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Recent advances in machine learning applications to computational fluid dynamics (CFD): models, challenges and future perspectives

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Abstract

Integrating machine learning (ML) techniques into computational fluid dynamics (CFD) has emerged as a promising model to speed up simulations, enhance turbulence modelling, improve prediction accuracies, and enable real-time flow analysis Comparative performance is also examined Critical analysis of previous work reveals current challenges, including limited generalization in flow regimes, high data requirements, and lack of robust uncertainty quantification The paper also outlines future approaches, including hybrid physics data-driven frameworks, transfer learning, interpretability, and open collaborative platforms Emphasis is By synthesizing developments and identifying research gaps, this study provides insights that can guide the development of ML–CFD towards robust, scalable, and industry-ready solutions

Keywords:- Machine Learning, Computational Fluid Dynamics, Turbulence Modelling, Hybrid Approaches, Uncertainty Quantification

Introduction

The integration of machine learning (ML) and computational fluid dynamics (CFD) has become one of the most dynamic and fast-growing research areas in computing science and engineering Accurate simulation of complex mechanical processes such as multiphase flow, heat transfer and turbulence – is possible by traditional CFD. Especially since simulation requires fine spatial/temporal discretization, advanced turbulence modelling, and large parallel processing it is also possible that this slow process hampers real-time decision processes and as engineering problems grow in size and complexity demand faster and more efficient methods that can overcome traditional CFD limitations

In this context, machine learning offers a transformative approach. Leveraging the ability of ML algorithms to detect patterns from data, detect nonlinear input-output maps, and assimilate complex correlations, researchers develop models that can replace or supplement traditional solvers, and reconstruct high-resolution solutions from raw or low-detail simulation results Unlike traditional purely physics-based numerical solvers, ML-based approaches can be trained directly on high-fidelity simulation data (such as direct numerical simulation – DNS, Large-Eddy-Simulation LES, or well-validated RANS models) and these models full physical equations at each step Without solutions, they reproduce complex flow behaviour by learning directly from the data. As a result, the combination of ML and CFD has opened up possibilities such as several times faster simulations, better prediction accuracy and real-time flow analysis compared to traditional methods

Research results over the last few years clearly show that the use of ML techniques in many sub-fields of CFD has proved highly scientifically and technically beneficial for example, surrogate modelling has been used in aerodynamics and fluid dynamics for rapid performance assessment, enabling extensive design optimization i.e. every possible size or geometry Deep neural network-based turbulence closure has been developed in the field of turbulence modelling to achieve the best design without expensive full-order simulations, which overcome the limitations of traditional Reynolds-averaged model by incorporating physical invariants in the

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model From (low-resolution) CFD results or sparse experimental data with the help of ML models such as convolution neural networks, generative anti-networks (GANs) and autoencoders these methods have obtained even finer scale structures than simulations done on macro networks You can also retrieve DNS-level details. This confluence of ML and CFD in application areas such as design optimization, turbulence modelling and super-resolution has brought new solutions beyond the limitations of traditional methods

Despite these advances, current ML-CFD integration faces several challenges. In particular, the generalizability of models is limited. Many ML models perform well in environments covered by their training data sets, but their accuracy and stability deteriorate when applied to unfamiliar flow conditions, different geometries, or boundary conditions And besides being expensive and time-consuming, the lack of uncertainty assessment in predictions obtained is a serious problem – most data-driven models results are "deterministic", not providing a reliable estimate of inherent uncertainty The above limitations (limited generalizability, reliance on big data, and lack of quantification of uncertainty) are major open challenges of the current research

To overcome these challenges, researchers will focus their future work in some new directions. Comparison of traditional physics-based methods and data-driven ML approaches has been reported. For example, systems such as physics-informed neural networks (PINNs) emerge, which incorporate ML model learning (loss functions) of the governing physical equations of flow Such physics-informed learning makes model prediction results physically more consistent and often perform better even on sparse data. In the same vein, uncertainty quantification (UQ) is being integrated into ML-CFD workflows to assess the reliability of model predictions and build confidence for industrial deployment can adopt these new techniques with confidence

Industrial integration is another forward direction in this area, where efforts to incorporate academic success into practical manufacturing processes and engineering design cycles are gaining momentum by integrating ML capabilities into existing CFD software infrastructure to enable real-time simulation-driven monitoring and control Mass customization will also be possible. Available research in 2023 suggests that hybrid physics data models, physics-informed approaches such as PINN, and uncertainty-inclusive reliable ML applications will together pave the way for the next generation of CFD tools Having made a definition.

Prior Methodologies in ML–CFD Research

Data Driven Surrogate Models

Data-driven surrogate models are an approach designed to incorporate machine learning (ML) into computational fluid dynamics (CFD). These models act as efficient estimators of CO and time-consuming astronomy, solving entire wearable datasets without aero and time-consuming displays learning complex execution sources from high fidelity (high fidelity) data sets such as direct numerical plant (DNS), large eddy astronomy (LES) or Stahl RANS calculations Derived from modelling, surrogate models can significantly reduce computational costs, and allow direct applications optimized to the design of plants

Ling, Kurzavsky, and Templeton (2016) were among the earliest researchers to demonstrate the potential of deep neural networks (DNNs) in turbulence closure model Their work incorporated invariant features such as Galilean invariance into the network architecture, so as to surrogate model traditional linear vortex viscosity closure Expectation can predict the Reynolds stress tensor more accurately Although the results showed a significant improvement in prediction accuracy, the model was limited to only those flow conditions that were included in the training dataset, thereby limiting its generalizability

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In a comprehensive review, Duraisamy, Iaccarino, and Xiao (2019) classified existing surrogate model approaches to turbulence modelling and flow forecasting and highlighted the advantages of combining data-only models with physics-based constraints show poor exclusion performance when applied to geometries

Methodologically, surrogate modelling has evolved from regression-based methods to advanced deep learning architectures capable of handling high-dimensional nonlinear flow features For example, Brunton, Proctor, and Kutz (2020) developed the Sparse Identification of Nonlinear Dynamics (SINDy) method, which directly CFD This method, which extracts governing equations from the data, was successful under some flow conditions, but faced difficulties under highly nonlinear and high-dimensional turbulent conditions.

Another important achievement was the work of Thuri and colleagues (2020), in which they used convolutional neural networks (CNNs) for turbulence super-resolution mesh refinement Their surrogate models were able to convert macro simulations into high-resolution predictions, much to capture fine-scale turbulent structures Lower computational costs were allowed but these models still required large, diverse, and high-quality data sets to ensure robustness under different flow conditions.

In the area of unsteady flow forecasting, Xie et al. (2020) developed Tempo GAN, a GAN-driven surrogate model designed to enhance temporal coherence in turbulent flow reconstruction. This approach was able to accurately capture complex spatial patterns as well as subtle temporal variations in flow. Building on similar goals, Fukami, Fukagata, and Taira (2021) used convolutional autoencoders to transform coarse CFD data into high-resolution turbulent-field representations Their method not only provided impressive reconstruction accuracy but of integrating deep learning techniques with CFD to significantly speed simulation processes Promising roles also underlined.

Surrogate modelling has also been used in design optimization work. Bhatnagar and colleagues (2019) used a CNN-based surrogate model to rapidly evaluate aerodynamic shapes during the optimization loop, greatly reducing the number of full CFD runs required but like many other surrogate models, their method shows a decrease in accuracy when applied to geometries outside the training set. Zhang, Wang, and Li (2022) solved this problem by integrating machine learning with reduced-order modelling (ROM) for unsteady aerodynamic analysis, improving prediction accuracy while maintaining computational efficiency

Recent research (2023) focuses on hybrid surrogate models that incorporate physical constraints directly into a machine learning framework so that predictions match conservation laws Transfer learning techniques are also popular, allowing pretrained surrogate models to adapt to new flow regimes with minimal redundant data. Furthermore, adaptive surrogate frameworks, in which the model iteratively refines its predictions based on feedback from the solver, emerge as a promising direction for industrial applications

Despite these advances, achieving generalization to varying flow conditions, reducing reliance on large high-fidelity data sets, and ensuring physical interpretability of surrogate predictions are still major challenges that need to be addressed that data-driven surrogate models from academic research to routine industrial CFD practice Per transferable In summary, these models have evolved from simple regression-based approaches to complex hybrid deep learning architectures capable of accelerating CFD workflows while maintaining high accuracy although issues related to generalization, data requirements, and physical compatibility still remain show a clear path to scalable, industry-ready surrogate models for CFD applications that are quickly becoming possible (Ling et al., 2016; Duraisamy et al., 2019; Thuerey et al., 2019; Thuerey et al.,, 2020;Fukami et al., 2021;

Physics Informed Neural Networks (PINNs)

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Physics-informed neural networks (PINNs) have emerged as a revolutionary approach to combine machine learning (ML) techniques with computational fluid dynamics (CFD), overcoming some major limitations of the data-driven model alone Unlike traditional ML methods that rely solely on high-fidelity data sets, PINNs Directly incorporate the governing physical equations, such as the Navier-Stokes equations, into their loss function This enables the network to find solutions that are data efficient and physically consistent, making them suitable for solving forward-reversal problems in CFD

The concept was first formalized by Raisi, Perdicaris, and Karniadakis (2019), who demonstrated that the inclusion of partial differential equations (PDEs) in the training process enables PINNs to solve nonlinear flow problems with minimal labelled data. In forward problems, PINNs predict fluid fields based on known initial boundary conditions, while in inverse problems estimate unknown parameters or boundary conditions from sparse observations were limited to relatively simple geometric structures

Subsequent research extended the scope of PINNs to more complex CFD problems. the sun and so on. (2020) used physically controlled deep learning to reconstruct velocity and pressure fields from sparse measurement data. Leveraging embedded physics constraints, their PINN models achieved greater stability and accuracy than data-only methods, although their use was still limited to flows of moderate complexity Mao, Jagtap, and Karniadakis (2020) extended the method to high-speed polyphasic flows, including fluid–structure interactions; These extensions, which also incorporated thermal effects into the network, demonstrated the adaptability of PINNs, but increased the computational burden and training complexity.

Several algorithmic innovations have been made to improve the scalability and robustness of PINNs. Lu and so on. (2021) presented adaptive loss balancing techniques, while Cai et al. (2021) proposed domain decomposition strategies to handle large computational domains. These advances have made it possible to apply PINNs to more challenging problems, but the modelling of high Reynolds number turbulence is still an unsolved challenge Jin et al. (2021) demonstrated that PINNs can be used to super-resolve the flow field, recovering fine scale structures from sparse data. However, PINNs often require careful tuning of hyperparameters, making them more complex to implement in practice than traditional solvers.

Applications of PINNs have extended beyond traditional CFD into more specialized areas. Kissas and others. (2020) applied PINNs to cardiac flow modelling, reconstructing hemodynamic fields in arterial networks from limited clinical measurements. Wang, Yu, and Perdicaris (2021) analysed training instabilities in PINNs in terms of neural tangent kernels, and provided a theoretical insight into why PINNs sometimes fail to converge. Dwivedi, Srinivasan, and Karniadakis (2021) proposed distributed PNNs to efficiently solve polyphasic problems, enabling scalable solutions for large fluid systems

Recent work has continued to address the major limitations of PINNs. Wassing et al. (2023) introduced an adaptive viscosity model, Wong et al. (2023) developed multi-case PINN frameworks for biomedical tube flows, and Ang et al. (2023) proposed a memory-efficient solution for low Reynolds number flows. These innovations aim to enhance the computational efficiency of PINNs and improve their suitability for industrial CFD applications.

Key advantages of PINNs include data efficiency, which allows accurate predictions even on limited labelled data using physical constraints; mesh-free structure, which works without predefined discretization and provides flexibility in handling complex geometric structures; and dual-use capabilities, through which forward and reverse problems can be solved in one framework. However, scalability, training time reduction, and automation of hyperparameter selection remain challenges in turbulent flows with high Reynolds number

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Current research is increasingly exploring hybrid PINN frameworks, in which data-dependent turbulence closure or surrogate model is integrated into PINN to increase generalizability and reduce computational burden. PINNs represent a powerful hybrid model that combines the interpretability and physical consistency of numerical solvers with the flexibility and data efficiency of machine learning Although their use in industrial CFD is still in its infancy, continued advances in scalability, robustness, and hybridization strengthen the possibility that PINNs are the next generation of the future can be an important component in CFD workflows (Raissi et al., 2019; Sun et al., 2020; Lu et al., 2021; Jin et al., 2021).

ML Assisted Numerical Solvers

Machine Learning (ML)-assisted numerical solvers represent an important development in integrating data-driven methods into traditional computational fluid dynamics (CFD) workflows Unlike purely alternative models that completely replace numerical solvers, ML-aided approaches synergize with traditional solvers such Methods that speed computations, increase stability, or improve accuracies by embedding ML modules directly in specific Steps in the CFD pipeline such as turbulence closure, mesh optimization, or iterative solution acceleration can leverage the predictive capabilities of ML without sacrificing the proven robustness of physics-based discretization schemes

Major advances in this area were demonstrated by Fukami et al. (2021), who used convolutional autoencoders and generative adversarial networks (GANs) to reconstruct high-resolution turbulent flow fields from coarse CFD simulation In this framework, the coarse-mesh CFD solver provided the baseline flow field while the ML model learned its super-resolution Computationally bypassed the need for expensive fine mesh simulations The approach Physical coherence was preserved across reconstructed areas, but accuracy depended on the diversity and fidelity of the training dataset

Similarly, Zhang et al. (2022) integrated ML techniques with reduced-order modelling (ROM) to accelerate unsteady aerodynamics simulations. Using ML to enhance ROM prediction, the authors achieved improved time accuracy and stability in long-term simulations, while maintaining computational efficiency

Besides super-resolution and ROM enhancement, other ML-assisted solver strategies have emerged in recent years. For example, neural network models for predicting optimal initial guesses or convergence accelerator parameters are integrated into iterative linear solvers to reduce the number of iterations required for pressure and velocity coupling in incompressible flow solvers and for optimal time step and mesh refinement control Reinforcement-learning frameworks are proposed, where the ML agent dynamically adjusts the solver parameters to balance accuracy and efficiency during runtime

The main advantage of ML-assisted solvers lies in their incremental adoption. Unlike fully data-driven models, they can be integrated into existing CFD codes with minimal disruption, making them particularly attractive for industrial applications where solver validation and reliability are top priority When applied, models often trained for a particular geometry or Reynolds number show performance degradation Ensuring physical stability, so that ML components obey conservation laws and avoid unphysical artifacts even when coupled with a numerical solver; and training data requirements, which, even lower than standalone ML models, still require high-quality training data sets (often generated from DNS or LES) to ensure reliable performance is also constrained This not only ensures physiological accuracy but also reduces the dependence on detailed training data. In addition, integrating transfer learning makes it possible to adapt pretrained ML models to new flow configurations with minimal retraining, significantly improving scalability for industrial use Overall, ML-assisted numerical solvers bridge the gap between purely physics-based methods and fully

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data-driven approaches By doing so, and providing a viable way to integrate ML into mainstream CFD workflows by accelerating simulations without compromising accuracy, these hybrid approaches are set to play a key role in next-generation CFD tools in areas such as optimization, design iteration and real-time decision making

Mesh Optimization and Adaptation

Mesh optimization and optimisation are critical components in the CFD workflow, directly affecting the accuracy, stability, and computational cost of simulations. Traditional mesh refinement methods often rely on heuristic or physics-based error indicators to determine areas requiring higher resolution. While effective, these methods can be computationally expensive and fail to optimally allocate computational resources, particularly in highly unsteady or multi-phase flows. Recent advances in machine learning have introduced new strategies for predicting mesh optimisation patterns, offering the potential to significantly reduce computational requirements while maintaining solution reliability.

Thuery et al. (2020) demonstrated one of the earliest deep learning-based methods for mesh refinement in CFD. Their method used convolutional neural networks (CNNs) to predict optimal areas for refinement directly from coarse-grid simulation data. By finding spatial features associated with high-error regions, the model was able to guide adaptive mesh refinement (AMR) without relying solely on traditional error estimators This greatly reduced computation cost and also maintained fine-scale feature accuracy, especially in turbulence-dominated flows It was, and generalizing flows outside of the training set remained a challenge

In a related development, Bhatnagar et al. (2019) indirectly contributed to grid optimization through their CNN-based aerodynamic coefficient estimation framework. Although their primary focus was on aerodynamic performance prediction, surrogate models facilitated more targeted mesh refinement strategies by identifying critical flow areas affecting aerodynamic forces, this integration of ML-driven flow analysis with mesh optimization offers a promising direction for optimizing solver performance in design-oriented simulations

Beyond image-based CNN approaches, emerging strategies in 2023 explored the use of graph neural networks (GNNs) and reinforcement learning (RL) for network optimization, this is especially beneficial in unstructured network environments, where RL-based methods for connection information solution accuracy plays an important role, on the other hand, enabling mesh optimization as a sequential decision problem to iteratively adjust mesh density based on simulation feedback to optimize the accuracy cost trade-off

A major advantage of ML-driven network optimization is that it can be implemented as an online integration within CFD solvers. Rather than generating a precomputed refinement model, ML models can dynamically adjust the network based on the evolution of flow features during runtime. This is particularly beneficial for transient simulations such as vortex deposition, burning, or shock–boundary layer interaction, where the location of critical flow regions changes over time but despite these advances it is still a challenge to ensure physical consistency and robustness in different flow regimes. Over-refinement in non-critical areas or over-refinement in dynamically emerging areas can affect solution fidelity. Besides, the need for training data is still great, especially when the objective is to generalize to various geometries and boundary conditions To overcome these challenges, recent research trends focus on hybrid approaches that combine physics-based error estimators and ML estimators f Emerging as a powerful tool to balance computational efficiency and predictive accuracy in CFD By integrating ML-based inferences into adaptive refinement loops, these methods

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promise to significantly accelerate simulation workflows, especially in large-scale and real-time applications (Thuerey et al., 2020; Bhatnagar et al., 2019).

Applications Documented in Previous Studies

Turbulence modelling

modeming turbulence is one of the major and widely researched applications of machine learning (ML) in computational fluid dynamics (CFD), as the multi-scale and chaotic nature of turbulent flow makes fluid mechanics a complex and long-term challenge Applied, yet often forced to compromise between computational cost and prediction accuracy Machine learning offers an opportunity to overcome this limitation, as it can learn complex closure relationships directly from high-fidelity datasets, such as direct numerical simulation (DNS) results by Ling, Kurzawski, and Templeton (2016). Pioneering work has been done integrating deep neural networks (DNNs) into RANS-based turbulence closure modeming, incorporating physical invariants such as Galilean invariants and rotational invariants directly into the network architecture to predict the Reynolds stress tensor The models can be more accurate than traditional linear eddy viscosity. Although this model produced good results under trained flow conditions, its generalization to flows outside the range of training data was limited, which is still a challenge in many turbulence-based ML applications Low-resolution CFD data reconstructed high-fidelity turbulence fields, where DNS-level accuracy was achieved at low cost using convolutional neural networks (CNNs) and generative anti-networks (GANs) This approach coarse-grid CFD solvers fine-scale without expensive mesh refinement were able to capture turbulent structures, which is particularly attractive for speeding up transient simulations, although large high-quality training data sets are still needed Sub grid scale (SGS) modelling in LES has also been improved by ML, where data-based SGS models trained on DNS data than static empirical coefficients Adjust dissipation levels based on local flow characteristics to better capture energy spectra and fine-scale dynamics, although ensuring physical consistency is still challenging Recent research has moved beyond pure data-based predictions to physics-informed machine learning approaches, in the loss of ML models Incorporating the Navier-Stokes equations, so that predicted turbulence fields obey conservation laws and fundamental principles of fluid dynamics such hybrid models combine the data efficiency of PINNs (Physics-Informed Neural Networks) and the accuracy of DNS-trained surrogates to provide better generalizations for unseen flow scenarios In addition, adapting pretrained turbulence models through transfer learning works for new Reynolds numbers, geometries, or flow conditions, reducing the need for extensive retraining which is very useful in industrial applications. Similarly, reinforcement learning has been used in adaptive turbulence closure selection, allowing the solver to dynamically choose the most appropriate turbulence model during simulation based on flow characteristics Lack of DNS data hinders their widespread use to overcome these problems, current research trends are moving towards a hybrid turbulence modelling framework where ML is used. In summary, machine learning has transformed turbulence modelling from static, empirical closure methods to dynamic, data-driven frameworks capable of capturing fine-scale flow structures with greater accuracy and less, and although their fully generalizable and interpretable forms are still in development. With the integration of hybrid modelling, they are very likely to be widely adopted in industrial CFD applications (Ling et al., 2016; Fukami et al., 2021).

Aerodynamic Design Optimization

Aerodynamic design optimization is a key area of integrated application of machine learning (ML) and computational fluid dynamics (CFD), where aerodynamic shapes such as air foils, wing(s) and vehicle bodies are traditionally optimized by a combination of iterative CFD simulations and optimization algorithms ML-based approaches address this challenge by developing surrogate models and hybrid frameworks, which enable rapid evaluation while maintaining predictive accuracy Bhatnagar et al. (2019) presented a convolutional neural network (CNN) based aerodynamic shape optimization framework, which significantly reduced the computational burden of traditional design procedures In this study, CNN model was trained on high-fidelity CFD dataset to predict aerodynamic properties like lift and drag directly from shape parameters could evaluate many times faster than traditional CFD, allowing them to be easily integrated into global optimization loops Although, this approach was quite accurate in trained geometries, its performance decreased in geometries different from the training set to improve, and prediction, etc. by enabling faster detection of gust response, flutter and other dynamic design scenarios. This hybrid approach balanced the speed of ROM with the corrective capacity of ML ROM Baseline quality remained a limiting factor, as inaccuracies in reduced-order solutions could creep into ML-based estimates by 2023. Recent research has made aerodynamic design optimization more effective using active learning strategies Increases, while decreasing the number runs expensive CFD. At the same time, multi-fidelity modelling approaches have emerged, incorporating ML to integrate low-fidelity analytical models and high-fidelity CFD data, harnessing the power of both to accelerate optimization without losing accuracy Reduces These physics-informed surrogates are particularly valuable in an industrial approach, where optimization tasks meeting safety-critical performance criteria with high confidence are presented as sequential decision problems and the RL agent gradually changes geometry to maximize efficiency objectives (e.g. lift-to-drag ratio), and design constraints Follows Such methods have yielded encouraging early-level results for multi-objective optimization in complex designs, involving combination Aerodynamic and structural considerations but despite these advances generalize to new geometries, manage high-dimensional parameter space, ensure interpretability of ML-based design process F Still Challenges Current research in this direction focuses on hybrid approaches that combine the interpretability of physics-based models and the efficiency of ML representatives to pave the way for more reliable extensible aerodynamic optimization workflows There are multi-objective problems that are capable of making complex uncontrollable and unstable, greatly speeding up the design cycle while maintaining high accuracy (Bhatnagar et al., 2019; Zhang et al., 2022).

Over resolution and flow reconstruction

Super-resolution and flow reconstruction emerged as a transformative application of machine learning (ML) that made it possible to retrieve high-fidelity flow fields from low-resolution or incomplete data in Computational Fluid Dynamics (CFD) Using data-driven models to achieve DNS-level resolution, super-resolution methods Reconstruct missing flow features that can upscale coarse simulation results, improve spatial and temporal resolution, and physically consistently One of the most important contributions in this field is Tempo GAN by Xie, Franz, Chu, and Thuy (2020). Generative anti-network (GAN)-based approach developed for super-resolution in turbulent flow simulations Different from traditional imaging super-resolution techniques, Tempo GAN incorporates time organization in the training process to reconstruct fine-scale turbulence structures with good temporal consistency Transient simulation is particularly feasible for occurrence, where time-asymmetry can produce physically unrealistic results although this method was very effective to recover fine scale features Greatly reduced This lets engineers integrate ML-based super-resolution modules directly into CFD workflows to run coarse simulations, and post-processing DNS-near quality and used in situations where data is sparse or incomplete such as velocity or pressure field reconstruction from limited sensor measurements Can be done through Informed Neural Networks (PINNs) In combination with physical law learning these models ensure that reconstructed fields follow governing

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equations, enhance reliability of engineering applications From 2023 recent studies integrating multi-scale learning architectures have further advanced these methods Since then, using transfer learning methods Pre-trained super-resolution models applied to new flow configurations with minimal retraining, reducing reliance on large data sets This Adaptability is important in industrial workflows where training data is often limited. Another emerging trend is that super-resolution methods can produce visually realistic but physically incorrect reconstructions ML super-resolution methods to identify potential artifacts or overfitting caused by models to ensure reconstructed field reliability. Furthermore, the need for a high-quality training dataset generated from an often-expensive DNS is still a barrier to large-scale adoption. To address these problems, current research develops hybrid approaches that combine data-based over resolution with physical conservation principles to ensure efficiency and adherence to physical conservation principles In summary, the difference between ML data needed for high-fidelity engineering analysis of course, inexpensive simulations, these methods Monitoring is poised to play a central role in the future of CFD post-processing, experimental data assimilation, and real-time streaming (Xie et al., 2020; Fukami et al., 2021).

Comparative analysis of previous works

Ling, Kurzawski, and Templeton (2016) first applied deep neural networks (DNNs) to model turbulence closure, incorporating physical properties such as Galilean invariance in the network architecture Their model made predictions of the Reynolds stress tensor physically more consistent than traditional rotational viscosity models the demonstration was done. However, it had the limitation of being limited to only those flow conditions that were included in the training data and its accuracy decreased in unseen flows or novel geometries (Ling et al., 2016).

Raissi, Perdikaris, and Karniadakis (2019) developed physics-informed neural networks (PINNs). This approach ensured data efficiency and physical consistency by incorporating the Navier-Stokes equations directly into the loss function. PINNs have succeeded in solving forward and inverse CFD problems even with limited sparse data. However, their application in turbulent flows with high Reynolds numbers has been difficult and its extension to the industrial scale is still limited (Raissi et al., 2019).

Thuerey et al. (2020) presented a CNN-based mesh refinement and super-resolution technique. This model showed the ability to identify high-error regions in CFD results and transform them into higher resolution ones, thereby reducing computational cost and making it possible to capture turbulence structures at the microscopic level. However, its major limitation is that it requires large, diverse, and high-quality datasets and its generalization outside the training domain is uncertain (Thuerey et al., 2020).

Fukami, Fukagata, and Taira (2021) presented a combined framework based on CNN and GAN. The method reconstructed turbulent flows from low-resolution CFD data with DNS-level accuracy and preserved energy spectra and vorticity. However, its performance remained highly dependent on high-fidelity and representative training data and its performance was unstable under different flow conditions (Fukami et al., 2021).

Zhang, Wang, and Li (2022) improved unsteady aerodynamic analysis using ML-enhanced reduced-order modelling (ROM). It increased the accuracy and temporal stability of the ROM and accelerated CFD simulations for aeroelasticity and optimization problems. However, its performance depended on the underlying quality of the ROM, and if there were errors in the original ROM, they were also transferred to the ML-enhanced predictions (Zhang et al., 2022).

Holistic Insights

Comparative analysis of these studies shows that data-driven methods such as DNN, CNN and GAN provide high accuracy under specific conditions, but require large and high-quality datasets. In contrast, physics-informed models (PINNs) can work even with relatively less data, but their computational complexity increases at flows with high Reynolds numbers.

Additionally, differences were also observed between generalization and specialization: PINNs showed better generalization ability while surrogate models such as CNN/DNN/GANs proved to be excellent in specialized tasks, such as super-resolution or turbulence modelling.

From a computational balance point of view, mesh refinement and ROM-based hybrid models are helpful in saving costs, but their performance depends on the quality of the underlying data and models. From an industrial point of view, all these models still need further development, especially in the areas of uncertainty quantification, interpretability, and adaptability to different flow conditions.

Challenges identified in previous studies

Analysis of previous research makes clear that despite significant progress in integrating machine learning (ML) and computational fluid dynamics (CFD) several serious and interrelated challenges still exist that affect model accuracy, reliability, and industrial utility and whether performs equally accurately in unseen scenarios For example, deep neural networks (Ling et al., 2016) or CNN-based super-resolution models (Fukami et al., 2021) perform well in their training domain, but their prediction accuracy decreases rapidly at different Reynolds numbers, sizes, or turbulence levels Their multipurpose capability is limited in industrial applications The second major issue is physical consistency & interpretability, as data-only models can sometimes violate fundamental physical laws like mass motion or energy conservation, and when PINNs (Raissi et al., 2019) this problem by incorporating these laws in the training process partially resolved, it remains very computationally valuable to accurately capture high Reynolds numbers and large-scale turbulence. Moreover, ML models act as “black boxes”, making it difficult to understand their decision reasons, and this is a major obstacle to adoption in safety-sensitive areas such as aerospace or biomedical flows A fourth problem, especially for complex multiphase or high Reynolds number flows, is scalability at the industrial scenario, as existing models do not work effectively without retraining due to complex geometry, Multiphysics coupling, and changing operating conditions in real industrial scenarios. A fifth challenge is computational balancing in hybrid models, where methods like ROM–ML or ML-assisted solvers are hard to balance between accuracy and speed, as their performance largely depends on the quality of the baseline physics-based model Lack of (UQ) is a major obstacle, as it is risky to rely on producing models without clear confidence limits, especially when data are sparse or need extrapolation Although in recent years some research has begun to incorporate probabilistic or Bayesian approaches in ML–CFD frameworks UQ mechanisms are needed

Future Perspectives

ML CFD models need to be transparent to achieve widespread adoption, especially in safety-sensitive fields like aerospace, automotive, and energy Current high-performance machine-learning architectures often act as “black boxes,” making it difficult for engineers to understand what factors or flow characteristics or predictions are liable to future emphasis on interpretive AI (XAI) approaches Explaining which flow patterns or physical parameters influence model output will not only increase confidence but also help researchers debug models, identify biases, and ensure compliance with regulatory standards. Similarly, uncertainty quantification (UQ) will be important for industrial engineers to clearly distinguish between high-risk and high-confidence areas to know the extent of their prediction reliability This will use probability-based modelling, Bayesian neural networks, and ensemble-based methods a long-term goal To become a standard part of industrial pipelines is for ML CFD methods, which need seamless integration with existing CFD codes, active flow control, rapid design iterations, and simulation to enable real-time or near-real-time applications such as monitoring. Macroscopic scale phenomena will extend the ability to efficiently combine processes such as chemical reactions, multiphase flow with fluid dynamics, and precisely measuring microscopy effects Availability of high-quality, standardized, open data sets and community-based collaborative research platforms to ensure reproducibility and accelerate innovation MLCFD will be required to integrate with open-source CFD solvers. Quantifying uncertainty to aid decision making, and play key roles will move towards seamless integration of real industrial impacts If these directions are pursued systematically, ML CFD frameworks will evolve from specialized research tools to fundamental components of engineering simulation This will also enable deeper understanding

Conclusion

Integration of machine learning (ML) and computational fluid dynamics (CFD) is revolutionizing fluid simulation, enabling faster, more efficient and in many cases more accurate predictions Advances in recent years have proven its potential application in turbulence modelling, surrogate modelling and real-time flow analysis improved the quality of engineering decisions by saving time and resources yet challenges such as limited generalizability, physical discrepancies, large need for high quality data, lack of uncertainty quantification still hinder its widespread industrial adoption Future direction Towards hybrid physical–data-based approaches; is to interpretable transparent models, and open and standardized data sets, supported by collaborative interdisciplinary research If continued organized efforts in these areas, ML–CFD methods will evolve from research prototype level to robust, industrial-scale tools for simulating and solving not only fluid flow problems will redefine process, but also take design, customization and decision-making capabilities in the industry to new heights

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