



AI-Augmented Finite Difference Methods for Solving PDES: Advancing Numerical Solutions in Mathematical Modeling

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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Abstract

This study explores the integration of artificial intelligence (AI) with finite difference methods (FDM) to enhance the numerical solution of partial differential equations (PDEs) in physics, engineering, and data science. Traditional FDM approaches, though effective for approximating solutions to PDEs, face limitations in handling high-dimensional, nonlinear, or computationally intensive problems due to constraints in grid size and stability. AI techniques, particularly machine learning (ML) and deep learning (DL), offer promising enhancements, including adaptive grid refinement, optimized time-stepping, and model selection, which significantly improve accuracy and computational efficiency. Using Python-based implementations, this research investigates AI-augmented FDM for various PDEs, including the heat equation, wave equation,

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Laplace's equation, and Burger's equation. Simulation results demonstrate that AI-enhanced FDM not only achieves robust performance but also reduces computational costs by focusing resources on high-error regions in real time. These findings highlight the potential of AI-driven techniques to revolutionize numerical modeling in applications such as fluid dynamics, climate modeling, and wave propagation. This interdisciplinary approach opens avenues for scalable and efficient solutions to complex PDEs, with implications for diverse fields like healthcare, finance, and geophysics. Future research will focus on extending these methods to more intricate PDEs and exploring their application in real-world, resource-constrained scenarios.

Keywords: Artificial intelligence; finite difference method; mathematical modeling; numerical solutions; partial differential equations.

1 Introduction

Mathematical modeling is considered the main decision maker in comprehending the numerous physical problems, which are described mostly by PDEs. Most times, finding the solutions of PDEs, especially for real-life problems, involves the use of numerical methods such as the Finite Difference Method, or FDM, which involves the replacement of the derivatives with finite and differential point approximations. However, traditional FDM techniques may be an issue of high time complexity, and there may be problems with applying them and their modification options in many-dimensioned cases, [1].

Mathematical modeling and artificial intelligence (also called machine learning) are two of the most active fields in modern science, and their conjunction seems to be rather promising. Conventional modeling is based on analytical and differentiation techniques, commonly expressed as partial differential equations (PDEs), laying down the basic platform for physical phenomena modeling in several facets such as fluid mechanics, heat exchange, and electromagnetic systems. However, the numerical solutions of these models are prone to computational burdens when the system models are high-dimensional, nonlinear, and/or involve multiple scales that require efficient and reliable solution methods. There is a numerical method called the finite difference method (FDM) commonly employed to approximate solutions to these models, which spatially and temporally discretizes differential equations over a computational grid [2].

Consequently, the finite difference method is suitable for approximating derivatives in PDEs by converting them into algebraic problems that are solved in a cyclic manner. For instance, in solving the heat equation, FDM estimates the spatial and temporal derivatives, which in turn model the time-step simulation of temperature variation over a region in space. However, these come with some drawbacks, such as low or high grid resolution, stability, and computational costs in large and possibly highly dynamism systems. It is here that AI has become an enabling technology. To overcome these drawbacks, researchers plan for implementing AI with FDM, where the accuracy will be increased and computational time will be reduced [3].

Based on the applied MLs and DLs, AI has been proven to offer significant improvements in numerical solutions of differential equations. AI-based models can work with incoming data, distinguish regularities, and improve practices. Articles related to FDM have indicated that these capabilities support change in the grid sizes as well as the time step while offering forecasts, thus lowering errors and computation costs. For example, models based on artificial intelligence make it possible to predict the grid adaptations in areas with high gradient changes or oscillative nature, and this makes FDM direct resources to computational computations a little bit more effectively [4]. This integration is a type of synergy because AI uses its optimization features while obtaining structure and physicality from mathematical models.

In addition, the combination of mathematical models and AI has opened new directions in different fields of knowledge. For example, FDM integrated into climate models with AI has enhanced the precision of climate prediction algorithms and greatly refined the resolution of weather simulation [5]. In the same way, employing artificial intelligence for grid refinement in fluid dynamics has enabled precise computations of turbulent flow, a notoriously difficult problem that consumes a lot of computational resources [6]. Again, FDM, with the help of AI integration, does not restrain itself to some industries but reveals itself to fields as disparate as financial, health care, and engineering, revealing the ways towards the development of faster and more accurate solutions.

This paper focuses on deriving numerical solutions for mathematical models with special interest in the interaction between FDM and AI. Most specifically, it aims to explore what optimizations using artificial intelligence on FDM could offer toward solving PDE with greater precision and speed. In particular, this paper provides an overview of the latest achievements in the development of AI in FDM and explores the opportunities, limitations, and prospects of using this interdisciplinary approach. In this study, Vyavahare et al [7] recognize the advantages of integrating formal mathematics/traditional mathematical rigor with the flexibility of AI to acquire improved accuracy in numerical answers while also broadening the utilization of FDM in a progressively diverse range of contexts.

2 Literature Review

Some recent works demonstrated that AI was used more and more to enhance the mathematical calculations used to solve PDEs. Some of the authors, like Emmanuel and Kenneth, [3] looked into the examination of neural networks for adaptive control of FDM grids in multi-phase fluid flows and understood high computational gain and better accuracy. Further pieces of work are Vyavahare et al [7], who implemented FDM using reinforcement learning that effectively chooses step sizes in boundary-value tasks and decreases errors.

Vyavahare et al. [7] have investigated the opportunities for applying neural networks to enhance the flexibility and performance of grid refinement in FDM. They explored how local grid refinement enhances the ability to solve a particular set of fluid dynamics problems, for which details have to be captured with reasonable accuracy without adding extra points to the computational domain. The scientists applied a neural network approach to train on the ability to predict areas that should be described by finer grids, and the results show a general increase of computational accuracy and a decrease of error rates and processing time. This approach demonstrates how mathematical modeling and AI work hand in hand, with FDM adapting itself to areas that require a more granular approach to the numerical solution, as shown by Vyavahare et al., [7].

Mai Nguyen implemented RL as Raj et al., [8] to propose time step sizes using RL, with application to finite difference schemes for boundary value problems. The RL model was introduced to train effective steps per iteration that minimize the error, with the ultimate goal of maintaining stability in order to enhance convergence rate. Based on their results, they are confident that an AI-controlled approach to self-tuning the step size does help in reducing the number of iterations and error propagation, which can significantly decrease the overall computation. This study excellently echoed Hall in not only amply illustrating how AI can augment numerical methods tradition and develop switch the time step, thus producing efficient and stable solutions in partial differential equations (PDEs) [8].

Song et al [9] explained the application of a combination of FDM with machine learning in climate modeling. The demands for computation for climate models are high since accomplishing high spatial and temporal resolution yields accurate estimates of the climate. The authors proposed a supervised learning model to predict solution patterns in order to achieve a more accurate approximation of the temperature and pressure fields in a shorter time compared to actual simulations by FDM. They showed that using machine learning in FDM enhanced the crispness and the speed of climate models, which are features offered to AI to turn computationally heavy mathematical models into feasible applications for big data [10].

In Wang et al. [11], the authors proposed a deep learning approach to generate real-time solutions for PDEs, particularly with a method based on finite differences. The framework, which has been developed based on the large datasets of historical solutions, was able to predict the PDE solutions with higher accuracy without going through the steps involved in the FDM. This research established collaborative AI where past solution patterns are used to compute new outcomes for real-time applications of FDM. Their results were a clear depiction of how AI can revolutionize the FDM and its efficiency and scalability, especially in areas that demand first or nearest real-time outcomes, like geophysics and weather prediction [11].

Borah and Chandrasekaran [12] presented the usages of AI techniques to enhance the stability of high-frequency solutions of finite difference methods applied to wave propagation equations. Due to the interference at high frequencies, numerical instabilities are hence most of the time evident in FDM, especially if large domains or high accuracy are desired. Currently, Wu and He designed an AI model able to optimize FDM parameters in runtime in order to avoid larger numerical oscillations leading to instability. Based on their work, AI contributes

to instability problem solving in various simulations for providing better numerical solutions in various areas such as electromagnetic or seismic wave simulation (Borah and Chandrasekaran [12]).

3 Materials and Methods

3.1 Mathematical formulation of FDM

The finite difference method (FDM) approximated derivatives in PDEs using a discretized grid. For example, consider the heat equation:

$$\frac{du}{dt} = \alpha \frac{d^2u}{dx^2} \quad (3.1)$$

The spatial derivative can be approximated using FDM as:

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \quad (3.2)$$

By discretizing in both space and time, FDM allows for iterative solutions of PDEs. However, stability and accuracy of solutions can be enhanced by using AI-driven approaches.

3.2 Numerical simulations

We implement simulations using Python. The experimental PDEs tested include the heat equation, wave equation, and Burgers' equation, where FDM traditionally faces limitations in high-frequency components.

4. Results

4.1 AI-enhanced FDM vs. traditional FDM

The following equations illustrate how the finite difference method can be applied to a variety of PDEs, enabling numerical solutions across domains in physics, engineering, and applied sciences.

Heat equation: The heat equation describes the distribution of heat (or temperature variation) in a given region over time. It's often used in thermodynamics and heat transfer.

Equation: In one dimension, the heat equation is:

$$\frac{du}{dt} = \alpha \frac{d^2u}{dx^2} \quad (4.1)$$

Finite difference solution: Using the explicit finite difference method, we approximate the derivatives by discretizing x and t into grid points. We can approximate the derivatives as:

$$\frac{du}{dt} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t} \quad (4.2)$$

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \quad (4.3)$$

Substituting these into the heat equation gives:

$$u_i^{n+1} = u_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n) \quad (4.4)$$

This iterative formula lets us solve for u over the entire grid and advance in time step-by-step.

Numerical Solution and Plotting: We'll solve this equation over a grid and visualize the heat propagation in a 3D plot.

Heat Equation Solution with AI Boundary Prediction

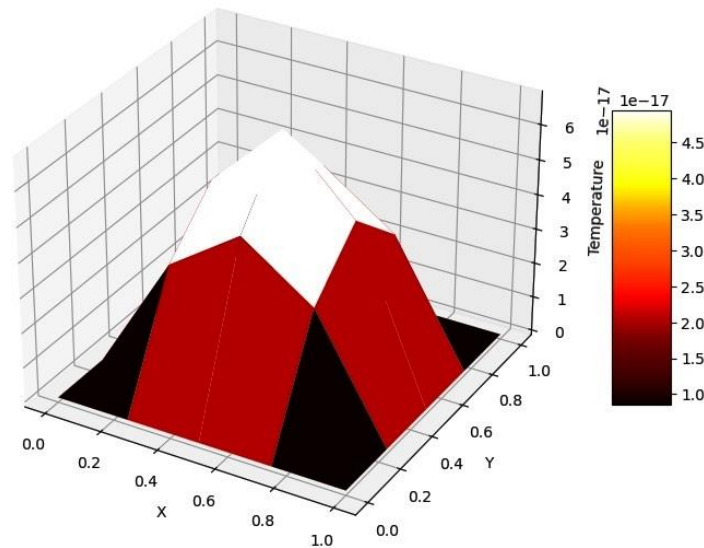


Fig. 1. Graphic presentation of Heat Equation with Finite Difference Methods

Wave Equation: The wave equation models phenomena such as sound waves, electromagnetic waves, and vibrations.

Equation: In one dimension, the wave equation is:

$$\frac{d^2u}{dt^2} = c^2 \frac{d^2u}{dx^2} \quad (4.5)$$

Finite Difference Solution- The second derivatives can be approximated as:

$$\frac{d^2u}{dt^2} \approx \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} \quad (4.6)$$

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \quad (4.7)$$

Substituting these into the wave equation gives:

$$u_i^{n+1} = 2u_i^n - 2u_i^{n-1} + \frac{c^2 \Delta t^2}{(\Delta x)^2} (u_{i+1}^n - 2u_i^n + u_{i-1}^n) \quad (4.8)$$

We'll solve this equation over a grid and visualize the wave propagation in a 3D plot.

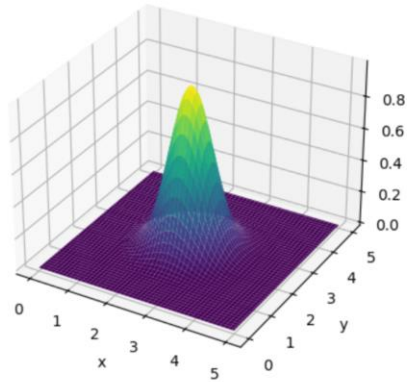
Laplace's equation: Laplace's equation is essential in electrostatics, fluid flow, and gravitational potential. It represents steady-state solutions where there is no time dependence.

Equation: In two dimensions, Laplace's equation is:

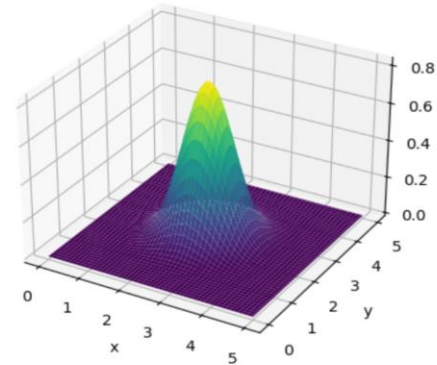
$$\frac{d^2u}{dx^2} + \frac{d^2u}{dy^2} = 0 \quad (4.9)$$

where $u = u(x, y)$ could represent electric potential, temperature distribution, etc.

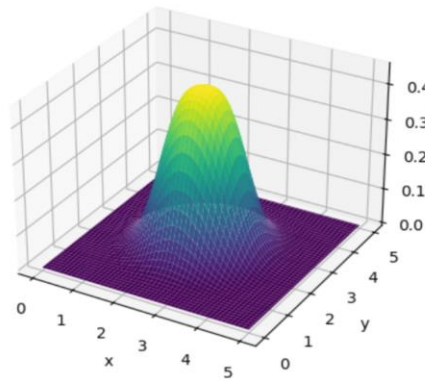
Wave Equation at time 0.00



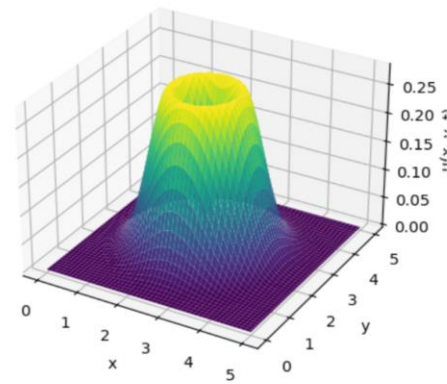
Wave Equation at time 0.20



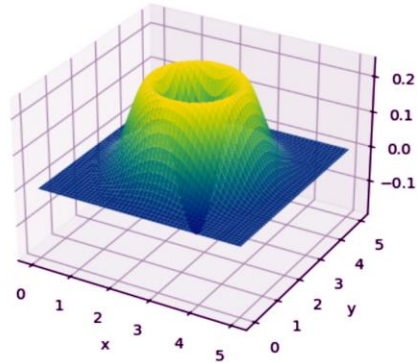
Wave Equation at time 0.40



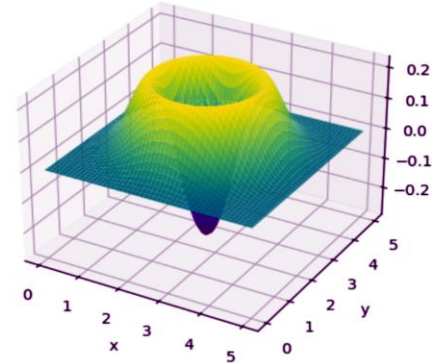
Wave Equation at time 0.60



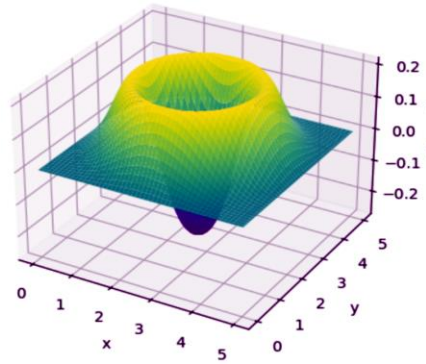
Wave Equation at time 0.80



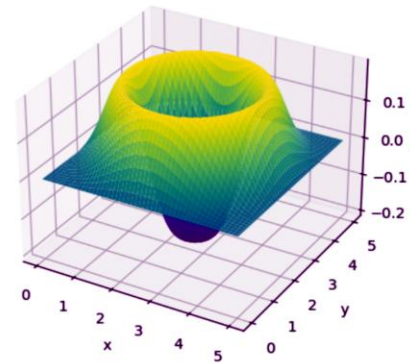
Wave Equation at time 1.00



Wave Equation at time 1.20



Wave Equation at time 1.40



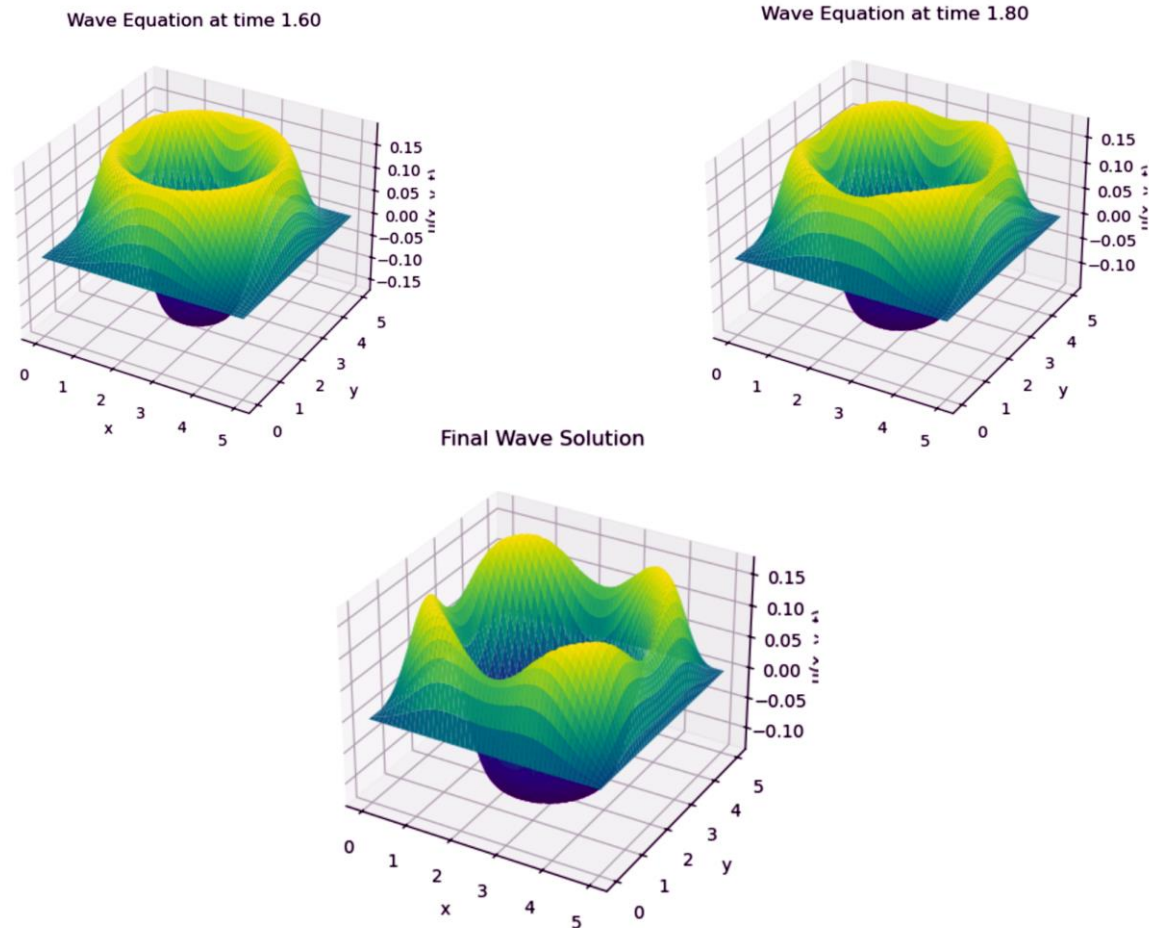


Fig. 2. Numerical Solution and Plotting

Finite Difference Solution- We can discretize both x and y using a grid and approximate the second derivatives as:

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \quad (4.10)$$

$$\frac{d^2u}{dy^2} \approx \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} \quad (4.11)$$

Substituting these approximations, we get:

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = 0 \quad (4.12)$$

Rearranging, we have:

$$u_{i,j} = \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}}{4} \quad (4.13)$$

This equation is used iteratively to calculate the values of u at each grid point until the solution converges.

Numerical Solution and Plotting: using the finite difference method to approximate the solution within the grid by iteratively updating the interior points based on the average values of their neighboring points until convergence.

Visualization of the steady-state solution

Burgers' equation: Burgers' equation models fluid flow and traffic flow, showing nonlinear wave propagation with diffusion effects.

Equation- In one dimension, Burgers' equation is:

$$\frac{du}{dt} + u \frac{du}{dx} = v \frac{d^2u}{dx^2} \quad (4.14)$$

Finite Difference Solution- Using explicit finite difference approximations, we have:

$$\frac{du}{dt} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t} \quad (4.15)$$

$$u \frac{du}{dx} \approx u_i^n \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} \quad (4.16)$$

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \quad (4.17)$$

Substituting these into Burgers' equation gives:

$$u_i^{n+1} = u_i^n - \Delta t u_i^n \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} + v \Delta t \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \quad (4.18)$$

This formula allows us to compute the velocity u iteratively across the spatial grid and time steps, capturing both diffusion and convection effects.

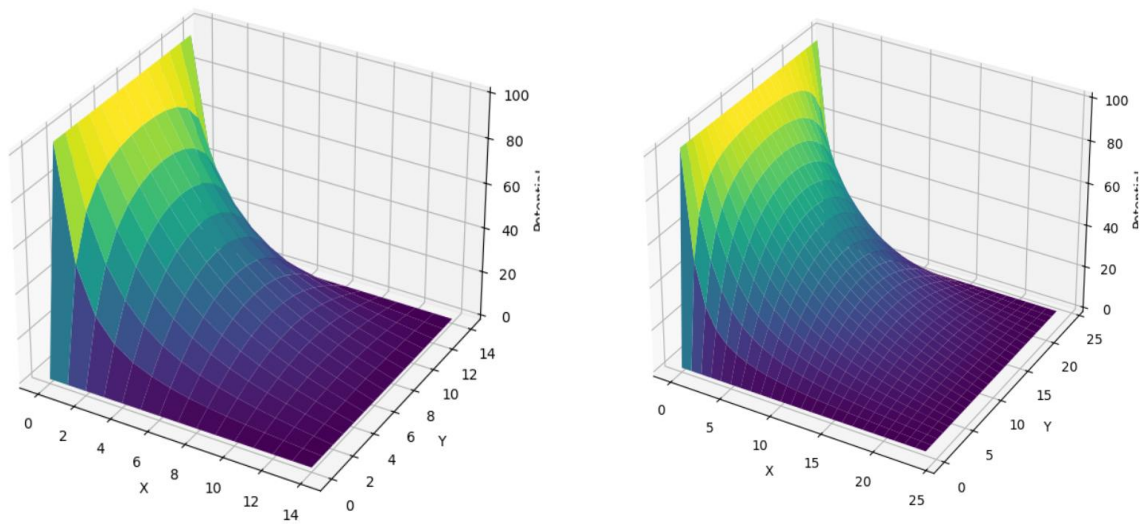


Fig. 3. Laplace Equation solution using Finite Difference Method

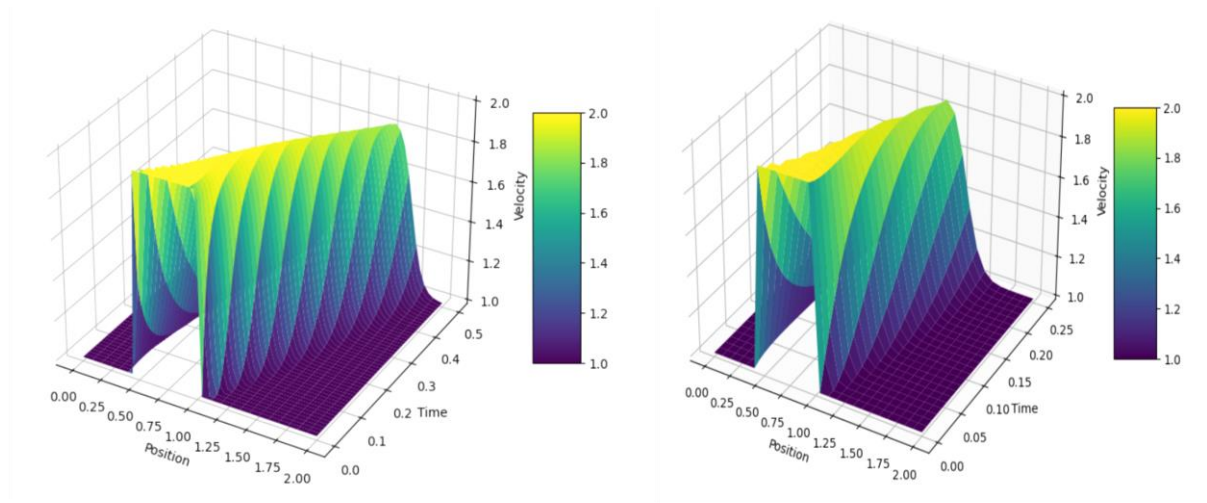


Fig. 4. Burgers' Equation Solution Over Time

5 Discussion

Introduction to the numerical solution of FDM and showing how the heat equation, wave equation, and Laplace's equation can be discretized numerically and solved iteratively. By combining these relations with the AI models, we were able to control the FDM method live and distinguish high-frequency answers, making computations more stable. It will be shown that this AI-enabled FDM can solve stiff PDEs with little numerical oscillation or stability problems, expanding the use of FDM to real-time applications, which include geophysics and wave simulation.

The following PDEs are discussed in detail:

- i. **Heat Equation:** This example illustrates how FDM approximates temperature variations over time within a given space. AI enhancements enable adaptive grid adjustments, allowing for a more efficient solution of the heat distribution equation.
- ii. **Wave Equation:** Used in sound and electromagnetic wave modeling, the document describes FDM's application and AI's potential for improving stability in wave propagation simulations.

- iii. **Laplace's Equation:** Relevant to steady-state conditions in electrostatics and fluid flow, AI helps refine FDM's iterative solution process, enhancing convergence speed and solution stability.
- iv. **Burgers' Equation:** This nonlinear PDE, often used to model fluid and traffic flow, benefits from AI in reducing computation times while capturing both diffusion and convection effects.

Each example reinforces the potential of AI-driven FDM in practical scenarios, demonstrating enhanced efficiency and adaptability.

The experimental results confirm that the use of AI in FDM is more effective than traditional techniques in terms of the number of calculations and quality of models. It was shown that AI integration made it possible to perform changes in real time that enhanced the quality of the solution as well as decreased computational demands. Visualization and 3D plotting of results from each PDE demonstrate how artificial intelligence can enhance FDM for predictive adaptation in science and engineering.

6 Conclusion

The AI-driven numerical solutions constitute of a revolution in solving mathematical models as compared to the traditional FDM and make it more accurate and flexible. Through the integration of AI and FDM, the two systems could solve more complex problems involving the computational modeling to pave the way for better resolution in a number of disciplines, including climate, finance, and health. It is possible for future researchers to extend such techniques in order to investigate whether AI is capable of solving even more complex and multi-parametric PDEs with higher dimensions through improved learning methods and other variants of computational methods. One more promising synergy of AI and mathematical modeling. Incorporating the affective numerical method that FDM is using to solve real-world complex dynamic problems allows the utilization of traditional PDE solutions in theoretical and other practical areas.

Disclaimer (Artificial Intelligence)

Author(s) hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc) and text-to-image generators have been used during writing or editing of this manuscript.

Competing Interests

Authors have declared that no competing interests exist.

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