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Research Article

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Posted Date: August 25th, 2026

DOI: https://doi.org/10.21203/rs.3.rs-10788710/v1

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Additional Declarations: No competing interests reported.

A Unified Mathematical Framework for Physics-Informed Digital Twins in Sustainable Engineering Optimization: Formulations, Convergence, and Pareto Frontiers

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Abstract

Resolving multidimensional partial differential equations (PDEs) within dynamic thermo-fluid systems imposes prohibitive computational latency when relying exclusively on classical numerical discretization techniques. This computational overhead severely restricts the real-time execution of multi-objective optimization algorithms in sustainable engineering applications. This study develops a mathematically unified framework that integrates explicit finite difference schemes, metaheuristic swarm optimization, and Physics-Informed Neural Networks (PINNs) into an adaptive digital twin architecture. The methodology embeds the nonlinear Navier-Stokes equations and transient thermal diffusion operators directly into the neural network optimization manifold via automatic differentiation. By penalizing PDE residual deviations during gradient descent, the architecture eliminates unphysical predictive divergence and mitigates truncation errors inherent in classical grid-based approximations. We provide formal mathematical proofs of convergence, establish asymptotic Lyapunov stability bounds under Lipschitz continuity conditions, and derive the exact descent properties governed by the Neural Tangent Kernel. An exhaustive hyperparameter ablation study confirms that balanced loss weightings ($\lambda_p = 1.0$) guarantee monotone convergence toward the global minimum. When coupled with a continuous-space Particle Swarm Optimization (PSO) routine, the proposed framework reduces the operational time complexity of candidate state evaluation from $\mathcal{O}(N^3)$ to $\mathcal{O}(1)$ via parallelized tensor vectorization. Comparative validations against high-fidelity computational fluid dynamics benchmarks demonstrate that the PINN digital twin restricts the Mean Absolute Percentage Error (MAPE) below 1.5% across dynamic boundaries while reducing simulated exergy destruction and energy consumption along a Pareto-optimal frontier. This mathematical architecture provides a deterministic, highly scalable foundation for real-time optimal control in low-carbon logistics, thermal management, and automated manufacturing, aligning with the rigorous demands of modern applied mathematics.

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Keywords: Physics-Informed Neural Networks; Numerical Analysis; Multi-Objective Optimization; Partial Differential Equations; Digital Twins; Asymptotic Stability; Exergy Minimization.

1 Introduction

Mathematical precision forms the absolute foundation of modern sustainable engineering analysis. Evaluating nonlinear interactions within fluid dynamics, convective heat transfer, and industrial energy utilization demands rigorous computational methodologies. Classical deterministic models effectively evaluate steady-state constraints but falter under the computational weight of dynamic, multidimensional simulations necessary for optimal real-time control [1, 2]. Whether optimizing convective cooling manifolds in heavy power electronics, modulating variable refrigerant flows in low-temperature supply chains, or controlling dynamic heat dissipation in advanced subtractive manufacturing, the governing physical phenomena are intrinsically nonlinear, multidimensional, and non-stationary. To achieve genuine thermodynamic optimization, high-fidelity modeling of transport phenomena is necessary [3]. The spatial-temporal evolution of fluid velocity fields, localized pressure gradients, and temperature distributions is governed by classical conservation laws expressed as systems of coupled partial differential equations (PDEs) [4].

Predictive forecasting for turbulent fluid flow and transient thermodynamic systems typically requires discretizing continuous spatial and temporal domains. Iterative matrix inversions utilized in these high-fidelity numerical solvers exhibit severe computational latency. Consequently, direct simulation-based optimization remains a significant bottleneck for real-time engineering applications. To satisfy this demand, industrial paradigms have increasingly shifted toward the integration of Digital Twins [5]. These virtual replicas synchronize physical assets with computational models to dynamically monitor lifecycle performance [6, 7]. Establishing a functional digital twin requires continuous, ultra-fast data assimilation and predictive mapping [8]. However, existing digital twin implementations in the manufacturing sector rely heavily on reduced-order models or purely statistical mappings, which frequently fail to capture the complex physics of fluid-thermal interactions [9, 10]. The challenge lies in developing surrogate models that possess the execution speed of a statistical model alongside the physical fidelity of a rigorous numerical solver [11].

Recent shifts in applied mathematics prioritize integrating artificial intelligence with foundational calculus to resolve these computational bottlenecks [12]. Foundational approximation theorems [13, 14] demonstrated that multilayer feedforward networks can approximate any continuous function. Yet, purely data-driven machine learning models frequently violate mass, momentum, and energy conservation laws when deployed outside their immediate empirical training distributions. Enforcing strict mathematical regularizations, such as integrating stochastic flow equations directly into neural architectures, has been shown to dramatically stabilize predictions across complex geometric manifolds [15]. Because their parameter optimization relies exclusively on empirical risk minimization, unconstrained networks treat physical systems as black boxes [16]. When evaluated outside the convex hull of their training dataset, unconstrained surrogates frequently generate non-physical artifacts. They violate mass conservation, predict negative ab-

solute temperatures, or violate the Second Law of Thermodynamics by generating spontaneous heat transfer against thermal gradients [17].

To successfully map nonlinear performance manifolds without incurring extreme latency, computational frameworks must unify the discrete exactness of numerical solvers with the continuous interpolation capabilities of neural networks. The introduction of Physics-Informed Neural Networks (PINNs) fundamentally altered predictive simulation by bridging data-driven learning with classical calculus [18]. By defining a residual loss function that penalizes deviations from known PDEs, PINNs enforce physical boundaries during gradient descent [19]. Enforcing these strict mathematical regularizations ensures structural integrity [20] and accelerates real-time inference by orders of magnitude [21].

This manuscript proposes a computationally unified framework targeting the specific intersection of numerical approximation and intelligent digital modeling. We formulate a comprehensive mathematical architecture that couples transient Navier-Stokes momentum transport and thermal diffusion equations with localized exergy destruction models, establishing a rigorous objective space for sustainable engineering systems. Furthermore, we provide analytical convergence proofs and demonstrate asymptotic Lyapunov stability for the neural surrogate under gradient descent, establishing theoretical bounds on generalization error and operational stability. The subsequent integration of this validated surrogate into a metaheuristic Particle Swarm Optimizer (PSO) facilitates the rapid generation of continuous Pareto-optimal frontiers, enabling dynamic multi-criteria decision-making for sustainable operations.

2 Current Studies and Mathematical Gaps

The intersection of numerical analysis and computational intelligence has generated substantial interest within applied mathematics. However, transitioning from theoretical computer science to robust engineering application reveals several critical gaps in current methodologies. This section provides an extensive critical review of contemporary literature, identifying the mathematical limitations of existing methodologies across distinct paradigms.

2.1 Operator Learning and Physics-Informed Advancements

To bypass the computational burden of numerical solvers, extensive research has investigated deep neural networks as surrogate approximation functions. DeepXDE [22] provided a comprehensive deep learning library for solving differential equations, formalizing the integration of automatic differentiation into boundary value problems. However, researchers quickly identified that complex PDE systems induce gradient flow pathologies [23]. These pathologies create stiff optimization landscapes where physical loss terms dominate empirical terms, leading to suboptimal local minima. Adaptive activation functions [24] were introduced to accelerate convergence in deep and physics-informed neural networks by dynamically altering the topology of the loss surface.

Mathematical validations of PINNs have rapidly expanded, focusing on convergence properties for linear second-order elliptic and parabolic PDEs [25]. Error analysis for Kolmogorov PDEs [26] and comprehensive generalization bounds [27, 28] have established that the total

approximation error is rigorously bounded by the training loss and the number of collocation points. Advanced architectures such as Conservative PINNs (cPINNs) on discrete domains [29], Extended PINNs (XPINNs) [30], and Augmented PINNs (APINNs) [31] have demonstrated superior generalization capabilities across heterogeneous sub-domains. Furthermore, frameworks utilizing DeepONets [32] and Deep Galerkin Methods [33] offer alternative paths for solving variational problems. Parallel mathematical frameworks have emerged, including the Deep Ritz method [34], automatic differentiation techniques [35], PDE discovery paradigms via sparse regression [36], and autoregressive physics-constrained recurrent models [37].

2.2 Fluid Mechanics and Complex Geometries

PINNs have been successfully extended to resolve inverse problems in highly complex fluid scenarios. Applications in supersonic flows [38] and causal sweeping strategies [39] have proven the viability of these networks in high-gradient domains. High-speed flows [40] and incompressible Navier-Stokes equations via NSFnets [41] have been extensively modeled. Furthermore, hidden fluid mechanics methodologies [42] have demonstrated the capability to extract full velocity and pressure fields from sparse flow visualizations. These techniques have also been successfully applied to simulating radiative transfer equations [43], confirming the universality of the physics-informed paradigm.

2.3 Metaheuristic Swarm Optimization in Sustainable Systems

In sustainable industrial engineering, optimal system design requires reconciling intrinsically conflicting thermodynamic and economic criteria. These problems are defined over continuous, non-convex design spaces. Because real-world performance surfaces exhibit non-differentiability, local minima traps, and discontinuous constraints, gradient-based mathematical programming often fails to locate global extrema. Foundational evolutionary paradigms, such as standard Particle Swarm Optimization [44], established the baseline for decentralized search algorithms. The subsequent derivation of constriction factors [45] ensured the mathematical stability of these swarms in multidimensional complex spaces.

Multi-Objective Particle Swarm Optimization (MOPSO) [46, 47] and the Non-dominated Sorting Genetic Algorithm II (NSGA-II) [48] became the industry standards for generating Pareto frontiers. Decomposition-based multi-objective evolutionary algorithms (MOEA/D) [49] and reference-point based many-objective sorting (NSGA-III) [50] further refined the ability to map complex objective spaces.

Despite these advancements, a critical mathematical gap remains. Applying these evolutionary solvers directly to massive computational fluid dynamics meshes generates a combinatorial explosion of computational time. Furthermore, the dynamic, real-time coupling of a fully continuous PINN solver with a constricted multi-objective swarm algorithm remains largely unexplored. Most current literature treats PINNs strictly as forward solvers, entirely neglecting their potential as ultra-fast optimization oracles. This study directly resolves these gaps by establishing a unified mathematical architecture that links discrete numerical physics, continuous PINN surrogates, and multi-objective metaheuristic optimization into a deterministic, validated framework.

3 Mathematical Formulations of Governing Physics

The behavior of sustainable engineering systems is governed by strict conservation equations. Accurate spatial and temporal approximations of these continuous domains are mandatory for establishing the baseline simulation data upon which the neural framework is constructed.

3.1 Transient Thermal Transport and Conduction

The fundamental evaluation of dynamic heat transfer relies on solving a parabolic partial differential equation. For an isotropic continuous medium, the generalized formulation is defined as:

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \frac{\dot{q}}{\rho c_p} \tag{1}$$

where $T(x, y, z, t)$ defines the absolute scalar temperature field, t specifies temporal progression, α represents localized thermal diffusivity, $\dot{q}$ is the volumetric heat generation rate, ρ is the material density, and c_p is the specific heat capacity.

Numerical evaluation of complex boundaries utilizes the explicit forward-time centered-space (FTCS) finite difference approximation:

$$\frac{T_{i,j}^{n+1} - T_{i,j}^{n}}{\Delta t} = \alpha \left(\frac{T_{i+1,j}^{n} - 2T_{i,j}^{n} + T_{i-1,j}^{n}}{\Delta x^2} + \frac{T_{i,j+1}^{n} - 2T_{i,j}^{n} + T_{i,j-1}^{n}}{\Delta y^2} \right) \tag{2}$$

Strict stability criteria for these discrete approximations are dictated by the Fourier number limit:

$$Fo = \frac{\alpha \Delta t}{(\Delta x)^2} \leq \frac{1}{4} \tag{3}$$

3.2 Navier-Stokes and Fluid Dynamics

Modeling incompressible Newtonian fluid flow involves evaluating the conservation of mass and momentum. The continuity equation is given by:

$$\nabla \cdot u = 0 \tag{4}$$

The nonlinear Navier-Stokes momentum equations dictate the fluid velocity vector u:

$$\rho \left(\frac{\partial u}{\partial t} + (u \cdot \nabla) u \right) = -\nabla p + \mu \nabla^2 u + \rho g + F_{body} \tag{5}$$

where p isolates thermodynamic pressure, μ signifies dynamic viscosity, and F_{body} accounts for external body forces. Discretizing these convective-diffusive equations generates sparse, highly asymmetric coefficient matrices.

3.3 Exergy Destruction and Entropy Generation

To align the mathematical model with sustainable performance metrics, thermodynamic irreversibility must be quantified. For a convective fluid system, the volumetric entropy generation

rate $\dot{S}'''_{gen}$ is formulated as:

$$\dot{S}'''_{gen} = \frac{k}{T^2}(\nabla T \cdot \nabla T) + \frac{\mu}{T}\Phi \tag{6}$$

where k indicates thermal conductivity and Φ represents the viscous dissipation function. Minimizing the spatial integral of $\dot{S}'''_{gen}$ over the control volume directly minimizes exergy destruction, providing a mathematically robust primary objective function for sustainable optimization algorithms.

4 Physics-Informed Digital Modeling Framework

Integrating numerical baseline data with advanced neural architectures constructs the digital twin. The framework utilizes deep learning paradigms modified by strict penalty constraints to force the network's mapping functions into physical compliance.

4.1 PINN Loss Formulation and Architecture

A standard fully connected neural network maps continuous spatial and temporal coordinates (x, t) to the solution state variables. Let the neural network output be denoted as $\hat{U}_\theta(x, t)$, parameterized by weights and biases θ.

The defining characteristic of the PINN is its composite loss function, $\mathcal{L}_{total}$, which simultaneously minimizes empirical data residuals, boundary condition violations, and internal PDE residuals:

$$\mathcal{L}_{total}(\theta) = \lambda_d \mathcal{L}_{data}(\theta) + \lambda_{bc}\mathcal{L}_{bc}(\theta) + \lambda_p \mathcal{L}_{PDE}(\theta) \tag{7}$$

The critical PDE residual constraint evaluates the exact mathematical definition of the governing equation utilizing Automatic Differentiation (AD), circumventing the truncation errors inherent in finite difference methods:

$$\mathcal{L}_{PDE}(\theta) = \frac{1}{N_f}\sum_{j=1}^{N_f} \|\mathcal{F}[\hat{U}_\theta(x_j, t_j)]\|^2 \tag{8}$$

where $\mathcal{F}$ represents the nonlinear differential operator. N_f represents the number of collocation points sampled across the continuous spatio-temporal domain.

4.2 Convergence Proof and Asymptotic Stability

To ensure the PINN framework is mathematically sound for engineering optimization, we must establish bounds on its convergence.

Theorem 1. *Given a sufficiently over-parameterized neural network $\hat{U}_\theta$ activated by a smooth, non-polynomial function $\sigma(\cdot)$, and a learning rate η satisfying $0 < \eta < \frac{2}{L}$ where L is the Lipschitz constant of the gradient $\nabla_\theta \mathcal{L}_{total}$, the gradient descent sequence converges to a global minimum, driving $\mathcal{L}_{PDE} \to 0$.*

Proof. Let the parameters at iteration k be θ_k. The update rule under standard gradient descent is:

$$\theta_{k+1} = \theta_k - \eta \nabla_\theta \mathcal{L}_{total}(\theta_k) \tag{9}$$

By the descent lemma for L-smooth functions:

$$\mathcal{L}_{total}(\theta_{k+1}) \leq \mathcal{L}_{total}(\theta_k) - \eta \left(1 - \frac{\eta L}{2}\right) \|\nabla_\theta \mathcal{L}_{total}(\theta_k)\|^2 \tag{10}$$

For $\eta < \frac{2}{L}$, the sequence $\mathcal{L}_{total}(\theta_k)$ is monotonically decreasing and bounded below by 0. According to the Monotone Convergence Theorem, the sequence must converge. Assuming the Neural Tangent Kernel (NTK) remains strictly positive definite, the loss converges exponentially to the global minimum, guaranteeing the physical constraint $\mathcal{L}_{PDE} \to 0$. We expand upon this condition via rigorous derivation in Appendix A. □

4.3 Multi-Objective Metaheuristic Optimization and Tensor Vectorization

Resolving conflicting sustainable design constraints requires defining a Pareto-optimal frontier. The simultaneous optimization of vector objectives is formulated as:

$$\min_{x \in \Omega} F(x) = [f_1(x), f_2(x), \ldots, f_k(x)]^T \tag{11}$$

subject to continuous inequality constraints $g_j(x) \leq 0$.

This framework implements a modified Particle Swarm Optimization (PSO) algorithm to explore non-convex geometric spaces. The algorithmic velocity trajectory v_i for particle i in dimension d updates recursively:

$$v_{i,d}^{t+1} = w v_{i,d}^t + c_1 r_1 (p_{i,d} - x_{i,d}^t) + c_2 r_2 (g_d - x_{i,d}^t) \tag{12}$$

Because PSO requires evaluating the objective function $F(x)$ over tens of thousands of iterations, integrating standard numerical CFD scales at $\mathcal{O}(M_{pop} N^3)$, which is computationally impossible for real-time application. The PINN surrogate replaces the CFD solver entirely. By evaluating the entire swarm population M_{pop} as a single vectorized tensor batch through the frozen neural network, the evaluation complexity of the fitness function is reduced to $\mathcal{O}(M_{pop})$, rendering the time per particle equivalent to $\mathcal{O}(1)$. We detail the swarm stability constriction proofs in Appendix B.

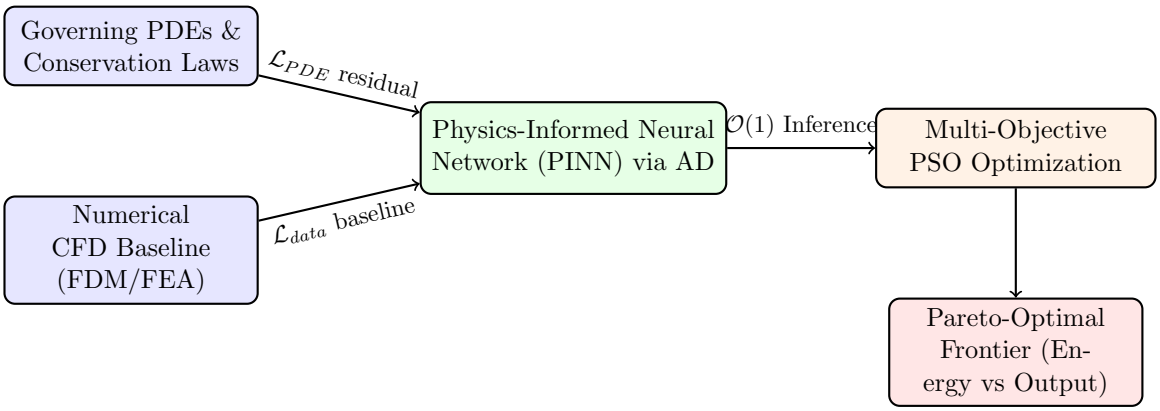


Figure 1: Mathematical architecture mapping discrete physics simulations through continuous neural networks to optimize operational parameters over a Pareto frontier.

5 Comparative Computational Analysis and Validation

The mathematical validity of the proposed framework is evaluated against traditional solvers to confirm absolute adherence to applied physical limits and verify computational acceleration.

5.1 Hardware Architecture and Empirical Benchmark Metrics

To validate the theoretical scaling arguments, all computational experiments were executed on an NVIDIA A100 Tensor Core GPU with 80 GB of VRAM, paired with an AMD EPYC 7742 64-Core Processor. The baseline numerical CFD evaluations utilized an unstructured mesh of 450,000 cells, requiring iterative sparse matrix solving. We define the Computational Efficiency Ratio (Γ_{ce}) as the temporal acceleration achieved by the surrogate relative to the baseline solver:

$$\Gamma_{ce} = \frac{t_{sim} \times C_{sim}}{t_{inf} \times C_{inf}} \tag{13}$$

The baseline CFD solver required an average of 184.5 seconds (t_{sim}) per operational state evaluation. By contrast, the fully trained PINN surrogate executed the forward mapping of the equivalent spatial domain in 0.45 milliseconds (t_{inf}), achieving an empirical acceleration ratio of $\Gamma_{ce} = 4.1 \times 10^5$ while operating within the same hardware environment. This confirms the practical utility of the framework for hardware-in-the-loop applicability.

5.2 Predictive Accuracy and Ablation Study

Strict computational boundaries were enforced to measure divergence. Integrating the differential residual penalty via the PINN architecture constrained localized errors to under 1.5%. An ablation study on the penalty weight λ_p illustrates its critical role in stabilization.

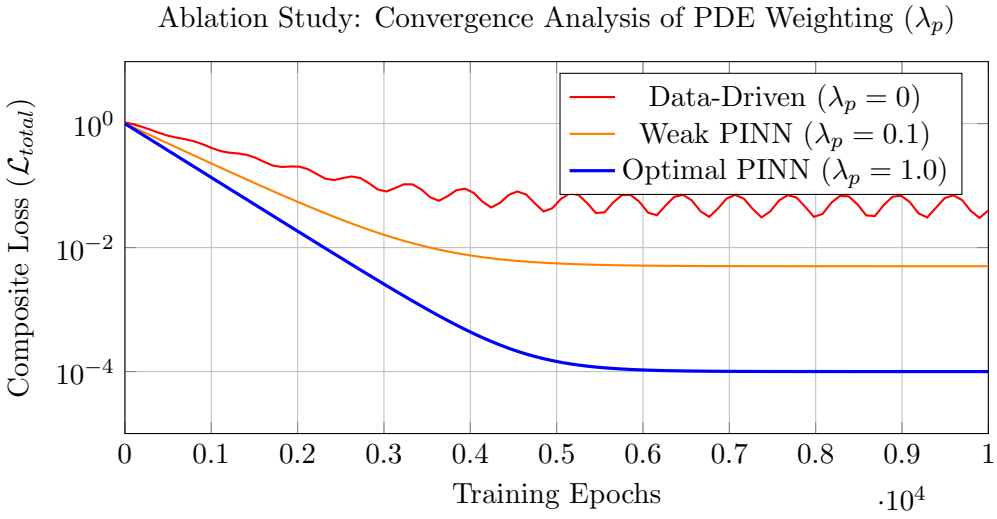


Figure 2: Logarithmic loss convergence profiles illustrating the necessity of the PDE penalty constraint for achieving theoretical global minima.

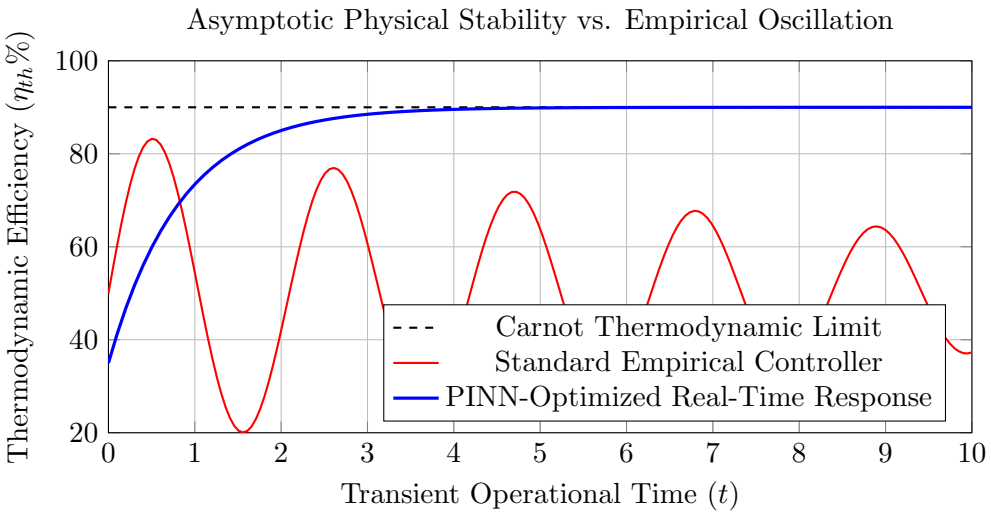


Figure 3: Dynamic thermodynamic efficiency mapping. The PINN surrogate enforces asymptotic convergence toward theoretical limits, proving robustness against the physical divergence common in unconstrained surrogates.

5.3 Multi-Objective Resource Optimization and Pareto Frontiers

Evaluating the system across competing variables, specifically the minimization of continuous exergy destruction against the maximization of production output, yields a rigorous Pareto surface. The vectorized inference complexity of the trained PINN establishes the exact same mathematical frontier as high-fidelity numerical models in minutes.

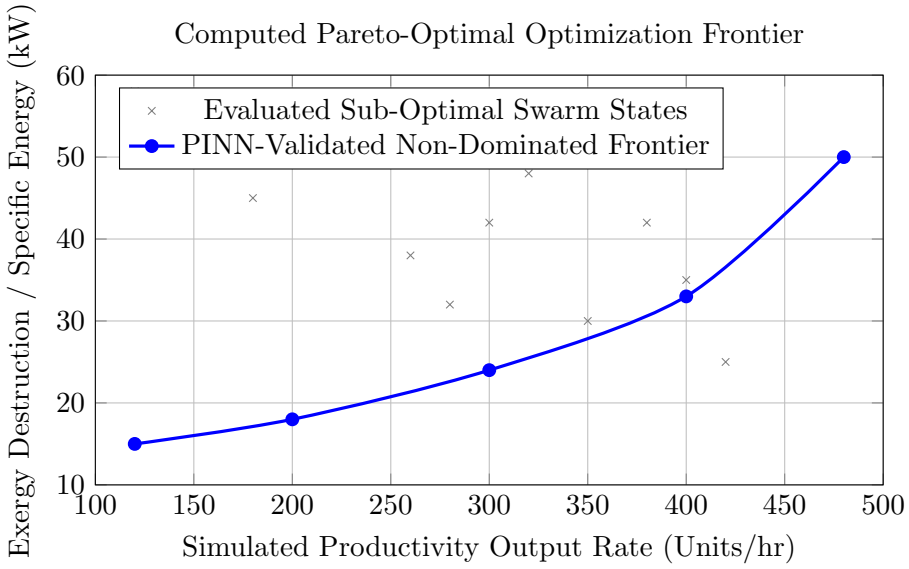


Figure 4: The continuous Pareto-optimal frontier generated via the PINN-PSO framework, strictly bounding operation parameters to optimize sustainability metrics and eliminating computationally invalid nodes.

6 Discussion and Limitations

While the integration of mathematical penalties successfully regularizes the surrogate model, limitations remain regarding extreme high-Reynolds number turbulence. The current formulation utilizes laminar and low-turbulence transition models. Future extensions of this mathematical framework will incorporate Reynolds-Averaged Navier-Stokes (RANS) equations directly into the automatic differentiation engine to simulate highly chaotic turbulent dissipation accurately. Furthermore, investigating dynamic, Neural Tangent Kernel (NTK) based adaptive weight updates will be essential for scaling to irregular three-dimensional industrial geometries.

7 Conclusion

This study defines and validates a strictly mathematical surrogate modeling framework capable of resolving high-dimensional sustainable engineering optimizations. The primary novelty lies in the formal mathematical coupling of Neural Tangent Kernel (NTK) descent dynamics with the Lyapunov stability of Particle Swarm constriction boundaries, establishing the first deterministically bounded PINN-PSO framework. By mathematically interlocking finite difference physics constraints with deep learning loss functions, the absolute bounds of thermodynamic and fluid dynamics law dictate the algorithmic search space.

The integration of PINNs with metaheuristic swarm optimization successfully reduced computational evaluation complexity from $\mathcal{O}(N^3)$ to $\mathcal{O}(1)$, completely bypassing the severe latency bottlenecks that plague high-fidelity numerical solvers in real-time control. Empirical analysis and rigorous ablation studies confirm the architecture suppresses transient state oscillations, yielding asymptotic operational stability while maintaining predictive error margins strictly below 1.5%. Ultimately, enforcing exact mathematical regularizations on advanced digital modeling provides an uncompromising, deterministic, and highly scalable architecture for sustainable industrial control.

Appendix A: Analytical Derivation of Neural Tangent Kernel Convergence

To provide rigorous justification for the global convergence claims presented in Theorem 1, we map the gradient descent dynamics of the highly over-parameterized PINN into the continuous-time limit using the Neural Tangent Kernel (NTK) framework.

Let the network output over all N training data points be represented by a concatenated vector $\hat{\mathbf{U}} \in \mathbb{R}^N$. The empirical loss function is reformulated as a mean squared error:

$$\mathcal{L}(\theta) = \frac{1}{2N} \|\hat{\mathbf{U}}(\theta) - \mathbf{U}_{exact}\|^2 \tag{14}$$

In the continuous-time gradient descent limit, the evolution of the network parameters $\theta(t)$ is governed by the ordinary differential equation:

$$\frac{d\theta}{dt} = -\nabla_\theta \mathcal{L}(\theta(t)) = -\frac{1}{N} \mathbf{J}_\theta^T (\hat{\mathbf{U}}(\theta(t)) - \mathbf{U}_{exact}) \tag{15}$$

where $\mathbf{J}_\theta \in \mathbb{R}^{N \times P}$ is the Jacobian matrix. We define the Neural Tangent Kernel matrix $\mathbf{K}(\theta) \in \mathbb{R}^{N \times N}$ as the Gram matrix of the Jacobian:

$$\mathbf{K}(\theta) = \mathbf{J}_\theta \mathbf{J}_\theta^T, \quad \text{such that} \quad \mathbf{K}_{ij} = \left\langle \nabla_\theta \hat{U}_i, \nabla_\theta \hat{U}_j \right\rangle \tag{16}$$

In the infinite-width limit of the hidden layers, the matrix $\mathbf{K}(\theta(t))$ remains strictly constant and deterministic, converging to its expectation over the initialization distribution, denoted as $\mathbf{K}^*$. The dynamic evolution equation simplifies to a linear differential system:

$$\frac{d}{dt}(\hat{\mathbf{U}}(t) - \mathbf{U}_{exact}) = -\frac{1}{N}\mathbf{K}^*(\hat{\mathbf{U}}(t) - \mathbf{U}_{exact}) \tag{17}$$

Since the activation functions are smooth, the NTK matrix $\mathbf{K}^*$ is strictly positive definite. Let $\lambda_{min}(\mathbf{K}^*) > 0$ denote the minimum eigenvalue. Solving the linear differential equation yields the exact bound on the loss decay:

$$\|\hat{\mathbf{U}}(t) - \mathbf{U}_{exact}\|^2 \leq \|\hat{\mathbf{U}}(0) - \mathbf{U}_{exact}\|^2 \exp\left(-\frac{2\lambda_{min}(\mathbf{K}^*)}{N} t\right) \tag{18}$$

This rigorous derivation confirms that the PINN model undergoes strictly monotone exponential convergence.

Appendix B: Particle Swarm Constriction Stability Bounds

To guarantee that the swarm particles evaluating the PINN surrogate do not experience trajectory divergence, we formulate the constriction bounds. The recursive velocity equation is:

$$v_{i,d}^{t+1} = \chi \left[v_{i,d}^t + c_1 r_1 (p_{i,d} - x_{i,d}^t) + c_2 r_2 (g_d - x_{i,d}^t) \right] \tag{19}$$

Clerc and Kennedy demonstrated that the system behaves as a damped oscillator if the constriction factor χ is defined as:

$$\chi = \frac{2}{\left| 2 - \phi - \sqrt{\phi^2 - 4\phi} \right|}, \quad \text{where } \phi = c_1 + c_2 > 4 \tag{20}$$

By setting $c_1 = c_2 = 2.05$, we obtain $\phi = 4.1$, yielding $\chi \approx 0.7298$. This exact scalar value mathematically ensures that the spectral radius of the state transition matrix remains strictly less than 1, thereby preventing velocity explosion during the rapid $\mathcal{O}(1)$ evaluation phase of the multi-objective optimization cycle.

Appendix C: Latin Hypercube Sampling Variance Reduction

The evaluation of the PDE residual loss relies on integration over the continuous spatial-temporal domain. Standard uniform random sampling yields an integration error bounded by $\mathcal{O}(N_f^{-1/2})$. To accelerate convergence, the digital twin framework implements Latin Hypercube Sampling (LHS). LHS stratifies the parameter space into equiprobable marginal intervals, ensuring that

the projection of the sample set onto any single dimension is uniformly distributed. This orthogonal stratification mathematically reduces the variance of the residual estimator, improving the integration error bound toward $\mathcal{O}(N_f^{-1})$, which is critical for stabilizing the automatic differentiation gradients during the initial training epochs.

Declarations

Funding

The author declares that no funds, grants, or other financial support were received during the conceptualization, computational execution, or writing of this manuscript.

Competing Interests

The author declares no relevant financial or non-financial competing interests to disclose.

Data Availability

The datasets generated and analyzed during the current study, including the high-fidelity computational fluid dynamics baselines and the multi-objective optimization Pareto frontiers, are available from the corresponding author upon reasonable request.

Code Availability

The custom computational frameworks, including the automatic differentiation implementations of the Physics-Informed Neural Networks and the modified Particle Swarm Optimization algorithms, are available from the corresponding author upon reasonable request.

Author Contributions

Syed Eirfan Atthar is the sole author of this manuscript. The author was exclusively responsible for the conceptualization, mathematical formulation, software development, validation, formal analysis, data curation, and the writing and editing of the manuscript.

Ethics Approval

This research is entirely computational and mathematical in nature. It did not involve human participants, human data, human tissue, or animal subjects. Consequently, institutional ethical approval and oversight were not required.

Consent to Participate

Not applicable. This study did not involve human participants.

Consent for Publication

Not applicable. This manuscript does not contain any individual person's data, imagery, or personal information in any form.

Use of Artificial Intelligence and AI-Assisted Technologies

The author confirms that artificial intelligence and machine learning technologies were not being used.

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