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Physics-Informed Machine Learning for Compressible Nozzle Flow Simulation: A Review of Advances and Research Opportunities

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Abstract: *Compressible nozzle flows represent a challenge in aerospace engineering, requiring computational resources to resolve shock structures and turbulent transitions. This paper provides a review of Physics-Informed Machine Learning as a framework to address computational bottlenecks in Computational Fluid Dynamics (CFD). Principles of Physics-Informed Neural Networks are detailed, alongside methodological advances in loss engineering, dynamic weighting strategies, and the integration of artificial viscosity to stabilize shock wave resolution. The review examines hybrid and multi-fidelity architectures, such as DeepONet and extended PINNs, which enable flow prediction and geometry-aware generalization across irregular grids. Applications are analysed, including forward simulation of subsonic and supersonic branches, inverse estimation of fluid parameters, and the reconstruction of flow fields from sparse, noisy sensor data. Although PIML offers advantages in data efficiency and design acceleration, challenges remain in resolving discontinuities at high Reynolds numbers and ensuring training robustness. The conclusion identifies research opportunities in shock-aware learning, Bayesian uncertainty quantification, and scalable domain decomposition, offering a roadmap for the deployment of physics-informed tools in industrial nozzle design.*

Keywords

Physics-informed machine learning, PINNs, compressible flow, nozzle flow, hybrid CFD, inverse problems, uncertainty quantification.

INTRODUCTION

The simulation and optimisation of compressible nozzle flows are fundamental to the advancement of aerospace propulsion, supersonic aviation, and rocket engine design(Khan et al., 2021; Li et al., 2025). These flows are characterized by high-velocity regimes where compressibility effects, such as expansion waves and shock waves, dominate the fluid dynamics (Liang et al., 2024; Mizuno et al., 2026). Traditionally, these phenomena are modelled using the compressible Euler or Navier-Stokes equations, which present significant computational challenges due to their nonlinear and hyperbolic nature(Bernardini et al., 2021; Gassner & Winters, 2021). While classical Computational Fluid Dynamics methods, such as shock-capturing or shock-fitting schemes, have matured significantly, they often require extensive computational resources and high-fidelity mesh generation(Yang et al., 2025). Furthermore, they can suffer from numerical artifacts such as the Gibbs phenomenon or excessive diffusion near discontinuities (Eikelder et al., 2023).

In recent years, the emergence of Physics-Informed Machine Learning, and specifically Physics-Informed Neural Networks, has offered a transformative alternative to traditional numerical solvers(Luo et al., 2025). PINNs integrate the governing partial differential equations directly into the neural network's loss function, allowing the model to learn surrogate solutions that satisfy physical laws without the strict requirement for a computational mesh(Serebrennikova et al., 2022). This paradigm is particularly advantageous for nozzle flows, where geometry-dependent analytical solutions can be complex and flow regimes can transition abruptly from subsonic to supersonic states(Liang et al., 2024). Recent studies have demonstrated that PINNs can accurately identify shock locations in converging-diverging nozzles and provide sharp profiles for transitions without the need for exogenous training data (Liang et al., 2024).

Despite these advantages, applying PINNs to high-speed compressible flows introduces unique methodological hurdles. The presence of discontinuities (shocks) often leads to training instabilities, as the original PINN formulation struggles with hyperbolic conservation laws(Ryck et al., 2024; Thodi et al., 2024). To address this, researchers have introduced advanced techniques such as weighted loss functions, domain decomposition strategies like Extended PINNs, and the enforcement of entropy-inspired artificial viscosity to ensure physical consistency(He et al., 2023; Nath et al., 2023; Wassing et al., 2023). Furthermore, innovations such as clustering training points near shock regions and utilizing higher-order neural units have shown promise in improving the resolution of complex flow features(Kovář & Fürst, 2024; Liang et al., 2024).

The field is also expanding toward multi-fidelity and hybrid approaches. For instance, recent work has explored the integration of low-fidelity data to generate high-fidelity solutions within seconds of inference time (Rui et al., 2023), as well as the potential of Hybrid Quantum Physics-Informed Neural Networks to overcome the computational costs (Leong et al., 2025). Given this rapid evolution, there is a critical need for a comprehensive review that synthesizes these methodological advances and identifies remaining gaps.

This review aims to provide a structured overview of the current state of PIML for compressible nozzle flows. We examine the foundations of physics-informed learning, evaluate recent breakthroughs in loss engineering and domain-adapted architectures, and discuss the practical applications of these models in real-time design and flow reconstruction (Kovář & Fürst, 2024; Molnar et al., 2023). Finally, we highlight the open challenges, including shock resolution, turbulence modelling, and scalability that must be addressed to transition these tools into standard industrial workflows.

Compressible Nozzle Flow Physics

The simulation of nozzle flows is governed by the conservation laws of mass, momentum, and energy, typically expressed through the Euler or Navier-Stokes equations. These equations, representing mass (F_1), momentum (F_2), energy (F_3), and the state equation (F_4), are incorporated as residuals in a neural network's loss function for solving nozzle flows (Liang et al., 2024). Key phenomena in these systems include choking, where the flow reaches Mach 1 at the nozzle throat, and the formation of expansion fans and shocks depending on the back-pressure conditions (Giehler et al., 2023).

When the nozzle operates in overexpanded or underexpanded regimes, the flow must adjust to the ambient conditions through complex wave patterns. Normal shocks represent a particular challenge because they manifest as sharp discontinuities in density, pressure, and velocity. In contrast to ideal inviscid behavior, viscous and turbulent effects must be considered in practical applications, especially at large Reynolds numbers where high-resolution shock-capturing technology becomes essential for reliable results (Boiron et al., 2008). PIML frameworks are specifically designed to identify these shock locations accurately while providing sharp solutions (Liang et al., 2023).

Physics-Informed Learning Foundations

The core methodology of physics-informed learning involves the use of Physics-Informed Neural Networks (PINNs) to recast the flow simulation as an optimization problem(Jagtap et al., 2022). This is achieved by defining a composite loss function that includes residuals from the governing partial differential equations, initial conditions, and boundary conditions (Liang et al., 2024).

Current research distinguishes between soft and hard constraint formulations. Soft constraints treat physical laws as penalty terms in the loss function, which offers flexibility however provides no absolute guarantee that the physical laws or boundary conditions will be satisfied outside the training space (Mohan et al., 2020). In contrast, hard constraints structurally enforce these conditions by embedding them into the neural network architecture itself, often through differentiable layers or specific distance functions (Pan et al., 2024). While hard constraints can be more computationally expensive to implement, they are often necessary for achieving accurate solutions in complex geometries with curved boundaries (Xiao et al., 2024). Furthermore, these frameworks (CITE_33, CITE_34) are uniquely suited for inverse problems, such as estimating unknown specific-heat ratios or flow parameters from sparse experimental data, without the need for the costly data assimilation techniques of traditional CFD (Jagtap et al., 2022).

Methodological Advances

The application of physics-informed machine learning to compressible nozzle flows has necessitated significant departures from standard neural network frameworks (Li et al., 2024). Because these flows are governed by hyperbolic conservation laws, traditional PINN formulations often struggle with the sharp gradients and discontinuities characteristic of supersonic regimes (Lorin & Novruzi, 2024). Recent research has focused on enhancing these models through specialized formulations, loss function optimization, and hybrid architectures that integrate classical computational fluid dynamics (Liang et al., 2024),

Physics-Informed Neural Networks

Physics-informed neural networks (PINNs) provide a meshless framework for solving the Euler and Navier-Stokes equations by embedding these governing laws directly into the network training process (Wassing et al., 2023). In the context of converging-diverging nozzles, PINNs have demonstrated the ability to resolve complex flow features including subsonic, supersonic, and mixed regimes with normal shocks (Liang et al., 2023). While classical numerical methods often require complex shock-capturing or shock-fitting schemes, PINNs can identify shock locations and provide sharp transition profiles without manual grid refinement (Liang et al., 2024).

Recent studies have explored both steady and unsteady flow conditions within nozzle geometries. For steady-state simulations, PINNs have been shown to accurately predict different flow branches based on the ratio of back pressure to stagnation pressure(Liang et al., 2024). In unsteady scenarios, networks with increased neuron counts and higher training point densities can track time-dependent flow developments until reaching a steady state (Liang et al., 2024). Beyond forward simulation, the PINN framework can be used for inverse problems, such as identifying unknown physical properties like the specific-heat ratio (Liang et al., 2024). However, the original PINNs can sometimes struggle with the hyperbolic nonlinear partial differential equations unless specific adjustments are made to produce physical solutions and avoid trivial solutions (Liang et al., 2023).

Loss Engineering and Constraints

A major challenge in training PINNs for high-speed flows is the imbalance between different components of the loss function (Jahaninasab & Bijarchi, 2024). It has been observed that optimizers may prioritize smooth, incorrect solutions over discontinuous physical solutions to minimize effort during the descent process (Liang et al., 2023). To counteract this, researchers have implemented weighted loss functions where specific equations, such as the momentum balance, are assigned significantly higher weights (Liang et al., 2023). Dynamic weighting strategies have also been proposed to balance gradients across different loss components automatically, which helps mitigate gradient vanishing during training (Liang et al., 2023)

Stability is further enhanced by enforcing hard boundary conditions and introducing artificial dissipation. For nozzle flows, enforcing hard constraints on pressure boundaries ensures the network adheres to physical limits at the inlet and outlet (Liang et al., 2024). Furthermore, incorporating adaptive artificial viscosity has proven essential for stabilizing shock waves in transonic and supersonic regimes (Wassing et al., 2025). This technique, inspired by classical numerical dissipation, allows the network to find physically reasonable entropy solutions by locally smoothing discontinuities during the early stages of training before reducing the viscosity for higher accuracy (Bard & Dorelli, 2021). These strategies, combined with residual-based sampling and self-adaptive weighting, prevent any single loss term dominating the optimisation process, thereby improving convergence in the presence of stiff residuals (Aygun & Karakus, 2024).

Hybrid and Multi-Fidelity Models

To reduce the high computational cost of generating training data and improve accuracy, hybrid frameworks combine physics-informed learning with available CFD data. Multi-fidelity strategies leverage large amounts of low-fidelity data, such as results from 2D Euler simulations alongside sparse high-fidelity data from 3D CFD or experimental measurements , (Rui et al., 2023). These models use specialized sub-networks to capture both linear and non-linear correlations between the different data fidelities, allowing for precise flow reconstruction even with limited expensive measurements (Li & Montomoli, 2024).

Transfer learning and operator learning have also emerged as powerful tools for nozzle design optimization (Chen & Liu, 2022). Frameworks like DeepONet can approximate nonlinear operators and predict complex fields, such as velocity and temperature, several orders of magnitude faster than conventional CFD solvers (Mao et al., 2020). Once trained, these models can be used in a readily integrable manner to assimilate sparse measurements and provide real-time aerothermal assessments (Mao et al., 2020). Additionally, machine learning models can be used to provide a pre-computed initialization for traditional CFD simulations, significantly accelerating the convergence of iterative solvers by providing a physically consistent initial guess (Fuchi et al., 2022).

Domain-Adapted Architectures

The geometric complexity of nozzles and the presence of sharp gradients require network architectures that are adapted to the specific domain physics. Coordinate and mesh transformations are frequently used to precondition the network, allowing it to handle flow around curved nozzle walls and within varying cross-sections more effectively (Oldenburg et al., 2022). For problems involving multiple physical scales or complex shock structures, extended PINNs use space-time domain decomposition to partition the flow field into simpler sub-domains, which improves predictive accuracy (Jagtap et al., 2022).

Architectural innovations also include the use of conservative formulations and adaptive activation functions. Formulating the governing equations in their conservative form helps the network maintain physical consistency across shocks and discontinuities(Liang et al., 2024). Adaptive activation functions, which allow the network to tune its own response during training, have been shown to outperform fixed functions in resolving the expansion waves and oblique shocks common in supersonic nozzle exhausts(Jagtap et al., 2022). These domain-adapted approaches ensure that the network can accurately capture the multiscale dynamics of high-speed compressible flows (Mao et al., 2020).

Applications in Nozzle Flows

The integration of physics-informed neural networks into the study of nozzle flows has transformed the modeling of complex compressible phenomena(Luo et al., 2024). By embedding the governing equations of fluid dynamics directly into the learning process, these models bridge the gap between traditional computational fluid dynamics and purely data-driven approaches(Li et al., 2024),(He et al., 2023).

Forward Flow Prediction

Forward flow prediction in converging-diverging nozzles involves the determination of state variables such as pressure, density, velocity, and temperature based on known geometry and boundary conditions(Liang et al., 2024). Traditional PINN frameworks often struggle with the hyperbolic nature of the Euler equations, particularly when discontinuities like shock waves are present(Liang et al., 2023). Recent advancements have addressed these challenges by implementing specific weight balancing strategies in the loss function to avoid trivial solutions and capture the correct physics of the flow(Liang et al., 2023). In CD nozzle simulations, PINNs have demonstrated the capability to identify shock locations accurately and provide well-resolved solutions for various pressure ratios without requiring any auxiliary training data (Liang et al., 2023). For instance, researchers have successfully predicted subsonic, transonic, and supersonic regimes by enforcing strict constraints on boundary conditions and adjusting the weights of momentum loss components (Liang et al., 2024). Beyond steady-state solutions, these models have been extended to unsteady flows, capturing the transition from rest to steady-state conditions where analytical solutions are typically unavailable (Liang et al., 2024).

Inverse Design and Parameter Estimation

Inverse problems in nozzle flows are often ill-posed and computationally expensive with traditional numerical methods (Jagtap et al., 2022). Physics-informed machine learning offers a more efficient alternative for inferring hidden parameters or optimizing nozzle geometry from limited observations (Jagtap et al., 2022). A significant application in this area is the estimation of material properties or fluid constants (Mahmoudabadbozchelou & Jamali, 2021). For example, PINNs have effectively determined the unknown specific heat ratio (γ) of a gas by training the network on a small set of interior solution points (Liang et al., 2024).

The inference of boundary conditions and operating states is another critical area where PINNs excel. In supersonic flow scenarios, these models can infer full flow fields from density gradient data, obtained via Schlieren photography(Molnar et al., 2023). By minimising the residual between the physical laws and available measurement data, researchers can determine the optimal geometry required to achieve specific flow characteristics(Kovář & Fürst, 2024). This capability is particularly valuable for rocket nozzle design optimisation, where the actual performance must be aligned with design specifications under varying operating conditions(Xiao et al., 2026).

Benchmarking and Evaluation

Standardized benchmarking is essential to validate the reliability of physics-informed models against established numerical methods(Mohammadi et al., 2023; Sharma et al., 2023).

Evaluation typically focuses on the model's ability to minimize the L_2 norm of the total error(Kim et al., 2021) and various residual-based metrics(Urbán et al., 2023). In compressible nozzle applications, specific metrics such as root-mean-square error are used to assess the accuracy of velocity and pressure field reconstructions(Molnar et al., 2023). For flows containing discontinuities, performance is often evaluated using metrics such as shock location error and the sharpness of the transition profile(Assonitis et al., 2021; Flaszyński et al., 2021). Unlike low-order CFD methods that may require grid refinement at the shock or high-order methods that suffer from the Gibbs phenomenon, optimized PINNs have shown the ability to identify shock locations accurately without such drawbacks (Liang et al., 2024). Researchers also emphasize the importance of "conservation residuals," which assess the extent to which the neural network satisfies the integral forms of the governing equations (Thodi et al., 2024).

Table 1: Summarizes Representative Studies in this Domain

Study	**Geometry**	**Flow Regime**	**Data Type**	**Key Performance Metric**
(Liang et al., 2024)	CD Nozzle	Subsonic/Supersonic/Shock	Physics-only	Profile sharpness
(Wassing et al., 2023)	Parametric boundary shapes	Transonic Euler	Parametric physics	Shock angle accuracy < 1 deg
(Peyvan & Kumar, 2025)	Hypersonic and supersonic flows	Geometry-dependent hypersonic and supersonic flows	Scarce high-fidelity data	Flows on arbitrary grids
(Hosseini & Shiri, 2024)		Reconstruction study	Sensor measurements	R^2 and RMSE

Research Opportunities

Shock-Aware Learning

Handling discontinuities remains a primary obstacle for PINNs in compressible nozzle simulations. Standard optimizers often converge sub optimally, tending toward smooth solutions, even when the physics dictate a sharp shock (Liang et al., 2023). To address this, researchers have explored adjusting the weights of loss function components, such as applying significantly higher weights to the momentum equation, thereby forcing the discovery of discontinuous solutions (Liang et al., 2024).

Other emerging techniques include the introduction of artificial dissipation to stabilize shock waves, like classical numerical schemes such as Weighted Essentially Non-Oscillatory methods (Wassing et al., 2025). Recent models such as DGNet and Separated-Transfer PINNs utilize the Rankine-Hugoniot relation as a physical constraint or employ velocity-dependent weights to identify and resolve discontinuities without *a priori* knowledge of the shock location (Wang et al., 2025). These "shock-capturing" loss functions are critical for accurately predicting the non-smooth residual landscapes typical of nozzle flows.

Generalization Across Geometries

PINNs typically require retraining for new scenarios such as different boundary conditions, initial conditions, geometry, or new parameter values (Nguyen et al., 2024). Current research is shifting toward "geometry-aware" neural operators, such as DeepONet and Fusion-DeepONet, which map geometry-dependent features to flow fields using shared parameters (He et al., 2024), (Peyvan & Kumar, 2025). These models can handle both uniform and irregular grids, outperforming traditional mesh-based neural networks in scalability and efficiency (Peyvan & Kumar, 2025).

Transfer learning has also proven effective, in which parameters from a network trained on one geometric description are transferred to a new design, requiring only minimal fine-tuning (Goraya et al., 2022). This approach drastically reduces the training epochs needed to obtain accurate solutions for varying Reynolds numbers or nozzle shapes (Goraya et al., 2022). Furthermore, the development of PI-GANO allows simultaneous generalization across both PDE parameters and domain geometries, eliminating the high computational cost of generating synthetic training data for every new design (Zhong & Meidani, 2024).

Uncertainty Quantification

For engineering certification, it is not enough for a model to be fast; it must also be able to quantify the confidence of its predictions. Bayesian Physics-Informed Neural Networks address this by treating network weights as probability distributions rather than point estimates(Pensoneault & Zhu, 2024). These networks (Liu et al., 2024) are particularly robust when dealing with the high-level noise typical of experimental nozzle measurements, as they provide a comprehensive uncertainty quantification for the reconstructed velocity and pressure fields.

Ensemble learning offers an alternative strategy, where the variance between multiple standard PINN predictions serves as a proxy for uncertainty (Liu et al., 2024). These methods are vital for identifying regions in the nozzle where the model may be struggling, such as shock-boundary layer interactions or areas with sparse sensor coverage (Mousavi & Eldredge, 2025).

Data Efficiency and Experiment Integration

The synergy between sparse experimental data and physical laws is a major frontier for nozzle research. PINNs can act as advanced data assimilation tools, reconstructing high-resolution flow fields from a limited number of sensors around a nozzle wall or cylinder. For instance, studies have shown that more than 28 sensors can successfully reconstruct a velocity field with high precision (Hosseini & Shiri, 2024).

Recent methodological improvements, such as sensitivity-based adaptive sampling, help identify optimal sensor placements that maximize information gain for model training (Chang et al., 2025). By integrating direct sensor data inputs into the network architecture rather than just the loss function, models become significantly more robust to structural uncertainties and unseen flow conditions (Chang et al., 2025). This data efficiency is crucial for combining low-resolution experimental visualisations, such as Particle Image Velocimetry, with high-resolution requirements (Cai et al., 2024).

Limitations and Open Challenges

Despite the rapid evolution of physics-informed machine learning, several fundamental barriers continue to hinder its seamless integration into industrial nozzle-design workflows. These challenges span from the mathematical nature of the optimization problem to the physical complexities of high-speed compressible flows (Xiao et al., 2026).

Training Instability and Loss Weighting Sensitivity

A primary bottleneck in training Physics-Informed Neural Networks is the inherent difficulty in balancing competing objectives within the multi-term loss function. Traditional formulations that use static, uniform weights often fail because they do not account for the disparate scales of the partial differential equation residuals versus boundary and initial condition errors (Maddu et al., 2021). Research indicates that successful training requires meticulous selection of loss weights to ensure simultaneous convergence of all terms (Dreisbach et al., 2024). To mitigate this, dynamic weighting schemes such as "Soft-Adapt" (Dreisbach et al., 2024) and "Inverse-Dirichlet weighting" (Maddu et al., 2021) have been proposed to adaptively adjust the influence of each loss component during the training process. Furthermore, the choice of non-dimensionalisation significantly impacts performance, as it acts as a form of normalization that can either facilitate or obstruct the network’s ability to learn high-frequency physical features (Raghu et al., 2024).

Challenges in Shock Resolution and Discontinuities

Compressible nozzle flows are frequently characterized by discontinuities, such as shock waves(Liang et al., 2024) and expansion fans(Vesper et al., 2021). PINNs struggle to approximate these sharp gradients because neural networks typically favor smooth, continuous functions(Lai et al., 2025). However, traditional high-order numerical methods are often plagued by the Gibbs phenomenon or instabilities near shocks (Liang et al., 2024). Current evidence suggests that PINNs perform better when PDEs are expressed in their simple differential form rather than the conservative one favored by classical solvers, primarily owing to automatic differentiation (Liang et al., 2023). To improve resolution, some researchers have successfully integrated the Equation of State directly into the loss function (Mizuno et al., 2026) or utilized artificial viscosity, though the latter remains highly sensitive to the viscosity coefficient (Wassing et al., 2024).

Conclusions

The integration of physics-informed machine learning into the simulation of compressible nozzle flows represents a significant paradigm shift in computational fluid dynamics. This review has demonstrated that by embedding governing physical laws directly into the learning process, these models can offer robust solutions even in scenarios where experimental or high-fidelity data are scarce. The ability of PINNs to act as continuous solvers without the need for traditional mesh discretization provides a flexible alternative for complex internal flow geometries.

However, the path to widespread adoption is contingent upon overcoming several key technical hurdles. Future research must prioritize the development of sophisticated shock-capturing techniques that do not sacrifice the simplicity of the neural architecture, such as those accurately capturing sharp discontinuities. Additionally, more efficient dynamic weighting schemes will be essential for improving training stability. As the field moves towards more parametric and geometry-aware architectures, physics-informed methods are poised to become a cornerstone of real-time design and uncertainty quantification in aerospace engineering. Ultimately, fostering a culture of reproducibility through standardized benchmarks will be the catalyst for moving these powerful tools from academic research into industrial nozzle design.

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