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APPLICATION OF AN ADAPTIVE NEURAL NETWORK FOR THE IDENTIFICATION OF FRACTIONAL PARAMETERS OF HEAT AND MOISTURE TRANSFER PROCESSES IN FRACTAL MEDIA

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Abstract. Physics-Informed Neural Networks (PINN) represent a powerful approach in machine learning that enables the solution of forward, inverse, and parameter identification problems related to models governed by fractional differential equations. This is achieved by incorporating residuals of operator equations, boundary, and initial conditions into the objective function during training. The proposed approach focuses on an adaptive inverse fractal-oriented PINN designed for modeling heat and moisture transfer in capillary-porous materials with a fractal structure and identifying unknown fractional parameters. The core idea is to first construct a fractal neural network for solving the forward problem and then extend its application by transforming fractional derivative orders into trainable variables for optimization. Additionally, synthetic data are incorporated into the objective function to ensure the necessary conditions for solving the identification problem. To ensure that the approximate solution accurately reproduces the physical behavior of the system, the components of the loss function such as deviations from synthetic data, initial and boundary conditions, and residuals of differential equations are adaptively weighted at each training epoch. Similarly, the gradients of trainable parameters are scaled accordingly during the training process. To confirm the effectiveness and reliability of this approach, several examples obtained using the developed software are presented. These examples illustrate its application in various specific scenarios and demonstrate the ability of the adaptive fractal PINN to successfully solve heat and mass transfer problems in fractal capillary-porous structures, as well as accurately identify fractional parameters.

Keywords: neural network, fractional derivatives, fractal media, parameter identification problem, heat and moisture transfer processes, adaptive learning, capillary-porous materials.

Introduction

Porous structures play a significant role in technology, industry, and the natural sciences, as their effective parameters determine the macroscopic behavior of systems. Particular attention is given to capillary-porous materials, in which fine, interconnected pores or channels lead to the dominance of capillary effects. These materials exhibit fractal characteristics due to their multilevel self-organization and complex structure, which provides a high capacity for adsorption, permeability, and moisture distribution factors that, in turn, influence their operational properties, such as durability and structural strength.

The determination of characteristics such as permeability, hydraulic and moisture conductivity, as well as fractional parameters of thermophysical and rheological processes, is typically achieved through the solution of inverse problems, since direct measurement of these parameters is complex, costly, and labor-intensive. The use of more readily computable indicators in differential and fractional-differential models significantly enhances the accuracy of parameter estimations.

It should also be noted that precise determination of the parameters of porous materials is crucial for accurate modeling of their behavior, particularly in systems such as tissues, bones, vascular networks, concrete, wood, and other construction materials. For instance, the coefficient of saturated hydraulic conductivity greatly affects soil moisture regimes and can vary by several orders of magnitude.

Due to their complex multiscale structure, heterogeneity, and the scarcity of homogeneous data, data-driven approaches, notably PINN, have rapidly gained popularity in these fields. Recent studies also demonstrate that PINN are effectively employed to determine the key characteristics of porous media.

Objectives and Problems of Research

In this study, we employ a modified neural network approach based on the fractal PINN architecture [1-3] for the identification of fractional-differential parameters governing non-isothermal moisture transfer in fractal capillary-porous media. This approach enhances the accuracy of unknown parameter estimation, ensures numerical stability, and optimizes the modeling of heat and moisture transfer processes.

The object of the study is the processes of non-isothermal moisture transfer in fractal capillary-porous media.

The subject of the study is a modified neural network approach based on the fractal PINN architecture for the identification of fractional parameters in heat and moisture transfer processes.

The main objective of this research is to develop and implement a fractal neural network-based approach that improves the accuracy of fractional parameter identification, ensures numerical stability, and optimizes the modeling of heat and moisture transfer processes. To achieve this objective, the following sub-tasks have been defined:

- to investigate the theoretical foundations of fractional derivatives based on the Caputo and Grünwald-Letnikov approaches, which form the basis of the mathematical model of non-isothermal moisture transfer in fractal media, and to analyze their applicability within the fPINN framework;
- to develop an algorithm for identifying fractional parameters that regulate heat and moisture transfer processes using the fractal neural network approach;
- to implement a software solution for the fractional parameter identification algorithm;
- to conduct numerical studies to evaluate the adequacy and effectiveness of the proposed algorithm;
- to analyze the obtained data and formulate conclusions regarding the feasibility of applying an adapted fractal neural network for parameter identification in non-isothermal moisture transfer in capillary-porous media with self-similar organization.

The practical significance of this study lies in the direct applicability of the developed approach to technological problems that require precise and rapid analysis of heat and moisture transfer processes in materials with a fractal structure. This method enhances the accuracy of modeling heat and moisture transport in complex fractal geometries, optimizes the management of technological processes by enabling rapid recovery of unknown parameters, and reduces computational costs compared to traditional methods. Furthermore, the results obtained pave the way for further research on multiphysics processes in complex heterogeneous media and expand the scope of applied developments across various scientific and industrial domains.

Review of Modern Information Sources on the Subject of the Paper

The development of mathematical models for simulating the behavior and describing nonequilibrium physical phenomena in fractal porous systems with complex spatiotemporal organization necessitates the use of fractional differentiation methods.

Fractional calculus extends the classical approach to differentiation and integration by allowing non-integer orders of derivatives. Its historical origins date back to the 17th century and are associated with Leibniz, who first posed the question of defining a derivative of an arbitrary order [4]. Since then, numerous mathematicians have contributed to the formation of the theoretical foundations of this field. In recent years, interest in fractional calculus among engineers and researchers has significantly increased. This is due to its ability to accurately represent complex processes in various domains, such as semiconductor technologies, electromagnetism, aerogels, biology, and fluid mechanics [5-9].

The use of fractional derivatives enables the modeling of memory effects and nonlocal properties of systems, which are often beyond the scope of classical differentiation. However, fractional models typically involve a substantial number of parameters (e.g., fractional orders or specific coefficients) that are not always easily measurable directly [10, 11]. As a result, inverse problems aimed at determining these fractional parameters and physical coefficients present significant challenges, including instability, solution ambiguity, and high computational costs.

Against this backdrop, Physics-Informed Neural Networks (PINN) [12] have emerged as an effective computational tool. The key advantage of this approach lies in integrating physical laws encoded in differential equations with the neural network's ability to efficiently interpolate complex dependencies. PINNs serve as a flexible alternative to traditional methods, including finite difference methods, finite element methods, variational techniques, and spectral analysis [13-15]. Although these "classical" schemes are well-established, they often face difficulties when dealing with highly nonlinear problems, high-dimensional spaces, or parameter uncertainty. In response to these challenges, data-driven approaches are actively being explored. These methods have been successfully applied to solve forward problems in various domains, such as fluid mechanics and mass transfer [16-21]. Moreover, PINNs play a crucial role in solving inverse problems and identifying unknown parameters.

Inverse problems are often more complex than forward problems due to their ill-posed nature there may be multiple solutions, or no solution may exist at all. Additionally, they are further complicated by data scarcity, incomplete information, and specific geometric constraints [22].

There are two primary approaches to constructing inverse PINNs for recovering unknown parameters. In the first approach, variables and unknown parameters are treated as input features for the neural network. In the second approach, unknown physical quantities are directly embedded into the network as trainable parameters and incorporated into the loss function through the residuals of the governing equations. These inverse PINN formulations have already been validated in several significant engineering applications [23-27], including the reconstruction of differential equation structures and heat transfer in porous media [22], [28].

However, most existing PINN implementations are designed specifically for integer-order derivatives, which are typically computed using automatic differentiation. At the same time, there is growing interest in extending PINNs to process fractional derivatives, which allow for a more accurate representation of complex phenomena. One of the recent advancements in this direction is fPINN (Fractional Physics-Informed Neural Networks), which employs finite difference methods to compute fractional derivatives [29]. This approach has already demonstrated success in modeling fractional-time diffusion with conformable derivatives [30] and turbulent flow modeling [31].

Overall, the application of neural networks to problems involving fractional dimensions particularly inverse problems and parameter identification remains in its early stages, with only a limited number of research studies published in this domain.

This study focuses on time-space fractional heat and moisture transfer equations, which describe the behavior of dynamic transport processes in capillary-porous materials with fractal organization. The primary objective is to propose a modified adaptive approach for inverse fractal PINNs, which involves developing an adaptive scaling procedure for loss function components and gradients of trainable parameters. This approach enables balanced optimization and ensures convergence in solving the fractional parameter identification problem.

Problem Statement

Classical heat transfer and moisture transport problems are typically described by integer-order differential equations. In addition to the standard behavior of heat and moisture exchange, phenomena of anomalous moisture and thermal conductivity characteristic of materials with unique structures such as capillary-porous media are frequently observed. Researchers have determined that, to adequately describe the anomalous phenomena inherent in these materials, integer-order differential equations prove insufficient, whereas the global correlation afforded by fractional differential operators holds the potential to more accurately capture their memory and intrinsic properties.

In this study, we focus on the examination of differential operators within the frameworks of the Caputo and Grünwald-Letnikov theories, as these approaches enable a more comprehensive description of the anomalous conductivity ranges characteristic of materials with fractional properties. They allow the use of fractional derivatives, which can effectively model memory, temporal, and nonlocal effects in such materials, thereby providing a better representation of their behavior compared to traditional approaches.

Below, we present the definitions of the Caputo and Grünwald-Letnikov differential operators [32].

For a function $f(t)$, the Caputo derivative of order α (where $n=\lceil \alpha \rceil$, i.e., the smallest integer not less than α) is defined as:

$$ {}^{C}D_{a}^{\alpha} f(x,t) = \frac{1}{\Gamma(n-\alpha)} \int_{a}^{t} (t-\tau)^{-\alpha+n-1} f^{(n)}(t) \partial\tau, \ 0<\alpha\le 1, \tag{1} $$

where $\Gamma(\cdot)$ denotes the gamma function, and $f^{(n)}(t)$ represents the n-th derivative of the function f with respect to the variable τ.

The Grünwald–Letnikov derivative of order α is defined by the limit of finite differences:

$$ {}^{GL}D_{x}^{\beta} f(x) = \lim_{h->0} \frac{1}{h^{\beta}} \sum_{k=0}^{\left[\frac{x-a}{h}\right]} (-1)^{k} \binom{\beta}{k} (x-kh), \tag{2} $$

where h is the discretization step, $\lfloor\cdot\rfloor$ denotes the floor function, and $\binom{\alpha}{k}$ is the generalized binomial coefficient, defined as:

$$ \binom{\alpha}{k} = \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)}. $$

Thus, considering the application of fractional calculus, the heat and mass transfer processes in a capillary-porous material with a fractal structure can be mathematically described by a system of fractional differential equations (3) – (9):

$$ {}^{C}D_{\tau}^{\alpha} T = a\, {}^{GL}D_{x}^{\beta} T + \frac{\varepsilon \rho_0 r}{c\rho} {}^{C}D_{\tau}^{\alpha} U, \tag{3} $$

$$ {}^{C}D_{\tau}^{\alpha} U = d\, {}^{GL}D_{x_i}^{\beta} U + d\delta\, {}^{GL}D_{x_i}^{\beta} T, \tag{4} $$

$$ T\big|_{\tau=0} = T^{i}(x), U\big|_{\tau=0} = U^{i}(x), \tag{5} $$

$$ \lambda\, {}^{GL}D_{x}^{\upsilon} T\big|_{x=0} + \sigma\beta\left(U\big|_{x=0} - U_p\right) = \alpha^{*}\left(T\big|_{x=0} - t_c\right), \tag{6} $$

$$ \lambda\, {}^{GL}D_{x}^{\upsilon} T\big|_{x=l} + \sigma\beta\left(U\big|_{x=l} - U_p\right) = \alpha^{*}\left(T\big|_{x=l} - t_c\right), \tag{7} $$

$$ d\, {}^{GL}D_{x}^{\upsilon} U\big|_{x=0} + d\delta\, {}^{GL}D_{x}^{\upsilon} T\big|_{x=0} = \beta^{*}\left(U_p - U\big|_{x=0}\right), \tag{8} $$

$$ d\, {}^{GL}D_{x}^{\upsilon} U\big|_{x=l} + d\delta\, {}^{GL}D_{x}^{\upsilon} T\big|_{x=l} = \beta^{*}\left(U_p - U\big|_{x=l}\right), \tag{9} $$

where x is the spatial coordinate; t is the temporal coordinate, with $(t,x)\in G, G=[0,T]\times[0,l]$; $U(t,x)$ is the moisture function to be determined; $T(t,x)$ is the temperature function to be determined; $c(T,U)$ is the specific heat capacity; a is the thermal diffusivity of the medium; $d(U,T)$ is the moisture diffusivity coefficient; $\lambda(T,U)$ is the thermal conductivity coefficient; ρ is the density; $\sigma=\rho_0(1-\varepsilon)$, where ρ_0 is the base density; r is the specific heat of vaporization; $U_p(t_c,\varphi)$ represents the equilibrium moisture content; t_c is the environmental temperature; φ is the relative humidity of the external environment; $U_i(x)$ is the initial moisture content; $T_i(x)$ is the initial temperature; β^{*},α^{*} is the moisture and heat exchange coefficient; ${}^{C}D_{\tau}^{\alpha}$, ${}^{GL}D_{x_i}^{\beta}$ and ${}^{GL}D_{x_i}^{\upsilon}$ are the fractional-order differential operators defined in the sense of Caputo and Grünwald-Letnikov, respectively; $\alpha(0<\alpha\le1)$ is the fractional order of the time derivative; $\beta(1<\beta\le2)$ and $\gamma(0<\gamma\le1)$ are the fractional orders of the spatial derivatives.

The problem described by equations (3) - (9) is a typical forward problem, where the model is applied to predict the behavior of the system given known parameters (including the fractional orders α,β,γ). The objective is to determine the spatial and temporal distribution of temperature and moisture using the corresponding governing equations (3) - (4), initial conditions (5), and boundary conditions (6) - (9).

The objective of the inverse problem is to identify the model parameters, specifically the fractional orders α,β,γ, in cases where output data (such as synthetic or experimental temperature and moisture values) are available. The identification problem is inherently more complex, as it is often ill-posed in the sense of Hadamard [33], necessitating the use of additional regularization and optimization techniques to obtain a stable and accurate solution.

Thus, the approach begins by solving the forward problem to model the distribution fields $U(t,x)$ and $T(t,x)$ based on the given parameters. Subsequently, inverse methods are employed to refine the fractional orders α,β,γ to achieve the best possible agreement between the model and the experimental data.

Main Material Presentation

a. Direct problem

The fundamental idea behind the PINN approach is to directly incorporate both known physical laws and experimental data into the construction and training of a neural network. In problems governed by partial differential equations, the general form of the equations and certain physical principles are typically known and can be imposed as constraints. This allows the trained neural network to produce solutions that are consistent with physical laws while simultaneously leveraging measured data to enhance predictive accuracy.

To achieve this, PINN defines a composite loss function consisting of two key components: one part ensures consistency with available experimental data, while the other enforces physical constraints. In particular, partial differential equations are embedded into the model through the minimization of the loss function, which penalizes deviations between the neural network's output and the given governing equations. This is facilitated by automatic differentiation, which enables precise computation of integer-order derivatives in both space and time. However, when dealing with fractional derivatives, additional challenges arise, necessitating specialized numerical techniques.

In this study, we adapted and implemented the approach outlined in [29], where fractional operators in both time and space were approximated using numerical schemes (10) and (11) [32], [34].

$$^{C}D_t^{\alpha} f(x,t_n) = \mu^{-\alpha}\left[q_0 f(x,t_n) - q_{n-1} f(x,t_0) + \sum_{i=1}^{n-1}(q_i - q_{i-1}) f(x,t_{n-i})\right], \tag{10}$$

where $q_i = \left((i+1)^{1-\alpha} - i^{1-\alpha}\right)/\Gamma(2-\alpha), i = 0,1,\ldots,N-1;$ $\mu = \dfrac{T}{N}, N \in \mathbb{N}$, $t_n = n\mu, n = 0,\ldots,N.$

$$^{GL}D_x^{\beta} f(x,t) \approx \frac{1}{h^{\beta}} \sum_{i=0}^{n} g_i^{\beta} f(x_{n+1-i},t), \tag{11}$$

where $g_i = \dfrac{\Gamma(i-\beta)}{\Gamma(i+1)\Gamma(-\beta)}$, $h = x_n / i, n = 0,\ldots,N.$

As a next step, these approximations were incorporated into the loss function (12), (13) of the fractional neural network (Fig. 1). This integration enabled the effective incorporation of fractional derivatives into the optimization process, ensuring the proper consideration of the physical characteristics of the modeled phenomena.

$$L_{N_U}\left(\theta^U\right)=\frac{\eta_{U_r}}{N_r}\times\sum_{k=1}^{K}\sum_{n=1}^{N-1}\left[\mu^{-\alpha}[q_0U_{k,n}-q_{k-1}U_{0,n}+\sum_{j=1}^{k-1}\left(q_j-q_{j-1}\right)U_{k-j,n}]-\frac{d}{h_1^{\beta}}\sum_{j=0}^{n}g_j^{\beta}U_{k,n+1-j}-\frac{d\delta}{h_1^{\beta}}\sum_{j=0}^{n}g_j^{\beta}T_{k,n+1-j},\right]^2+$$

$$+\frac{\eta_{U_b}}{N_b}\times\left[\begin{array}{l}\sum_{k=1}^{K}\left(\frac{d}{h^{\gamma}}g_0^{\gamma}U_{k,1}+\frac{d\delta}{h^{\gamma}}g_0^{\gamma}T_{k,1}-\beta\left(U_p-U_{k,0}\right)\right)^2+\\+\sum_{k=1}^{K}\left(\frac{d}{h^{\gamma}}\sum_{j=0}^{N}\upsilon_j^{\gamma}U_{k,N+1-j}-\frac{d\delta}{h^{\gamma}}\sum_{i=0}^{N}\upsilon_j^{\gamma}T_{k,N+1-j}-\beta\left(U_p-U_{k,N}\right)\right)^2\end{array}\right]+ \qquad (12)$$

$$+\frac{\eta_{U_i}}{N_i}\sum_{n=0}^{N}\left(U_{0,n}-U_n^i\right)^2+\frac{\eta_{U_d}}{N_d}\sum_{j=1}^{N_d}\left(U_j-U_j^*\right)^2,$$

$$L_{N_T}\left(\theta^T\right)=$$

$$+\frac{\eta_{T_r}}{N_r}\times\sum_{k=1}^{K}\sum_{n=1}^{N-1}\left[\begin{array}{l}\mu^{-\alpha}[q_0T_{k,n}-q_{k-1}T_{0,n}+\sum_{j=1}^{k-1}\left(q_j-q_{j-1}\right)T_{k-j,n}]-\frac{a}{h^{\beta}}\sum_{j=0}^{n}g_j^{\beta}T_{k,n+1-j}-\\-\frac{\mu^{-\alpha}\varepsilon\rho_0 r}{c\rho}[q_0U_{k,n}-q_{k-1}U_{0,n}+\sum_{j=1}^{k-1}\left(q_j-q_{j-1}\right)U_{k-j,n}]\end{array}\right]^2+$$

$$+\frac{\eta_{T_b}}{N_b}\times\left[\sum_{k=1}^{K}\left(\frac{\lambda}{h^{\gamma}}g_0^{\gamma}T_{k,1}-\sigma\beta_1\left(U_{k,0}-U_p\right)-\alpha^*\left(T_{k,0}-t_c\right)\right)^2+\sum_{k=1}^{K}\left(\frac{\lambda}{h^{\gamma}}\sum_{j=0}^{N}g_j^{\gamma}T_{k,N+1-j}-\sigma\beta\left(U_{k,N}-U_p\right)-\alpha^*\left(T_{k,N}-t_c\right)\right)^2\right] \qquad (13)$$

$$+\frac{\eta_{T_i}}{N_i}\sum_{n=0}^{N}\left(T_{0,n}-T_n^i\right)^2+\frac{\eta_{T_d}}{N_d}\sum_{j=1}^{N_d}\left(T_j-T_j^*\right)^2,$$

where $\eta_{U_d},\eta_{U_r},\eta_{U_i},\eta_{U_b},\eta_{T_d},\eta_{T_r},\eta_{T_i},\eta_{T_b}$ are the weight coefficients and $U\left(t_k,x_n\right)=U_{k,n}$, $T\left(t_k,x_n\right)=T_{k,n}$.

The presence of two loss functions reflects the architecture of the network designed to solve both the forward problem and the parameter identification problem. This structure consists of two independent fully connected branches operating in parallel: a shared input layer receives the spatiotemporal variable, while the output layer integrates the results of both branches. Thus, the functions $U\left(t,x\right)$ and $T\left(t,x\right)$ are approximated by their respective values $U^N\left(t,x;\theta^U\right)$ and $T^N\left(t,x;\theta^T\right)$, obtained through a deep neural network.

The network parameters $\theta^U:=\left\{w^U,b^U\right\}$ and $\theta^T:=\left\{w^T,b^T\right\}$ are optimized by minimizing the loss functions, which ensure compliance with the differential equations (3), (4), initial conditions (5), and boundary conditions (6) – (9). The introduction of a penalty term for deviations from these conditions not only enhances the accuracy of the mathematical model's reproduction but also ensures that the obtained solution aligns with established physical laws.

The training process is structured so that each loss function of the two networks is minimized through an alternating parameter adjustment approach. First, the parameters of the first network are optimized while keeping those of the second network fixed. Then, the same procedure is applied to the second network while maintaining the parameters of the first. This cycle is repeated until either the specified number of iterations is reached or the desired level of accuracy is achieved [3].

At this stage, we have examined the solution of the forward problem and determined the distribution of temperature and moisture within the fractal-structured capillary-porous material based on the constructed model. We now proceed to the next task, which involves identifying the unknown physical parameters of the system that influence heat and moisture transfer processes in the fractal medium.

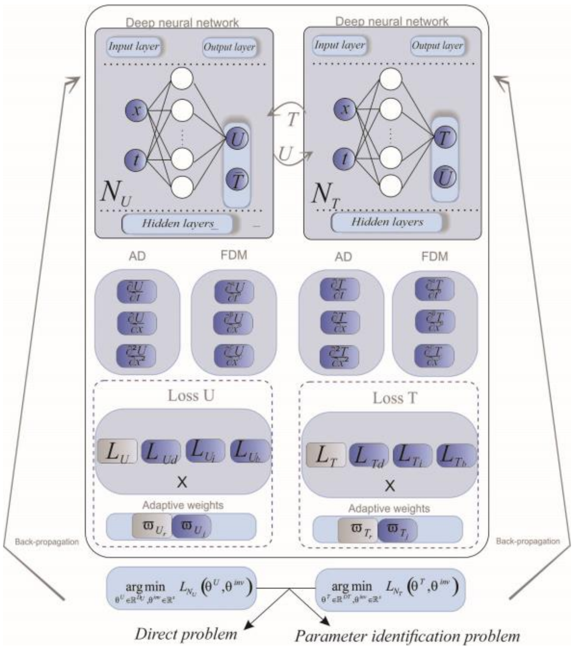

Fig. 1. Architecture of the Fractional Neural Network

b. Parameter identification problem

The identification problem may be ill-posed due to the limited number of experimental measurements available for the physical system described by fractional differential equations. This can lead to solution instability and high sensitivity to errors in the input data.

To overcome these challenges, it is necessary to employ specialized training strategies and regularization techniques that ensure the stability of the optimization process and the accuracy of the identified parameters. One such approach involves incorporating a penalty term into the loss function, which helps to mitigate the impact of noise and improve the consistency of the solution with physical laws (14), (15).

$$L_{N_U}^{INV}\left(\theta^U;\theta^{\theta^{inv}}\right)=L_{N_U}\left(\theta^U\right)+\eta_{inv}\times\sum_{i=1}^{s}\left(\theta_i^{inv}-\theta_i^{inv^*}\right)^2, \tag{14}$$

$$L_{N_T}^{INV}\left(\theta^T;\theta^{inv}\right)=L_{N_T}\left(\theta^T\right)+\eta_{inv}\times\sum_{i=1}^{s}\left(\theta_i^{inv}-\theta_i^{inv^*}\right)^2, \tag{15}$$

where $\theta^{inv}:=\{\alpha,\beta,\gamma\}$ represents the physical parameters, specifically the fractional orders of derivatives α,β,γ and η_{inv} is the weighting coefficient.

Additionally, a viable solution involves utilizing adaptive gradient balancing methods during training [2], [35], which helps to prevent conflicts between different components of the loss function.

To avoid limitations in problem formulation, it is necessary to conduct the search in a transformed parameter space using specialized functional transformations (16):

$$\begin{aligned}\alpha&=0.5\tanh\left(\alpha_i\right)+0.5,\\ \beta&=0.5\tanh\left(\beta_i\right)+1.5,\\ \gamma&=0.5\tanh\left(\gamma_i\right)+0.5,\end{aligned} \tag{16}$$

where $\alpha,\gamma\in(0;1)$, $\beta\in(1;2)$.

Such reparameterization enables optimization without imposing artificial constraints on the parameters, as the initial variables $\alpha_i,\beta_i,\gamma_i$ can take values across the entire real number domain, while their mapped representations automatically remain within permissible ranges.

Furthermore, this study employs an adaptive method proposed in [35], which allows for the dynamic adjustment of the training process based on the specific characteristics of the problem being solved. To ensure the convergence of the inverse fractional PINN, we introduce modified loss functions with weighting coefficients:

$$L_{N_U}^{INV}\left(\theta^U;\theta^{inv}\right)=\sum_{j=1}^{P}\left(\varpi_{Uj}^{\ e}\times(R_{Uj}^{\ i\times b\times d})^2+\varpi_{Ur}^{\ e}\times(R_{Uj}^{\ r})^2\right), \quad (17)$$

$$L_{T_U}^{INV}\left(\theta^T;\theta^{inv}\right)=\sum_{j=1}^{P}\left(\varpi_{Tj}^{\ e}\times(R_{Tj}^{\ i\times b\times d})^2+\varpi_{Tr}^{\ e}\times(R_{Tj}^{\ r})^2\right), \quad (18)$$

where P represents the set of training points, $R_{Uj}^{\ i\times b\times d}, R_{Tj}^{\ i\times b\times d}$ denotes the discrepancies between the network output, initial conditions, boundary conditions, and known data; $R_{Uj}^{\ r}, R_{Tj}^{\ r}$ corresponds to the residuals of the governing equations for humidity and temperature functions; $\varpi_{Uj}^{\ e}, \varpi_{Ur}^{\ e}, \varpi_{Tj}^{\ e}, \varpi_{Tr}^{\ e}$ are adaptive weights that adjust at each training iteration to balance the different components of the loss function.

The weight updates at each optimization step are governed by the following relationships:

$$\varpi_{Uj}^{\ e}=\frac{\hat{\varpi}_{U\ j}^{\ e}}{\sum_{i=1}^{P}\hat{\varpi}_{U\ i}^{\ e}+\hat{\varpi}_{U\ r}^{\ e}},\ \varpi_{Ur}^{\ e}=\frac{\hat{\varpi}_{U\ r}^{\ e}}{\sum_{i=1}^{P}\hat{\varpi}_{U\ i}^{\ e}+\hat{\varpi}_{U\ r}^{\ e}},\ \varpi_{Tj}^{\ e}=\frac{\hat{\varpi}_{T\ j}^{\ e}}{\sum_{i=1}^{P}\hat{\varpi}_{T\ i}^{\ e}+\hat{\varpi}_{T\ r}^{\ e}},\ \varpi_{Tr}^{\ e}=\frac{\hat{\varpi}_{T\ r}^{\ e}}{\sum_{i=1}^{P}\hat{\varpi}_{T\ i}^{\ e}+\hat{\varpi}_{T\ r}^{\ e}},\ j=1,\ldots,P, \quad (19)$$

where auxiliary quantities $\hat{\varpi}_{U\ j}^{\ e}, \hat{\varpi}_{U\ r}^{\ e}, \hat{\varpi}_{T\ j}^{\ e}, \hat{\varpi}_{T\ r}^{\ e}$ are introduced. In particular,

$$\hat{\varpi}_{U\ j}^{\ e}=\begin{cases}\eta_{U_b},\ if\ x_j\in\partial G\\ \eta_{U_i},\ if\ \tau_j=0\\ \varphi(e)\times\eta_{U_d},\ if\ \left(x_j,\tau_j\right)\in N_d\\ 0,\ in\ other\ cases,\end{cases},\quad j=1,\ldots,P$$
$$\hat{\varpi}_{T\ j}^{\ e}=\begin{cases}\eta_{T_b},\ if\ x_j\in\partial G\\ \eta_{T_i},\ if\ \tau_j=0\\ \varphi(e)\times\eta_{T_d},\ if\ \left(x_j,\tau_j\right)\in N_d\\ 0,\ in\ other\ cases\end{cases},\quad j=1,\ldots,P \quad (20)$$

$$\hat{\varpi}_{U\ r}^{\ e}=\begin{cases}1,\ if\ \left(x_j,\tau_j\right)\in G\\ 0,\ in\ other\ cases\end{cases},\ j=1,\ldots,P$$
$$\hat{\varpi}_{T\ r}^{\ e}=\begin{cases}1,\ if\ \left(x_j,\tau_j\right)\in G\\ 0,\ in\ other\ cases\end{cases},\ j=1,\ldots,P \quad (21)$$

where $\eta_{T_d}, \eta_{U_d}, \eta_{U_b}, \eta_{U_i}, \eta_{T_b}, \eta_{T_i}$ are constants that define the weight of the boundary conditions, initial conditions, and known experimental or synthetic data, respectively. The function $\varphi(e)$ increases with the epoch number e, starting from zero and approaching one, allowing the model to initially focus primarily on the residuals of the governing equations and later adjust to the available data. For example, it can be defined as:

$$\varphi(e)=\frac{\tanh\left(10\left(\frac{e-E/2-\tilde{E}}{E}\right)\right)}{2},\ e=1,\ldots,E,$$

where E is the total number of epochs, and $\tilde{E}$ is the epoch threshold after which the weight coefficients are significantly adjusted.

The computation of the gradients $\nabla_{\theta^U}L_{N_U}$, $\nabla_{\theta^{inv}}L_{N_U}$, $\nabla_{\theta^T}L_{N_T}$ and $\nabla_{\theta^{inv}}L_{N_T}$ is performed using the automatic differentiation algorithm. Additionally, the gradients with respect to the physical parameters are scaled by a factor of $\varphi(e)$. This scaling plays a crucial role in ensuring convergence: it prevents the physical parameters from being updated until the corresponding data begin to significantly influence the overall loss function. Once this condition is met, the parameters are updated using the Adam optimizer with an initial learning rate ν_i, which is adjusted dynamically based on the epoch number e, according to:

$$\nu_e = \nu_i \vartheta^{\left\lfloor \frac{e}{100} \right\rfloor},$$

where ϑ is a constant attenuation coefficient, with the condition that $0.9 < \vartheta < 0.99$.

The model training process is conducted iteratively, starting from the initial epoch. At each step, sequential parameter updates are performed, incorporating adaptive weight coefficient adjustments and gradient scaling. The training process continues until convergence is achieved or the maximum number of epochs is exceeded.

Thus, the algorithm ensures adaptive tuning of weight coefficients and controlled parameter updates, facilitating efficient learning, improving stability, and enhancing convergence. This, in turn, contributes to more accurate identification of fractional-order parameters.

Results and Discussion

This section presents a study that demonstrates the capabilities of the proposed fractal neural method for the numerical solution of both the forward problem and the parameter identification problem in modeling heat and moisture transfer processes (3) – (9) with fractional derivatives in spatial and temporal variables.

Numerical experiments were conducted on a hardware platform equipped with an Intel(R) Core(TM) i7-8750H processor, 16 GB of RAM, and running the Windows 10 operating system. To implement the proposed approach, a software code was developed, incorporating two independent fully connected neural networks implemented using the TensorFlow and Keras libraries. The optimization of network parameters and the identified fractional exponents was performed using an automatic differentiation mechanism.

The Adam algorithm was employed for loss function optimization, while the initial weight coefficients were configured using the Xavier initialization method. The primary training hyperparameters included the following: the number of hidden layers in each network 8, the number of neurons per layer 40, the initial learning rate 0.01, and the total number of iterations approximately 4000.

The experiments were conducted to model heat and moisture transfer in a capillary-porous material with a fractal structure, specifically wood with a baseline density of ρ = 460 kg/m^3. The initial conditions for the model were set as follows: sample temperature $T_0 = 20^\circ C$, ambient temperature $t_c = 70^\circ C$, initial moisture content $U_i = 0.5$ kg/kg, relative air humidity $\varphi = 65\%$, and drying agent velocity $v = 2$ m/s. The fractional parameters of the model were assigned specific values $\alpha = 0.9, \beta = 1.9, \gamma = 0.95$.

The visualization of the modeling results for the temperature and moisture dynamics using the fractal adaptive neural network method is presented in Figure 2.

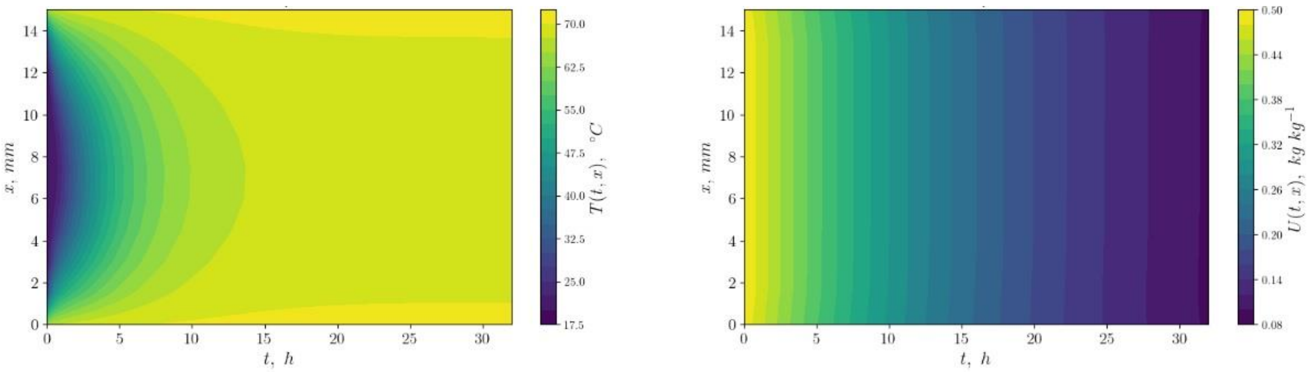

Fig. 2. Variation of Temperature and Moisture Fields

Fig. 3 illustrates the evolution of the weighted (c) and unweighted (a, b) loss functions during the training process of the PINN. The weighted loss function incorporates adaptive weight coefficients (19) – (21), which allow for differentiated emphasis on specific components of the loss function. During model training, these weight coefficients are updated at each iteration to maintain a balance between different types of errors, including discrepancies from differential equations, initial and boundary conditions, and known data.

In contrast, the unweighted loss function is computed with fixed weight coefficients, representing the baseline model error. Comparing these loss function graphs provides deeper insight into how the weight coefficients influence the training process.

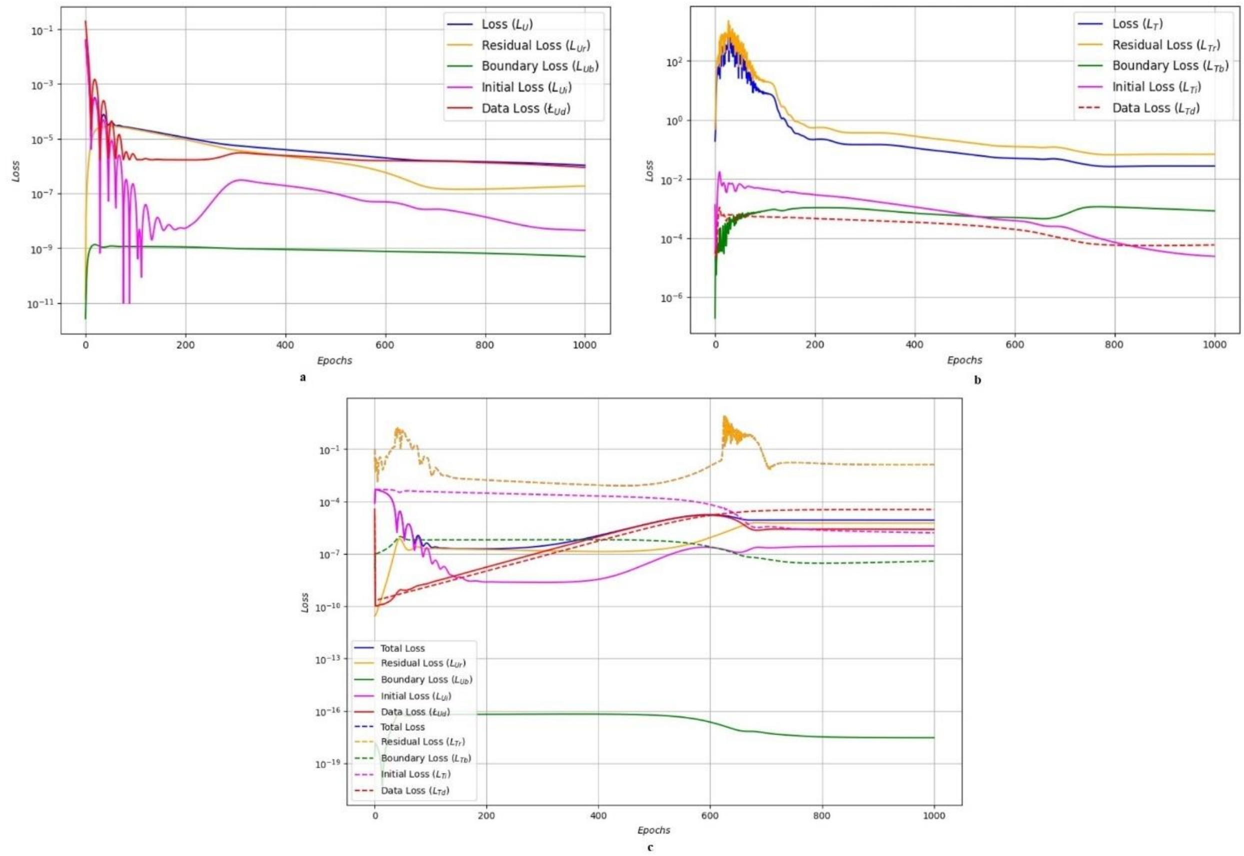

Fig. 3. Comparison of Loss Functions with Fixed and Adaptive Weights During the Training of a Fractal Neural Network

In cases (a) and (b) presented in Figure 3, it can be observed that different components of the loss function have varying magnitudes and may dominate at different stages of training, leading to uneven reduction of each component.

In contrast, case (c) employs an adaptive approach that dynamically scales the weights of the loss function components (17) – (18). This ensures a better balance of the different components throughout the training process, allowing for a more effective reduction of residual errors across all terms simultaneously. As a result, convergence occurs more uniformly, and the model achieves improved consistency with boundary and initial conditions, as well as with the available experimental data.

Let us now consider the "inverse" problem, in which the objective is to determine the unknown physical parameters that influence heat and moisture transfer processes in a fractal medium, specifically the fractional derivative indices of the model (3) – (9). The proposed neural network algorithm enables solving the parameter identification problem while utilizing essentially the same code base as for the forward formulation. However, this involves adding fractional parameters to the list of variables subject to optimization, along with incorporating additional penalty terms into the loss function (14), (15). The final modeling results are presented in Figure 4.

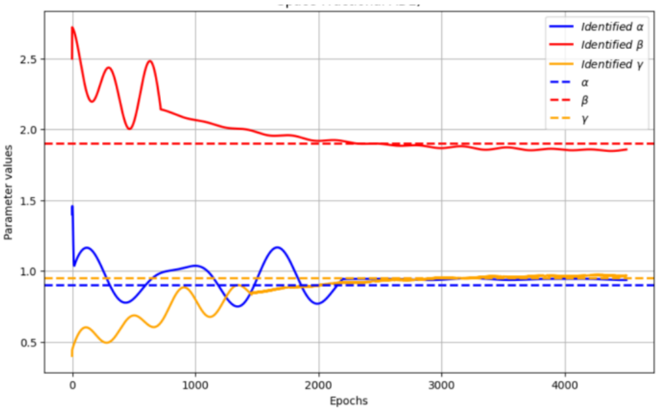

Fig. 4. Identification of fractional parameters with the inclusion of a penalty term in the loss function

The application of functional transformations (16) improves stability and convergence metrics (Figure 5). However, the best results are achieved by combining these strategies with the use of adaptive weights (19) – (21), as demonstrated by the modeling results presented in Figure 6.

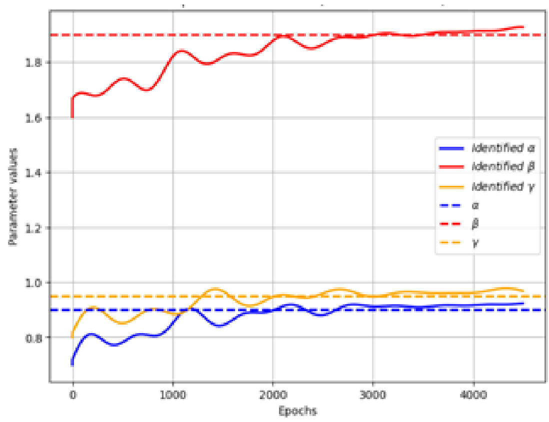

Fig. 5. Impact of functional transformations on the identification of fractional parameters

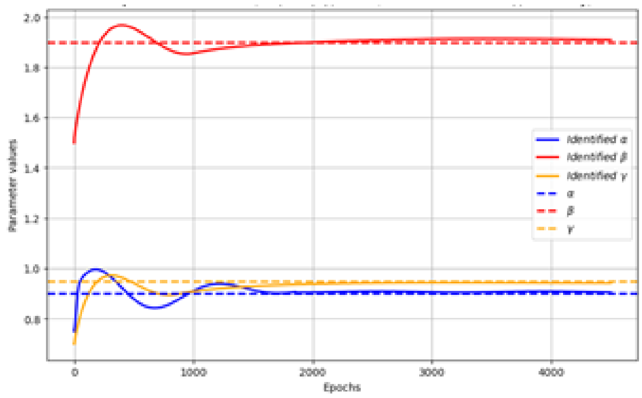

Fig. 6. Improvement of fractional parameter identification using adaptive weighting coefficients in the loss function

A comparison of the presented graphs illustrates how the stepwise addition of different types of regularization affects the accuracy and stability of fractional parameter identification within the inverse heat and moisture transfer problem in fractal media. The curves in Fig. 4 depict convergence; however, it is evident that the issue of local minima and the complex topology of loss functions is not always resolved. The graphs in Fig. 5 reflect the transformation of the parameter space, achieved through specialized functional transformations (16). This strategy helps "stretch" or "compress" the parameter space, making the loss function smoother and less prone to becoming trapped in local minima. As a result, the optimization problem becomes easier to solve, leading to more reliable parameter identification.

Figure 6 demonstrates another level of refinement introducing adaptive weighting coefficients into the loss functions. With this approach, during the initial training phase, the network primarily focuses on aligning with the governing equations before shifting toward approximating experimental data. Consequently, the model more effectively learns the underlying physics of the process, which enhances the accuracy of fractional parameter estimation and reduces the risk of imbalance toward one component of the loss function. Overall, this strategy enables a more robust and precise identification of fractional parameters in the heat and moisture transfer model for fractal media.

Conclusions

This study presents the application of an adaptive approach to an inverse fractional physics-informed neural network (PINN) for solving heat and moisture transfer problems and identifying unknown parameters in capillary-porous materials with a fractal structure. The proposed architecture of the fractional neural network and the training algorithm ensure the efficient resolution of both the forward problem and the parameter identification task, allowing the simultaneous determination of up to three parameters.

The further development of the method involves extending the approach to two-dimensional problems and incorporating a larger number of parameters. The key innovation of the proposed approach is the adaptive scaling of individual components of the loss function and gradients of trainable parameters, which plays a crucial role in ensuring the convergence of the identification problem. This strategy enables maintaining a balance between different components of the loss function and effectively managing weight updates, thereby ensuring the reliable convergence of the algorithm.

The numerical experiments conducted using the developed software confirm that the proposed adaptive architecture of the inverse fractional neural network is scalable, stable, and demonstrates high efficiency in solving partial heat and moisture transfer problems in materials with a fractal structure, as well as in the identification of fractional parameters.

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ЗАСТОСУВАННЯ АДАПТИВНОЇ НЕЙРОННОЇ МЕРЕЖІ ДЛЯ ІДЕНТИФІКАЦІЇ ДРОБОВИХ ПАРАМЕТРІВ ПРОЦЕСІВ ТЕПЛО- ТА ВОЛОГОПЕРЕНЕСЕННЯ У ФРАКТАЛЬНИХ СЕРЕДОВИЩАХ

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Анотація. Фізично обґрунтовані нейронні мережі (PINN) є потужним підходом у машинному навчанні, що дозволяє розв’язувати прямі, обернені задачі та задачі ідентифікації, пов’язані з моделями, що описуються дробовими диференціальними рівняннями, за рахунок включення залишків операторних рівнянь, граничних та початкових умов в цільову функцію під час навчання. У пропонованому підході зосереджено увагу на адаптивному оберненому фрактально-орієнтованому PINN, призначеному для моделювання тепло- та вологопереносу у капілярно-пористих матеріалах із фрактальною структурою та ідентифікації невідомих дробових параметрів. Основна ідея полягає в тому, щоб спершу побудувати фрактальну нейронну мережу для прямої задачі, а потім розширити її застосування, перетворивши показники дробових похідних на змінні, що підлягають оптимізації. Додатково до цільової функції включаються синтетичні дані, які забезпечують необхідні умови для розв’язання задачі ідентифікації. Щоб наближений розв’язок правильно відтворював фізичну поведінку системи, компоненти функції втрат (зокрема, відхилення від синтетичних даних, початкових та граничних умов, а також залишки диференціальних рівнянь) зважуються адаптивно на кожній епосі навчання. Аналогічним чином виконується й масштабування градієнтів параметрів, що залучені до процесу тренування. Для підтвердження ефективності та надійності цього підходу наведено декілька прикладів, отриманих за допомогою розробленого програмного забезпечення, що ілюструють його застосування в різнопланових часткових сценаріях і демонструють здатність адаптивного фрактального PINN успішно розв’язувати задачі тепло- та масопереносу у фрактальних капілярно-пористих структурах, а також ідентифікації дробових показників

Ключові слова: нейронна мережа, дробові похідні, фрактальні середовища, задача ідентифікації параметрів, процеси тепло- та вологообміну, адаптивне навчання, капілярно-пористі матеріали.