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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.

Major Findings: *(1) AI/ML/DL methods are transforming CFD by enabling efficient surrogate modelling, turbulence prediction, and inverse design with reduced computational costs. (2) Physics-informed and hybrid models ensure physical consistency, improving generalisation and trust in predictions. (3) Integration with digital twins and real-time systems paves the way for adaptive, intelligent control of fluid systems.*

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

1.0 Introduction

Computational Fluid Dynamics (CFD) is a powerful numerical tool widely used to analyse fluid flow, heat transfer, and related phenomena across various engineering disciplines, including aerospace, automotive, chemical processing, and environmental sciences[1]. By solving the governing equations of fluid motion, CFD

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enables detailed predictions of complex flow behaviour, facilitating design optimisation and performance evaluation. Despite advances in numerical methods and increasing computational power, high-fidelity CFD simulations, especially those involving turbulence, multiphase flows, or complex geometries, remain computationally expensive and time-consuming[2]. This limitation restricts their use in scenarios demanding rapid design iterations, real-time control, or large-scale parametric studies.

Traditional turbulence modelling approaches, such as Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES), often involve trade-offs between accuracy and computational cost, motivating the search for novel methods to improve model fidelity without prohibitive overhead[5]. Additionally, the complexity of Multiphysics flows and the growing volume of high-fidelity CFD data have spurred interest in data-driven methodologies capable of capturing underlying flow dynamics efficiently.

Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) have recently emerged as promising technologies to augment and accelerate traditional CFD workflows. These data-driven methods are capable of learning complex nonlinear relationships from simulation and experimental datasets, enabling faster surrogate modelling, improved turbulence closures, inverse design, and real-time flow prediction[3,4]. For instance, Convolutional Neural Networks (CNNs) have been applied for flow field[5] reconstruction and feature extraction, while Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) networks are used for predicting unsteady flows and temporal evolution[6,7]. Furthermore, Physics-Informed Neural Networks (PINNs) integrate governing equations directly into the learning process, improving generalisation and ensuring physically consistent predictions[3].

Recent works have demonstrated the potential of AI/ML in various CFD-related tasks. Guo *et al.*[4] showed that CNNs could approximate steady-state flow fields with high accuracy and reduced computational time. Rabault *et al.*[8] employed deep reinforcement learning to develop active flow control strategies for drag reduction in bluff body flows. Generative models like GANs have been explored for inverse design problems, enabling rapid exploration of design spaces previously inaccessible through classical optimization[9]. These advances underscore a shift towards hybrid CFD frameworks where data-driven models complement and accelerate physics-based simulations.

This review provides a comprehensive overview of the recent advances (2015–2025) in applying AI, ML, and DL techniques to CFD problems. Key application areas covered include turbulence modelling, heat transfer prediction and enhancement, surrogate modelling, inverse design and optimisation, as well as real-time flow control. The role of physics-informed machine learning, which embeds physical laws into AI models, is highlighted as a crucial development toward trustworthy and interpretable CFD predictions.

The paper is structured as follows: Section 2 introduces the fundamental concepts of AI, ML, and DL relevant to CFD applications. Section 3 reviews recent research progress in different CFD application domains. Section 4 discusses current challenges and future research opportunities, and Section 5 concludes with a summary of key insights and potential impacts.

2.0 Fundamentals of Artificial Intelligence, Machine Learning, and Deep Learning in CFD

2.1 Brief Overview of AI, ML, and DL Concepts

Artificial Intelligence (AI) refers to the broad field of creating machines capable of performing tasks that typically require human intelligence, such as reasoning, perception, and decision-making[10]. Machine Learning (ML), a subset of AI, focuses on developing algorithms that improve automatically through experience by learning from data without explicit programming[11]. Deep Learning (DL) is a specialised branch of ML that uses multi-layered artificial neural networks to model complex hierarchical patterns in large datasets, enabling superior performance in tasks like image recognition, natural language processing, and increasingly, fluid dynamics[12].

In the context of Computational Fluid Dynamics (CFD), AI/ML/DL methods serve as powerful tools for capturing complex nonlinear behaviours in fluid flow

without directly solving governing equations. They can learn from high-fidelity simulation data or experimental measurements to provide surrogate models, turbulence closures, or predictive frameworks that enhance or accelerate traditional CFD approaches[13,14].

2.2 Types of ML Models Used in CFD

A variety of ML architectures have been successfully applied in CFD, each suited for specific tasks depending on the nature of data and problem characteristics. Table 1 summarises key models, their functions, and typical CFD applications.

2.3 Data Requirements and Sources

Successful application of AI/ML/DL in CFD heavily depends on the quality, quantity, and diversity of data used for training. Common sources include:

- Simulation data: High-fidelity CFD simulations (DNS, LES, RANS) provide detailed flow field information across a wide parameter space. These datasets are essential for supervised learning, but their generation can be computationally expensive[21].
- Experimental data: Measurements from wind tunnels, Particle Image Velocimetry (PIV), Laser Doppler Velocimetry (LDV), and other instruments offer real-world flow information. Experimental data can help improve model generalizability and address discrepancies in numerical methods[22].
- Hybrid datasets: Combining simulation and experimental data provides richer datasets, allowing models to leverage the strengths of both sources and mitigate weaknesses such as noise and sparsity[23].

Data preprocessing such as normalisation, noise filtering, and dimensionality reduction (e.g., Proper Orthogonal Decomposition - POD) is commonly applied to enhance learning efficiency[24].

2.4 Challenges in Integrating AI with CFD

Despite promising advances, integrating AI with CFD faces several challenges:

- Data scarcity and quality: Generating sufficiently large and diverse high-fidelity datasets remains costly and time-consuming. Experimental data may be limited or noisy[25].
- Generalisation and extrapolation: AI/ML models often perform poorly outside their training domain, raising concerns about robustness and reliability for unseen flow conditions[26].

Table 1. Key model functions of CFD

Model Type	Description	CFD Applications	References
Artificial Neural Networks (ANN)	Basic feedforward networks that approximate nonlinear functions	Surrogate modelling, turbulence closure	4, 14, 16
Convolutional Neural Networks (CNN)	Networks that extract spatial features via convolutions	Flow field reconstruction, reduced-order modelling	5, 6, 17
Recurrent Neural Networks (RNN), LSTM	Models for sequential/temporal data	Unsteady flow prediction, time-series forecasting	7, 18
Generative Adversarial Networks (GAN)	Networks consisting of a generator and a discriminator for data generation	Inverse design, synthetic flow data generation	9, 20
Physics-Informed Neural Networks (PINNs)	Integrate governing PDEs as constraints during training	Turbulence modelling, solving inverse problems	3, 19
Reinforcement Learning (RL)	Learning control strategies via interaction and reward feedback	Active flow control, optimisation in real-time scenarios	8, 15

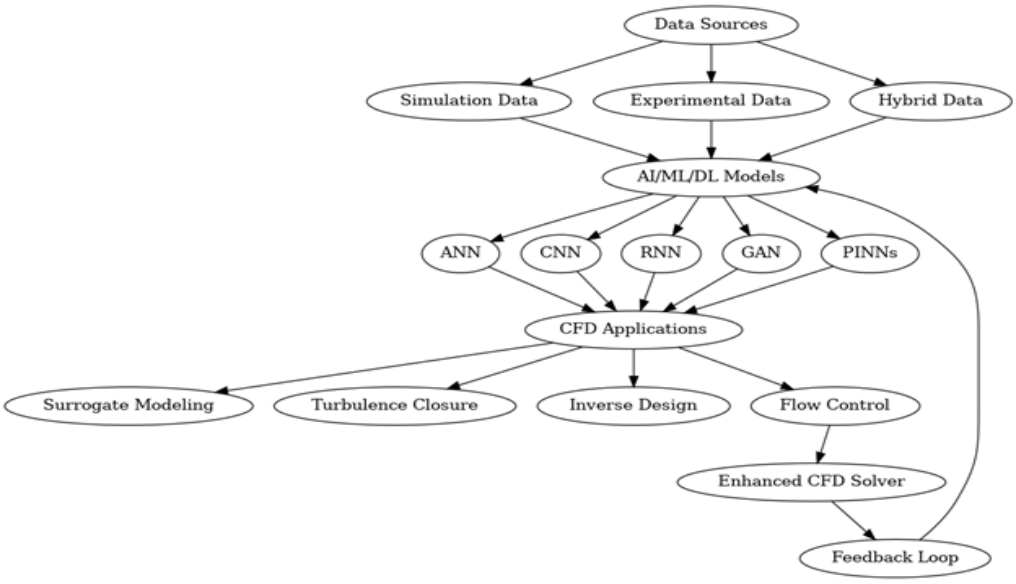


Figure 2. Integration of AI/ML/DL techniques with CFD workflows.

- Interpretability: Deep models, especially DL architectures, often act as "black boxes," making it difficult to understand the physical reasoning behind predictions[27].
- Physical consistency: Ensuring AI models respect fundamental physics (e.g., conservation laws) is crucial to avoid unphysical results, motivating the development of physics-informed methods[3].
- Computational cost: Training deep models on large datasets requires significant computational resources, though inference is typically faster than traditional CFD[28].

Addressing these challenges is essential to advancing AI-enhanced CFD toward widespread practical adoption. Figure 1 illustrates the integration of Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) techniques into Computational Fluid Dynamics (CFD), revolutionising the field by enhancing prediction accuracy and computational efficiency. This process begins with diverse data sources, including simulation, experimental, and hybrid datasets, which are essential for training various AI models such as Artificial Neural Networks (ANN), Convolutional Neural Networks (CNN), Recurrent Neural Networks (RNN), Generative Adversarial Networks (GAN), and Physics-Informed Neural Networks (PINNs). These trained models are applied to CFD tasks like surrogate modelling, turbulence closure, inverse design, and flow control, significantly improving solver performance. Notably, flow control strategies contribute to the development of enhanced CFD solvers, which continuously feed new data back into the AI models, creating a dynamic feedback loop that drives ongoing optimisation and refinement of both the models and CFD solutions.

3.0 Applications of AI/ML/DL in CFD

Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) have increasingly been integrated into various Computational Fluid Dynamics (CFD) applications to overcome limitations of traditional approaches and enable rapid, accurate predictions and control. This section reviews recent advances in key CFD domains empowered by AI techniques.

3.1 Turbulence Modelling

Traditional turbulence modelling challenges:
Classical turbulence models such as Reynolds-Averaged Navier-Stokes (RANS) equations rely on empirical closures that often lack generality and accuracy across complex flow regimes[29]. High-fidelity simulations like Direct Numerical Simulation (DNS) and Large Eddy

Simulation (LES) are computationally prohibitive for many practical engineering problems.

AI-based turbulence closures and Reynolds stress modelling:
ML models have been developed to learn Reynolds stress anisotropy directly from DNS/LES datasets, improving the prediction of turbulence quantities. For example, random forests, gradient boosting, and ANNs have been employed to augment or replace traditional closure terms[30].

Deep learning approaches and physics-informed models:
DL architectures like CNNs and PINNs are used to capture spatial correlations in turbulence and embed governing physical laws into the learning process. Physics-informed models improve robustness by ensuring mass, momentum, and energy conservation constraints are satisfied[31].

3.2 Heat Transfer Prediction and Enhancement

Use of ML/DL for predicting heat transfer coefficients and thermal fields:
ML algorithms, including ANNs and CNNs, predict local and global heat transfer coefficients based on input parameters such as geometry, flow velocity, and material properties, providing rapid alternatives to expensive simulations[32].

Surrogate models for conjugate heat transfer:
Surrogate modelling techniques trained on conjugate heat transfer simulations can estimate temperature distributions and heat fluxes efficiently, enabling quick design iterations[33].

Inverse design of thermal systems using DL:
Generative models like GANs and autoencoders facilitate inverse design by generating novel thermal system configurations that meet target heat transfer or thermal performance objectives[34].

3.3 Surrogate Modelling and Reduced-Order Models (ROMs)

Overview of surrogate modelling:
Surrogate models approximate the relationship between inputs and CFD outputs to reduce computational cost. These models enable rapid evaluations in design optimisation and uncertainty quantification[35]. The applications of CFD in various predictive models are shown in Figure 2.

AI-based ROMs for accelerating CFD simulations:
Autoencoders compress high-dimensional CFD data into low-dimensional latent spaces, capturing dominant flow features. LSTMs model temporal evolution in unsteady flows, and GANs generate synthetic yet realistic flow data[36].

3.4 Inverse Design and Optimisation

AI for aerodynamic and thermal system design:
AI-driven design frameworks optimise geometries to meet aerodynamic performance or thermal efficiency goals by learning from large CFD datasets and experimental results[37].

Generative models and reinforcement learning in inverse design:
GANs create design candidates that satisfy constraints, while reinforcement learning discovers optimal control strategies or shape modifications via interaction with CFD environments[38].

Hybrid AI-CFD optimisation frameworks:
Combining AI-based surrogate models with traditional CFD solvers in iterative loops enables faster convergence and improved accuracy in design optimisation workflows[39].

3.5 Real-Time Flow Control and Prediction

Deep reinforcement learning for active flow control: DRL agents have been trained to manipulate actuators in flow systems (e.g., synthetic jets, flaps) to reduce drag, suppress vortex shedding, or enhance mixing in real-time[40].

RNNs and LSTMs for real-time flow forecasting: Recurrent networks predict future flow states from past measurements, enabling fast and accurate forecasting for unsteady flows and aiding in control decision-making[41].

AI-assisted experimental flow control and sensing: AI methods assist in sensor placement, data assimilation, and control law identification in experiments, reducing experimental costs and enhancing flow control efficacy[42].

Table 2 represents a summary of the AI/ML/DL techniques applied on various CFD parameters. Figure 2 illustrates the integration of AI and ML with CFD data from simulations and experiments. Turbulence and heat transfer models are improved using ANNs, PINNs, CNNs, and GANs. Surrogate modelling reduces computational costs through simplified models. Inverse design and real-time control optimise geometry and dynamic flow systems. A feedback loop ensures continuous model refinement and data improvement.

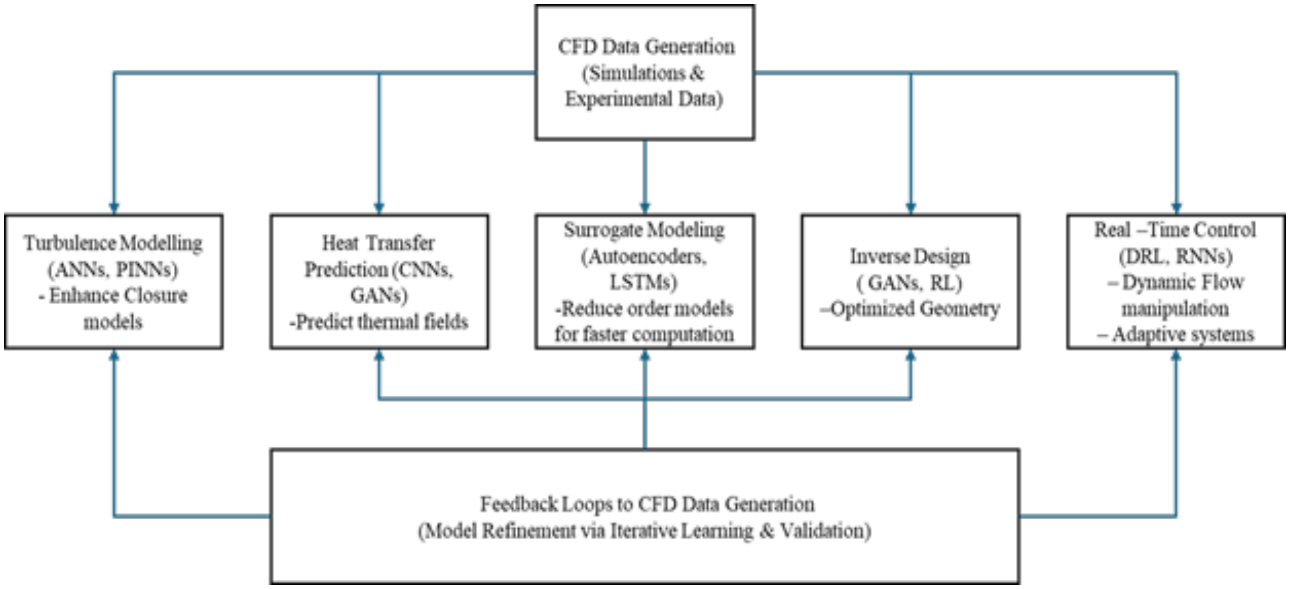


Figure 2. Overview of AI/ML/DL applications in CFD.

Table 2. Summary of AI/ML/DL applications in CFD

Application Domain	AI/ML/DL Techniques	Benefits	Representative References
Turbulence Modeling	ANN, CNN, PINNs	Improved closure models, accuracy	29, 30, 31
Heat Transfer Prediction	ANN, CNN, GAN	Rapid thermal predictions	32, 33, 34
Surrogate Modelling and ROMs	Autoencoders, LSTM, GAN	Computational efficiency	35, 36
Inverse Design and Optimisation	GAN, RL, hybrid AI-CFD frameworks	Efficient design exploration	37, 38, 39
Real-Time Flow Control	DRL, RNN, LSTM	Adaptive, fast control	40, 41, 42

4.0 Challenges and Future Perspectives

Despite the remarkable progress in integrating Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) into Computational Fluid Dynamics (CFD), several challenges must be addressed to fully exploit their potential. These challenges stem from both data-related and model-centric limitations, as well as broader concerns about generalizability, physical fidelity, and computational infrastructure. This section outlines the key bottlenecks and emerging research directions.

4.1 Data Quality and Quantity Issues

The success of AI/ML models in CFD largely depends on the availability of high-quality, diverse datasets. However, generating such datasets from DNS or high-resolution simulations is computationally expensive. Experimental data, while valuable, is often sparse and noisy, which limits its utility in training robust models[43]. Additionally, discrepancies between simulated and real-world conditions can lead to data-driven models that perform poorly in real scenarios.

Efforts to create hybrid datasets, combining synthetic and real-world data, and developing data augmentation strategies are ongoing to overcome these challenges[44].

4.2 Explainability and Physical Consistency of AI Models

The black-box nature of many AI models, particularly deep neural networks, poses a significant barrier in scientific domains like CFD, where interpretability and trust in predictions are critical[45]. Moreover, many ML models can produce outputs that violate fundamental physical laws such as conservation of mass or momentum.

Physics-Informed Neural Networks (PINNs) have emerged as a promising solution to enforce physical consistency, but their scalability and convergence still pose challenges[46].

4.3 Generalisation and Transfer Learning in CFD

Models trained on specific flow regimes or geometries often struggle to generalise to unseen conditions due to the high dimensionality and nonlinearity of fluid flows. Transfer learning, which leverages pre-trained models for new tasks, is under active investigation to improve adaptability and reduce data requirements[47].

However, transfer learning in CFD must carefully account for domain-specific differences (e.g., geometry, boundary conditions) to avoid performance degradation.

4.4 Integration with HPC and Digital Twins

Integrating AI/ML workflows into traditional High-Performance Computing (HPC) platforms remains a bottleneck, especially for real-time applications. The development of AI-powered digital twins—real-time virtual replicas of physical fluid systems—requires fast, reliable surrogate models and seamless coupling with CFD solvers[48].

This integration necessitates interdisciplinary collaboration among fluid dynamicists, data scientists, and software engineers to address issues like parallelisation, memory optimisation, and data exchange protocols.

4.5 Future Research Directions

To unlock the full potential of AI in CFD, several promising research avenues are being explored, and the integration diagram of AI-CFD is as displayed in Figure 3.

Hybrid modelling: Combining physics-based solvers with data-driven corrections to retain interpretability while enhancing performance[49].

Self-supervised and semi-supervised learning: Reducing reliance on labelled data through alternative training paradigms.

Continual learning: Developing models that adapt and learn from new simulations or experiments without forgetting previous knowledge.

Benchmark datasets and standardisation: Establishing open-access CFD benchmark datasets and evaluation protocols to accelerate model development and comparison[50].

Cross-domain applications: Extending CFD-AI frameworks to multiphysics problems (e.g., fluid-structure interaction, reactive flows). Table 3 represents the key challenges in AI-CFD integration for future.

Hybrid modelling approaches in computational sciences aim to leverage the strengths of both physics-

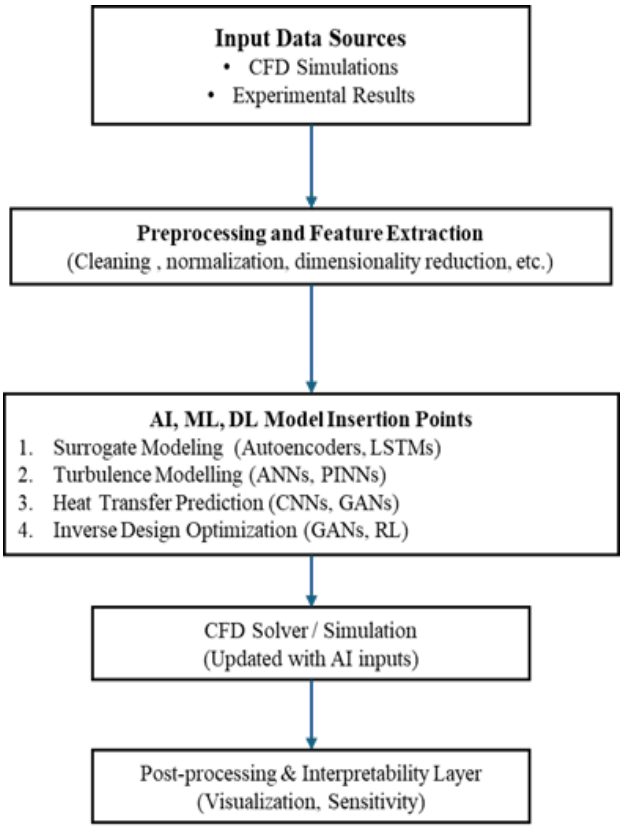


Figure 3. Schematic of AI-CFD integration workflow with challenges.

based and data-driven techniques to improve prediction accuracy, computational efficiency, and generalisation. Traditional physics-based models, such as Navier–Stokes solvers using Reynolds-Averaged Navier–Stokes (RANS), Large Eddy Simulation (LES), or Direct Numerical Simulation (DNS) and numerical schemes like Finite Volume or Finite Element methods, are grounded in first principles and offer interpretability but can be computationally expensive for complex systems.

On the other hand, AI-based models—including surrogate models and deep learning architectures—excel in learning patterns from data but often lack physical interpretability. Hybrid models bridge this gap by integrating physical laws with machine learning. Techniques such as Physics-Informed Neural Networks (PINNs) embed governing equations directly into neural networks, while grey-box modelling and Reduced Order Models (ROMs) enhanced with neural networks use simplified physics augmented by data-driven corrections.

These approaches offer promising solutions in areas where purely data-driven or purely physics-based models fall short, making them especially valuable in domains like CFD, where both fidelity and efficiency are critical. Figure 4 illustrates this approach.

A Digital Twin of a real-world fluid system—such as a pipeline—integrates physical processes with intelligent computational models to enable real-time monitoring, prediction, and control. The system begins with a sensor network (typically composed of IoT-based sensors) that continuously captures key parameters like pressure, temperature, and velocity.

This raw data undergoes pre-processing steps including filtering, noise removal, and temporal/spatial sampling to ensure data quality. The processed information feeds into an AI/ML module, which may include surrogate models for fast approximation, anomaly detection algorithms for

Table 3. Summary of key challenges and future directions in AI-CFD integration

Challenge/Direction	Description	References
Data scarcity and noise	Limited high-fidelity data; expensive simulations; experimental uncertainties	43, 44
Model explainability	Lack of transparency in predictions; trust issues	45, 46
Generalisation to new problems	Difficulty transferring models across domains or flow types	47
Integration with HPC/digital twins	Real-time capabilities and coupling with solvers are still under development	48
Hybrid/physics-informed learning	Merging ML and physics-based modelling for accuracy and trust	49, 50

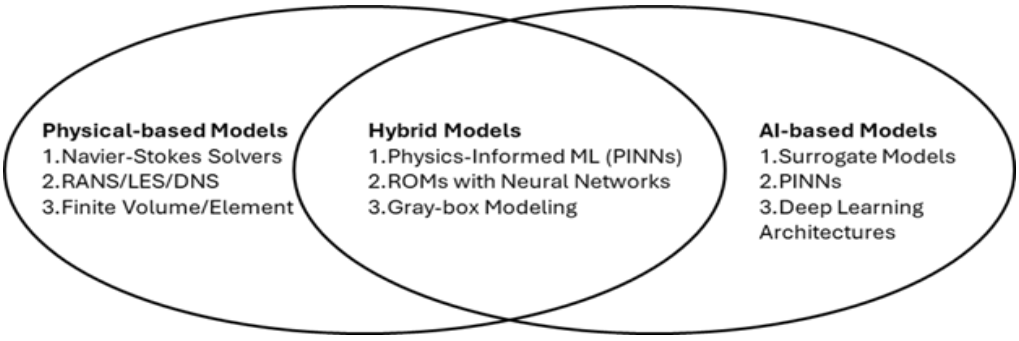


Figure 4. Venn diagram of hybrid modelling approaches.

identifying abnormal behaviour, and real-time inference engines for decision-making.

Complementing the AI module, a high-fidelity CFD solver serves as the physics core, validating and refining the predictions made by AI models through first-principles simulation. The integration of these components forms a Digital Twin interface, which synchronizes live sensor data with simulated outputs to provide real-time visualization, operational insights, and dynamic control.

This closed-loop system not only enhances the predictive capability and efficiency of fluid systems but also enables adaptive responses to evolving operational conditions. The architecture is illustrated in Figure 5.

5.0 Challenges and Future Perspectives

The integration of Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) into Computational Fluid Dynamics (CFD) marks a transformative shift in how fluid flow problems are addressed. This review has comprehensively highlighted recent advancements, applications, and challenges in

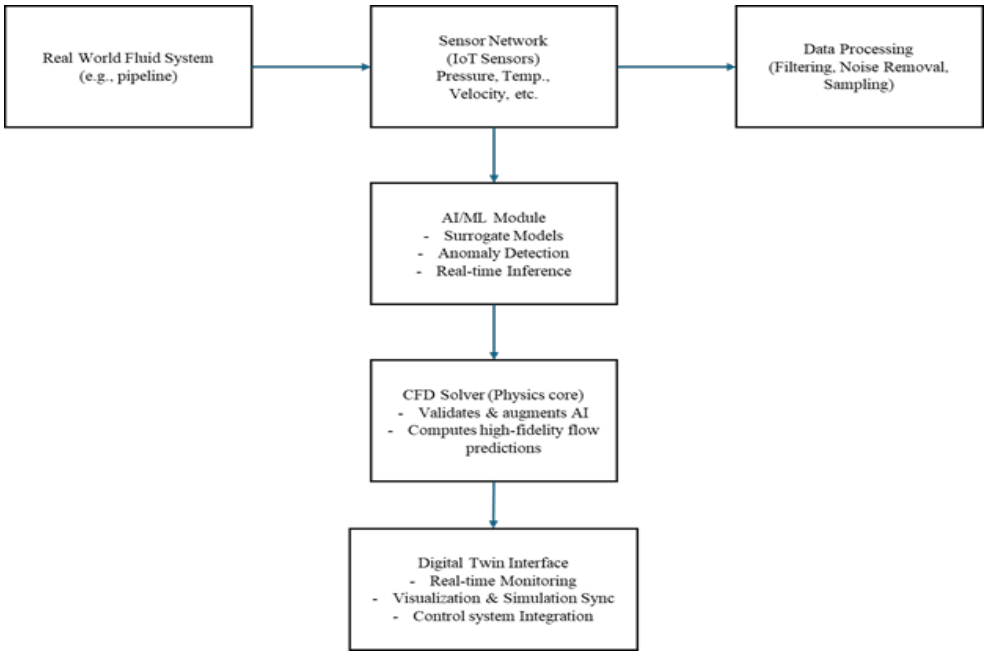


Figure 5. Conceptual architecture of a digital twin for CFD.

Table 4. List of future tools on CFD challenges over AI solution

Challenge	AI Solutions	Future Tools / Directions
Data Quality	• GANs (Data Augmentation) • CNNs (Noise Reduction)	• Synthetic Data Pipelines • Data Curation Standards
Model Interpretability	• PINNs (Physics Embedding) • SHAP/XAI Techniques	• Explainable AI (XAI) • Visualisation Dashboards
HPC Integration	• LSTMs with Parallelisation • Lightweight Surrogates	• Cloud-based CFD Platforms • Edge AI for CFD
Generalization	• Transfer Learning • Domain Adaptation Techniques	• Multi-fidelity Modelling • Cross-domain AI Libraries
Real-Time Constraints	• Surrogate Models (Autoencoders, LSTMs)	• Digital Twins • Reinforcement Learning Controllers

the domain, emphasising how AI/ML/DL methods are redefining CFD from both computational and modelling perspectives. Some of the promising AI-based tools for addressing future CFD challenges are summarized in Table 4.

5.1 Summary of Key Advances

- Over the past decade, AI/ML/DL have moved beyond proof-of-concept stages and are now enabling novel solutions to traditionally complex CFD problems. Key advancements include:
- Turbulence modelling using neural networks to predict Reynolds stresses and enhance RANS and LES frameworks[21,24].
- Heat transfer prediction and optimisation using DL-based surrogate models and inverse design strategies[28,31].
- Reduced-Order Models (ROMs) and surrogate models accelerated by autoencoders, GANs, and LSTMs for real-time simulation capabilities[33,35].
- Flow control and forecasting enabled by reinforcement learning and sequence modelling networks[39,40].
- These developments showcase a paradigm shift toward data-driven modelling, where learning-based approaches can complement or even replace parts of traditional numerical solvers.

5.2 Potential Impact on CFD and Engineering Design

The fusion of AI and CFD has the potential to significantly accelerate the pace of engineering design, optimisation, and decision-making. Surrogate models and ROMs can reduce computational time from hours or days to seconds, enabling rapid prototyping and real-time system control. AI-driven inverse design allows exploration of high-dimensional design spaces with unprecedented efficiency. Furthermore, the development of digital twins—real-time, AI-enhanced replicas of fluid systems—can revolutionise industries such as aerospace, automotive, biomedical engineering, and energy systems[48,50].

5.3 Call for Interdisciplinary Collaboration

While the progress is encouraging, the road to reliable, generalizable AI-driven CFD systems requires strong collaboration among fluid dynamicists, computer scientists, and engineers. Key areas for joint effort include:

- Establishing benchmark datasets and open platforms for reproducible research.
- Creating interpretable and physically consistent models.
- Integrating AI workflows into existing HPC infrastructures.
- Bridging the gap between data-driven models and physical understanding.

The convergence of data science and fluid mechanics is not merely a trend---it is a rapidly evolving discipline. Continued interdisciplinary collaboration is essential to fully realise the promise of AI-enhanced CFD.

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