

AI Methods, Especially Neural Networks (Like Physics-Informed Neural Networks, Pinns), Can Approximate Solutions to Complex ODEs/PDEs That Are Hard to Solve Analytically

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Abstract: Physics-Informed Neural Networks for Complex System Modeling Traditional numerical methods (e.g., Finite Element Method, Finite Difference Method) for solving complex ordinary and partial differential equations (ODEs/PDEs) often struggle with high-dimensional problems, irregular geometries, and inverse modeling, requiring extensive mesh generation and data. In this work, we present a Physics-Informed Neural Network (PINN) approach that offers a robust, mesh-free alternative to approximate solutions for complex, non-linear governing equations. By embedding the underlying physical laws—represented as differential equations—directly into the neural network's loss function, we enforce adherence to physical principles without the need for large, labeled datasets. Using automatic differentiation, the PINN architecture minimizes residuals of the differential equations, boundary conditions, and initial conditions simultaneously. Numerical experiments demonstrate that our proposed method successfully approximates complex solutions, showcasing strong generalization, efficiency in solving ill-posed inverse problems, and accuracy comparable to traditional solvers, even with sparse data.

Keywords -- Physics-Informer Neural Networks(PINNs), deep learning for scientific computing, mesh-free methods, residual-based optimization, and hybrid scientific computing.

I INTRODUCTION

Artificial Intelligence (AI) methods, particularly neural networks, have emerged as powerful tools for approximating solutions to complex differential equations. Among these approaches, Physics-Informed Neural Networks (PINNs) have gained significant attention. PINNs leverage the structure of the underlying physical laws— encoded as ordinary

differential equations (ODEs) or partial differential equations (PDEs)—to guide the training of neural networks. This allows them to approximate solutions even in cases where analytical methods are intractable or traditional numerical technique become computationally expensive. By integrating physical principles directly into the learning process, PINNs offer a flexible and efficient framework for tackling challenging problems in science and engineering.

II PHYSICS INFORMER NEURAL NETWORKS

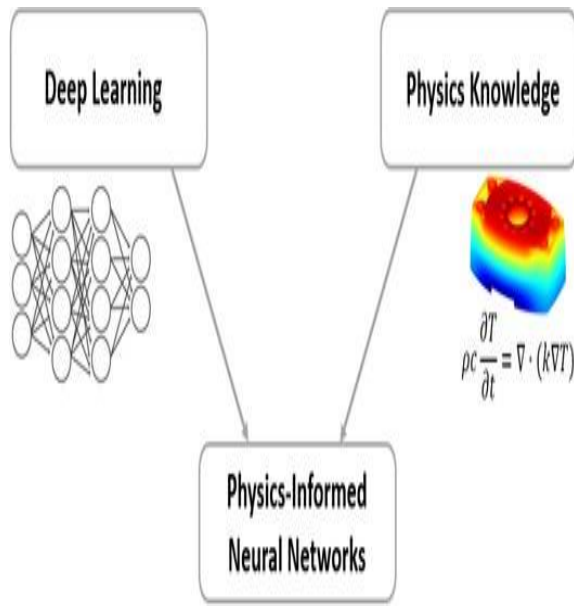
Physics-informed neural networks (PINNs) are neural networks that incorporate physical laws described by differential equations into their loss functions to guide the learning process toward solutions that are more consistent with the underlying physics. PINNs can be used to:

- Approximate solutions to partial differential equations(PDEs) and ordinary differential equations (ODEs).
- Solve inverse problems, such as estimating model parameters from limited data.

With Deep Learning Toolbox™, you can build and train PINNs, which enable rapid predictive analysis. You can integrate PINNs with MATLAB and Simulink for system-level simulation, control design, and design optimization.

III DEEP LEARNING FOR SCIENTIFIC COMPUTING

Scientific computing and numerical analysis Scientific Computing and Numerical Analysis are branches of applied mathematics that focus on the development and analysis of numerical algorithms for solving problems in continuous



IV. RESIDUAL BASED OPTIMIZATION

Residual-based optimization is an advanced technique in numerical simulation, machine learning, and signal processing that focuses on minimizing the residual—the difference between a predicted, approximated, or measured value and the true underlying function or ground truth. Instead of just optimizing the primary output, this method actively optimizes the error map(residual)to enhance accuracy, improve stability, and speed up convergence.

It is widely applied in complex scenarios, such as limited-angle CT reconstruction, PDE solving, and robust AI model training. Residual-Based Optimization Residual Representation: Defining the residual as the error between the current approximation and the desired target.

Adaptive Learning: Utilizing residual information to guide the learning process or to change the structure of the solution (e.g., in RBF neural networks). Alternative Optimization Domain: Often, the optimization runs in both the original domain (image or signal) and the residual domain to ensure better constraint satisfaction. Y brid scientific computing integrates diverse computing paradigms—such as quantum- classical, CPU-GPU, or AI-physics models—to enhance simulation accuracy and speed. These systems leverage specialized accelerators (like GPUs or QPUs) alongside traditional HPC for complex tasks, ranging from molecular modeling to climate simulations, offering superior speed and precision.

Key Types of Hybrid Scientific Computing:

Quantum-Classical Computing: Combines classical High-Performance Computing (HPC) with Quantum Processing Units (QPUs). The QPU handles specific hard, complex tasks (e.g., optimization, molecular modeling),while the CPU/GPU handles data pre-processing and management, sometimes referred to as quantum-centric supercomputing.

CPU+ GPU Co-processing: Leverages high-performance CPUs and GPUs in tandem. This setup is common for accelerating computational fluid dynamics and imaging tasks, utilizing parallel processing power to solve large data sets,.

AI and Physics-Based Modeling: Combines machine learning (data-driven models) with traditional simulation (first-principles modeling). This hybrid approach blends the speed of AI with the accuracy of physics, crucial for

Hybrid Infrastructure (HPC/Cloud/Grid): Combines on-premise clusters with cloud resources (e.g., AWS, Azure) to handle fluctuating workloads and provide scalable computing, a concept known as" Elastic Clusters, "according to Science Direct.

V CONCLUSION

- **Physics-Aware Learning:** PINNs minimize a loss function comprising both data mismatch and PDE residual, ensuring the solution adheres to physical principles rather than just fitting data.

mathematics, such as PDEs. Scientific Computing & Numerical Analysis “The study of numerical algorithms for the problems of continuous mathematics” NLA Diff Eqns Optim Sys of Eqns $Ax = b$, A sq Least Squares $\|Ax - b\|$, A rect Eigs & SVD $Ax = \lambda x$ ODEs $-u'' = f$ PDEs $u_t = u_{xx}$ Convex $\inf_{x \in \mathbb{R}^n} c^T x$ Non convex $\inf_{x \in \mathbb{R}^n} f(x)$ When a PDE is linear, This creates a natural connection between PDEs and Numerical Linear Algebra (NLA). Linear PDE Linear Algebra discretize Sometimes, when an energy functional exists for a problem (e.g., PDEs with coercive bilinear forms like the Laplace equation), we can also apply optimization techniques to solve it effectively. A typical approach to solving nonlinear PDEs involves transforming the problem into a sequence of linear problems, through linearization and iteration. In this way, nonlinear PDEs are reduced to linear algebra problems. Nonlinear PDE Linear Algebra linearize + iterate discretize 2 Machine learning for scientific computing and numerical analysis SciML is a recent research field based on both machine learning and scientific computing. Its goal is the development of robust, efficient, and interpretable methods to solve problems in science and engineering, such as PDEs, parameter identification, or inverse problems. In SciML, a common approach to solving nonlinear PDEs starts with generating training data, typically using standard numerical solvers, where the training data consists of reference solutions. This data is then used to construct a cost function that quantifies the training error, while the solution or solution operator is discretized using a neural network. The goal is to minimize this cost function through optimization to learn the optimal network weights. Nonlinear PDE Optimization generate training data discretize This brings optimization back to the core of the numerical solutions of PDEs.

- **Handling Complexity:** They are particularly useful for complex, non-linear, or high-dimensional systems where traditional numerical solvers (e.g., Finite Element Method) struggle with meshing or high computational costs.
- **Inverse Problem Solver:** Beyond solving for unknown field variables (forward problems), PINNs are highly efficient at identifying unknown parameters, boundary conditions, or constitutive models from noisy, limited data.
- **Overcoming Data Scarcity:** By leveraging the inherent physics, PINNs require less labeled data to achieve reliable, interpretable approximations, mitigating over-fitting issues, notes this Taylor & Francis Online article.

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