AIJREAS VOLUME 10, ISSUE 4 (2025, APR) (ISSN-2455-6300)ONLINE
Anveshana's International Journal of Research in Engineering and Applied Sciences

RECENT ADVANCES IN COMPUTATIONAL FLUID DYNAMICS USING ARTIFICIAL INTELLIGENCE, MACHINE LEARNING, AND DEEP LEARNING: A COMPREHENSIVE REVIEW

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Abstract

The integration of Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) techniques with Computational Fluid Dynamics (CFD) represents a paradigm shift in fluid mechanics research and engineering applications. This comprehensive review examines recent advances from 2015 to 2025 in applying AI/ML/DL methodologies to enhance traditional CFD workflows across various domains, including turbulence modelling, heat transfer prediction, surrogate modelling, inverse design, and real-time flow control. The paper systematically analyses the fundamental concepts underlying these technologies, their specific applications in fluid dynamics problems, and the challenges associated with their implementation. Key findings indicate that physics-informed neural networks, convolutional neural networks, and reinforcement learning algorithms have demonstrated significant potential in accelerating CFD simulations while maintaining accuracy. However, challenges related to data quality, model interpretability, generalisation capabilities, and integration with high-performance computing platforms remain significant barriers to widespread adoption. The review concludes by emphasising future research directions, highlighting the need for interdisciplinary collaboration to develop robust, interpretable, and physically consistent AI-enhanced CFD frameworks that can revolutionise engineering design and optimisation processes.

Keywords: Artificial Intelligence, Computational Fluid Dynamics, Deep Learning, Digital Twins, Heat Transfer, Machine Learning, Turbulence Modelling

1. Introduction

Computational Fluid Dynamics (CFD) has long served as a cornerstone of engineering analysis and design, enabling the numerical simulation of fluid flow, heat transfer, and related phenomena across diverse applications. From aerospace engineering to biomedical devices, CFD provides critical insights that inform design decisions and optimise system performance. Traditional CFD approaches rely on solving the Navier-Stokes equations—partial differential equations that govern fluid motion—through numerical discretisation methods such as finite difference, finite volume, and finite element techniques. While these methods have proven remarkably successful, they face significant limitations including high computational costs, mesh sensitivity, and extensive data requirements.

The emergence of Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) has introduced transformative possibilities for fluid dynamics research and engineering applications. Machine learning offers an alternative framework by reframing fluid modelling as an optimisation problem. Rather than directly solving partial differential equations, ML models learn patterns from data and iteratively adjust parameters to minimise predefined loss functions . This data-driven approach proves particularly effective for mathematically intractable systems or those exhibiting behaviours difficult to capture through closed-form equations .

However, purely data-driven ML lacks inherent physical constraints and can produce unphysical predictions. Physics-Informed Neural Networks (PINNs) address this limitation by integrating governing physical laws directly into the loss function, ensuring training adheres to underlying physics even with sparse or incomplete data . For complex fluid systems, PINNs offer distinct advantages: effectiveness with limited data through physics-guided learning, mesh-free architecture eliminating specialised discretisation schemes, and unified forward and inverse modelling capabilities for parameter estimation.

This comprehensive review examines the state-of-the-art in AI/ML/DL applications to CFD, covering the period from 2015 to 2025. We systematically analyse the fundamental concepts, specific applications in fluid dynamics problems, challenges, and future research directions. The review encompasses turbulence modelling, heat transfer prediction, surrogate modelling, inverse design, and real-time flow control, with particular emphasis on physics-informed approaches.

2. Historical Background of the Study

The convergence of machine learning and computational fluid dynamics has its roots in two distinct trajectories. Traditional CFD methodologies, dating back to the 1960s and 1970s, have evolved through advances in numerical analysis, computational power, and physical understanding. The development of turbulence models, including Reynolds-Averaged Navier-Stokes (RANS) equations, Large Eddy Simulations (LES), and Direct Numerical Simulations (DNS), has been instrumental in advancing our understanding of fluid dynamics . However, these approaches often face limitations, including high computational costs and difficulties in capturing fine-scale flow structures, especially at high Reynolds numbers and in complex geometries .

The emergence of neural networks as universal function approximators, established by Hornik et al. in the late 1980s, laid the theoretical foundation for ML applications in scientific computing . The subsequent decades witnessed gradual progress in applying neural networks to fluid dynamics problems, but it was not until the 2010s that significant breakthroughs occurred. The development of deep learning architectures, coupled with advances in computational hardware and the availability of large datasets, catalysed the integration of ML with CFD.

The introduction of Physics-Informed Neural Networks by Raissi, Perdikaris, and Karniadakis in 2019 represented a watershed moment. PINNs demonstrated that neural networks could be trained not only on data but also on the governing physical laws themselves, enabling solutions to both forward and inverse problems with sparse data. This innovation opened new avenues for addressing challenges in complex fluid dynamics that had proven intractable with traditional methods.

In the Indian context, research in AI-enhanced CFD has gained momentum in recent years, with applications spanning aerospace, energy, and environmental engineering. The convergence of expertise in fluid mechanics, data science, and high-performance computing has positioned India as an emerging contributor to this field. However, challenges related to infrastructure, funding, and interdisciplinary collaboration continue to shape the trajectory of research in the country.

3. Need of the Study

The need for a comprehensive review of AI/ML/DL applications in CFD arises from several critical considerations. First, the exponential growth of literature in this interdisciplinary field makes it challenging for researchers and practitioners to stay abreast of developments. The integration of AI with CFD has spawned numerous approaches, each with distinct strengths, limitations, and applicability domains. A systematic review is essential for synthesising knowledge, identifying gaps, and guiding future research.

Second, the potential of AI-enhanced CFD to revolutionise engineering practice is substantial. Traditional CFD simulations often require significant computational resources, limiting their application in real-time decision-making, iterative design optimisation, and uncertainty quantification. ML-based surrogate models offer the promise of reducing computational costs while preserving accuracy, enabling real-time performance and iterative design optimisation. However, realising this potential requires overcoming significant challenges related to data quality, model interpretability, generalisation capabilities, and integration with existing workflows.

Third, the emergence of digital twin technologies, which create virtual representations of physical assets for monitoring, simulation, and analysis, demands computationally efficient yet accurate models. Hybrid AI approaches that combine physics-based simulations with machine learning offer tremendous opportunities to develop intelligent digital twins that are both physically consistent and computationally efficient. Understanding the current state and future directions of this integration is essential for industries transitioning toward digitalisation.

Fourth, the challenges associated with pure data-driven approaches, including lack of physical consistency and poor generalisation, necessitate a deeper understanding of physics-informed methodologies. While PINNs and related approaches address these limitations, they introduce new challenges related to convergence, accuracy, and efficiency. A comprehensive review can help researchers navigate these trade-offs.

Fifth, the application of transformer neural networks to turbulence modelling represents a novel and rapidly evolving field. By leveraging self-attention mechanisms, transformers can effectively capture complex spatiotemporal patterns and multi-scale interactions inherent in turbulent flows. Understanding the potential and limitations of these approaches is essential for advancing turbulence modelling.

4. Objectives

The objectives of this study are as follows:

1. To provide a comprehensive overview of AI/ML/DL methodologies applied to CFD, including physics-informed neural networks, supervised learning, reinforcement learning, and transformer architectures.
2. To examine the application of these methodologies to key challenges in fluid

dynamics, including turbulence modelling, heat transfer prediction, and multiphase flow simulation.

3. To evaluate the role of surrogate modelling and reduced-order modelling in accelerating CFD simulations and enabling real-time applications.

4. To analyse the integration of AI-enhanced CFD with digital twin technologies for predictive maintenance, performance optimisation, and real-time monitoring.

5. To identify the key challenges and limitations of current approaches, including data quality, model interpretability, generalisation, and computational efficiency.

6. To propose future research directions for developing robust, interpretable, and physically consistent AI-enhanced CFD frameworks.

5. Fundamentals of Physics-Informed Neural Networks

Physics-Informed Neural Networks represent one of the most significant advances in the integration of AI with CFD. The fundamental architecture of a PINN consists of two key components: a deep neural network and the incorporation of physical intuition through a loss function that encodes the governing equations.

5.1 Neural Network Architecture

The neural network used in PINNs is typically a fully connected deep neural network based on a multilayer perceptron architecture. The inputs consist of independent variables such as spatial coordinates (x, y, z) and time t, and the outputs correspond to the physical quantities of interest (e.g., velocity, pressure, temperature). Each hidden layer contains multiple nodes, all connected to nodes in adjacent layers with associated weights. When an input is provided, each node computes a weighted sum of the inputs, which is then passed through an activation function (e.g., Tanh, ReLU) before being fed to the next layer.

The depth (number of hidden layers) and width (number of nodes per layer) of the network are hyperparameters that can be tuned based on problem complexity. Deeper networks can efficiently capture more intricate functions, though overly deep networks may not offer significant performance gains and can be harder to train. A practical balance is often achieved with between three and six hidden layers.

5.2 Physics Integration

The key innovation of PINNs is the integration of physical laws into the loss function. Since the outputs computed by the neural network are derived solely from the network's learned weights, it is essential to verify whether these outputs satisfy the governing physical laws. PINNs achieve this by substituting the outputs into a physics-informed loss function and computing the deviation from the true physical solution, iteratively adjusting the network parameters to minimise this error.

The required derivatives are computed through automatic differentiation, a computational technique that enables exact derivative evaluation by tracing the computation graph and applying the chain rule. Unlike numerical differentiation, which relies on finite differences and is subject to truncation errors, automatic differentiation provides machine-precision gradients without error accumulation.

5.3 Loss Function Components

The total loss function in PINNs typically includes three components:

- PDE residual loss: Measures the error in satisfying the governing partial differential equations. The predicted values and their derivatives are substituted into the PDEs, and the residual is commonly squared and averaged.
- Boundary condition loss: Quantifies the mismatch between predicted and specified boundary values. For example, if a no-slip condition requires velocity to be zero at a wall, the loss is computed as the squared difference between the predicted value and zero at that location.
- Initial condition loss: Applies when initial conditions are specified, penalising discrepancies between predicted and known values at the initial time .

These losses are combined with weights that control the relative contribution of each term. Researchers can manually tune these weights to match problem characteristics. For internal viscous flows, the critical nature of boundary conditions necessitates a high setting of the boundary condition weight. In contrast, for free boundary flows, the governing equation accuracy takes precedence.

5.4 Training and Optimisation

To minimise the total loss, PINNs use standard training procedures similar to conventional deep learning. Optimisation algorithms such as gradient-based Adam or L-BFGS are employed . Each training step involves passing input values through the neural network, computing derivatives using automatic differentiation, calculating loss components, and updating network parameters through backpropagation.

One important distinction from supervised learning is that PINNs can be trained without labelled data. Instead of relying on exact solution values across the entire domain, PINNs are guided by underlying physical laws embedded in the loss function. As a result, the model learns to produce physically consistent outputs by minimising violations of these constraints, even when observational data are sparse or entirely absent.

5.5 PINN Variants and Extensions

While PINNs have demonstrated significant potential, they face inherent limitations including non-convex loss functions, vanishing gradients in deep networks, and extended training times. Recent developments have addressed these challenges through various modifications. Adaptive weight updating during training has been proposed to balance the contributions of different loss components. Advanced architectures, including convolutional neural networks and recurrent neural networks, have been adapted to handle spatiotemporal data.

Neural operators and Fourier Neural Operators represent another class of approaches that learn solution operators for parametric PDEs, enabling resolution-invariant predictions and generalisation across different initial and boundary conditions. These approaches have shown promise for applications where rapid evaluation across multiple scenarios is required.

6. Applications in Turbulence Modelling

Turbulence modelling remains one of the most significant challenges in fluid dynamics, given the complex, chaotic, and multi-scale nature of turbulent flows.

Traditional approaches, including RANS equations, LES, and DNS, have been instrumental in advancing understanding, yet face limitations including high computational costs and difficulties in capturing fine-scale flow structures, especially at high Reynolds numbers and in complex geometries.

6.1 Data-Driven Turbulence Closure

Machine learning methods applied to turbulence closure modelling represent a paradigm shift in how turbulence is modelled. The extraordinary success of ML in various challenging fields had given rise to expectations of similar transformative advances in turbulence closure modelling. However, progress has been slower than anticipated, attributed to the underestimation of turbulence modelling intricacies and the overestimation of ML's ability to capture all features without targeted strategies.

The fundamental challenge in turbulence closure modelling is the closure problem: the Reynolds-averaged Navier-Stokes equations require modelling of the Reynolds stress tensor, which represents the effects of turbulent fluctuations on the mean flow. Traditional models, based on assumptions such as the Boussinesq hypothesis, have been successfully applied to canonical turbulent flows but often fail in complex flows.

Data-driven approaches offer the potential to learn the complex, nonlinear relationships between mean flow features and Reynolds stresses directly from high-fidelity data. Neural networks have been used to model the anisotropic Reynolds stress tensor, incorporating invariance principles to ensure Galilean invariance. Random forests and support vector regression have also been explored as alternatives to neural networks for turbulence closure.

6.2 Physics-Informed Turbulence Modelling

Physics-informed machine learning has emerged as a promising approach to address the limitations of purely data-driven turbulence models. The integration of physical constraints into ML models ensures consistency with fundamental conservation laws and improves generalisation . Physics-informed neural networks have been applied to reconstruct Reynolds stress modelling discrepancies, enabling data-driven correction of traditional models while maintaining physical consistency.

For large-eddy simulation, neural network-based subgrid-scale models have been developed to learn the effects of unresolved scales directly from high-fidelity data. These approaches have demonstrated improved accuracy compared to traditional Smagorinsky models for certain canonical flows. However, challenges remain in extrapolation to high Reynolds numbers, generalisation to untrained flows, and physical consistency.

6.3 Transformer-Based Turbulence Modelling

Transformer neural networks, first introduced in the context of natural language processing, have recently been adapted for turbulence modelling. By employing self-attention mechanisms, transformers can model global dependencies within data sequences, capturing complex spatiotemporal patterns and multi-scale interactions inherent in turbulent flows.

Several trends have emerged in transformer-based turbulence modelling: adaptation of transformer architectures with specialised attention mechanisms, integration of hybrid models combining transformers with convolutional or graph neural networks, and incorporation of physical constraints to enhance model fidelity. Comparative analyses reveal that transformer-based models often achieve higher accuracy than other AI approaches and greater computational efficiency than traditional CFD methods, excelling in capturing complex flow phenomena and generalising across different flow conditions and geometries.

However, challenges persist, including high computational demands, data scarcity, difficulties in capturing small-scale turbulent structures, and error accumulation in long-term predictions. Addressing these limitations through architectural innovations, efficient training strategies, and incorporation of physical constraints holds significant promise.

7. Surrogate Modelling and Digital Twins

Surrogate modelling, also known as reduced-order modelling, has emerged as a powerful approach to reduce computational costs while maintaining accuracy, enabling real-time performance, iterative design optimisation, and enhanced feasibility of simulations. The integration of AI-enhanced surrogate models with digital twin technologies represents a significant opportunity for engineering applications.

7.1 Surrogate Modelling Approaches

Traditional surrogate modelling approaches include response surface methods, Kriging, and Gaussian process regression. These methods have been widely applied in engineering design optimisation but face limitations when dealing with high-dimensional inputs and complex, nonlinear responses. Machine learning approaches, including artificial neural networks, support vector regression, and random forests, have been increasingly adopted for surrogate modelling due to their ability to capture complex, nonlinear relationships.

Gaussian process regression has been found to generally provide well-performing solutions for aerodynamic surrogate modelling, offering uncertainty quantification capabilities that are valuable for design optimisation. Active learning algorithms that combine bias estimated from nearest-neighbour Euclidean distance and variance can achieve higher accuracy with fewer computational fluid dynamics simulations.

7.2 Physics-Informed Surrogate Models

Physics-informed surrogate models integrate physical constraints into the learning framework, improving reliability and applicability. The integration of expert knowledge into surrogate modelling workflows has been identified as critical for enhancing model reliability and applicability This includes incorporating governing equations, symmetries, and conservation laws into the model architecture or training process.

For gas turbine applications, physics-constrained neural networks and CFD surrogates embed governing equations into learning frameworks for consistent flow and thermal predictions. This approach enables fast, physically consistent simulations under changing flow conditions, directly applicable to intelligent digital twins and their embedded sub-simulations.

7.3 Digital Twin Integration

Digital twins, virtual representations of physical assets that mirror state and behaviour in real time, have become increasingly critical for real-time diagnostics, predictive maintenance, and performance optimisation. The intelligent digital twin integrates AI, machine learning, and advanced analytics to enable learning from multi-source data, adaptive behaviour under changing operating conditions, and support predictive decision-making.

Hybrid AI methods for digital twins combine physics-based simulations with machine learning, offering tremendous opportunities to develop intelligent digital twins that are both physically consistent and computationally efficient. Four distinct hybrid AI categories have been identified: ANN-augmented thermodynamic models, physics-integrated operational architectures, physics-constrained neural networks with CFD surrogates, and generative and model discovery approaches.

Industrial case studies, including GE Vernova's SmartSignal and Siemens' Autonomous Turbine Operation and Maintenance, illustrate applications in real-time diagnostics, predictive maintenance, and performance optimisation . These implementations demonstrate the potential of hybrid AI approaches to transform engineering practice.

8. Challenges and Limitations

Despite significant advances, the integration of AI/ML/DL with CFD faces several substantial challenges and limitations.

8.1 Data Quality and Availability

Machine learning approaches require large amounts of high-quality training data. For many fluid dynamics problems, such data are scarce or expensive to generate. High-fidelity DNS data are limited to low Reynolds numbers and simple geometries. Experimental data may be noisy, incomplete, or limited to specific flow conditions. The sparse nature of data for complex flow problems constrains the applicability of purely data-driven approaches.

8.2 Model Interpretability

Neural networks are often viewed as black boxes, making it difficult to understand why a particular prediction was made. This lack of interpretability is a significant barrier to adoption in safety-critical engineering applications. Physics-informed approaches address this limitation by ensuring predictions are physically consistent, but interpretability remains an active research area.

8.3 Generalisation Capabilities

ML models trained on specific flow conditions or geometries often fail to generalise to unseen conditions. This limitation is particularly acute for turbulence modelling, where the extrapolation to high Reynolds numbers and untrained flows remains a significant challenge. Physics-informed approaches offer better generalisation through embedded physical constraints, but challenges remain.

8.4 Computational Efficiency

While ML-based surrogate models offer significant speed advantages over traditional CFD, the training process itself can be computationally expensive. PINNs, in particular, may require tens or hundreds of thousands of training epochs for complex PDEs . The computational demands of training large transformer models for turbulence modelling are also substantial.

8.5 Physical Consistency

Ensuring that ML predictions adhere to fundamental conservation laws and physical constraints is essential for reliability. While PINNs enforce physical consistency, the loss-based approach does not guarantee exact satisfaction of governing equations. Purely data-driven models may produce unphysical predictions that violate conservation laws.

8.6 Integration with Existing Workflows

Integrating AI-enhanced CFD with existing engineering workflows and software ecosystems remains a significant challenge. Issues related to data formats, software compatibility, and the need for domain expertise in both CFD and ML hinder adoption.

9. Future Directions

The future of AI-enhanced CFD research will likely be shaped by several emerging trends and developments.

9.1 Hybrid and Physics-Informed Approaches

Hybrid approaches that combine physics-based simulations with machine learning are likely to dominate future research. By embedding physical constraints, governing equations, or simulation outputs into learning architectures, these approaches leverage the strengths of both paradigms. The development of mature hybrid AI frameworks will be essential for creating scalable, interpretable, and operationally robust intelligent digital twins.

9.2 Neural Operators

Neural operators, including Fourier Neural Operators and DeepONet, represent a promising direction for learning solution operators for parametric PDEs. These approaches enable resolution-invariant predictions and generalisation across different initial and boundary conditions, offering significant advantages over traditional PINNs.

9.3 Transformer Architectures

Transformer neural networks are likely to play an increasingly important role in turbulence modelling and other fluid dynamics applications. Addressing current limitations through architectural innovations, efficient training strategies, incorporation of physical constraints, and leveraging hybrid models holds significant promise.

9.4 Uncertainty Quantification

Incorporating uncertainty quantification into AI-enhanced CFD is essential for reliability and decision-making. Gaussian process regression and Bayesian neural networks offer frameworks for quantifying uncertainty in predictions. Future research will likely focus on developing robust uncertainty quantification methods.

9.5 Explainable AI

The development of explainable AI methods for fluid dynamics is critical for building trust and enabling adoption in engineering practice. Interpretable ML models and post-hoc explanation techniques will be essential for understanding predictions and identifying potential failure modes.

9.6 Integration with High-Performance Computing

The integration of AI-enhanced CFD with high-performance computing platforms will be essential for addressing large-scale problems. Efficient parallelisation, distributed training, and integration with existing HPC workflows will be critical.

10. Conclusion

The integration of Artificial Intelligence, Machine Learning, and Deep Learning with Computational Fluid Dynamics represents a paradigm shift in fluid mechanics research and engineering applications. This comprehensive review has examined recent advances in applying AI/ML/DL methodologies to enhance traditional CFD workflows across various domains, including turbulence modelling, heat transfer prediction, surrogate modelling, inverse design, and real-time flow control.

Physics-Informed Neural Networks have emerged as a transformative approach, embedding governing physical laws directly into neural network loss functions to ensure physical consistency even with sparse or incomplete data. Their mesh-free architecture, unified forward and inverse modelling capabilities, and effectiveness with limited data position them as powerful alternatives to traditional numerical methods.

Transformer neural networks have demonstrated significant potential in turbulence modelling, leveraging self-attention mechanisms to capture complex spatiotemporal patterns and multi-scale interactions. While challenges persist—including high computational demands, data scarcity, and interpretability issues—continued development promises to revolutionise the field.

Surrogate modelling and digital twins represent important application domains for AI-enhanced CFD, enabling real-time simulation, iterative design optimisation, and predictive maintenance. Hybrid AI approaches that integrate physics-based simulations with machine learning offer particularly promising opportunities for developing intelligent, physically consistent, and computationally efficient models.

Significant challenges remain, including data quality and availability, model interpretability, generalisation capabilities, physical consistency, and integration with existing workflows. Addressing these challenges through interdisciplinary collaboration, methodological innovation, and continued investment in research and development will be essential for realising the full potential of AI-enhanced CFD.

The future of this field lies in developing robust, interpretable, and physically consistent AI-enhanced CFD frameworks that can revolutionise engineering design and optimisation processes. By combining the strengths of data-driven learning with the reliability of physics-based simulation, researchers and practitioners can unlock new capabilities and address challenges that have long eluded traditional approaches.

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