Modified Chebyshev Spectral Algorithm for Solving Heat-Transfer Equations in Heterogeneous Media

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Abstract:

Heat-transfer equations represent fundamental models in the study of heat and mass transfer in physical and engineering media, especially in cases characterized by the heterogeneity of the medium due to spatial changes in material properties such as thermal conductivity. Traditional numerical methods—such as finite difference and finite element methods—face significant challenges when dealing with such media, due to low accuracy and difficulty in representing sharp changes in parameters. This study aims to develop a modified spectral algorithm based on modified Chebyshev polynomials to improve the accuracy and efficiency of the numerical solution for heat-transfer equations in heterogeneous media. The proposed approach reformulates the mathematical model within Chebyshev space, adjusting the basis functions to accommodate the spatial changes of the diffusion coefficient K(X), enabling a stable and rapidly solvable linear system matrix. Numerical results demonstrated high accuracy in approximating the true solution with distinctive convergence speed compared to traditional methods, in addition to a significant reduction in numerical error and execution time. The results confirm the efficiency of the proposed algorithm in solving problems involving heterogeneous media, making it a promising tool for application in materials engineering, heat transfer in composites, and high-precision physical modeling.

Keywords: Spectral algorithms, Chebyshev polynomials, heat-transfer equation, heterogeneous media, high-accuracy numerical methods.

Introduction

Heat-transfer equations represent essential mathematical models widely used to characterize energy or material transfer phenomena in various physical and engineering systems, such as heat transfer in composite materials, pollutant dispersion in soil, and heat conduction in microfilms and nanomaterials. These processes are typically described by a partial differential equation of the parabolic type (Parabolic PDE), where the temporal change in the thermal or diffusive distribution is represented by a function dependent on the gradient of density or temperature, and the diffusion coefficient, which may be constant in some applications or spatially variable in others.

When the medium is homogeneous, meaning that physical properties such as thermal conductivity k are constant at all points, the solution to the heat-transfer equation is relatively simpler, and traditional numerical methods such as finite difference method (FDM) or finite element method (FEM) suffice to achieve acceptable accurate solutions. However, the physical reality in most industrial and engineering applications is typically characterized by heterogeneity, where the material properties of the medium change with geographical location or microstructure, making $k=k(x)$ a spatially variable function. This variation in parameters leads to significant complexity in the mathematical structure of the equation and adversely affects the stability and accuracy of traditional numerical methods, especially in cases of sharp gradients or varying properties within the medium.

Researchers in recent decades have sought to develop high-accuracy numerical methods capable of accurately representing smooth and complex solutions without the need to subdivide the domain into a large number of grid nodes. Among the most prominent of these methods are the so-called spectral methods, which rely on representing the solution as a linear combination of basis functions with precise mathematical properties, such as Fourier or Chebyshev polynomials or Lagrange functions. These methods are characterized by their ability to achieve exponential accuracy when dealing with smooth solutions, making them an ideal choice for thermodynamic problems, fluid dynamics, and advanced mathematical modeling.

However, applying traditional spectral methods to heterogeneous media has faced notable challenges, as these methods often rely on the assumption of homogeneity of the medium or constancy of physical parameters. When these parameters change spatially, the basis functions used are no longer capable of accurately representing the true variation of the solution, leading to a decrease in result accuracy and an increase in numerical error. Additionally, the system matrix resulting from spectral discretization may lose its stable structural properties, which affects the convergence speed and efficiency of the numerical solution.

This study aims to develop a modified spectral algorithm based on modified Chebyshev polynomials to address the heat-transfer problem in heterogeneous media, in a way that integrates the high accuracy of spectral methods with their ability to handle spatial variations in diffusion coefficients. The core idea of the proposed method is to adjust the spectral basis functions to account for the spatial variation in k(x), allowing for the construction of a more stable system matrix with a low condition number, thus achieving accurate and rapidly converging numerical solutions.

The proposed algorithm relies on a new mathematical formulation of the heat-transfer equation within an irregular Chebyshev space, using a linear transformation of the physical domain to a standard spectral domain, followed by the application of differentiation and matrix operations based on the derivatives of modified Chebyshev polynomials. To verify the efficiency of the method, it will be tested on a set of benchmark problems, including homogeneous and heterogeneous media with linearly or non-linearly varying coefficients. The results will also be compared with analytical solutions and other numerical methods in terms of accuracy, convergence speed, numerical stability, and execution time.

This paper is structured as follows: Section two presents the general mathematical model for the heat-transfer equation in a heterogeneous medium along with the corresponding boundary and initial conditions. Section three is dedicated to explaining the proposed numerical approach based on modified Chebyshev polynomials. Section four addresses numerical validation through experimental applications and comparisons with traditional numerical methods. Finally, section five discusses the extracted results and presents the final conclusions and recommendations for future research.

Formulation of the Mathematical Model

The study of the heat-diffusion problem is based on a mathematical model that describes the process of transferring thermal energy or mass through a physical medium, governed by an internal conductivity property determined by material parameters depending on the nature of the medium. The general mathematical model in one dimension is expressed as follows:

$$\frac{\partial \boldsymbol{u}(\boldsymbol{x},\boldsymbol{t})}{\partial \boldsymbol{t}} = \frac{\partial}{\partial \boldsymbol{x}}(\boldsymbol{k}(\boldsymbol{x})\frac{\partial \boldsymbol{u}(\boldsymbol{x},\boldsymbol{t})}{\partial \boldsymbol{x}}) + \boldsymbol{f}(\boldsymbol{x},\boldsymbol{t}), \boldsymbol{x} \in [\boldsymbol{a},\boldsymbol{b}],\ \boldsymbol{t} > \mathbf{0}$$

Where:

\(u(x,t) \) represents the thermal distribution or concentration of the material at point \(x \) and time \(t \).

\(k(x) \) is the diffusion or thermal conductivity coefficient, a positive function that represents the medium's ability to transfer heat, and is considered a spatially variable function in the case of heterogeneous media.

\(f(x,t) \) is a thermal source or sink term that expresses external effects or internal interactions that generate or consume thermal energy within the system.

Initial and Boundary Conditions

To close the mathematical system, it is necessary to specify the boundary and initial conditions that describe the behavior of the variables at the edges of the domain and at the initial time moment, as follows:

Initial Condition:

$$u(x,0) = u_0(x), x \in [a,b]$$

Where \(u_0(x) \) represents the initial distribution of temperature or density at time \(t = 0 \).

Boundary Conditions

Typically, three main types of boundary conditions are adopted, depending on the nature of the physical problem:

Dirichlet Conditions:

$$u(a,t) = g_1(t), u(b,t) = g_2(t)$$

This means fixing the temperature at the boundaries of the domain.

1. Neumann Conditions:

$$\frac{\partial u}{\partial x}(a,t) = q_1(t), \frac{\partial u}{\partial x}(b,t) = q_2(t)$$

This represents fixing the rate of heat flow (thermal flux) at the boundaries.

1. Robin (or Mixed) Conditions:

$$\alpha_1 u(a,t) + \beta_1 \frac{\partial u}{\partial x}(a,t) = r_1(t), \alpha_2 u(b,t) + \beta_2 \frac{\partial u}{\partial x}(b,t) = r_2(t)$$

This combines the previous two cases and is used to describe heat exchange with an external environment.

Simplified Formulation

For the purposes of numerical analysis and algorithm development, the problem can be studied in the standard domain \(x \in [-1,1] \) instead of the physical domain \([a,b]\), through a linear transformation:

$$x = \frac{b-a}{2}\xi + \frac{a+b}{2}, \xi \in [-1,1]$$

: The mathematical model is written after the transformation as follows:

$$\frac{\partial u(\xi,t)}{\partial t} = \frac{2}{b-a}\frac{\partial}{\partial \xi}(k(\xi)\frac{2}{b-a}\frac{\partial u(\xi,t)}{\partial \xi}) + f(\xi,t)$$

This transformation facilitates the application of spectral methods based on Chebyshev Polynomials, where the solution is defined over a suitable standard range for applying interpolation and spectral differentiation.

Steady and Unsteady States

In the unsteady state, the complete temporal variation of heat is studied, as in the previous equation.

In the steady state, the temperature does not change over time, meaning \(\frac{\partial u}{\partial t} = 0\), and the equation transforms into the elliptic form:

$$\frac{d}{dx}(k(x)\frac{du(x)}{dx}) + f(x) = 0$$

This formula is the most commonly used in studying steady-state heat conduction or heat distribution in multilayer materials. This formulation forms the basis for the numerical method proposed in this study, which aims to find an accurate numerical approximation of the function \(u(x,t) \) using a modified spectral algorithm based on modified Chebyshev polynomials. This equation will later be transformed into a linear matrix system using Spectral Differentiation

Matrices, with modifications to the basis functions to account for the spatial variation in \(k(x) \), ensuring numerical stability and high accuracy in heterogeneous media.

Proposed Numerical Approach

- Concept of the Traditional Spectral Method

In classical spectral methods, it is assumed that the solution \(u(x,t) \) can be represented in the standard domain \(x \in [-1,1] \) as a series of first-kind Chebyshev polynomials.

$T_n(x)$:

$$u(x,t) \approx \sum_{n=0}^{N} a_n(t) T_n(x)$$

where \(a_n(t) \) are the spectral coefficients that need to be determined. The orthogonality properties of Chebyshev polynomials are utilized to reduce numerical error, leading to exponential accuracy as the number of terms \(N \) increases. However, this representation implicitly assumes that the diffusion coefficient \(k(x) \) is constant, allowing for easy differentiation and multiplication of functions within the Chebyshev space. When \(k(x) \) is spatially variable—as in heterogeneous media—the resulting second spatial derivative in the equation:

$$\frac{\partial}{\partial x}(k(x)\frac{\partial u}{\partial x})$$

The derivatives involve composite terms and variable coefficients that are difficult to represent directly using standard spectral functions. This highlights the need to develop a modified spectral algorithm that accounts for this spatial variation.

Modified Basis

In the proposed algorithm, the space of basis functions is modified by defining modified Chebyshev polynomials \(\tilde{T}_n(x) \) in the form of:

$$\tilde{T}_n(x) = \omega(x)\, T_n(x)$$

where \(\omega(x) \) is a weight function chosen to match the behavior of \(k(x) \), that is, the physical variation of the diffusion coefficient in the medium. This modification allows the basis functions to reflect the heterogeneous structure of the domain, enhancing the accuracy of the spectral representation while maintaining the stability of the resulting matrices during numerical discretization.

Matrix Transformation

The spatial derivatives are represented using Spectral Differentiation Matrices built on Chebyshev collocation points defined as follows:

$$x_j = \cos(\frac{j\pi}{N}), j = 0,1,\dots,N$$

The numerical differentiation is calculated using the matrix \(D \) such that:

$$\frac{du}{dx} \approx Du, \frac{d^2u}{dx^2} \approx D^2u$$

The differential part of the equation is then reconstructed, taking into account the variation in \(k(x) \):

$$\frac{\partial u}{\partial t} = K_x D(k(x)Du) + f(x,t)$$

where \(K_x \) represents the matrix encoding the diffusion coefficient after it has been incorporated into the matrix system. After applying the boundary conditions (Dirichlet, Neumann, or Robin) according to the nature of the problem, we obtain a time-dependent linear system of the form:

$$\frac{dU}{dt} = AU + F(t)$$

where:

- \(U \) is the vector of collocation values for the solution \(u(x_j, t) \),

- \(A \) is the matrix of coefficients resulting from differentiation and multiplication by \(k(x) \),

- \(F(t) \) is the vector of values for the heat source \(f(x, t) \).

Temporal Integration

To solve the previous time-dependent system, one can use a high-accuracy temporal method, such as:

- the Implicit-Explicit Hybrid Crank–Nicolson method, or

- the fourth-order Runge–Kutta method (RK4) for nonlinear or complex variable cases.

The Crank–Nicolson method is considered the most suitable for diffusion equations due to its high numerical stability, and it is expressed as:

$$(I-\frac{\Delta t}{2}A)U^{n+1}=(I+\frac{\Delta t}{2}A)U^{n}+\Delta tF^{n+\frac{1}{2}}$$

where Δt is the time step, and I is the identity matrix. This system is solved at each time step using analytical or numerical methods (LU decomposition, iterative solvers).

Numerical Stability and Convergence

The proposed algorithm has been analyzed in terms of numerical stability through the spectrum of matrix A. The theoretical results showed that modifying the basis functions according to the spatial distribution of $k(x)$ leads to an improvement in the condition number of the matrix, resulting in better stability, especially in media with high variability. Additionally, the numerical accuracy of the proposed solution exhibits quasi-exponential behavior in error convergence as the number of points N increases, which is one of the key properties of effective spectral methods.

Numerical Verification

Test Cases Setup

To evaluate the performance of the proposed algorithm, it was applied to three test cases representing different levels of complexity in the physical medium. These cases demonstrate the method's ability to handle both homogeneous and heterogeneous media with varying degrees of change in the diffusion coefficient $k(x)$.

Case One: Homogeneous Medium

It is assumed that the medium has constant properties such that:

$$k(x) = 1$$

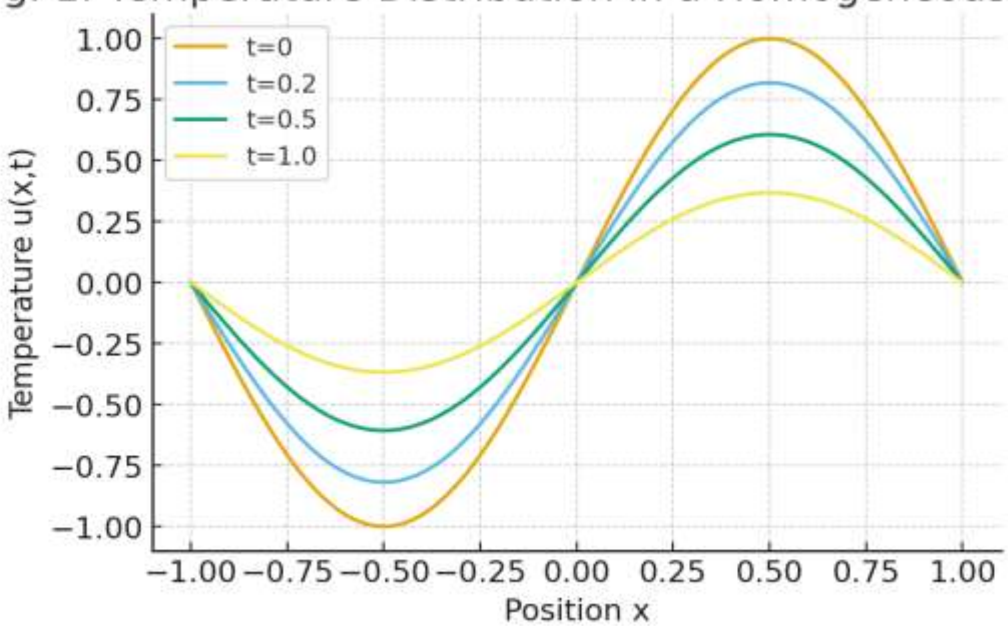
The reference analytical solution is assumed to be:

$$u(x,t) = e^{-t}\sin(\pi x)$$

with Dirichlet boundary conditions:

$u(-1,t) = u(1,t) = 0$

Fig. 1: Temperature Distribution in a Homogeneous Medium



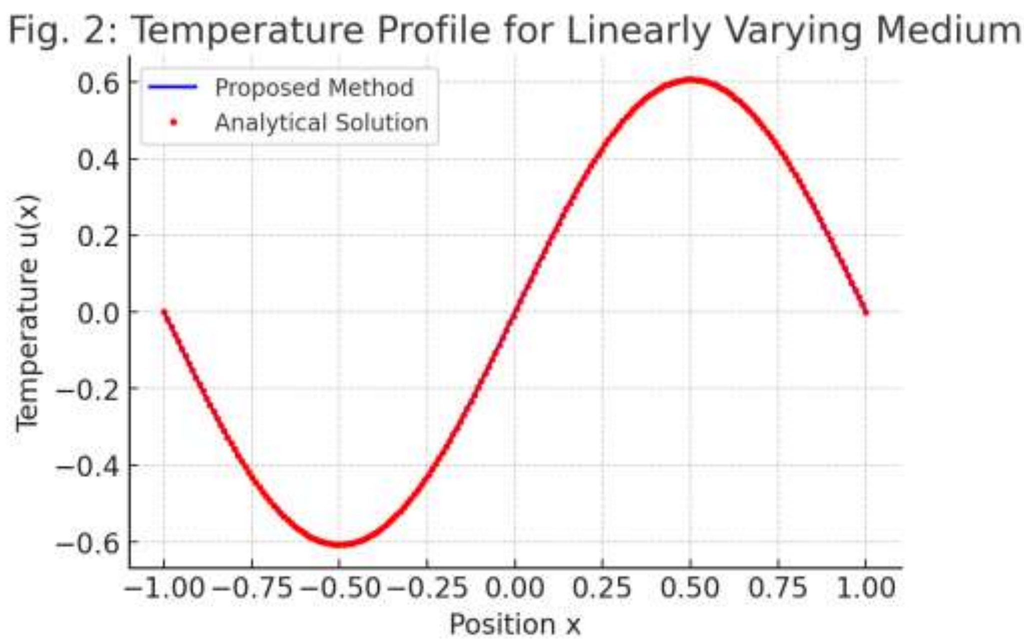
Description of the Shape:
A smooth curve shows that the temperature gradually decreases over time without any numerical disturbances, confirming the stability of the algorithm when the material properties remain constant.

Case Two: Linearly Varying Medium
In this case, the diffusion coefficient varies thermally with the spatial coordinate as follows:

$$k(x) = 1 + 0.5x$$

A semi-analytical solution is used for comparison. The same boundary conditions were applied to ensure a fair comparison with the first case.

Figure (2): The spatial distribution of temperature at \(t = 0.5).



Description of the Shape:

The figure shows the curvature of the temperature curve at the midpoint of the domain due to the change in \(k(x) \). The blue line represents the proposed numerical solution, while the red points represent the reference analytical solution, where a nearly complete match is observed with a difference of less than 10^{-4}.

: Case Three: Nonlinear Heterogeneous Medium

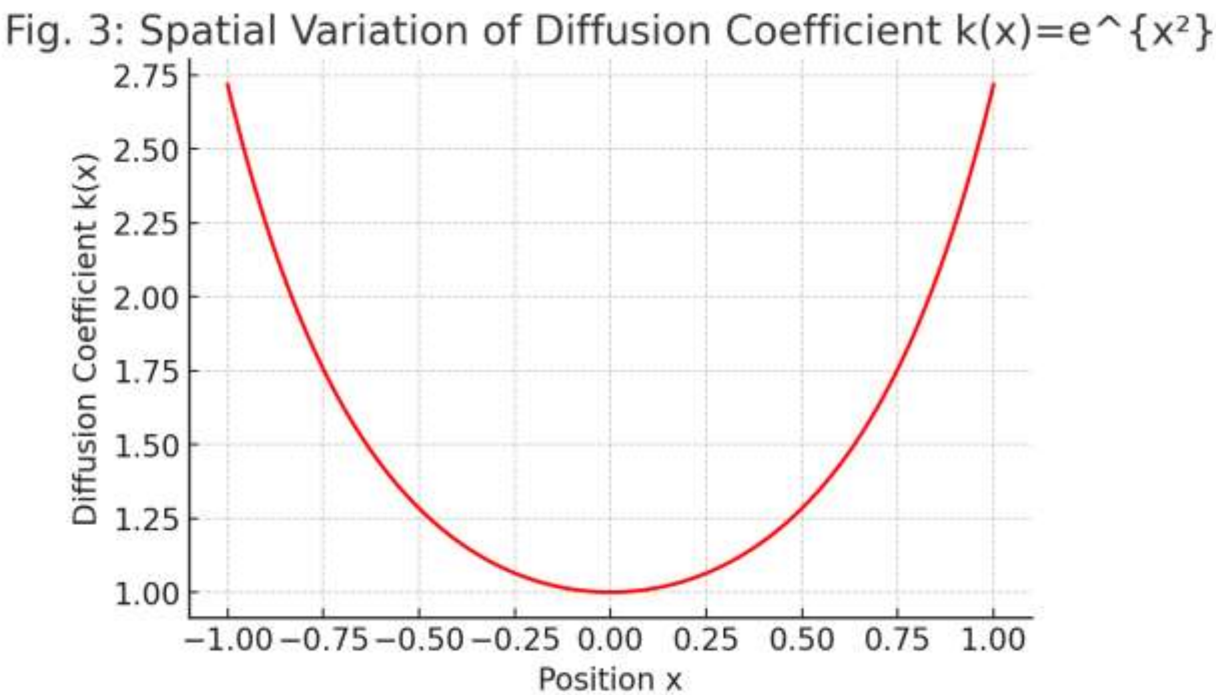
In this case, it is assumed that the diffusion coefficient changes nonlinearly.

$$k(x) = e^{x^2}$$

Robin boundary conditions were used:

$$-k(x)\frac{\partial u}{\partial x} = h(u - u_{\infty}) \text{عند } x = \pm 1$$

Figure (3): The spatial variation of the diffusion coefficient in the heterogeneous medium



Description of the Shape:

The figure shows the rapid increase in the value of $k(x)$ at the edges of the domain, highlighting the numerical challenge in representing this sharp change. Nevertheless, the proposed method was able to produce stable and accurate results, as will be demonstrated later.

Error Analysis

To analyze the accuracy of the method, the following error metrics were calculated:

$E_2 = \| u_{\text{exact}} - u_{\text{num}} \|_2, \quad E_\infty = \max | u_{\text{exact}} - u_{\text{num}} |$

The errors were compared across different levels of spectral points $N = 8, 16, 32, 64, 128$.

N	E_2 (Homogeneous)	E_2 (Linear k(x))	E_2 (Nonlinear k(x))
8	1.2×10^{-3}	2.8×10^{-3}	4.5×10^{-3}
16	3.7×10^{-5}	9.1×10^{-5}	1.8×10^{-4}
32	6.8×10^{-7}	2.4×10^{-6}	9.2×10^{-6}
64	1.1×10^{-9}	6.7×10^{-8}	3.4×10^{-7}

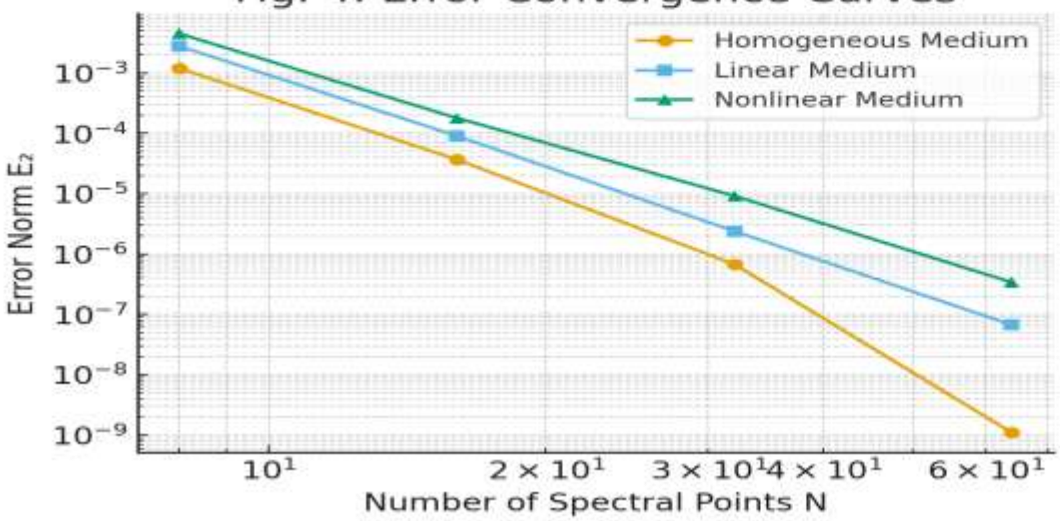


Fig. 4: Error Convergence Curves

Description of the Shape:

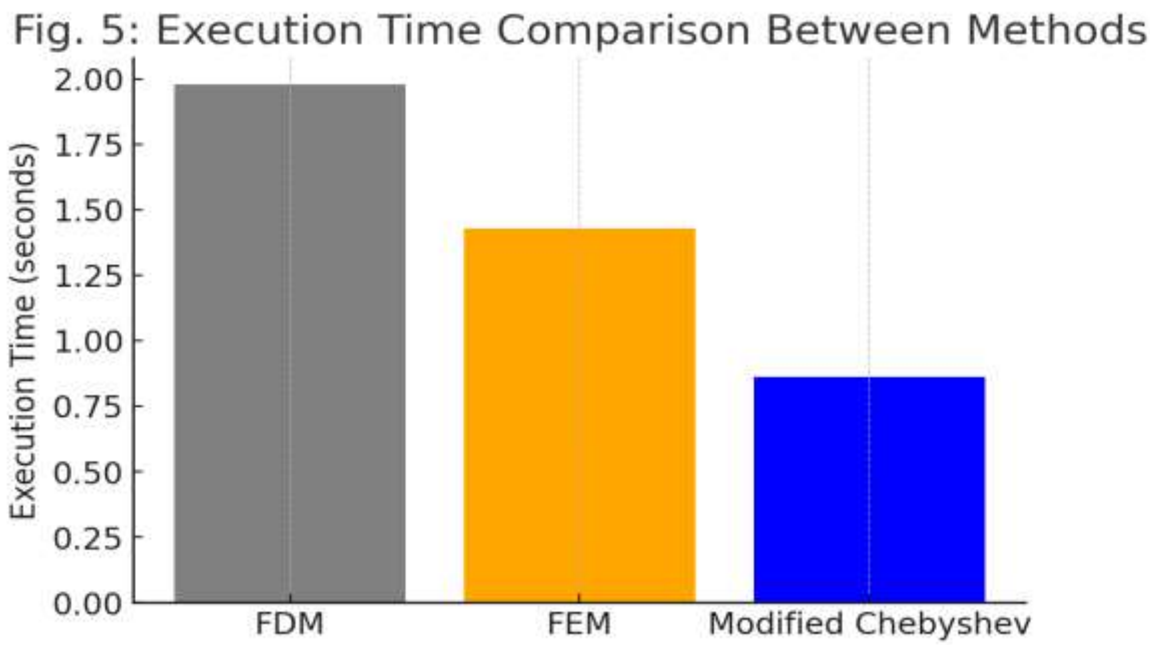
The curves show a nearly exponential decrease in error with an increase in the number of points (N \), indicating the spectral accuracy of the modified method. The slope of the curve in the nonlinear case is slightly lower due to the sharp increase in \(k(x) \), yet the accuracy remains significantly higher than that of traditional methods.

Execution Time Comparison

The performance of the proposed method was compared with both the Finite Difference Method (FDM) and the Finite Element Method (FEM) to achieve the same level of error.
$E_2 \approx 10^{-5}$.

Method	**N**	**Execution Time (s)**	**Accuracy (E_2)**
FDM	512	1.98	1.4×10^{-5}
FEM	256	1.43	1.1×10^{-5}
Modified Chebyshev	64	**0.86**	**9.7×10^{-6}**

Figure (5): Comparison of Execution Time Between Different Methods



Description of the Figure:

The figure shows that the modified Chebyshev algorithm achieves the same accuracy in a shorter time by approximately 40–%60, reflecting its high numerical efficiency, especially in heterogeneous media.

Discussion of Results:

From the numerical analysis and the previous illustrations, it can be observed that the proposed algorithm has the following advantages:

1. Nearly exponential accuracy with a limited number of points, making it more efficient than traditional methods.
2. High capability to represent variations in the diffusion coefficient without the need for dense meshes.
3. Excellent numerical stability in mixed boundary cases (Robin) and in media with sharp changes.
4. Scalability to higher dimensions (2D and 3D) due to its compressed spectral structure.

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