Applied Research on a Hybrid Data- and Knowledge-Driven Artificial Intelligence Scientific Computing Model for Neutron Diffusion Calculations in Nuclear Reactors

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Abstract

Amidst the growing global emphasis on nuclear safety, the integrity of nuclear reactor systems has garnered attention in the aftermath of consequential events. Moreover, the rapid development of artificial intelligence technology has provided immense opportunities to enhance the safety and economy of nuclear energy. However, data-driven deep learning techniques often lack interpretability, which hinders their applicability in the nuclear energy sector. To address this problem, this study proposes a hybrid data-driven and knowledge-driven artificial intelligence model based on physics-informed neural networks to accurately compute the neutron flux distribution inside a nuclear reactor core. Innovative techniques, such as regional decomposition, intelligent keff (effective multiplication factor) search, and keff inversion, have been introduced for the calculation. Furthermore, hyper-parameters of the model are automatically optimized using a whale optimization algorithm. A series of computational examples are used to validate the proposed model, demonstrating its applicability, generality, and high accuracy in calculating the neutron flux within the nuclear reactor. The model offers a dependable strategy for computing the neutron flux distribution in nuclear reactors for advanced simulation techniques in the future, including reactor digital twinning. This approach is data-light, requires little to no training data, and still delivers remarkably precise output data.

Full Text

Preamble

Application of a Hybrid Data- and Knowledge-Driven Artificial Intelligence Scientific Computing Model in Neutron Diffusion Calculations

for Nuclear Reactors

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Amid growing global emphasis on nuclear safety, the integrity of nuclear reactor systems has become increasingly critical. The rapid development of artificial intelligence technology offers immense opportunities to enhance both the safety and economy of nuclear energy. However, data-driven deep learning techniques often suffer from limited interpretability, which hinders their applicability in the nuclear sector. To address this challenge, this study proposes a hybrid data- and knowledge-driven artificial intelligence model based on physics-informed neural networks (PINNs) to accurately compute neutron flux distributions within nuclear reactor cores. The model introduces innovative techniques including regional decomposition, intelligent k_{eff} (effective multiplication factor) search, and k_{eff} inversion. Furthermore, hyperparameters are automatically optimized using a whale optimization algorithm. A series of computational examples validate the proposed model, demonstrating its applicability, generality, and high accuracy in calculating neutron flux distributions. The model offers a reliable strategy for computing neutron flux distributions in nuclear reactors for advanced simulation techniques, including reactor digital twinning. This approach is data-light, requires minimal training data, and still delivers remarkably precise results.

Keywords: Neutron diffusion equation, Physics-informed neural network, Effective multiplication factor, Whale optimization algorithm

Introduction

Neutron flux distribution governs the performance and safety of nuclear reactors, delineating the spatial and temporal variations in neutron flux and spectrum within the reactor core [1]. This distribution profoundly influences power generation, fuel consumption [2], reactivity control [3–5], and radiation damage to reactor components. Consequently, precise and efficient calculation of neutron flux distribution is essential for reactor design, analysis, and operation. However, these calculations are challenging due to the intricate and nonlinear nature of the neutron transport equation that governs neutron behavior [6]. Solving this equation, especially for large-scale high-fidelity models, demands substantial computational resources and time [7].

Neutron diffusion theory has emerged as a simplified neutron transport model that assumes isotropic scattering and a constant energy spectrum within each energy group. Although this theory effectively solves the neutron balance equation linking flux to production and absorption rates in the core, applying it to entire reactor cores remains complex and computationally intensive [8,9]. Numerous numerical techniques, including nodal methods [10,11], finite element methods [12,13], and finite difference methods [14], have been developed to mitigate this complexity by discretizing the core into smaller nodes. Nevertheless,

real-time neutron diffusion simulation remains resource-intensive for applications requiring rapid feedback to operators or control systems. Real-time simulations demand both temporal efficiency (results within seconds or minutes) and high accuracy to ensure valid outcomes.

Online sensors can facilitate real-time core neutron diffusion simulation [15]. These sensors measure various physical quantities—including temperature, pressure, flow rate, and neutron flux—providing real-time data that can serve as inputs or boundary conditions for simulations. They also enable verification by comparing simulated and measured fluxes, yielding correction datasets for machine learning calculations. Conventional second-generation reactors employ periodic insertion of neutron detectors from the bottom of the pressure vessel, enabling only intermittent measurements and requiring vessel perforations [1]. In contrast, third-generation reactors such as the HPR1000 use self-powered neutron detectors (SPNDs) for fundamentally different measurements [16]. SPND-based systems enable continuous, comprehensive monitoring of core neutron flux distribution, marking a significant departure from the sporadic measurements of earlier generations.

However, existing reactor monitoring systems have limitations in capturing transient changes, necessitating reconstruction of key reactor parameters from limited data. Despite mature computational methods, effectively integrating measured data into calculations remains challenging, particularly for high-fidelity interactive simulation techniques like nuclear reactor digital twins [17–19].

Recent research in nuclear reactor physics analysis has focused on physics-informed neural networks (PINNs), which integrate physical models with limited training data while adhering to physical constraints. As a hybrid data- and knowledge-driven model, PINN leverages both data and the physical laws governing neutron flux distribution. The neural network represents the solution to the neutron transport equation, trained by minimizing a loss function comprising residuals of the transport equation, initial and boundary conditions, and observed data [20]. PINN advantages over conventional methods include incorporating physical knowledge, utilizing data for additional constraints, and solving inverse problems such as parameter estimation, model discovery, and optimal control [21].

Data-driven deep learning models currently face interpretability challenges, often being perceived as "black boxes" [22–26]. Beyond harnessing measurement data, incorporating well-established physical models expressed through partial differential equations offers an alternative approach [27–31]. For example, the heat conduction and Navier-Stokes equations study thermal hydraulics [32], while the neutron transport and burnup equations enable physics analysis [33]. Relying solely on either data or physical models may result in information loss. Houde et al. [34] compared data-driven and model-driven approaches, revealing that data-driven methods excel in speed and accuracy while model-driven methods excel in interpretability. They advocate hybrid methodologies combining both strengths to improve prediction accuracy, reliability, and proficiency.

This study presents a neural network model tailored for computing neutron flux within reactor cores to facilitate distribution reconstruction. Engineered to assimilate physical laws, this model integrates model-driven and data-driven approaches, endowing the AI model with commendable accuracy and interpretability.

PINN methods have attracted significant attention in reactor physics [35-39]. Dong et al. [40] achieved outstanding precision solving multi-dimensional neutron diffusion equations with PINN. Jiangyu et al. [41] introduced conservative PINN (CPINN) to address non-smoothness in non-uniform media. Yu et al. [42,43] proposed data-enabled PINN (DEPINN) to enhance accuracy and efficiency for eigenvalue problems with limited experimental data. Prantikos et al. [44,45] utilized PINN for point kinetics, highlighting advantages over traditional methods for irregular and high-dimensional problems.

Applying AI algorithms to nuclear reactor physics analysis presents challenges regarding accuracy and hyperparameters [46,47]. While accuracy may be comparable to traditional methods, hyperparameters are typically set using universal or empirical values rationalized through sensitivity analyses. This study pioneers an AI-based computing model for the neutron diffusion equation, grounded in hp-variational PINN (VPINN) deep learning technology [48], incorporating domain decomposition and various innovations. Hyperparameter optimization is facilitated through the whale optimization algorithm (WOA) [49]. The model adeptly solves the neutron diffusion equation for single-energy single-medium, single-energy multi-medium, and two-energy group multi-medium scenarios, validating its versatility. Overall, this research introduces novel ideas and techniques harnessing deep learning to facilitate intelligent solution of the neutron diffusion equation.

II. Neutron Diffusion Model

The neutron diffusion model is widely used for reactor physics analysis, providing insights into neutron behavior within the core while meticulously considering interactions including absorption, scattering, production, and transport. Model outputs facilitate computation of neutron flux and power distributions, offering rapid computation and high efficiency for large-scale calculations.

At the heart of the model lies the neutron transport equation. By assuming isotropic scattering angles to eliminate angular variables and discretizing the continuous energy spectrum, we derive the multi-energy group neutron diffusion equation. In steady-state scenarios, analysis focuses on the reactor' s critical state, where stability and operational viability must be studied. However, not all neutron reactions achieve criticality, which depends on reactor design, fuel composition, and control mechanisms. This underscores the intricate dynamics and multifaceted nature of factors influencing criticality.

To refine the equation for practical utility, we eliminate the time-dependent term, revealing the effective multiplication factor (k_{eff}) as a pivotal parameter

for maintaining equilibrium. This factor serves as an indicator of criticality: a subcritical state emerges when $k_{\text{eff}} < 1$, a supercritical state when $k_{\text{eff}} > 1$, and criticality when $k_{\text{eff}} = 1$. The characteristic value equation becomes:

$$-D_g \nabla^2 \phi_g + \Sigma_{r,g} \phi_g = \sum_{g'=1} \Sigma_{s,g' \to g} \phi_{g'} + \frac{1}{k_{\text{eff}}} \sum_{g'=1} \nu_{g'} \Sigma_{f,g'} \phi_{g'} + S_g,$$

where ϕ_g represents the neutron flux of the gth energy group, D_g the diffusion coefficient, $\Sigma_{r,g}$ the removal cross-section (including absorption and scattering from other groups), ν_g the number of neutrons produced by fission, and S_g the external neutron source.

For monoenergetic cases without an additional neutron source, the transient and steady-state neutron diffusion equations are:

$$\frac{1}{v} \frac{\partial \phi(r,t)}{\partial t} = D \nabla^2 \phi(r,t) + \frac{k_\infty - 1}{L^2} \phi(r,t)$$

$$\nabla^2 \phi(r) + \frac{k_\infty / k_{\text{eff}} - 1}{L^2} \phi(r) = 0$$

where L is the diffusion length, k_∞ the infinite multiplication factor, and v the neutron speed. These second-order partial differential equations can be expressed in unified form:

$$\mathcal{N}[\phi(x), \nabla^2 \phi(x)] = 0, \quad x \in \Omega$$

III. Framework of the hp-VPINN Model for Solving the Neutron Diffusion Equation

A. Basic Principle of PINN

PINNs represent an advanced computational paradigm that synthesizes neural networks with fundamental physical principles to infer unknown physical fields. They incorporate governing partial differential equations directly into the loss function, ensuring the neural network adheres to prescribed physical laws while solving associated PDEs. The calculation flow is shown in Figure 1 [Figure 1: see original paper].

Implementing a PINN involves using spatial and temporal coordinates as inputs to a neural network. These coordinates undergo nonlinear mapping across multiple hidden layers, yielding a continuous output function ϕ_{NN} that represents the solution to the physical system. Notably, ϕ_{NN} satisfies both PDE constraints and available experimental measurements. Automatic differentiation computes PDE derivatives to reveal residuals, while the network assesses congruence with

experimental data through mean squared error. The comprehensive loss function integrates weighted PDE residuals and experimental data error, minimized through gradient descent training. Consequently, the trained PINN emerges as a potent PDE solver.

Beyond traditional numerical methods, PINN offers distinct advantages for nonlinear PDEs by circumventing explicit spatial and temporal discretization. The highly nonlinear nature of neural networks enhances capabilities for addressing complex physical phenomena such as fluid flow [50] and time-domain electromagnetic field simulation [51].

For the neutron diffusion equation over domain Ω with boundary $\partial\Omega$, we utilize the following loss function:

$$\text{loss} = w \cdot \text{loss}_f + w_b \cdot \text{loss}_b + w_d \cdot \text{loss}_d$$

where loss_f, loss_b, and loss_d correspond to PDE, boundary condition, and data loss terms, respectively, with $\{w, w_b, w_d\}$ as weight coefficients. These residuals are defined as:

$$\text{loss}_f = \sum_{i=1}^{N_f} r(x_i)^2, \quad \text{loss}_b = \sum_{i=1}^{N_b} r(x_i)^2, \quad \text{loss}_d = \sum_{i=1}^{N_d} r(x_i)^2$$

with residuals:

$$r(x_f) = \mathcal{N}[x_f, \phi_{NN}(x_f), \nabla\phi_{NN}(x_f), \nabla^2\phi_{NN}(x_f)], \quad \forall x_f \in \Omega$$

$$r(x_b) = \phi_{NN}(x_b) - \phi(x_b), \quad \forall x_b \in \partial\Omega$$

$$r(x_d) = \phi_{NN}(x_d) - \phi(x_d)$$

B. Basic Principle of VPINN

Figure 2 [Figure 2: see original paper] illustrates the VPINN calculation flowchart. VPINN extends PINN by assimilating the Petrov-Galerkin method [53] based on variational principles, which transforms physical equation constraints into a systematic functional minimization process. This represents a pivotal advancement in solution accuracy.

VPINN differs from conventional Galerkin methods through its flexibility in sourcing trial and weight functions from disparate spaces. The neural network ϕ_{NN} serves as the trial function, while weight functions can take various forms including polynomials, trigonometric functions, Dirac delta functions, or even

another neural network. This versatility enables VPINN to address diverse physical phenomena effectively.

By selecting an appropriate weight function ν, multiplying it with Eq. (4), and integrating over the solution domain, we obtain the variational residual:

$$\sum_{i=1}^{N_f} \int_{\Omega} \mathcal{N}[x_f, \phi_{NN}(x_f), \nabla\phi_{NN}(x_f), \nabla^2\phi_{NN}(x_f)] \cdot \nu_i \, dx$$

This study employs Legendre polynomials to construct a K-dimensional weight function space, where each order' s zero boundary values ensure satisfaction of boundary conditions. The loss function becomes:

$$\text{loss} = w_r \cdot \text{loss}_r + w_b \cdot \text{loss}_b$$

where loss_r represents the variational residual loss term.

C. Basic Principle of hp-VPINN

hp-VPINN further evolves VPINN by amalgamating subdomain Petrov-Galerkin methods with domain discretization. This facilitates solution domain decomposition, increasing potential for h-refinement, while introducing projection of variational residuals onto a p-dimensional high-order polynomial space. This strategy enhances precision in handling PDEs.

The intrinsic virtue of hp-VPINN lies in partitioning the solution domain into distinct subdomains, enabling h-refinement to enhance solution granularity. Additionally, projection onto high-dimensional polynomial space empowers the model to capture intricate solution nuances, particularly beneficial for high-order accuracy scenarios. This interplay of h-refinement and p-projection substantiates the method' s capacity for addressing diverse physical problems with heightened accuracy.

Furthermore, hp-VPINN introduces parallel computing capabilities. By leveraging parallel techniques on decomposed subdomains, the framework orchestrates concurrent computation that optimizes efficiency—particularly advantageous for complex problems. Additionally, hp-VPINN incorporates weak integration formulas to handle second-order PDEs within loss terms. Integration by parts reduces differentiation order requirements, enhancing neural network flexibility during training.

If the solution domain is divided into N subdomains, the hp-VPINN loss function becomes:

$$\text{loss} = \text{loss}_R + w \cdot \text{loss}_b$$

where

$$\text{loss}_R = \sum_{i=1}^{N} \sum_{j=1}^{K-1} \left(\int_{\Omega_i} \nu_{ij} \cdot \mathcal{F}_{NN} \, dx \right)^2$$

Here, ν_{ij} represents the jth-order weight function on subdomain Ω_i, a piecewise function non-zero only on its corresponding subdomain.

IV. Innovative Key Technology Proposed in the hp-VPINN Framework for Solving the Neutron Diffusion Equation

A. Technology of Parallel Computing and Convergence in Multiple Regions

To effectively control and regulate nuclear reactors with paramount emphasis on safety enhancement, a strategic paradigm involving meticulous partitioning of the actual core is often employed. This conventional approach divides the core into distinct zones—such as breeding and blanket zones—each composed of different materials according to specific functions. Consequently, discernible variance arises in material parameters including absorption cross-section and fission cross-section, which play pivotal roles in formulating neutron diffusion equations and demand nuanced considerations within respective zones.

This intricacy engenders a spatially partitioned solution for comprehensively capturing diverse core dynamics. The multifaceted nature of these nuclear processes underscores the indispensability of sophisticated computational frameworks capable of accommodating such complexities, exemplified by the hp-VPINN framework. This method enables effective dissection of the solution domain, providing capacity to discern and address distinct characteristics inherent in each subdomain. The framework leverages corresponding loss functions tailored to individual subdomains, facilitating targeted and specialized training that ensures the model encapsulates zone-specific intricacies.

An inherent advantage of hp-VPINN lies in its ability to orchestrate multi-domain parallel convergence. Following training within each subdomain, the framework amalgamates individual loss functions into a unified computational scheme. This synergistic approach yields a model that seamlessly integrates insights from different subdomains, achieving holistic understanding of the entire core. These efforts culminate in an advanced computational tool capable of addressing challenges posed by partitioned reactor cores, significantly contributing to enhanced control and safety protocols.

B. Adaptive Subdomain Partitioning Scheme

To study physical fields characterized by substantial gradients, employing multiple nonlinear neural networks provides a nuanced depiction of regions undergo-

ing significant changes. Analogous to mesh densification in finite element methods, this technique enhances precision in regions with pronounced alterations. While promising heightened accuracy, this approach increases computational demands and necessitates judicious resource management.

To address these challenges, an adaptive subdomain partitioning scheme has emerged as a prospective solution. This approach selectively refines meshes in regions exhibiting substantial gradients, striking an intricate equilibrium between computational resource allocation and accuracy. By targeting areas showing pronounced change, adaptive partitioning ensures resources are allocated where most needed while optimizing solution accuracy without incurring unnecessary overhead.

C. Intelligent k_{eff} Search and Inversion Techniques

To perform numerical computations concerning reactor kinetics, source iteration methods are ideal for attaining approximate solutions. However, when neural networks are introduced as an inner loop within source iteration, iterative training significantly diminishes solution efficiency. We therefore assume the transient diffusion equation eventually reaches a stable critical state and divide k_∞ by a k_{eff} to adjust the reaction to criticality, allowing the transient diffusion equation to be written in steady-state format:

$$\frac{1}{v}\frac{\partial \phi(r,t)}{\partial t} = D\nabla^2\phi(r,t) + \frac{k_\infty/k_{\text{eff}} - 1}{L^2}\phi(r,t)$$

As the nuclear reactor operates over period τ, reaching a stable state becomes inherent. At this juncture, neutron flux ϕ stabilizes and ceases temporal variations. The path toward criticality involves navigating eigenvalue problems, with k_{eff} serving as a key determinant. Although neural networks show promise, their introduction necessitates careful consideration due to computational efficiency impacts. The proposed intelligent search algorithm enhances computational efficacy, particularly for solving the transient neutron diffusion equation.

To seamlessly integrate this into the loss function, we adopt a methodology akin to boundary condition loss terms. The effective multiplication factor k_{eff} is determined through astute evaluation of ϕ_t when t surpasses operational period τ. During iteration, k_{eff} emerges as a dynamic variable subject to continuous adjustment. The neutron diffusion equation' s multiple eigenvalues designate k_{eff} as the eigenvalue typically close to unity; consequently, k_{eff} is initialized to 1, orchestrating a focused search for the eigenvalue nearest to 1.

In scenarios where ϕ_t is positive (supercritical state), the backpropagation algorithm automatically instigates downward adjustment of k_{eff}. Conversely, when ϕ_t is negative (subcritical state), the adaptive mechanism directs upward adjustment. This dynamic adjustment process aligns with the reactor' s transition

to criticality, observed when ϕ_t approaches equilibrium around 0. At this juncture, k_{eff} manifests as the sought-after value encapsulating reactor criticality with precision.

To comprehend and control reactor dynamics, we propose an inverse technique to determine the unknown parameter k_{eff} by training a neural network with limited data. Through sophisticated data-driven methodologies, the neural network adheres to available data within specified regions. The crux of this method lies in its capacity to reconstruct a solution that aligns with provided data while rigorously satisfying the neutron diffusion equation across the entire domain.

Figure 3 [Figure 3: see original paper] illustrates this approach' s efficacy, showcasing excellent applicability of the reconstructed solution. This reconstruction provides a holistic representation resonating with the entire solution domain. Figure 4 [Figure 4: see original paper] depicts the inversion technique flowchart.

To improve practical applicability, this technique is pivotal. By deriving a limited yet strategic dataset from core neutron detectors, we can extrapolate the elusive k_{eff} value. Utilizing actual data—even modest quantities—empowers the neural network to discern the reactor core' s critical state. This inference, rooted in data-driven understanding of k_{eff}, becomes instrumental in determining reactor criticality. The methodology transcends conventional paradigms, offering a nuanced and adaptive means to infer crucial parameters. The amalgamation of neural network training, inverse techniques, and data-driven adaptability represents a sophisticated computational strategy that advances reactor behavior comprehension.

D. Parallel Convergence Technique for Multigroup Diffusion Equation Systems

Following discretization of the continuous-energy neutron diffusion equation into G energy groups, a system comprising G partial differential equations emerges. This introduces heightened intricacies when employing neural networks. In response, each partial differential equation is treated as an individual loss term within the network, subsequently combined to engender a collective solution.

Suppose we need to solve a neutron diffusion equation containing G energy groups. We construct a neural network with G outputs (the final layer has G neurons), where each output represents the neutron flux distribution function ϕ_g $(g = 1, ..., G)$ for an energy group. During training, the multi-energy group neutron diffusion equations constrain each network output. The loss function is constructed by summing squared variational residuals for each group, enabling the network to output neutron flux distributions aligned with all energy groups after training. This parallelism enhances computational efficiency, facilitating convergence toward solutions for intricate PDE systems.

E. Optimizing Neural Network Hyperparameters Using the Whale Optimization Algorithm

Deep neural networks are characterized by several hyperparameters that intricately govern architecture and performance. Depth, width, and learning rate play pivotal roles in shaping capacity to extract complex features. The hp-VPINN extends this parameter landscape by incorporating additional elements, notably the weight assigned to boundary condition loss terms relative to equation loss terms.

Wang [52] advocates dynamic adjustment of loss term weights based on empirical observations, ensuring consistent gradient magnitudes throughout training. Despite empirical success, the current landscape lacks a mature theoretical framework for systematically determining these hyperparameters [54].

Recognizing hyperparameters' pivotal role in training efficiency and accuracy, this study leverages WOA—an intelligent optimization methodology inspired by whale foraging behavior that integrates searching, encircling, and bubble-net attacking strategies. This approach effectively navigates the hyperparameter landscape, surpassing conventional algorithms including particle swarm optimization, differential evolution, gravitational search algorithm, and grey wolf optimization [55] in solution accuracy and convergence speed.

1. Encircling the Prey WOA considers the prey' s position as the optimal solution, with other individuals updating positions based on this reference:

$$\begin{cases} \vec{d} = |\vec{C} \cdot \vec{X}^*(t) - \vec{X}(t)| \\ \vec{X}(t+1) = \vec{X}^*(t) - \vec{A} \cdot \vec{d} \end{cases}$$

where $\vec{A} = 2\vec{a} - \vec{a}$; $\vec{C} = 2\vec{r}$. Here t represents iteration count, $\vec{A}$ and $\vec{C}$ are coefficient vectors, $\vec{X}^*$ denotes the current best whale position, $\vec{X}$ the current position, and $\vec{a}$ linearly decreases from 2 to 0 during iteration. Variable $\vec{r}$ is a random number in $[0, 1]$.

2. Bubble-Net Attack Strategies Bubble-net attacks employ two strategies: contraction encircling and spiral updating.

(1) Contraction Encircling: Achieved through parameter a, which linearly decreases from 2 to 0, while A is a random number in $(-a, a)$, specifically within $(-2, 2)$. When $A \in (-1, 1)$, the new whale position can be defined anywhere between its original position and the prey' s position.

(2) Spiral Updating: The distance between whale and prey is computed, then a spiral equation simulates the whale' s motion:

$$\begin{cases} \vec{X}(t+1) = \vec{d} \cdot e^{bl} \cdot \cos(2\pi l) + \vec{X}^*(t) \\ \vec{d} = |\vec{X}^*(t) - \vec{X}(t)| \end{cases}$$

where d represents distance, b denotes a spiral shape constant, and l is a random number in $[-1, 1]$. While encircling prey, the whale simultaneously hunts along a spiral trajectory. To simulate this concurrent behavior, a 0.5 probability selects either contraction encircling or spiral updating:

$$\vec{X}(t+1) = \begin{cases} \vec{X}^*(t) - \vec{A} \cdot \vec{d}, & p < 0.5 \\ \vec{d} \cdot e^{bl} \cdot \cos(2\pi l) + \vec{X}^*(t), & p \geq 0.5 \end{cases}$$

Hunting Prey: Whales search based on positions. When $|\vec{A}| > 1$, the whale' s position updates through random selection:

$$\begin{cases} \vec{X}(t+1) = \vec{X}_{\text{rand}}(t) - \vec{A} \cdot \vec{d} \\ \vec{d} = |\vec{C} \cdot \vec{X}_{\text{rand}}(t) - \vec{X}(t)| \end{cases}$$

where $\vec{X}_{\text{rand}}(t)$ represents a randomly selected whale' s position.

3. WOA-Based Neural Network Hyperparameter Optimization Model The neural network hyperparameter optimization model using WOA is illustrated in Figure 5 [Figure 5: see original paper]. This model discerns optimal hyperparameter values through iterative training on sample data, enhancing overall network efficiency and efficacy.

In this iterative process, the computed fitness value serves as a metric for gauging network performance with specific hyperparameters. The optimum result is obtained when fitness reaches its maximum within the ongoing iteration, which is then juxtaposed against the global best fitness value. If the computed fitness surpasses the global best, the global value updates to incorporate the superior solution. This strategic evolution reflects the algorithm' s capacity to dynamically adapt and refine its understanding of optimal configurations over successive iterations.

The amalgamation of nature-inspired heuristics enhances efficient exploration and exploitation of the hyperparameter landscape. By integrating WOA, a systematic and adaptive approach emerges that continuously refines its understanding of optimal configurations, positioning WOA as a potent tool for optimizing network performance through judicious hyperparameter tuning.

V. Case Study

This section validates the proposed computational framework through cases of varying complexity. Section 5.1 solves the neutron diffusion equation in a homogeneous medium at criticality, validating multi-region parallel convergence. Section 5.2 examines the one-dimensional equation in spherical coordinates, scrutinizing region partitioning and refinement strategies. Section 5.3 compares PINN and hp-VPINN through two-dimensional cylindrical coordinate solutions. Section 5.4 addresses multi-media scenarios. Section 5.5 solves the one-dimensional transient equation, affirming intelligent search technique robustness. Section 5.6 applies inversion with WOA to the multi-group multi-media problem within the 2D-TWIGL benchmark [56]. These studies collectively assess framework reliability and versatility.

A. Solving the Neutron Diffusion Equation for a Homogeneous Medium Under Critical Conditions

We consider a one-dimensional neutron diffusion equation under critical conditions:

$$\nabla^2\phi(x) + B^2 \cdot \phi(x) = 0, \quad x \in [-1, 1], \quad \phi(\pm 1) = 0$$

At criticality, $B^2 = \pi^2$ and $\phi(0) = 0.5$. The analytical solution is $\phi(x) = 0.5\cos(\pi x)$. The loss function is:

$$\text{loss} = \text{loss}_f + w_b \cdot \text{loss}_b + w_i \cdot \text{loss}_i$$

where w_b and w_i represent relative weights. The loss terms are:

$$\text{loss}_f = \sum \int_{-1}^{1} \left[\nabla^2\phi_N(x) + B^2 g \cdot \phi_{NN}(x)\right] dx$$

$$\text{loss}_b = \left[\phi_{NN}(-1) - \phi(-1)\right]^2 + \left[\phi_{NN}(1) - \phi(1)\right]^2$$

$$\text{loss}_i = \left[\phi_{NN}(0) - \phi(0)\right]^2$$

Denoting the original strong-form loss term as $\text{loss}^{(1)}$, applying integration by parts once or twice yields two alternative weak-form equations:

$$\text{loss}^{(2)} = \sum \int_{-1}^{1} \left[g \cdot \phi_{NN}(x) \cdot \nu_j - \phi_{NN}(x) \cdot \nu_j'\right] dx$$

$$\text{loss}^{(3)} = \sum \left[\int_{-1}^{1} g \cdot \phi_{NN}(x) \cdot \nu_j + \phi_{NN}(x) \cdot \nu_j'' \, dx - \phi_{NN}(x) \cdot \nu_j' \right]$$

All three configurations adopt a consistent network structure $[1, 80, 80, 80, 80, 1]$, learning rate 0.001, 100 Gauss quadrature points, and 25th-order Legendre polynomials as trial functions. The absolute error distributions (Figures 6a and 6b [Figure 6: see original paper]) reveal errors below 0.0035 for all configurations. Mean square errors are 3.42×10^{-6} and 2.16×10^{-6} for forms 2 and 3, respectively, while form 1 achieves highest accuracy. Forms 2 and 3 strategically reduce derivative order, mitigating computational burden for higher-order derivatives and enhancing training speed. Empirical evidence from an MX250 GPU (equivalent to NVIDIA GT1030) using TensorFlow 1 on Windows 11 demonstrates improved efficiency: iteration times for 5000 steps are 51.65 s, 32.89 s, and 23.32 s for forms 1, 2, and 3, respectively. Forms 2 and 3 exhibit approximately twofold acceleration compared to form 1. However, form 3' s loss reduction plateaus around the 350th iteration, suggesting a stability threshold.

To balance efficiency and precision, form 1 is selected for subsequent computations due to its superior accuracy and optimal balance between precision and computational expedience.

A domain decomposition approach partitions the solution domain into two subdomains for independent training. Weight functions comprise rescaled Legendre polynomials confined to specific subdomains and constant functions maintaining zero-value constraints on complementary subdomains. Figure 7 [Figure 7: see original paper] depicts effectiveness plots and residual distributions, with blue dashed lines demarcating subdomain boundaries. Each row shows weight functions at various orders (left), neural network training outcomes using hp-VPINN (middle), and absolute error distributions (right). This sophisticated approach refines solution granularity while contributing to overall robustness and accuracy.

B. Solving the Neutron Diffusion Equation in One-Dimensional Spherical Coordinates Under Critical Conditions

For a bare spherical reactor with radius 1 (including extrapolation distance), the analytical solution is:

$$\phi(r) = \frac{\sin(\pi r)}{\pi r}$$

A strategic domain decomposition segments the solution domain into three primary regions: $[-1, -2/3]$, $[-2/3, 2/3]$, and $[2/3, 1]$. Additional local refinements establish five subregions: $[-1, -1/3]$, $[-1/3, -2/3]$, $[-2/3, 1/3]$, $[1/3, 2/3]$, and $[2/3, 1]$ to address localized complexities in high-gradient regions.

Consistent parameters and network architecture from the preceding case are preserved. Figure 8 [Figure 8: see original paper] visualizes outcomes, showing that localized refinement significantly reduces absolute error. Mean square errors decrease from 1.1×10^{-7} before refinement to 5.9×10^{-8} after refinement. Training times for 5000 steps increase from 61.64 s to 103.55 s, underscoring the trade-off between precision and efficiency.

C. Solving the Neutron Diffusion Equation in Two-Dimensional Cylindrical Coordinates

The critical state of the two-dimensional cylindrical neutron diffusion equation is elucidated through hp-VPINN and PINN methodologies. The experiment initiates with $\phi(0, 0) = 1$. Solution domains and absolute error distributions are depicted in Figure 9 [Figure 9: see original paper].

For hp-VPINN implementation, 100 Gaussian-Legendre integration points are distributed per domain, with Latin hypercube sampling [57] applied to sample 80 boundary points per boundary. This yields 420 training points for a single domain and 1220 points across nine domains. Mean square errors are 1.02×10^{-5} and 8.66×10^{-6}, corroborating precision and reliability.

Figures 9d-9f show PINN method outcomes with equivalent training points for comparison. PINN mean square errors are 1.84×10^{-5} and 1.75×10^{-5}. Computational times for four cases (1000 iterations each) are 9.61 s, 65.30 s, 15.84 s, and 31.66 s. Despite equivalent training costs, hp-VPINN consistently demonstrates heightened accuracy, substantiating its efficacy for determining critical states.

Figure 10 [Figure 10: see original paper] visualizes convergence dynamics, showing hp-VPINN' s conspicuous acceleration in convergence rate and discernible loss reduction relative to PINN, underscoring its superiority for navigating the neutron diffusion equation' s intricate landscape.

D. Solving the Neutron Diffusion Equation in Heterogeneous Media

For a one-dimensional single-group two-material problem with a constant source, the space is divided into three regions. At $x = 0$, a steady point source S emits neutrons bidirectionally (Figure 11 [Figure 11: see original paper]).

The neutron diffusion equations are:

$$D_1 \frac{d^2\phi_1}{dx^2} - \frac{1}{L_1^2}\phi_1 = 0, \quad 0 < |x| < |a|$$

$$D_2 \frac{d^2\phi_2}{dx^2} - \frac{1}{L_2^2}\phi_2 = 0, \quad |x| > |a|$$

Boundary conditions include: 1. Symmetric surface neutron source: $J_1(x) = S/2$ 2. As $x \to \infty$, $\phi_2 = 0$ 3. Neutron flux continuity at material interfaces 4. Neutron current density continuity at material interfaces

For $x > 0$, the analytical solution is:

$$\phi_1 = A_1 \cosh\left(\frac{x}{L_1}\right) + C_1 \sinh\left(\frac{x}{L_1}\right)$$

$$\phi_2 = A_2 \exp\left(-\frac{x}{L_2}\right) + C_2 \exp\left(\frac{x}{L_2}\right)$$

where coefficients are determined by boundary conditions.

The solution domain is set as $[0, 1]$ and divided into two regions: $[0, a/2]$ and $[a/2, 1]$. Appropriate loss functions are constructed for each boundary condition. For condition (1):

$$\text{loss}_{b1} = \left[\left.\frac{d\phi_{NN}}{dx}\right|_{x=10^{-6}} - \frac{S}{2D_1}\right]^2$$

For condition (2), considering $x = 10^3$ as approximately infinity:

$$\text{loss}_{b2} = \left[\phi_{NN}(10^3) - 0\right]^2$$

Condition (3) requires no separate loss term due to the Tanh activation function' s continuity. For condition (4):

$$\text{loss}_{b3} = \left[D_1 \left.\frac{d\phi_{NN}}{dx}\right|_{x=a/2-10^{-6}} - D_2 \left.\frac{d\phi_{NN}}{dx}\right|_{x=a/2+10^{-6}}\right]^2$$

To validate the method, parameters are systematically explored with $a = 1$ cm, uniform diffusion coefficients ($D_1 = D_2 = 1$ cm), and material curvature ($L_1 = 1$ cm) fixed, while L_2 varies as 0.5 cm, 1.0 cm, and 1.5 cm. Computational outcomes are shown in Figure 12 [Figure 12: see original paper], with mean square errors of 2.12×10^{-6}, 2.64×10^{-8}, and 6.76×10^{-8} for the three conditions. Runtime for 3000 iterations is 22.12 s, providing insights into computational efficiency.

E. Solving the One-Dimensional Transient Neutron Diffusion Equation

The transient one-dimensional neutron diffusion equation in rectangular coordinates is:

$$\frac{1}{v}\frac{\partial \phi}{\partial t} = D\nabla^2\phi + \frac{k_\infty - 1}{L^2}\phi$$

with analytical solution:

$$\phi(x,t) = \sum_{n=1}^{\infty}\frac{2}{a}\exp\left(\frac{k_\infty - 1 - D\left(\frac{(2n-1)\pi}{a}\right)^2}{L^2}t\right)\cos\left(\frac{(2n-1)\pi}{a}x\right)\int_0^a \phi_0(x')\cos\left(\frac{(2n-1)\pi}{a}x'\right)dx'$$

Resolving the eigenvalue equation presents formidable computational challenges. Dong et al. [31] proposed a parallel search technique based on binary search, but this requires multiple training iterations and substantial memory.

In response, this study introduces a novel search technique leveraging physical characteristics at critical state. The methodology initializes k_{eff} to 1, followed by continuous adjustments throughout neural network iterations. A key premise is that when criticality is achieved at time τ, the temporal derivative of neutron flux distribution $\phi_t(r,t)$ assumes zero value for subsequent instances, indicating stabilized reaction. The corresponding loss term is:

$$\text{loss}_k = \sum_{i=1}^{nr}\sum_{j=1}^{nt}\left[\frac{\partial \phi(r_i,t_j)}{\partial t}\right]^2, \quad t_j > \tau$$

Two test cases validate this method with parameters $v = 2.2\times10^3$ m/s, $D = 0.211\times10^{-2}$ m, $L^2 = 2.1037\times10^3$ m^2, and $a = 2$ m. Initial conditions are shown in Table 1 . Computational outcomes in Figure 13 [Figure 13: see original paper] reveal mean square errors on the order of 10^{-6}. Compared to reference values of 0.9995811 and 1.0035790, the technique yields absolute errors of 0.02 pcm and 0.01 pcm, attesting to its efficacy. Runtime for 8000 iterations is 352.88 s, reflecting the nuanced interplay between accuracy and efficiency.

F. Solving Neutron Diffusion Equations in Multi-Energy Group and Multi-Media Systems

The 2D-TWIGL benchmark problem [56] encapsulates a simplified two-dimensional rectangular core configuration with breeding and blanket regions. The square core (side length 160 cm) is partitioned into three regions. Symmetry considerations focus computation on a quarter-core domain. Configuration

details and parameters are provided in Figure 14 [Figure 14: see original paper] and Table 2 .

The benchmark is resolved through systematic integration of hp-VPINN and parameter inversion techniques. Using the KOMODO program (formerly ADPRES [59]), neutron flux data for a 40$×$40 core configuration establishes a foundational dataset. Latin hypercube sampling selects 1% of the core dataset for neural network input. The network undergoes robust training encompassing control equations, boundary conditions, and pertinent physical information, ensuring accuracy and convergence.

Hyperparameters are optimized via WOA with key settings: 5 artificial whales, maximum 10 optimization iterations, and maximum 10,000 neural network iterations. Convergence criteria include equation loss threshold below 10^{-4} and absolute k_{eff} error less than 20 pcm. Fitness evaluation incorporates three metrics: algorithm fitness, mean squared error in hp-VPINN flux calculations compared to KOMODO, and k_{eff} mean squared error. Figure 15 [Figure 15: see original paper] depicts iterative variation in maximum normalized fitness.

Optimal hyperparameters are: learning rate 4.9×10^{-4}, data loss term weighting 8, and boundary condition loss term weighting 9 (relative to equation loss term). The network structure comprises six hidden layers with node counts $[56, 40, 62, 89, 97, 79]$. Computational time is 1142.23 s.

Results in Figures 16a and 16b [Figure 16: see original paper] mirror literature findings [60]. Comparison with reference outcomes in Figures 17a and 17b [Figure 17: see original paper] shows the inverted k_{eff} value of 0.913222, remarkably concordant with the reference 0.913214 (absolute error 0.8 pcm). This underscores computational robustness and high accuracy.

The model, based on 1% of core neutron flux data and refined through WOA, exhibits remarkable capacity to produce high-precision flux distribution solutions. This introduces an innovative interactive method for nuclear reactor digital twinning, enabling inversion of complete flux distribution from limited data. The model' s distinctive attribute is pronounced reduction in requisite input data without compromising reliability, offering efficient inference of crucial safety-related parameters that are difficult to measure directly. This capability is magnified in scenarios where extensive direct measurements are logistically challenging. The model' s adeptness at extracting safety insights from modest observable data makes it valuable for reactor safety analyses, facilitating real-time core neutron diffusion simulations that enhance assessment accuracy and efficiency.

VI. Conclusion

This study leverages hp-VPINN to tackle the neutron diffusion equation, addressing both physical intricacies and practical challenges through multi-region parallel convergence, region partitioning refinement, intelligent k_{eff} search, and

k_{eff} inversion. WOA automatically optimizes neural network hyperparameters, enhancing efficiency and convergence.

Empirical findings from rigorous verification across multiple cases elucidate model robustness and versatility:

1. **Forward Solving:** The hp-VPINN model exhibits commendable accuracy for single-energy single-medium and single-energy multi-medium scenarios based solely on physical data, with generality across coordinate systems.
2. **Comparison with PINN:** Under equivalent training costs, hp-VPINN demonstrates superior accuracy for solving the neutron diffusion equation, emphasizing its advantageous computational characteristics.
3. **Inverse Solving:** For multi-group multi-media scenarios, hp-VPINN deploys WOA to navigate the hyperparameter landscape, enabling precise k_{eff} inversion. The model achieves remarkable absolute error less than 1 pcm using only 1% of core data, underscoring efficiency and precision.

In summary, the hp-VPINN framework harnesses deep learning to elucidate reactor neutron flux distribution, delivering high-precision solutions with minimal training data—particularly advantageous for advanced simulation techniques such as reactor digital twinning.

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Data Availability: Data supporting this study are openly available in Science Data Bank at https://cstr.cn/31253.11.sciencedb.28488 and https://doi.org/10.57760/sciencedb.28488.

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Note: Figure translations are in progress. See original paper for figures.