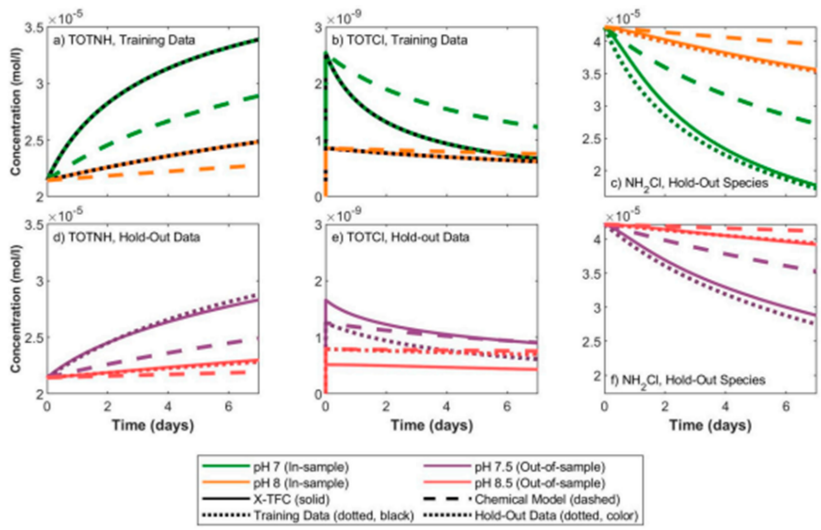

Figure 10: X-TFC model results using training data for TOTNH and TOTCl (Frankel et al. [2024]).

The ability of PINNs to model chemical systems without the need for complex grid generation or mesh-based methods is another key advantage. This mesh-free approach reduces the computational overhead typically associated with traditional numerical methods, such as finite element or finite difference methods, making PINNs particularly advantageous for systems where grid-based methods are difficult or impractical to implement (Zhang et al. [2024], Tarkhov et al. [2023]). For example, in autocatalytic reactions within tubular reactors, where system complexity makes grid generation challenging, PINNs offer a more flexible and efficient alternative. The mesh-free nature of PINNs allows them to model these systems with greater ease and accuracy, reducing computational costs and improving the scalability of simulations (Giampaolo et al. [2022]).

Despite these advancements, several challenges remain in fully realizing the potential of PINNs. One major challenge is the slow convergence of training, particularly when derivative constraints are used to improve model accuracy. Techniques like logarithmic-normalized transformations address some of the issues related to stiffness, but they require careful implementation to avoid numerical instabilities. Moreover, while frameworks like X-TFC improve stability, they are not universally applicable across all types of systems, and their generalization remains an ongoing area of research (Sun et al. [2023], Hao et al. [2023]). Scaling PINNs to handle large, high-dimensional systems is still a significant challenge, and optimizing the training process to ensure faster convergence and more efficient learning (Chen et al. [2024], Frankel et al. [2024]) is a crucial area of development.

The scalability of PINNs is particularly challenging for large systems with numerous interacting variables. Despite innovations like MOE and CRK-PINNs, these models still require significant computational resources, especially for real-world systems involving multiple scales and complex interactions. As the size and complexity of chemical systems increase, the training time and resources required for PINNs grow exponentially. Developing efficient algorithms capable of handling these large-scale systems is essential for expanding their practical applications.

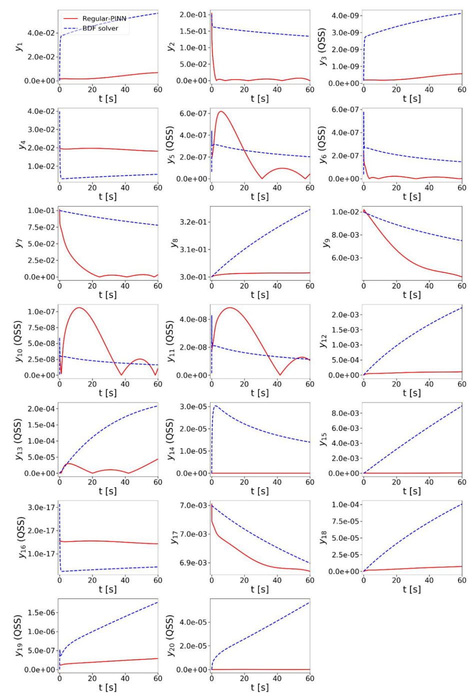

Figure 11: Training results of regular-PINN for the POLLU problem (Ji et al. [2021])

Overall, the evolution of PINNs in the context of chemical kinetics and reaction dynamics is transformative. Through groundbreaking innovations, PINNs have become indispensable for solving complex chemical engineering problems (Nikolaienko et al. [2024], Ji et al. [2021], Serebrennikova et al. [2024]). From combustion reaction kinetics to reaction-diffusion systems, catalysis, and environmental monitoring, the versatility and power of PINNs are evident. As research continues to address challenges like scaling and training, and as methodologies like X-TFC, MOE, and CRK-PINNs evolve, PINNs are poised to become integral to computational chemistry and chemical engineering (Nikolaienko et al. [2024], Ji et al. [2021]). With their ability to integrate physical laws, optimize complex systems, and provide accurate predictions in real time, PINNs have the potential to drive significant advances in industries ranging from energy production to materials science and environmental sustainability (Sun et al. [2023]).

6 Applications in Catalysis and Reactor Modeling

Physics-Informed Neural Networks (PINNs) are rapidly transforming the field of catalysis and reactor modeling, offering a novel and powerful framework for understanding and optimizing chemical processes. These systems, often at the heart of industrial chemical manufacturing, rely on complex interactions between chemical reactions, mass transfer, and species diffusion (Raissi et al. [2019]). Traditional methods of modeling these interactions, though valuable, face limitations when attempting to capture the intricate and dynamic behaviors that arise in reaction-diffusion systems, particularly at the microscale (Giampaolo et al. [2022]). These traditional approaches struggle with the steep gradients and non-linear interactions inherent in these systems, leading to less accurate and sometimes inefficient simulations (Tarkhov et al. [2023], Zhang et al. [2024]). However, the emergence of PINNs offers a breakthrough by embedding governing physical and chemical equations directly into the neural network training process, enabling a more accurate and efficient way to simulate catalytic systems.

At the core of many catalytic processes is the challenge of understanding the behavior of reactants and products within porous catalyst pellets. These pellets, which serve as the surface where reactions occur, are inherently complex due to the competitive nature of reaction rates and species diffusion (Chen et al. [2024]). The reaction kinetics and the rate at which reactants diffuse through the porous material interact in subtle ways that are difficult to model accurately. Traditional methods rely on simplifying assumptions, such as homogeneity and constant properties, which may not capture the fine-scale behavior within the catalyst (Ji et al. [2021]). In contrast, PINNs offer a revolutionary approach by directly incorporating the relevant conservation laws, mass transfer equations, and reaction rate laws into the loss functions of the neural network. This allows for the modeling of the distribution of chemical species across the pellet with unprecedented detail and accuracy (Sun et al. [2023]).

The ability of PINNs to balance diffusion and reaction kinetics offers significant advantages in optimizing catalyst performance. For instance, by modeling how reactants and products are transported and transformed within the porous structure of a catalyst, PINNs provide engineers with valuable insights into optimal parameters such as pellet size, porosity, and surface area (Zhang et al. [2024]). This capability allows for a more targeted approach to catalyst design and reactor optimization, reducing energy consumption and improving overall efficiency. Moreover, this alignment with sustainability goals in industrial processes makes PINNs an essential tool for advancing green chemistry, where minimizing energy waste and resource consumption is critical (Xiao and Wu [2023], Zhang et al. [2024]).

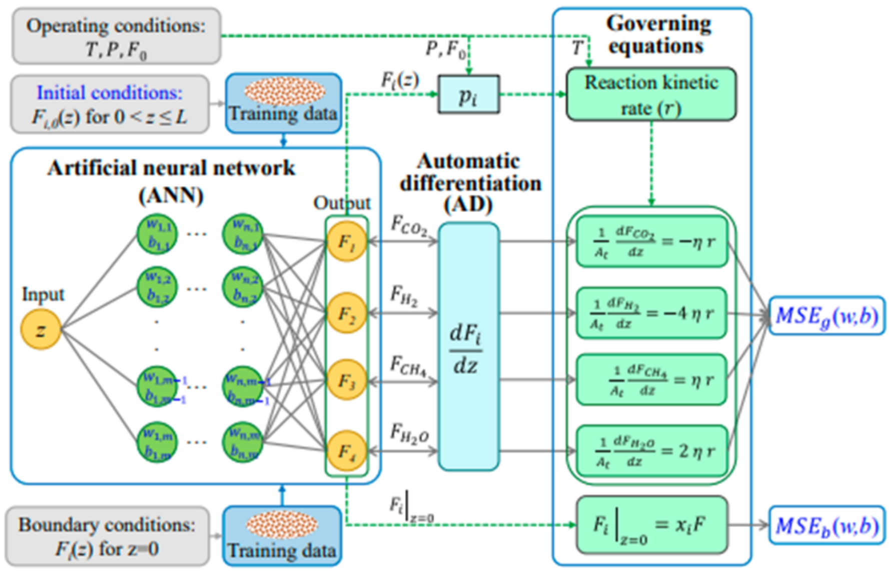

Figure 12: Architecture of the physics-informed neural network (PINN) forward problem for CO2 methanation in an isothermal fixed-bed (IFB) reactor (Ngo and Lim [2021])

The optimized weights and biases (w^* and b^*) were obtained from the following optimization problem:

$$
\begin{aligned}
\{w^*, b^*\} &= \arg\min_{w,b}\{\text{Loss} = \text{MSE}_g(w,b) + \text{MSE}_b(w,b)\} \\
\text{MSE}_g(w,b) &= \frac{1}{N_{\text{train}}} \sum_{j=1}^{N_{\text{train}}} \sum_{i=1}^{N_{\text{comp}}} \left| \frac{1}{A_t} \left(\frac{dF_i}{dz} \right)_j - \eta \nu_i r_j \right|^2 \\
\text{MSE}_b(w,b) &= \frac{1}{N_{\text{bnd}}} \sum_{k=1}^{N_{\text{bnd}}} \sum_{i=1}^{N_{\text{comp}}} \left| F_{i,k}|_{z=0} - x_{i,0} F_0 \right|^2
\end{aligned}
\tag{21}
$$

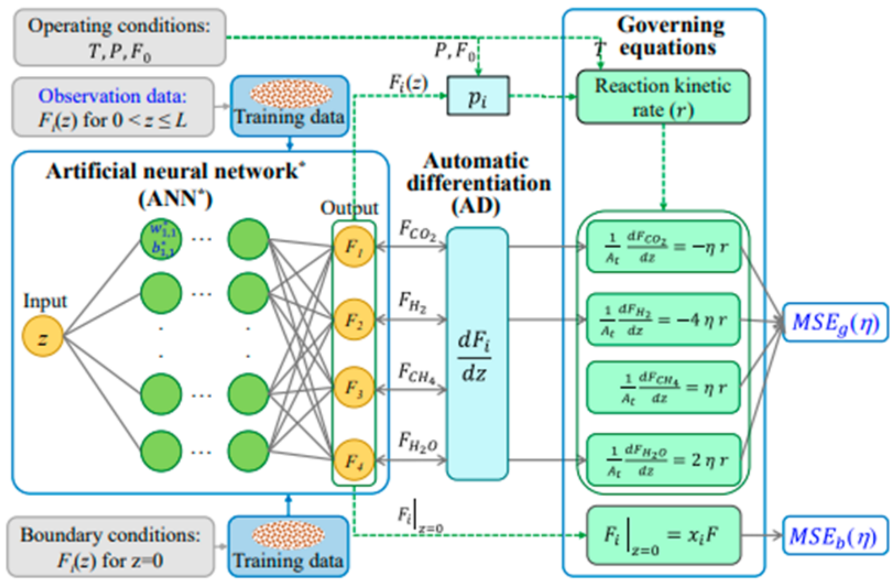

Figure 13: Architecture of the physics-informed neural networks (PINN) inverse problem for CO2 methanation in an isothermal fixed-bed (IFB) reactor (Ngo and Lim [2021]).

In the inverse PINN, the effectiveness factor (η) as an unknown model parameter was identified using the following optimization with a loss function:

$$
\begin{aligned}
\{\eta^*\} &= \arg\min_{\eta}\{\text{Loss} = \text{MSE}_g(\eta) + \text{MSE}_b(\eta)\} \\
\text{MSE}_g(\eta) &= \frac{1}{N_{\text{obs}}}\sum_{j=1}^{N_{\text{obs}}}\sum_{i=1}^{N_{\text{comp}}}\left|\frac{1}{A_t}\left(\frac{dF_i}{dz}\right)_j - \eta\nu_i r_j\right|^2 \\
\text{MSE}_b(\eta) &= \frac{1}{N_{\text{bnd}}}\sum_{k=1}^{N_{\text{bnd}}}\sum_{i=1}^{N_{\text{comp}}}\left|F_{i,k}|_{z=0} - x_{i,0}F_0\right|^2
\end{aligned}
\tag{22}
$$

Solution and Parameter Identification of a Fixed-Bed Reactor Model for Catalytic CO2 Methanation Using Physics-Informed Neural Networks (Ngo and Lim [2021]).

PINNs extend their utility beyond catalyst pellets to solving complex reaction-diffusion equations that govern the behavior of chemical species under the combined influence of chemical reactions and mass transfer. These equations, which are central to the operation of catalytic systems, are notoriously difficult to solve due to their nonlinear nature and the need for high computational accuracy (**?**). PINNs overcome these challenges by incorporating the relevant physical laws directly into the network's training process. This ensures that every prediction made by the model respects the fundamental principles of mass conservation, reaction dynamics, and thermodynamic constraints (Chen et al. [2024]), providing highly accurate simulations of catalytic systems. As a result, researchers can simulate catalytic processes with a level of precision that was previously unattainable, enabling the design of reactors that are both stable and efficient, even under fluctuating or harsh operating conditions (Sun et al. [2023]).

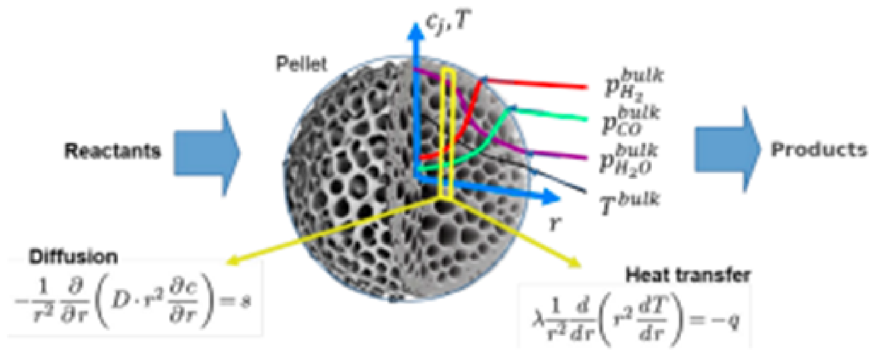

Figure 14: Schematic representation of the catalytic particle as an element of chemical reactor performing FischerTropsch synthesis. The mass and heat transport in the particle is modeled by diffusion and heat transfer equations, in which the source terms result from the kinetics of underlying reactions (Nikolaienko et al. [2024]).

One of the most significant impacts of PINNs in catalysis and reactor modeling is their ability to provide real-time optimization and predictive capabilities (Chen et al. [2024], Xiao and Wu [2023]). In industrial settings, such as large-scale chemical manufacturing plants, reaction conditions can change unexpectedly due to fluctuations in feedstock, temperature, pressure, or other variables. The ability to dynamically model and optimize systems in real time is crucial for minimizing downtime and maximizing production efficiency (Frankel et al. [2024]). PINNs facilitate this by offering rapid, yet precise, simulations of chemical reactions and transport phenomena, allowing engineers to make adjustments on-the-fly and avoid costly disruptions (Zhang et al. [2024]). Furthermore, because PINNs do not require the generation of complex computational grids, they reduce computational overhead, making simulations faster and more cost-effective (Ji et al. [2021]).

In practice, the speed and efficiency of PINNs make them an invaluable tool in industries where time and cost are critical factors. The ability to perform these complex simulations quickly translates into tangible benefits for businesses. For example, in chemical manufacturing, real-time predictive capabilities can help avoid costly reactor failures, reduce waste, and improve product consistency. Similarly, the faster convergence of PINNs enables more frequent and detailed simulations, allowing for continuous improvement in system performance and the rapid development of new processes and technologies (Tarkhov et al. [2023]).

Looking to the future, the integration of PINNs into broader industrial workflows has the potential to revolutionize the field of chemical engineering. As these models continue to evolve, they will likely become even more integrated with real-time data collection and decision-making systems. This evolution could lead to fully autonomous systems capable of designing and optimizing catalytic processes with minimal human intervention (Tarkhov et al. [2023]). Furthermore, PINNs can be combined with other advanced technologies such as machine learning, optimization algorithms, and experimental data integration, creating hybrid models that offer even greater accuracy, efficiency, and scalability (Chen et al. [2024]).

Physics-Informed Neural Networks (PINNs) offer transformative potential in fields like catalysis, reactor modeling, and polymer science. However, significant challenges impede their seamless integration into real-world applications. A major limitation is the difficulty in handling high-dimensional systems, where the complexity of physical interactions and multi-scale phenomena can overwhelm the computational framework. Training stability is another pressing issue, as the inclusion of derivative constraints and boundary conditions often leads to ill-conditioned optimization problems. Sparse data availability further complicates the training process, making it difficult to achieve robust model generalization. To address these challenges, researchers are leveraging strategies such as adaptive learning rates, pretraining using traditional numerical methods, and integrating domain-specific knowledge into loss functions. Additionally, real-world implementations often reveal practical constraints like computational resource limitations and the need for domain expertise to ensure accurate model interpretations. By addressing these gaps, PINNs can unlock unprecedented capabilities in modeling and optimizing complex chemical systems, enabling advancements in material science, environmental sustainability, and industrial efficiency.

The growing role of PINNs in catalysis and reactor modeling is not just a technical advancement; it is a catalyst for innovation in the chemical industry. By enabling more accurate, efficient, and real-time simulations, PINNs hold the promise of driving the next wave of breakthroughs in chemical process optimization. These advancements align with the global push toward sustainability, offering a pathway for industries to reduce their environmental impact while improving performance and reducing costs (Raissi et al. [2019]). As the capabilities of PINNs continue to expand, they are poised to redefine the boundaries of what is possible in chemical engineering, creating new opportunities for innovation, efficiency, and sustainability in the chemical industry.

Recent innovations in PINN methodologies have introduced techniques such as gradient-enhanced PINNs, multi-fidelity PINNs, and adaptive PINNs, which significantly enhance the flexibility and precision of these networks. Gradient-enhanced PINNs leverage higher-order derivatives in their loss functions, ensuring sharper gradient resolution in simulations of chemical reactions and boundary-layer dynamics. Multi-fidelity PINNs integrate low-fidelity and high-fidelity data sources to improve computational efficiency without compromising accuracy, making them ideal for multiscale systems. Adaptive PINNs, on the other hand, adjust learning rates and loss weights dynamically during training to address challenges such as stiffness in chemical kinetics or high-dimensional interactions in multi-component systems. These advancements not only expand the scope of PINNs across domains but also accelerate convergence and improve the robustness of models, enabling breakthroughs in catalysis, environmental modeling, and reaction-diffusion processes.

PINNs represent a paradigm shift in the way we approach catalysis and reactor modeling. By embedding fundamental physical laws directly into neural network architectures, these models provide a more accurate, efficient, and sustainable way to simulate complex chemical systems. With their growing role in industrial applications, PINNs are transforming how we understand chemical reactions.

7 Non-Equilibrium Flows and Hypersonic Applications

Physics-Informed Neural Networks (PINNs) are at the forefront of transforming computational modeling across a wide range of fields, from chemical kinetics to aerospace engineering. These innovative models have proven themselves as essential tools for solving complex, high-dimensional systems by embedding fundamental physical laws into the neural network architecture (Raissi et al. [2019]). One of the most advanced and promising extensions of PINNs is Physics-Informed DeepONets (PI-DeepONets), which further enhance the capability of traditional PINNs. PI-DeepONets are designed to solve parametric partial differential equations (PDEs) without requiring paired input-output data, thus overcoming some of the major limitations of traditional approaches. This advancement opens up new possibilities for efficiently addressing problems in turbulence, hypersonic flow, and reaction dynamics—areas where computational demand and accuracy are often major hurdles (Zanardi et al. [2023, 2022]).

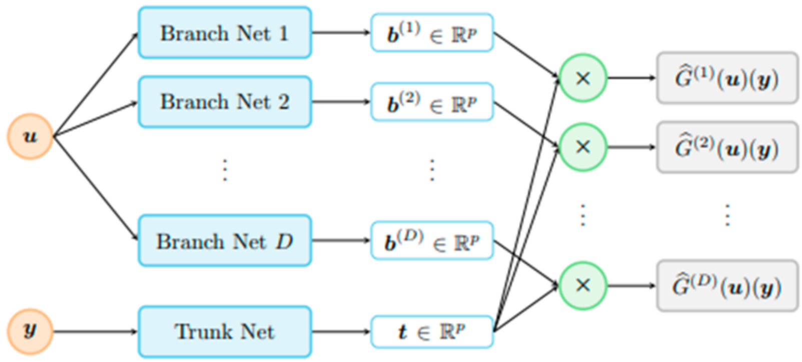

Figure 15: Multi-output DeepONet: The modified architecture consists of multiple "branch nets" (one for each output) for extracting latent representations of the input functions, and one "trunk net" for extracting latent representations of the input coordinates at which the output functions are evaluated (Zanardi et al. [2022]).

A modified DeepONet G prediction of a function u evaluated at y can be expressed by

$$\hat{G}(u)(y) = \begin{bmatrix} \sum_{k=1}^{P} b_k^{(1)}(u(x_1), u(x_2), ..., u(x_m))t_k(y) + b_0^{(1)} \\ \sum_{k=1}^{P} b_k^{(2)}(u(x_1), u(x_2), ..., u(x_m))t_k(y) + b_0^{(2)} \\ \vdots \\ \sum_{k=1}^{P} b_k^{(D)}(u(x_1), u(x_2), ..., u(x_m))t_k(y) + b_0^{(D)} \end{bmatrix}. \tag{23}$$

All the trainable parameters, denoted by $L_{Data}(\theta)$, can be optimized by minimizing the following loss

$$\mathcal{L}_{data}(\theta) = \frac{1}{NP} \sum_{d=1}^{D} \sum_{i=1}^{N} \sum_{j=1}^{P} \left| G^{(d)}(u_i)(y_{i,j}) - \hat{G}^{(d)}(u_i)(y_{i,j}) \right|^2 \tag{24}$$

Physics-informed neural networks (PINNs) can integrate data and physical governing laws by adding residuals of PDEs in the loss function of a neural network using automatic differentiation. Specifically, we consider minimizing the following composite loss function

$$\mathcal{L}(\theta) = \mathcal{L}_{data}(\theta) + \mathcal{L}_{phy}(\theta) \tag{25}$$

where $L_{data}(\theta)$ is calculated over a given "anchors" data points defined by the triplet $(u_i, y_{ij}, \hat{G}(u_i)(y_{ij}))$, while

$$\mathcal{L}_N(\theta) = \frac{1}{NQm} \sum_{d=1}^{D} \sum_{i=1}^{N} \sum_{j=1}^{Q} \sum_{k=1}^{m} \left| \mathcal{N}^{(d)} \left(u_i(x_k), \widehat{G}(u_i)(y_{i,j}) \right) \right|^2 \quad (26)$$

$$\mathcal{L}_{IC}(\theta) + \mathcal{L}_{BC}(\theta) = \frac{1}{NBm} \sum_{d=1}^{D} \sum_{i=1}^{N} \sum_{j=1}^{B} \sum_{k=1}^{m} \left| \mathcal{B}^{(d)} \left(u_i(x_k), \widehat{G}(u_i)(y_{i,j}) \right) \right|^2 \quad (27)$$

Since the master equations is a set of first-order differential equations without any external inputs, the input function u will be represented by different initial conditions (IC), while the independent variable y of $G(u)$ will be time

$$u = [T, \rho, \mathbf{Y}_0] \in \mathbb{R}^{N_{G+3}} \quad (28)$$

$$y = t \in \mathbb{R}^1 \quad (29)$$

$$\widehat{G}(u)(y) = \widehat{\mathbf{Y}}_u(t) \in \mathbb{R}^{N_{G+1}} \quad (30)$$

Towards Efficient Simulations of Non-Equilibrium Chemistry in Hypersonic Flows: A Physics-Informed Neural Network Framework (Zanardi et al. [2022]).

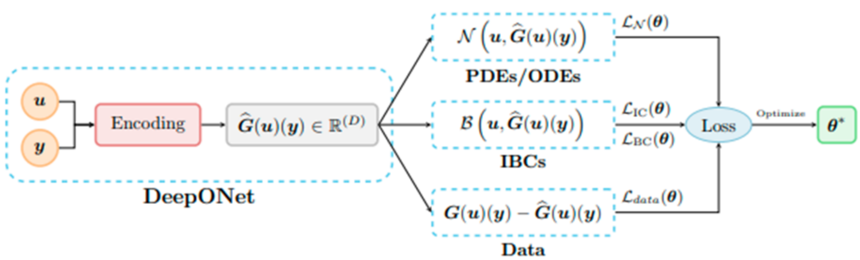

Figure 16: Physics-informed DeepONet: Automatic differentiation can be employed to formulate appropriate regularization mechanisms for biasing the DeepONet outputs to satisfy a given system of PDEs/ODEs (Zanardi et al. [2022])

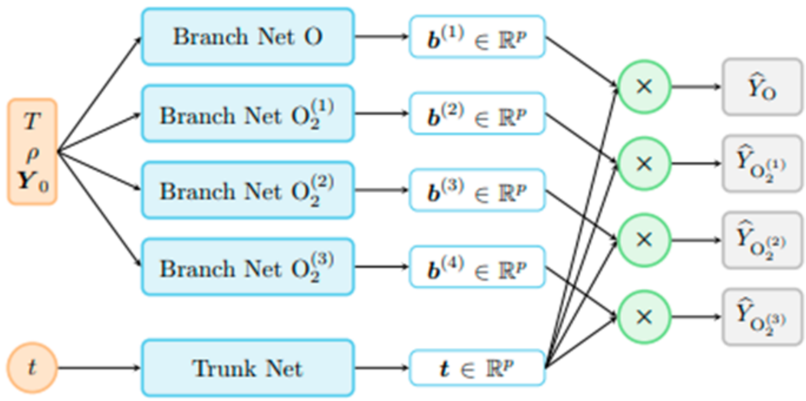

Figure 17: DeepONet for Master Equations (Zanardi et al. [2023])

In the field of chemical kinetics and reaction dynamics, PINNs have proven to be particularly valuable. Stiff reaction networks, which involve rapid changes in concentration and energy states, pose significant challenges for conventional modeling techniques. However, by incorporating mass and energy conservation laws directly into the neural network framework, PINNs ensure both stability and precision in simulations (Ji et al. [2021]). This makes them indispensable for tackling complex chemical systems like combustion and catalysis. Their ability to predict reaction intermediates and rates with remarkable accuracy has profound implications for improving industrial processes and energy systems, especially in the optimization of reactors and the design of more efficient catalysts (Ngo and Lim [2021]).

Moreover, PINNs excel in solving reaction-diffusion equations, which describe the spatiotemporal evolution of chemical species under the influence of chemical reactions and mass transfer. These equations are central to understanding diffusion and transport phenomena in various systems, including chemical reactors and environmental remediation processes. By coupling reaction kinetics with molecular diffusion, PINNs can provide highly detailed simulations that aid in the design of catalysts, the optimization of pollution control techniques, and advancements in materials science. This coupling allows engineers and researchers to predict the behavior of chemical species in real time, ensuring that reactors operate at peak efficiency and reducing energy consumption in industrial processes.

The potential applications of PINNs extend far beyond chemical engineering. In the realm of aerospace, PINNs are revolutionizing the design and simulation of hypersonic flows, which are characterized by extremely high speeds and non-equilibrium thermodynamic conditions. Traditional Computational Fluid Dynamics (CFD) methods often struggle to accurately model such flows due to their complexity and the turbulent interactions between pressure, temperature, and chemical reactions. PINNs, on the other hand, excel in capturing these interactions with extraordinary precision, making them an invaluable tool for hypersonic flight design (Hao et al. [2023]). By enabling more accurate simulations, PINNs help ensure the development of safer, more efficient aerospace vehicles and propulsion systems, ultimately accelerating the advancement of next-generation aerospace technologies (Zanardi et al. [2022, 2023]).The ability to infer the missing fields will be evaluated for:

Case 1: Complete data

In this case, full data of ρ, υ, ν are available, thus the total loss function has the form:

$$\mathcal{L} = \underbrace{\frac{1}{N_s} \sum_{i \in \Omega_s} [(\rho_i - \rho_i^*)^2 + (u_i - u_i^*)^2 + (v_i - v_i^*)^2]}_{\text{Data loss}} + \underbrace{\frac{1}{N_c} \sum_{i \in \Omega_c} |e_i|^2}_{\text{Physics loss}}. \tag{31}$$

Case 2(a): Missing perturbation velocity

$$\mathcal{L} = \frac{1}{N_s} \sum_{i \in \Omega_s} [(\rho_i - \rho_i)^2 + (v_i - v_i)^2] + \frac{1}{N_c} \sum_{i \in \Omega_c} |e_i|^2 \tag{32}$$

Case 2(b): Missing perturbation density

$$\mathcal{L} = \frac{1}{N_s} \sum_{i \in \Omega_s} [(u_i - u_i)^2 + (v_i - v_i)^2] + \frac{1}{N_c} \sum_{i \in \Omega_c} |e_i|^2 \tag{33}$$

Case 2(c): Sparse data of p

$$\mathcal{L} = \frac{1}{N_s} \sum_{i \in \Omega_s} [(u_i - u_i)^2 + (v_i - v_i)^2] + \frac{1}{N_c} \sum_{i \in \Omega_c} |e_i|^2 \tag{34}$$

Case 3: Numerical schlieren data

$$\mathcal{L} = \frac{1}{N_s} \sum_{i \in \Omega_s} \left[\left(\frac{\partial \rho_i}{\partial y} - \frac{\partial \rho_i^*}{\partial y} \right)^2 + (u_i - u_i^*)^2 + (v_i - v_i^*)^2 \right] + \frac{1}{N_c} \sum_{i \in \Omega_c} |e_i|^2. \tag{35}$$

Instability-wave prediction in hypersonic boundary layers with physics-informed neural operators (Hao et al. [2023]).

Beyond their applications in catalysis and aerospace, PINNs are also making significant strides in the modeling of complex polymer systems and multi-component materials. In polymerization processes, where molecular interactions at both micro and macro scales govern the behavior of materials, PINNs offer a powerful framework for simulating these intricate processes (Lin and Yu [2022]). This capability is essential for controlling the synthesis of polymers and designing advanced materials with tailored properties. PINN's flexibility and ability to handle high-dimensional, stiff systems make them particularly suited for complex environmental modeling, reactor design, and sustainable material development (Chen et al. [2023]). Their ability to balance accuracy with computational efficiency opens up new avenues for solving challenges that were once computationally prohibitive.

Despite their transformative potential, PINNs face several challenges, particularly in training. The process often requires extensive hyperparameter tuning and sophisticated strategies to balance competing phenomena in multi-physics problems. High-dimensional systems can also lead to overfitting, where the model performs well on training data but fails to generalize to new situations. To address these issues, researchers are employing adaptive training techniques, improved initialization methods, and the integration of domain-specific knowledge (Krishnapriyan et al. [2021]). These strategies help guide the training process, enhancing the stability and reliability of the model while ensuring that it delivers accurate solutions across a wide range of applications.

The advantages of PINNs over traditional methods are significant and far-reaching. One of the most compelling aspects of PINNs is their ability to drastically reduce computational costs. In fields like chemical engineering and fluid dynamics, PINNs have been shown to outperform conventional CFD approaches, especially in high-stakes scenarios such as turbulent reacting flows (Liu et al. [2024]). In many cases, PINNs can achieve accuracy within 5% of ground truth data while completing simulations orders of magnitude faster. This makes them invaluable tools for real-time decision-making, where speed and accuracy are paramount. By integrating new innovations such as PI-DeepONets and microkinetic modeling, PINNs are further enhancing their ability to tackle nonlinear, multi-parameter systems with greater ease (Frankel et al. [2024]).

PINNs are not just reshaping individual domains—they are bridging the gap between machine learning and physical laws, leading to a paradigm shift in how we approach computational modeling. Their ability to model complex, high-dimensional systems with speed and precision is transforming industries ranging from chemical engineering to aerospace. As PINNs continue to evolve and improve, their applications will expand, driving further advancements in efficiency, sustainability, and technological progress. In the future, PINNs could become an essential tool in nearly every scientific and industrial domain, offering faster, more accurate, and more reliable simulations that will help solve some of the world's most pressing challenges.

Physics-Informed Neural Networks, and particularly their advanced form in PI-DeepONets, are poised to revolutionize computational modeling across a broad spectrum of scientific fields. By embedding physical laws directly into the neural network architecture, PINNs offer a powerful approach to solving complex, high-dimensional problems that were once deemed too computationally intensive. Their applications in catalysis, aerospace, polymer science, and beyond highlight their transformative potential, offering solutions that are faster, more accurate, and more sustainable (Branca and Pallottini [2022]). As research into PINNs continues to advance, these models will undoubtedly become a significant contributing factor in the future of scientific and industrial innovation, driving progress across numerous fields of study and application.

8 Polymer and Complex System Modeling

The integration of Physics-Informed Neural Networks (PINNs) into polymer and complex system modeling represents a groundbreaking advancement in material science and engineering. PINNs uniquely blend deep learning techniques with the fundamental laws of physics, offering a powerful framework that enables the accurate simulation, optimization, and understanding of complex, multi-scale phenomena (Raissi et al. [2019]). This innovative approach has been transformative, allowing researchers to explore and solve problems that were previously intractable or computationally expensive using traditional methods.

Historically, complex systems in polymer science and material engineering were modeled using conventional numerical techniques such as finite element methods (FEM) and finite difference methods (FDM). While these approaches have been invaluable, they often fall short when dealing with high-dimensional partial differential equations (PDEs) and multi-scale phenomena, which are inherent in polymer systems. These challenges arise from the need to account for both macroscopic properties, like material strength and flexibility, and microscopic interactions, such as molecular dynamics and chemical bonding. Traditional methods are typically resource-intensive and computationally prohibitive, especially when simulating long-term processes or large systems with complex geometries. PINNs address these challenges by embedding physical laws directly into the neural network architecture, ensuring that the models not only learn from data but also respect conservation laws, boundary conditions, and system dynamics.

One of the standout features of PINNs is their ability to embed physics-based constraints, such as conservation of mass, energy, and momentum, directly into the training process. This enables accurate simulations of dynamic systems, including multi-component polymer systems where chemical reactions like polymerization and physical processes such as phase separation occur simultaneously. Advanced loss functions further enhance this capability by capturing the interplay between chemical and physical phenomena, as demonstrated in applications like the Gray-Scott reaction-diffusion model, showcasing PINNs' power in solving nonlinear, multi-dimensional problems across various domains (Giampaolo et al. [2022]).

1D GRAY SCOTT SYSTEMS:

In these cases, the loss functions is composed by two terms

$$\mathcal{L} = \omega_B \mathcal{L}_B + \omega_F \mathcal{L}_F \tag{36}$$

where L_F represents the loss component related to the dynamics and LB represents the loss component related to the initial/boundary conditions. The two terms can be written as follows:

$$\mathcal{L}_{\mathcal{B}} = \frac{1}{N_0} \sum i = 1^{N_0} ||\hat{u}(0, x_i) - h_0||^2 + \frac{1}{N_B} \sum_{i=1}^{N_B} ||\hat{u}(t, x_i) - h_B||^2 \tag{37}$$

$$\mathcal{L}_f = \frac{1}{N}\sum_{i=1}^{N}\left(||f_1((t,x)_i)||^2 + ||f_2((t,x)_i)||^2\right), \tag{38}$$

2D GRAY-SCOTT SYSTEM:

In the case under consideration the loss function consists of three terms: the first one is related to the initial conditions and to the boundary conditions, the second one relates to the dynamics of the system, and the third computes the error with respect to known data points:

$$\mathcal{L} = \omega_B \mathcal{L}_{\mathcal{F}} + \omega_{data}\mathcal{L}_{data} \tag{39}$$

each of the aforementioned components can be written as:

$$\mathcal{L}B = \frac{1}{N_0}\sum i = 1^{N_0}||\hat{u}(t,x,y)|t = 0 - h0, i||^2 + \frac{1}{N_b}\sum_{i=1}^{N_b}||\hat{u}(t,x,y)|x \in \partial\Omega - hB, i||^2 \tag{40}$$

$$\mathcal{L}_F = \frac{1}{N_f}\sum_{i=1}^{N_f}\left(||f_1((t,x,y)_i)||^2 + ||f_2((t,x,y)_i)||^2\right) \tag{41}$$

$$\mathcal{L}_{data} = \frac{1}{N_{data}}\sum_{i=1}^{N_{data}}||\tilde{u}((t,x,y)i) - h_{data,i}||^2 \tag{42}$$

Physics-informed neural networks approach for 1D and 2D Gray-Scott systems (Giampaolo et al. [2022]).

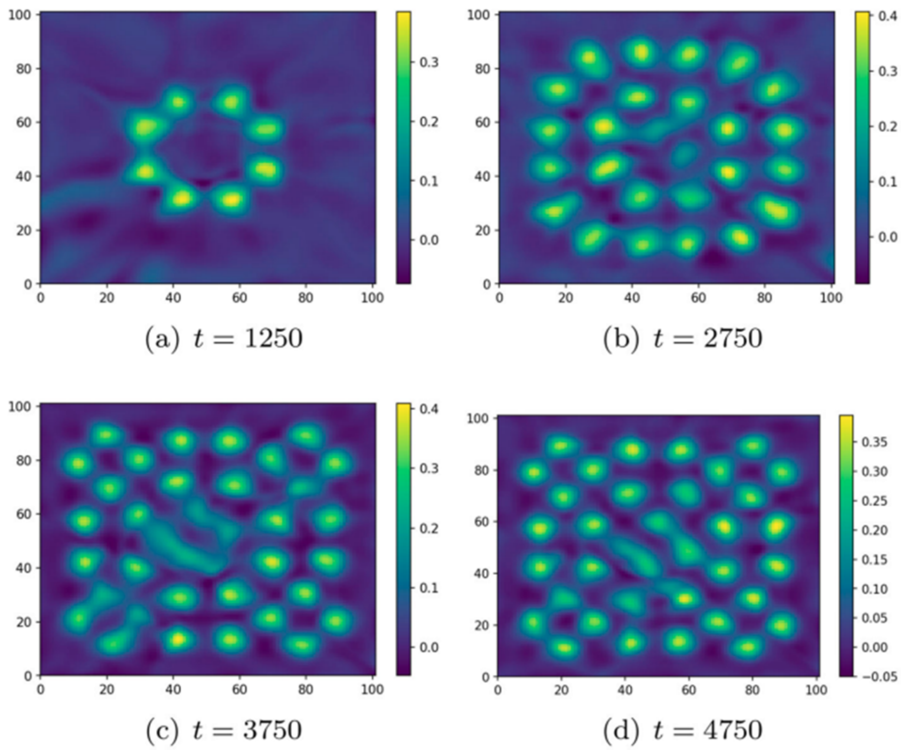

Figure 18: Example of Mitosis patterns. The parameters used in the (3) are F = 0.028 and K = 0.062. The times shown are: t = 1250, 2750, 3750, 4750 (Giampaolo et al. [2022])

Automatic differentiation, a technique used in neural networks to compute gradients efficiently, has also played a pivotal role in enhancing the computational efficiency of PINNs. By enabling the seamless calculation of gradients even through deep and complex neural network architectures, automatic differentiation allows PINNs to handle the high-dimensional PDEs that govern polymer systems. This capability ensures that PINNs can model multi-scale phenomena, bridging the gap between microscopic processes, such as molecular interactions, and macroscopic material properties, like strength, elasticity, and conductivity. The ability to solve these complex equations with fewer computational resources and faster convergence times makes PINNs highly advantageous over traditional numerical methods, especially for real-time applications such as material design and process optimization.

In addition to automatic differentiation, pretraining strategies have further enhanced the performance of PINNs. These strategies use data from traditional numerical methods like FEM or FDM as a starting point for training the neural networks. By leveraging this a priori knowledge, PINNs can converge more quickly and achieve higher accuracy, particularly when dealing with problems that involve complex geometries or dynamic boundary conditions. This combination of physics-informed constraints and data-driven learning provides a robust foundation for solving real-world problems in polymer science and material engineering.

In the field of polymer science, PINNs have shown tremendous promise in modeling and predicting the behavior of polymer blends, including phase separation, morphology, and interactions between different polymer components. These systems, often characterized by highly nonlinear behavior, pose significant challenges to traditional computational approaches. However, by leveraging the power of PINNs, researchers can accurately predict how different chemical species within a polymer blend will affect its phase behavior and mechanical properties. This has far-reaching implications for the design and optimization of advanced materials, such as lightweight composites for aerospace applications, biodegradable plastics for environmental sustainability, and polymers for biomedical uses.

One of the key applications of PINNs in polymer science is the modeling of block copolymers. Block copolymers are materials made up of two or more chemically distinct polymer blocks, and they have the unique ability to self-assemble into highly organized structures, such as lamellae, cylinders, or spheres. Understanding and controlling this self-assembly process is critical for designing materials with precise, tunable properties for a wide range of applications, including nanotechnology, photonics, and biomedical engineering. PINNs have been instrumental in solving the reaction-diffusion equations that govern the behavior of block copolymers, enabling researchers to predict and optimize self-assembled morphologies. This is essential for the fabrication of nanoscale devices, drug delivery systems, and photonic crystals, where the precise control of morphology is crucial to achieving desired functionalities (Lin and Yu [2022]).

Beyond modeling static properties, PINNs have also made significant strides in the simulation of dynamic polymerization processes. These processes, which are central to the synthesis of polymer materials, often involve complex reaction networks with multiple components and nonlinear interactions. Traditional numerical methods struggle to handle the computational demands of these systems, particularly when real-time predictions are required. However, PINNs have demonstrated the ability to efficiently and accurately model these dynamics. For instance, PINNs have been used to study controlled radical polymerization, a process in which the polymerization rate is carefully controlled through reversible termination steps. By modeling these processes, PINNs provide valuable insights into the kinetics of polymerization, molecular weight distribution, reaction rates, and other critical parameters. This knowledge is essential for the design of high-performance materials with well-defined molecular architectures and tailored properties.

Furthermore, PINNs have been applied to predict the mechanical, thermal, and optical properties of polymer materials. By combining physics-based models with data-driven approaches, PINNs allow for the optimization of polymer composites for specific applications, such as in the automotive, aerospace, medical, and consumer electronics industries. These materials must meet stringent requirements for reliability and durability, often under extreme environmental conditions. PINNs can simulate how materials respond to stress, temperature, and light, providing crucial insights that inform the design of next-generation polymer materials.

Despite the considerable advantages of PINNs, there remain challenges in applying them to complex systems, especially in polymer science. High-dimensional PDEs, multi-scale phenomena, and sparse data availability can complicate the training process. To overcome these challenges, researchers have employed several innovative strategies. Transfer learning, for example, allows PINNs to leverage knowledge gained from similar systems to accelerate the training process. By fine-tuning pretrained models for specific tasks, PINNs can adapt more quickly to new problems. Adaptive learning rates and advanced optimization techniques, such as stochastic gradient descent with warm restarts, have also been used to enhance convergence stability and avoid local minima.

Regularization techniques like weight decay and early stopping have been essential in preventing overfitting, ensuring that the models generalize well to unseen data. Furthermore, incorporating domain-specific constraints into the loss function ensures that the solutions respect the underlying physical principles, even in highly nonlinear systems. These strategies collectively help address the computational and methodological challenges inherent in modeling complex systems with PINNs.

Compared to traditional numerical methods, PINNs offer numerous advantages. They are computationally efficient, require less time and resources to generate accurate results, and integrate physical laws directly into the training process. This integration ensures that the predictions made by PINNs are physically consistent and adhere to fundamental conservation principles, making them more reliable for solving multi-physics problems. Moreover, the ability of PINNs to handle multi-scale phenomena, complex geometries, and dynamic boundary conditions makes them a superior tool for polymer science and engineering, offering a new paradigm for material design, optimization, and process modeling.

PINNs are revolutionizing the way researchers model and design advanced materials. By leveraging the power of deep learning and physics-based constraints, PINNs have the potential to solve some of the most challenging problems in polymer science and complex system modeling. As the technology continues to evolve PINNs will be enabling the design of next-generation materials with tailored properties for a wide range of applications. Through continued innovation and refinement, PINNs are set to become an indispensable tool for researchers and engineers working to create the materials of tomorrow.

9 Miscellaneous Applications of PINNs

The novel approach of PINNs has garnered increasing attention in a broad spectrum of scientific and engineering fields, ranging from chemistry and physics to bioengineering, materials science, and environmental science (Raissi et al.

[2019]). The reason for this rapid adoption lies in the ability of PINNs to embed physical laws—such as conservation of mass, energy, and momentum—directly into the architecture of neural networks. This integration allows PINNs to not only produce accurate and reliable predictions but also to ensure that those predictions are consistent with real-world phenomena, even when dealing with limited or noisy data. The incorporation of first-principles knowledge into the machine learning framework significantly reduces the need for extensive datasets, making it possible to generalize effectively across various complex systems. This ability is particularly important when traditional computational methods struggle with systems that are computationally expensive or difficult to model with conventional techniques.

PINNs have proven especially adept at modeling complex systems involving interacting subsystems, which is a common characteristic of many real-world phenomena. For example, Partially Connected Recurrent Neural Networks (PCRNNs) enhance PINNs by introducing process-structure knowledge that allows the model to account for high-dimensional interactions across multiple subsystems. This approach is crucial in tackling systems such as chemical reactors, where feedback mechanisms and intricate interactions between different components need to be captured. Similarly, environmental systems with interconnected biogeochemical processes can be modeled efficiently with PCRNNs, providing detailed and computationally feasible predictions of system behavior. These innovations have significantly expanded the versatility of PINNs, making them applicable to a wider range of scientific challenges, from industrial applications to environmental monitoring.

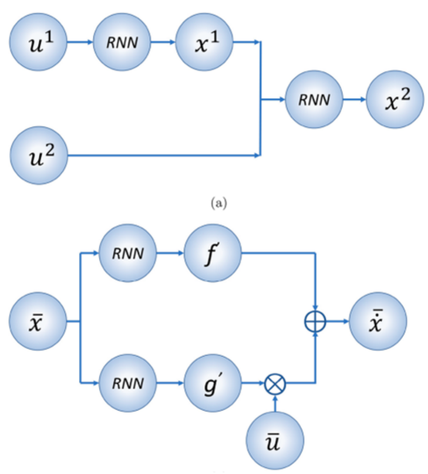

Figure 19: Structure of a partially connected RNN and a RNN model developed in the form of control-affine systems (Xiao and Wu [2023])

One of the most significant applications of PINNs is in solving ordinary differential equations (ODEs) and partial differential equations (PDEs). These equations are central to many scientific disciplines, including astrophysics, materials science, and environmental science. In astrophysics, for instance, PINNs have been employed to model the chemical and thermal evolution of the Interstellar Medium (ISM), offering insights into the processes that drive the formation of stars and planetary systems (Branca and Pallottini [2022]). By taking initial conditions such as density and temperature, PINNs are able to simulate the evolution of these variables over time, providing valuable predictions for astronomical phenomena. Likewise, in environmental science, PINNs have been applied to model the dispersion of pollutants in air and water, solving complex transport and reaction equations. By integrating real-time sensor data into these models, PINNs can predict pollutant dispersion under varying environmental conditions, assisting in the development of strategies for mitigating the effects of pollution.

In materials science, PINNs play a crucial role in predicting phase transitions and the formation of crystalline structures under different thermodynamic conditions. These capabilities are instrumental in the design and optimization of advanced materials such as catalysts, polymers, and superconductors, which require tailored properties for specific applications. By simulating how materials behave under various conditions, PINNs help scientists understand the underlying mechanisms governing material properties and phase behavior, paving the way for the development of new materials with enhanced performance characteristics. For example, PINNs have been used to predict the behavior of polymer blends, aiding in the design of lightweight composites for aerospace applications or biodegradable plastics for environmental sustainability.

As the applications of PINNs continue to grow, the methods used to improve their efficiency and accuracy have evolved significantly. One of the key advancements in this field is the Deep Galerkin Method (DGM), which has made it possible to solve high-dimensional PDEs more efficiently (Giampaolo et al. [2022]). By incorporating adaptive activation functions, annealing learning rates, and optimization algorithms like ADAM, DGM improves the accuracy and robustness of PINNs in solving complex equations. This is especially important when dealing with high-dimensional variables, which are often difficult for traditional numerical methods such as finite element or finite difference methods to handle. As a result, PINNs can be applied to even more complex systems that involve numerous interacting variables, such as those encountered in bioengineering.

Bioengineering has benefited greatly from the integration of PINNs, particularly in modeling complex biological and physiological processes. PINNs have been used to model drug delivery systems, tissue regeneration processes (Chen et al. [2023]), and the interactions between various biochemical components. These models solve reaction-diffusion equations that describe the movement of molecules within biological systems, providing insights into the dynamics of processes such as drug distribution or tissue healing. By improving the accuracy of these models, PINNs enable the optimization of therapeutic strategies and the design of advanced medical treatments, such as personalized drug delivery systems or regenerative medicine.

Despite their many advantages, the application of PINNs is not without challenges (Krishnapriyan et al. [2021]). One of the key difficulties lies in modeling highly nonlinear systems, where small changes in input parameters can lead to large and unpredictable changes in the output. Additionally, dealing with sparse or noisy datasets can be problematic, as it can reduce the accuracy and stability of the network. To address these challenges, several strategies have been proposed. Hybrid models that combine PINNs with traditional numerical methods, such as finite element or finite difference techniques, offer a way to improve the stability and accuracy of the results. Pretraining PINNs using data from traditional simulations has also proven effective in enhancing convergence rates, especially when the available data is limited or noisy.

Furthermore, adaptive training techniques such as adaptive activation functions and annealing learning rates have been used to improve the efficiency of PINNs, allowing them to handle more complex problems. These techniques help the network avoid common pitfalls such as slow convergence or overfitting, ensuring that the PINNs are able to generalize effectively to unseen data. Additionally, regularization methods like weight decay and early stopping can be used to prevent overfitting, further enhancing the robustness of PINNs.

The computational advantages of PINNs over traditional methods are substantial, particularly in fields like environmental science (Serebrennikova et al. [2024]) and materials engineering. PINNs require less time and computational resources to solve complex problems, making them more efficient than conventional methods. They also offer the advantage of being able to integrate domain-specific knowledge directly into the learning process. This enables PINNs to provide solutions that not only adhere to physical laws but also remain interpretable and reliable. In fields like environmental modeling, where real-time data integration is crucial, this feature is particularly valuable. In materials science, PINNs have enabled faster and more accurate discovery of materials with tailored properties, while in astrophysics, they have led to breakthroughs in understanding the formation and evolution of celestial bodies.

Physics-Informed Neural Networks represent a paradigm shift in the way we approach computational modeling. By combining the power of machine learning with the rigor of physical laws, PINNs offer a powerful tool for solving complex, high-dimensional problems across a wide range of scientific and engineering disciplines. As the field continues to evolve, PINNs are expected to drive significant advancements in fields such as environmental science, materials engineering, bioengineering, and astrophysics. With their ability to provide accurate, interpretable, and reliable predictions while adhering to physical principles, PINNs are poised to transform the landscape of computational science, offering new solutions to some of the most challenging problems in modern science and engineering.

10 Addressing limitations of PINNs

Physics-Informed Neural Networks (PINNs) are a promising tool for solving complex problems governed by physical laws, particularly in the realm of partial differential equations (PDEs) (Raissi et al. [2019]). While they offer significant advantages in terms of embedding domain-specific knowledge into the architecture of neural networks, their transition from theoretical frameworks to practical, real-world applications is hindered by several substantial challenges. These challenges, which stem from both the nature of the problems they aim to solve and the inherent limitations of current neural network architectures, must be addressed for PINNs to achieve widespread adoption and further advance the field (Krishnapriyan et al. [2021]).

One of the most pressing challenges in the deployment of PINNs is the training complexity associated with embedding physical laws into neural network architectures. The very feature that sets PINNs apart from traditional neural networks—their ability to incorporate domain-specific knowledge through the inclusion of governing equations, such as PDEs—also presents a significant computational bottleneck (Hao et al. [2023]). In particular, the process of computing the PDE residuals and enforcing boundary conditions is computationally expensive and often becomes a limiting factor, especially when dealing with high-dimensional systems. As the complexity of the underlying physical system increases, so too does the computational burden, making it increasingly difficult to scale PINNs to tackle more intricate problems in areas such as fluid dynamics, material science, and climate modeling (Zhang et al. [2024]). To overcome this, recent research has focused on developing more efficient algorithms that can reduce the computational cost of training. Additionally, parallel computing strategies, such as multi-GPU setups or distributed computing environments, are being explored to accelerate training processes and make them more feasible for large-scale systems. These advancements in computational techniques are critical for enabling PINNs to handle the demands of high-dimensional systems, offering the potential for solving more complex and realistic physical problems.

Another significant hurdle in the practical application of PINNs is their sensitivity to hyperparameter tuning. Like traditional neural networks, the performance of PINNs is highly dependent on the choice of architecture, activation functions, learning rates, and other hyperparameters. However, unlike standard machine learning models, the process of selecting these hyperparameters for PINNs is more nuanced due to the additional layer of physical constraints that must be integrated into the model. The tuning of these hyperparameters often requires significant experimentation, as there is no one-size-fits-all approach, and the optimal configuration can vary greatly depending on the specific problem at hand. This trial-and-error nature of hyperparameter selection can make the development of PINNs both time-consuming and resource-intensive. To mitigate this issue, researchers are increasingly turning to automated hyperparameter tuning methods, such as Bayesian optimization and reinforcement learning-based strategies. These methods aim to streamline the hyperparameter optimization process, reducing the need for manual intervention and enabling more efficient exploration of the hyperparameter space. By automating the tuning process, PINNs can be more easily adapted to different physical problems, improving both their efficiency and accuracy.

A more fundamental limitation of PINNs lies in their reliance on the accuracy and completeness of the governing physical equations that are embedded in the model. While PINNs are designed to work by incorporating known physical laws, they are inherently limited by the accuracy of the equations used. In many fields, especially those involving complex phenomena such as turbulence, chemical reactions, or biological processes, the underlying physical models may be incomplete, poorly characterized, or even approximate. This can lead to unreliable predictions, as the model is essentially constrained by the fidelity of the physical laws it encodes. Furthermore, the presence of incomplete or noisy data exacerbates this issue, as it can lead to incorrect boundary conditions or inaccurate representations of physical behavior. To address these challenges, researchers are exploring techniques such as uncertainty quantification and adaptive modeling. Uncertainty quantification involves incorporating uncertainty into the PINN framework, allowing the model to account for and propagate errors in the governing equations. Adaptive modeling, on the other hand, aims to dynamically adjust the model's complexity based on the available data, ensuring that PINNs remain robust even in the face of gaps or inaccuracies in the theoretical framework. These approaches are critical for ensuring that PINNs remain effective in fields where the underlying physics are not fully understood or are subject to frequent revisions.

Despite these challenges, the field of PINNs is advancing rapidly. Researchers are actively addressing the computational, architectural, and theoretical limitations that hinder their practical application. By developing more efficient algorithms, automating hyperparameter tuning, and incorporating techniques for handling uncertainty and incomplete models, the scientific community is steadily overcoming the barriers to widespread use. As these obstacles are mitigated, PINNs are poised to play an increasingly important role in solving complex real-world problems across a wide range of scientific and engineering disciplines. The continued refinement of these models will ultimately expand the scope of problems that can be tackled, paving the way for their broader application in areas such as climate modeling, materials science, and biomedical engineering (Serebrennikova et al. [2024], Lin and Yu [2022], Chen et al. [2023]).

11 FUTURE DIRECTIONS

The future of Physics-Informed Neural Networks (PINNs) in chemistry is marked by immense potential, with researchers exploring novel methods to enhance their capabilities and broaden their applicability. One promising direction is the integration of experimental data into PINN frameworks. Traditionally, PINNs rely heavily on theoretical formulations or simulations, which can sometimes be limited by incomplete or uncertain governing equations. By combining sparse, high-fidelity experimental datasets with PINNs, researchers can significantly improve model accuracy and reliability. This hybrid approach enables the simulation of systems where the underlying physics is not fully understood, making it particularly valuable in fields like reaction kinetics and catalytic processes (Sun et al. [2023], Ji et al. [2021]). By leveraging empirical insights, PINNs can bridge gaps in theoretical knowledge, ensuring simulations align closely with real-world behavior and providing more accurate predictions for complex chemical systems.

Another transformative area is the application of PINNs in multi-scale modeling. Chemical systems often operate across diverse scales, from the molecular to the macroscopic. PINNs can unify these scales into a single model, offering a comprehensive understanding of phenomena like chemical reactions, phase transitions, and transport mechanisms. For instance, PINNs could connect molecular dynamics simulations to the behavior of industrial reactors, providing holistic insights crucial for process optimization (Zhang et al. [2024], Xiao and Wu [2023]) . This capability is especially impactful in industries like pharmaceuticals, energy, and materials science, where multi-scale interactions play a vital role in innovation. By incorporating data from multiple scales, PINNs offer unparalleled opportunities to study and optimize complex systems, paving the way for more efficient and sustainable chemical processes.

The incorporation of uncertainty quantification (UQ) into PINNs represents another critical advancement. Chemical simulations often involve inherent uncertainties in parameters such as reaction rates or material properties. By integrating Bayesian frameworks and probabilistic modeling, PINNs can not only provide predictions but also quantify the confidence in those predictions (Chen et al. [2024]). This capability is essential in high-stakes scenarios, such as the design of chemical processes or environmental modeling, where variability can significantly impact outcomes. UQ methods enhance the reliability of PINN-based models, enabling better risk assessments and more informed decision-making. This approach ensures that PINNs remain robust and dependable tools for tackling real-world chemical challenges.

Advancements in training algorithms are also addressing longstanding hurdles in PINN development. Techniques like adaptive loss weighting, which dynamically adjusts the importance of different loss function components during training, help focus on the most critical aspects of the system, improving both efficiency and accuracy (Krishnapriyan et al. [2021]). Similarly, curriculum learning, where models are trained progressively on increasingly complex problems, enhances convergence rates and performance. These innovations are particularly valuable for stiff or multi-scale systems, ensuring that PINNs can effectively model even the most challenging chemical scenarios.

Hybrid approaches are further expanding the applicability of PINNs. By combining PINNs with traditional numerical methods, such as finite element analysis or molecular dynamics simulations, researchers can harness the strengths of both techniques to address complex, multi-faceted problems (Frankel et al. [2024]). These hybrid models are particularly useful in fields like catalysis and materials science, where high-fidelity simulations and empirical data are often needed. Such frameworks enhance the robustness and efficiency of PINNs, enabling their application to a broader range of chemical domains.

Looking to the future, PINNs are poised to make significant contributions to frontier areas like quantum chemistry and nanotechnology. In quantum chemistry, PINNs offer efficient approximations of complex quantum mechanical systems, facilitating the study of molecular interactions and reaction pathways (Raissi et al. [2019]). In nanotechnology, PINNs can model and optimize nanoscale systems, enabling breakthroughs in drug delivery, sensor design, and next-generation electronics. By tackling challenges at these frontiers, PINNs have the potential to revolutionize how we understand and manipulate chemical systems at the smallest scales.

Overall, the future of PINNs in chemistry is bright, with advancements in experimental integration, multi-scale modeling, uncertainty quantification, training algorithms, and hybrid approaches driving their evolution. These developments not only address current limitations but also unlock new opportunities, positioning PINNs as transformative tools for innovation in computational chemistry and beyond.

12 Conclusion

Physics-Informed Neural Networks (PINNs) represent a paradigm shift in computational chemistry by seamlessly integrating physical laws with machine learning frameworks. This survey has highlighted their transformative potential in addressing a wide range of chemical problems, from reaction kinetics to complex multi-scale systems. PINNs not only reduce computational costs but also enhance the accuracy and adaptability of models in real-world applications, making them invaluable tools for researchers and industry practitioners alike.

Despite their success, challenges such as computational intensity, hyperparameter optimization, and reliance on well-defined governing equations remain barriers to their broader adoption. Solutions like transfer learning, multi-fidelity modeling, and hybrid approaches hold promise for overcoming these limitations, paving the way for more robust and efficient PINN-based methodologies.

Looking forward, the integration of experimental data and advancements in uncertainty quantification will further strengthen PINN applications, ensuring their reliability and precision in practical settings. Additionally, their potential to tackle frontier areas such as quantum chemistry, nanotechnology, and molecular dynamics opens new doors for innovation, expanding the scope of PINNs in solving the most pressing challenges in chemistry.

By consolidating existing research and identifying key opportunities for growth, this survey serves as a valuable resource for researchers and practitioners aiming to leverage PINNs in their work. As the field continues to evolve, PINNs are poised to play a central role in advancing computational chemistry, contributing to deeper insights, more efficient solutions, and groundbreaking discoveries in the years to come.

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