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Application of Deep Learning and Physics-Informed Neural Networks to the Heat Transfer Problem within the Green–Naghdi Type II Theory

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Abstract. The paper considers the heat transfer problem within the framework of the Green–Naghdi type II theory, which accounts for the finite speed of thermal wave propagation. A comparison is made between the analytical solution, the numerical method based on a finite difference scheme, and the approach utilizing Physics-Informed Neural Networks (PINN). To validate the results, the parameters of duralumin are used in a dimensionless form. It is shown that the PINN method accurately reproduces the dynamics of thermal waves and demonstrates efficiency comparable to classical methods, while providing additional robustness to discretization errors. The results obtained confirm the prospects of applying PINN to solve both direct and inverse problems of hyperbolic heat conduction.

INTRODUCTION

The solution of hyperbolic heat conduction equations can be obtained using various methods. Analytical approaches, based on Fourier and Laplace transforms or Fourier series expansions, provide rigorous results but are applicable only to relatively simple geometries and boundary conditions. Numerical methods (finite-difference and finite-element schemes) make it possible to efficiently solve problems in complex domains and under arbitrary loading, but they require stability analysis, the coordination of time and space steps, as well as significant computational resources. In particular, methods based on second-order schemes in time and space have become widespread in solving dynamic heat conduction problems [5-6], [12-13], [23], [28-30].

In recent years, methods based on deep machine learning have been actively developed. Special attention has been drawn to the Physics-Informed Neural Networks (PINN) technology proposed in [20-22]. The main idea of PINN is the integration of physical laws into the neural network loss function, which makes it possible to obtain approximate solutions of partial differential equations without explicit discretization of the domain. This approach has proven effective for solving both direct and inverse problems, including heat conduction, elasticity, and acoustics [1-4], [7-11], [14-27]. Several studies have demonstrated that PINN is capable of reproducing complex dynamic processes and shows robustness to noisy data, which makes it a promising tool for engineering applications.

Of particular interest is the application of PINN to hyperbolic heat conduction models, in particular to the Green–Naghdi type II theory. Such formulations not only allow for a correct description of thermal wave propagation processes but also enable the solution of inverse problems related to the identification of material parameters or localization of heat sources.

In this paper, we consider a heat transfer problem within the framework of the Green–Naghdi type II theory with prescribed initial conditions and Dirichlet boundary conditions. Three solution approaches are compared: an analytical method (Fourier series expansion), a numerical method (second-order finite-difference scheme), and a neural network-based approach utilizing PINN. For verification purposes, a thermally conductive medium made of duralumin is considered, with its parameters given in dimensionless form. The main focus is placed on analyzing the accuracy, stability, and specific features of applying PINN to the modeling of thermal processes.

MATHEMATICAL FORMULATION OF THE PROBLEM

Let us consider the heat transfer problem in a homogeneous isotropic medium, described by the Green–Naghdi type II equation [3] (Fig. 1).

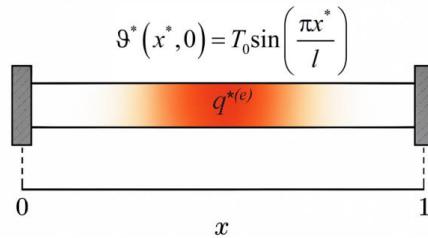


FIGURE 1. Illustration of the mathematical formulation of the problem.

In dimensional form, the governing equation can be written as:

$$\rho c_e \dot{\theta}^* = \tilde{\kappa}^* \square \theta^* + \rho q^{*(e)}, \quad (1)$$

where, ρ — is the material density, c_e — is the specific heat capacity at constant strain, T_0 — is the initial temperature, $\theta^*(x^*, t^*) = T^*(x^*, t^*) - T_0$ — is the temperature deviation from the initial value, $\tilde{\kappa}^*$ — is the thermal wave speed, $q^{*(e)}$ — is the volumetric heat source (the heat released per unit volume per unit time), and $\dot{q}^{*(e)}$ — is the rate of change of the heat source intensity with respect to time.

The Dirichlet boundary conditions are specified as:

$$\theta|_{x=0} = 0, \quad \theta|_{x=l} = 0, \quad (2)$$

and the initial conditions at $t^* = 0$:

$$\theta^*(x^*, 0) = T_0 \sin\left(\frac{\pi x^*}{l}\right), \quad \dot{\theta}^*(x^*, 0) = \frac{T_0 c_T}{l} \left(\frac{x^*}{l}\right) \left(\frac{x^*}{l} - 1\right), \quad (3)$$

For simplification of the analysis and for obtaining the canonical form of the governing equation, let us introduce dimensionless variables. As characteristic scales we choose the length l , the thermal wave propagation time l/c_T and the initial temperature T_0 . Then, the system of dimensionless variables takes the form:

$$x = \frac{x^*}{l}, \quad t = \frac{c_T t^*}{l}, \quad c_T^2 = \frac{\tilde{\kappa}}{\rho c_e}, \quad \theta = \frac{\theta^*}{T_0}, \quad q^{*(e)} = \frac{q^{*(e)} l}{c_e c_T T_0}. \quad (4)$$

where x, t — are the dimensionless spatial and temporal variables, θ — is the relative temperature deviation, c_T — is the thermal wave speed, and $q^{*(e)}$ — is the dimensionless external heat source.

Thus, the mathematical formulation of the problem in its dimensionless form is:

$$\ddot{\theta} - \square \theta = \dot{q}^{*(e)}, \quad x \in [0, 1], \quad t > 0, \quad (5)$$

with Dirichlet boundary conditions:

$$\theta|_{x=0} = \sin(\pi x), \quad \dot{\theta}|_{x=0} = x(x-1), \quad (6)$$

and initial conditions:

$$\theta|_{x=0} = 0, \quad \theta|_{x=l} = 0. \quad (7)$$

ANALYTICAL SOLUTION FOR THE GREEN–NAGHDI TYPE II HEAT CONDUCTION EQUATION

Let us consider the one-dimensional heat transfer problem within the framework of the Green–Naghdi type II theory in its dimensionless form (equations (5)–(7)). As an external heat source, we take the function:

$$q^{*(e)}(x, t) = 2xt, \quad (8)$$

which models a linearly increasing source in both space and time. In this case, the intensity of heat generation grows proportionally to the coordinate x and time t , which corresponds to a non-stationary process of localized heat release.

Then its time derivative, which enters the governing equation (5), takes the form:

$$\dot{q}(x, t) = 2x. \quad (9)$$

To solve the problem (5) – (7) we apply the method of separation of variables with the expansion of the desired function in terms of the eigenfunctions of the Sturm–Liouville boundary value problem:

$$\vartheta(x, t) = \sum_{n=1}^{\infty} a_n(t) \sin(\pi n x). \quad (10)$$

Substituting this representation into the governing equation leads to the following system for the coefficients:

$$a_n''(t) + (\pi n)^2 a_n(t) = F_n, \quad F_n = 4 \int_0^1 x \sin(\pi n x) dx = \frac{4(-1)^{n+1}}{\pi n}, \quad (11)$$

where F_n are the Fourier coefficients of the source term.

At $t = 0$ the temperature distribution in the rod is prescribed as a sinusoidal function (6). This condition corresponds to a perturbation in which the maximum temperature deviation from the initial value occurs at the middle of the domain, while at the ends $x = 0$ and $x = 1$ the temperature vanishes due to the imposed Dirichlet boundary conditions. In addition, (6) specifies the distribution of the initial rate of temperature change. This quadratic function is negative in the interval $0 \leq x \leq 1$ and vanishes at the boundaries, which is consistent with the end-fixing conditions. Thus, at time $t = 0$ the temperature is not only distributed according to a sinusoidal law, but also begins to change at a given rate, which reflects the dynamic nature of the problem statement.

When moving to the coefficients of expansion in eigenfunctions, the system of initial conditions takes the form

$$a_n(0) = \delta_{n1}, \quad a_n'(0) = \begin{cases} 0, & n - \text{even number}, \\ -\frac{8}{\pi^3 n^3}, & n - \text{odd number}, \end{cases} \quad (12)$$

where δ_{n1} — is the Kronecker delta, equal to 1 for $n = 1$ and 0 otherwise.

The solution for each coefficient a_n from (11) is:

$$a_n(t) = \left(\delta_{n1} - \frac{4(-1)^{n+1}}{\pi^3 n^3} \right) \cos(\pi n t) + \frac{4((-1)^n - 1)}{\pi^4 n^4} \sin(\pi n t) + \frac{4(-1)^{n+1}}{\pi^3 n^3}. \quad (13)$$

Thus, the general solution of the problem is represented as a Fourier series:

$$\vartheta(x, t) = \sum_{n=1}^{\infty} \left[\left(\delta_{n1} - \frac{4(-1)^{n+1}}{\pi^3 n^3} \right) \cos(\pi n t) + \frac{4((-1)^n - 1)}{\pi^4 n^4} \sin(\pi n t) + \frac{4(-1)^{n+1}}{\pi^3 n^3} \right] \sin(\pi n x). \quad (14)$$

NUMERICAL SOLUTION FOR THE GREEN–NAGHDI TYPE II HEAT CONDUCTION EQUATION

For the numerical solution of the one-dimensional heat transfer problem within the framework of the Green–Naghdi type II theory (equations (5)–(7)) we introduce uniform grids in the spatial coordinate and time:

$$x_j = j \Delta x, \quad j = 0, \dots, M, \quad t^n = n \Delta t, \quad n = 0, 1, \dots \quad (15)$$

and seek approximations $u_j^n \approx \vartheta(x_j, t^n)$. The second derivative with respect to space is approximated by a central difference of second order:

$$\vartheta_{xx}(x_j, t^n) \approx \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}. \quad (16)$$

Applying central differences in time leads to an explicit scheme of second-order accuracy:

$$u_j^{n+1} = 2u_j^n - u_j^{n-1} + \lambda^2 (u_{j+1}^n - 2u_j^n + u_{j-1}^n) + (\Delta t)^2 f_j, \quad j = 1, \dots, M-1, \quad (17)$$

where $\lambda = \Delta t / \Delta x$, and $f_j = 2x_j$. The Dirichlet boundary conditions are imposed explicitly:

$$u_0^n = 0, \quad u_M^n = 0, \quad n \geq 0. \quad (18)$$

To construct the first time layer, a Taylor expansion is used with account of the governing equation:

$$u_j^1 = u_j^0 + \Delta t, v_j^0 + \frac{1}{2}(\Delta t)^2 \left((\vartheta_{xx})_j^0 + f_j \right), \quad (19)$$

where $u_j^0 = \sin(\pi x_j)$, $v_j^0 = x_j(x_j - 1)$.

A Fourier analysis for the homogeneous equation shows that the scheme is stable under the Courant–Friedrichs–Lowy condition:

$$\lambda = \frac{\Delta t}{\Delta x} \leq 1. \quad (20)$$

Thus, the time step is selected from condition (20). The scheme has second-order accuracy in space and time.

To control accuracy, an analytical solution in the form of a Fourier series of eigenfunctions of the Dirichlet problem was used. Comparison of the numerical results with a truncated series (400 members) showed that the relative error in the norm of L_2 on the time interval $0 \leq t \leq 1.2$ does not exceed 10^{-6} . This confirms the correctness of the implementation and the second-order convergence with respect to the grid steps.

SOLUTION OF THE GREEN–NAGHDI TYPE II HEAT CONDUCTION EQUATION USING A NEURAL NETWORK

PINN approximation with exact enforcement of boundary and initial conditions

To satisfy the boundary and initial conditions exactly, a special representation of the solution is used, allowing them to be embedded directly into the model structure:

$$\vartheta(x, t) = g(x) + th(x) + t^2 S(x) N_\phi(x, t), \quad (21)$$

where $S(x) = x(1-x)$ vanishes at the boundary $x = 0, 1$, and $N_\phi : \mathbb{D}^2 \rightarrow \mathbb{D}$ — is the output of a fully connected neural network with parameters ϕ .

Verification of conditions:

Boundary conditions — $\vartheta(0, t) = g(0) + th(0) + t^2 S(0) N_\phi(0, t) = 0$ and similarly $\vartheta(1, t) = 0$.

Initial conditions — $\vartheta(x, 0) = g(x)$, because $t = 0$ vanishes the terms with $h(x)$ и N_ϕ ;

further $\vartheta_t(x, t) = h(x) + 2tS(x)N_\phi + t^2 S(x)\partial_t N_\phi$, where $\vartheta_t(x, 0) = h(x)$.

Thus, the loss function contains no additional penalty terms for boundary and initial conditions, and the training of the neural network is focused exclusively on the dynamics of the equation.

The approximating model is a fully connected neural network (Multi-Layer Perceptron, MLP). The inputs are the spatial and temporal coordinates $(x, t) \in \mathbb{D}^2$, which ensures joint modeling of the solution's dependence on both spatial and temporal variables. The output of the network is a scalar value $N_\phi(x, t)$, representing a part of the solution in the constructive form.

Network architecture and initialization

The network architecture includes five hidden layers with 128 neurons each, with the \tanh activation function. This choice is motivated by its properties: smoothness, boundedness, and the ability to adequately reproduce both low-frequency and moderately oscillatory components of the solution. Such a combination of depth and width provides sufficient approximation capacity while maintaining training stability.

Weights are initialized according to the Xavier (Glorot) scheme, which ensures a balanced scale of the initial parameters and promotes more stable convergence of the optimization process. For problems with a more complex spectral content (e.g., dominated by high-frequency components), alternative activation functions such as sinusoidal ones (SIREN), as well as an adapted weight initialization strategy, are preferable. This approach improves the ability of the model to reproduce oscillatory solution behavior, which is typical for hyperbolic-type problems.

Loss function and automatic differentiation

The training of the neural network model is based on minimizing the residual of the Green–Naghdi type II heat conduction equation [4]. The only functional used is the mean squared residual of the governing equation at the collocation points:

$$L_{\text{PDE}}(\phi) = \frac{1}{N_c} \sum_{i=1}^{N_c} \left[\vartheta_u(x_i, t_i; \phi) - \vartheta_{xx}(x_i, t_i; \phi) - \dot{q}^{(e)}(x_i, t_i) \right]^2, \quad (22)$$

where $\{(x_i, t_i)\}_{i=1}^{N_c}$ — is a sample of points from the region $x \in (0, 1), t \in (0, T]$, and the heat source has the form $\dot{q}^{(e)}(x, t) = 2x$.

The derivatives $\vartheta_t, \vartheta_u, \vartheta_x, \vartheta_{xx}$, are computed using automatic differentiation. In particular, in PyTorch this is implemented by successive calls of the *autograd.grad* function, which allows obtaining derivatives of any order with respect to spatial and temporal variables without explicit construction of finite-difference approximations. This significantly simplifies implementation and provides machine precision in computing gradients, which is necessary for training the network.

Special attention was paid to the stability of second derivative computations, since they are most sensitive to approximation errors and numerical artifacts. To improve accuracy, derivatives were computed in standard floating-point precision (float32), even when mixed precision (AMP) was used for acceleration.

It should be noted that mixed precision (AMP) can accelerate training on GPUs due to computations in float16/bfloat16 format. However, when calculating second derivatives, loss of accuracy and degradation of convergence are possible. Therefore, in the base configuration, AMP was disabled, and when enabled, additional quality control is required (e.g., comparison with reference values or fallback to float32 for derivative computation).

Thus, the loss function is formed solely by the residual of the equation, while the boundary and initial conditions are automatically satisfied through the special solution representation. This allows the optimization of network parameters to focus on approximating the equation dynamics, ensuring high accuracy and stability of training.

Strategy for generating collocation points

A key element of the PINN method is the generation of the set of collocation points $\{(x_i, t_i)\}_{i=1}^{N_c}$, at which the residual of the equation is evaluated. In the basic configuration, the points are uniformly sampled over the rectangular domain $(0, 1) \times (0, T]$. This approach ensures coverage of the entire integration domain and uniform distribution of errors in space and time.

To improve training stability, resampling is applied: at each training iteration, a new set of collocation points is generated. This makes it possible to:

- reduce correlation between successive batches,
- avoid “fitting” the solution to a fixed grid,
- increase robustness against trapping in local minima of the loss function.

In some cases, it is advisable to use more advanced point generation schemes, such as Latin Hypercube Sampling (LHS) or Sobol sequences. These methods provide better filling of the domain and allow for more uniform coverage of the variable space than simple uniform sampling.

When solving problems with pronounced solution fronts, characteristic of hyperbolic equations, local point refinement is useful. In particular, it is recommended to increase the density of collocation points:

- near the initial moment of time $t \approx 0$, where the solution is most sensitive to the initial perturbation,
- near the boundary points $x = 0, 1$, where strict boundary conditions are imposed.

Thus, an adaptive sampling strategy significantly improves the agreement of the PINN solution with the analytical reference and accelerates training convergence.

The training of the neural network model is carried out on a graphics processor and is organized in two phases:

– **Phase 1 (Adam).** At the first stage, the stochastic gradient optimizer Adam [24] is used with an initial learning rate $lr = 10^{-3}$. To control convergence, an adaptive scheduler ReduceLROnPlateau is applied, which automatically decreases the learning rate in the absence of noticeable progress. A minimum of 2000 epochs is allocated for the “warm-up” of the model, allowing the network to leave the random initialization state and to form a correct approximation.

– **Phase 2 (L-BFGS).** At the second stage, fine-tuning of the parameters is performed using the quasi-Newton method L-BFGS with line search according to the “strong Wolfe” condition. This method effectively minimizes quadratic functionals and allows achieving high solution accuracy near the optimum.

The transition between training phases is implemented using a combination of criteria:

- *early transition*: if the equation residual becomes smaller than the threshold $L_{PDE} < 10^{-4}$;
- *plateau detection*: if the improvement of the error is less than 10^{-5} for 800 consecutive epochs;
- *learning rate condition*: if the learning rate decreases below a prescribed threshold $lr < 5 \cdot 10^{-5}$.

Such a hybrid strategy adapts the training process to the dynamics of the specific problem: Adam ensures rapid descent in the initial stages, while L-BFGS refines the solution to high accuracy. As a result, computational resources are saved and a stable reduction of the residual is achieved while maintaining accuracy compared to analytical and numerical solutions.

CALCULATION RESULTS

To verify the correctness of the proposed PINN scheme, computational experiments were carried out for the one-dimensional heat transfer problem within the framework of the Green–Naghdi type II theory. As reference solutions, the following were used:

1. the analytical solution represented as a Fourier series in trigonometric functions (14);
2. an independent numerical solution (17), obtained by a finite-difference wave-type scheme.

The PINN model was trained on a graphics processor in a two-phase mode: in the first stage the Adam $lr = 10^{-3}$ algorithm with ReduceLROnPlateau learning rate reduction was applied, and in the second stage fine-tuning was performed using the L-BFGS method (Fig. 2).

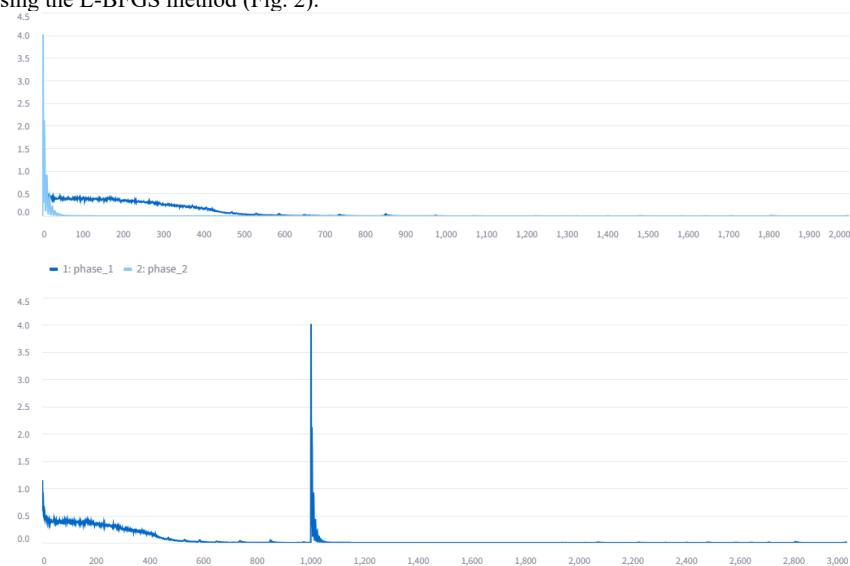


FIGURE 2. Loss function history during PINN training: Adam phase and fine-tuning with L-BFGS.

The minimization of the loss function was stable, with a monotonic decrease of the residual and achievement of the threshold value $L_{PDE} < 10^{-4}$.

Comparison of the solutions showed a high degree of agreement between the PINN results and the analytical and finite-difference solutions. For a quantitative assessment of accuracy, global relative errors in the L_2 – norm were calculated (Fig. 3):

$$\varepsilon_{FD/Analytic} \approx O(10^{-3}), \varepsilon_{PINN/Analytic} \approx O(10^{-4}), \varepsilon_{PINN/FD} \approx O(10^{-3}) \quad (23)$$

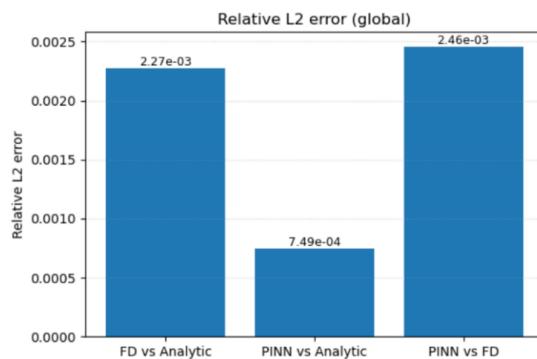


FIGURE 3. Relative L_2 - error between the analytical solution, finite-difference approximation, and the PINN model.

The obtained values demonstrate comparable accuracy of PINN and the classical finite-difference approximation, while PINN does not require explicit discretization of the domain.

The graphical results are presented as solution cross-sections with respect to spatial and temporal variables $\theta(x_0, t)$ at fixed values of x_0 and $\theta(x, t_0)$ at fixed instants of time t_0 (Fig. 4). In these graphs, the solutions obtained by different methods practically coincide.

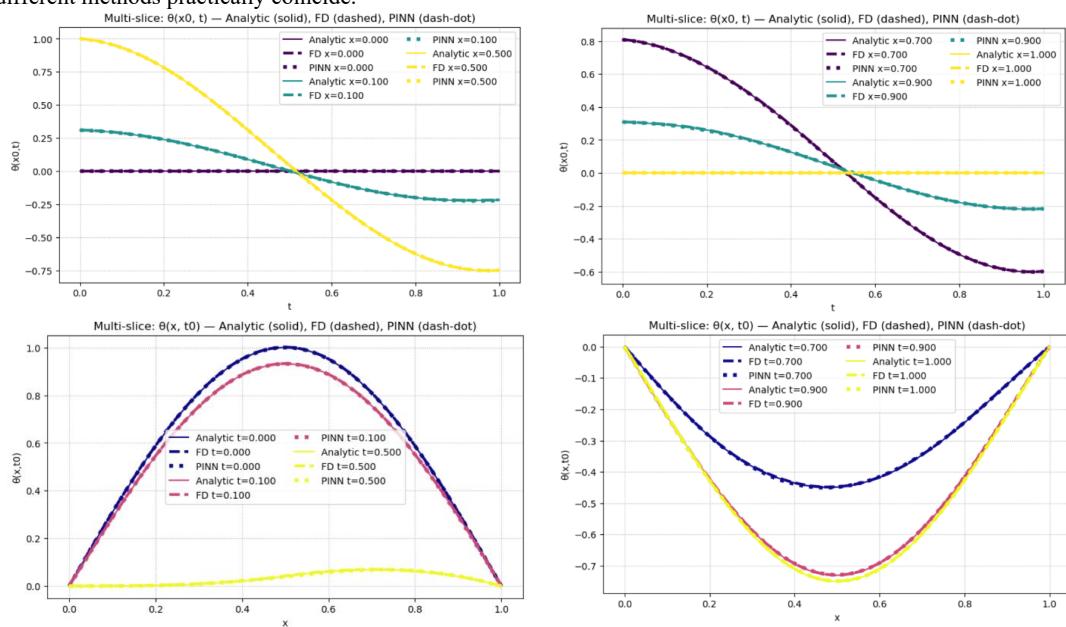


FIGURE 4. Temperature field $\theta(x_0, t)$ for fixed x_0 and $\theta(x, t_0)$ for fixed t_0 .

Additionally, three-dimensional surfaces $\theta(x, t)$ were constructed for both the PINN and analytical solutions (Fig. 5). The analysis of these visualizations confirms the correct reproduction by PINN of the wave nature of the Green–Naghdi type II model, including the finite propagation speed of thermal disturbances.

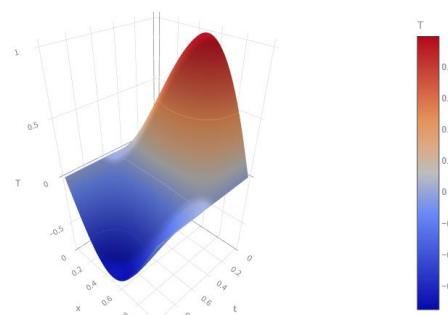


FIGURE 5. Three-dimensional surfaces of the temperature field $\theta(x, t)$, obtained using PINN and the analytical solution.

Thus, the performed calculations showed that the proposed approach provides high approximation accuracy and can be considered as an alternative tool to classical numerical schemes for solving hyperbolic heat conduction problems.

CONCLUSION

In this work, the one-dimensional heat transfer problem within the framework of the Green–Naghdi type II theory was considered using Physics-Informed Neural Networks (PINN). A neural network approximation of the solution was constructed based on a special representation that ensures exact satisfaction of the boundary and initial conditions. The mean squared residual of the governing equation, computed at collocation points using automatic differentiation, was employed as the loss function.

The conducted computational experiments showed that the proposed approach makes it possible to obtain a solution comparable in accuracy to the analytical Fourier series and the independent finite-difference method. The relative error in the L_2 – norm for PINN does not exceed 10^{-3} , which indicates the high accuracy of the method. Graphical analysis (cross-sections with respect to spatial and temporal variables, three-dimensional surfaces of the temperature field) confirmed the correct reproduction of the wave nature of the Green–Naghdi type II model.

The proposed two-phase training scheme with optimization Adam → L-BFGS and resampling of collocation points ensures stable convergence and effective reduction of the residual. Thus, PINN can be considered as a universal tool for solving hyperbolic heat conduction problems, combining the accuracy of analytical methods with the flexibility of numerical schemes.

Promising directions for further research include extending the proposed approach to multidimensional problems and more complex geometries, as well as the use of sinusoidal activations (SIREN), which improve the reproduction of high-frequency components of the solution. In addition, the method can be effectively applied to inverse problems of material parameter identification and heat source localization. Of particular interest is the analysis of the robustness of PINN to noisy data and the development of regularization schemes aimed at improving the reliability and accuracy of the approximation.

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