ABSTRACT
for the dissertation of Mustafin Maksat submitted for the degree of Doctor of Philosophy (PhD) in the educational program 8D06102 – Computer Engineering on the topic: "Adaptive structured grid generation by solving diffusion equation using physics-informed neural networks"

Relevance of the Research Topic. In recent years, there has been a significant increase in interest in adaptive mesh/grid generation methods in the field of numerical modeling and computational mathematics. This trend is closely related to the need for modeling multidimensional physical processes with high accuracy and efficient use of computational resources. The non-uniformity of the computational grid in complex geometries, boundary layers, and regions where localized phenomena occur directly affects the quality of the solution. Traditional uniform grids require an increase in grid resolution throughout the entire domain to achieve high accuracy, which, especially in multidimensional problems, leads to a sharp increase in the number of nodes, longer computation time, and inefficient use of memory resources. Such an approach results in redundant computations when high accuracy is needed only in limited regions. Adaptive grids, on the other hand, make it possible to efficiently allocate computational resources and optimize the computational load. In such cases, adaptive grids serve as a highly efficient tool that provides node density corresponding to the features of the solution.

The main goal of the grid generation process is to automatically determine the distribution of nodes adapted to the physical or geometrical complexity of the problem. Traditional approaches (iterative methods based on finite difference schemes), while accurate and reliable, have limitations regarding the implementation of boundary conditions, the description of multidimensional geometries, and the control of adaptation dynamics. Moreover, for differential equations that lack analytical solutions, the task of efficient grid generation remains an unsolved scientific and practical problem.

In this work, physics-informed neural networks (PINNs) are proposed as a new scientific paradigm. The distinctive feature of the PINN method is that it represents the coordinates of the computational domain through neural networks and includes the differential characteristics of the problem into the loss function. This allows the model to simultaneously satisfy the differential equations and boundary conditions, providing an autonomous adaptation process during training.

However, the classical PINN method also has shortcomings: inaccurate enforcement of boundary conditions, limited localized adaptation, and incomplete utilization of neural network architecture flexibility. Therefore, this study proposes a modified PINN architecture (MPINN), in which boundary conditions are directly incorporated at the architecture level, and the adaptation

process is localized using special mask functions. This approach is aimed at overcoming the weaknesses of the classical PINN and improving adaptation quality.

The relevance of this dissertation lies in the development of a new, efficient method for generating adaptive meshes using PINN and MPINN for solving diffusion-type equations. This method is particularly important for problems without analytical solutions and with complex geometries, where it is necessary to increase computational accuracy and reduce computational costs. Furthermore, the proposed method is suitable for use in computational domains of various dimensions, making it a universal computational tool for scientific and engineering applications.

Objective of the dissertation – to develop methods for generating adaptive structured grids using physics-informed neural networks (PINNs) in one- and two-dimensional computational domains with precise enforcement of boundary conditions.

Research Objectives

1. Conduct a review of the application of PINNs in grid generation problems.
2. Implement the numerical solution of an adaptive grid generation model based on one- and two-dimensional diffusion equations.
3. Apply the PINN method for adaptive grid generation.
4. Implement classical and modified PINN methods to ensure the enforcement of boundary conditions.
5. Compare and analyze the obtained results.

Object of the Research – problems based on one- and two-dimensional differential equations that require adaptive grid generation. A characteristic feature of these problems is the sharp variation or localization of the solution in certain regions, as well as the influence of the accuracy of boundary condition enforcement on the solution quality.

Subject of the Research

The methodology of applying neural network models (PINN and MPINN) for constructing adaptive coordinate systems in solving diffusion-type equations, including their architectural structure, training algorithms, loss functions, and numerical assessment of adaptation quality.

Scientific Novelty

- For the first time, adaptive grid generation based on the diffusion equation has been implemented using the PINN method, where the grid adaptation process is governed by differential equations.

- The exact matching of grid node boundaries with the computational domain is achieved using the modified MPINN method, which ensures strict enforcement of boundary conditions during grid adaptation.

Main Provisions Submitted for Defense

A PINN-based method is proposed for generating a one-dimensional adaptive computational grid based on the diffusion equation, the solution of

which shows high agreement with the analytical solution. During the study, the PINN results were compared with a test problem possessing an analytical solution, and the maximum deviation of the nodes was $5 \cdot 10^{-5}$, indicating the high accuracy of the generated adaptive grid.

By modifying the classical PINN method (MPINN), a new approach is proposed to ensure the immobility of the boundary nodes of the computational grid. In the new architecture, boundary conditions are directly embedded in the neural network using a mask function, preventing the displacement of boundary points during computation and improving adaptation stability.

Theoretical and Practical Significance of the Research

The theoretical significance of the work lies in combining diffusion equations with the PINN method for constructing adaptive computational grids and in proposing the MPINN model that enforces boundary conditions at the architectural level.

The practical significance lies in the applicability of the MPINN method for adaptive grid generation. The method allows efficient use of computational resources, improves accuracy and stability in complex problems, and can be applied to practical problems of numerical modeling.

Reliability of Scientific Results

The reliability of the obtained scientific results is confirmed by the theoretical justification of the proposed methods, the comparison of numerical results with analytical solutions, and the comparative analysis of the models. The effectiveness of the MPINN architecture was evaluated using RMSE, maximum deviation, and boundary condition compliance metrics. The stability of the results was verified through computational experiments under various initial parameters, neural network configurations, and convergence conditions.

Structure and Summary of the Work

The dissertation consists of an introduction, four main chapters, a conclusion, and a list of references.
The total volume of the work is 73 pages, including 41 figures, 8 tables, and 54 formulas.

The introduction substantiates the relevance of the topic, outlines the goals, objectives, scientific novelty, and structure of the work.

The first chapter provides an extensive review of domestic and foreign research on adaptive computational grid generation and its applications. Theoretical foundations, typology, and grid generation methods, as well as their use in solving differential equations, are discussed. The chapter also describes physics-informed neural networks (PINN), control functions for grid density management, and the role of the ADF mask function in adaptive grid generation. Based on the review, the research relevance and advantages of the PINN method are justified, and the theoretical and methodological foundation of the dissertation is established.

The second chapter presents the theoretical foundations of adaptive grid generation, the diffusion equation and its use in one-dimensional problems, characteristics of boundary conditions, and control functions. The formulation of two-dimensional adaptation equations and grid quality evaluation criteria is also described.

The third chapter presents the research methodology: comparison of finite-difference and PINN-based methods, descriptions of the PINN and MPINN architectures, neural network training algorithms, methods for soft and hard boundary condition enforcement, and the conceptual model of adaptation based on mask functions.

The fourth chapter analyzes the obtained results. Analytical and numerical solutions for one- and two-dimensional problems are compared, adaptation quality is assessed using RMSE and maximum deviation, and the advantages and limitations of the PINN and MPINN methods are identified.

The conclusion summarizes the main results of the study, describes their scientific and practical significance, and suggests directions for further research.

Publications Based on the Research Results

A total of 7 publications have been issued on the dissertation topic, including: 4 articles in journals recommended by the Committee for Quality Assurance in Science and Higher Education of the Ministry of Science and Higher Education of the Republic of Kazakhstan (CQASE MES RK); 2 papers in peer-reviewed journals indexed in international citation databases *Web of Science* and/or *SCOPUS*; 1 paper in international conference proceedings.

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