Stability of Finite Difference Schemes on the Diffusion Equation with Discontinuous Coefficients

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Abstract

The diffusion equation is one of the most fundamental partial differential equations, with widespread applications for analyzing heat and mass transport in a variety of media. When the diffusivity coefficient k is constant, von Neumann articulated a condition ensuring stability for explicit finite difference schemes approximating the diffusion equation. For materials with a variable continuous diffusivity coefficient $k(x)$, von Neumann's stability analysis methods can be extended by considering the maximum diffusivity value; this extension is known as the principle of frozen coefficients. Previously, it was not proven whether these conditions held for materials with a discontinuous diffusivity coefficient. In this work, we prove that the stability condition still holds for a conservative finite difference scheme with discontinuous coefficients in both one and two dimensions. We also provide numerical simulations that demonstrate the convergence and stability of both a conservative and non-conservative finite difference scheme on a variety of examples.

Summary

The mathematical model of diffusion has been commonly used to analyze heat and mass transport in various materials. In media with variable diffusivity, numerical approximation techniques, such as the finite difference method, can be used to calculate solutions of the diffusion equation. However, when a medium's diffusivity varies drastically, approximation errors may be greatly amplified. It has not been rigorously shown that these numerical approximation techniques, under drastically variable diffusivity conditions, would accurately converge to the correct values.

In this work, we analyze two different numerical approximations, a conservative and a non-conservative finite difference scheme, for both one-dimensional and two-dimensional media with variable diffusivity. The principle of frozen coefficients describes conditions guaranteeing stability for schemes on media with mildly varying diffusivity. We generalize this principle and prove stability, as well as convergence, for the conservative scheme on media with drastically varying diffusivity. We also provide numerical evidence, using computer simulations, for a similar stability condition in the non-conservative scheme. Thus, we demonstrate the utility of efficient mathematical methods to solve the diffusion equation in these general systems.

1 Introduction

Partial differential equations (PDEs) are essential to modelling many different physical phenomena, such as sound, heat, electrodynamics, and fluids. In *Théorie analytique de la chaleur*, Fourier proposed Equation (1.1) to model the conductive diffusion of heat:

$$\frac{\partial u}{\partial t} = \nabla \cdot (k(x)\nabla u), \tag{1.1}$$

where $u(x,t)$ is the temperature of a material at point x at time t, $k(x)$ is the diffusivity of said material at point x, and ∇ is the derivative in the dimension of space. This heat diffusion equation is a standard PDE taught to nearly every student of numerical analysis and differential equations due to its simplicity and vast application; it is related to the solutions of the Fokker-Planck equation for Brownian motion and the Black-Scholes equation in financial mathematics, and it is the standard introductory example to parabolic PDEs [1, 2, 3]. Equation (1.1) can be solved explicitly for $u(x,t)$ when k is constant, but this is not the case with most PDEs. In fact, when k is variable, no explicit solution exists to Equation (1.1). So, numerical approximation methods, such as the finite difference, finite volume, and finite element methods, are necessary to model functions described by PDEs.

The finite difference (FD) method is one of the most powerful tools in the numerical analysis of PDEs. Because of its intuitive approach and simple implementation of discretizing the function's domain to approximate its partial derivatives, the FD method has been popular throughout the societies of mathematics and engineering. However, explicit FD schemes, which are easily set up and quickly computed, are vulnerable to the oscillation and amplification of approximation errors. Thus, von Neumann introduced stability analysis, an equivalent of convergence analysis for well-posed PDEs [1]. Through the use of Fourier and eigenvalue techniques, von Neumann showed stability conditions for many FD and semi-discretization schemes. However, many well-known variable coefficient PDEs, including Equation (1.1), have not been rigorously analyzed for stability, due to the failure of common techniques. Von Neumann's Fourier techniques are applicable only when the approximated PDE is identical at every discretized point. Von Neumann's eigenvalue analysis is not applicable to the case of variable coefficients, due to the complexity of the linear equations produced by the FD scheme.

Currently, it is known that the method of frozen coefficients can be applied with heuristically successful results [1]. Many PDEs, including all first-order equations, have been proven to hold for stability conditions proposed by the principle of frozen coefficients [4]. However, this principle assumes a constant coefficient locally, which is reasonable due to its continuity. In the case of a discontinuous variable coefficient, this assumption is not true.

Thus, random-walk methods are used to approximate diffusion with a discontinuous coefficient [5, 6]. However, these methods have unavoidable errors. Using a stable explicit FD scheme instead, such errors can be bounded and avoided. Currently, stability conditions are still relatively unstudied for discontinuous coefficient PDEs [1]. We study conditions for stability of two explicit finite difference schemes for the diffusion equation, when the diffusivity coefficient is discontinuous.

In Section 2 we establish the background for this paper with notation (Section 2.1), preliminary knowledge (Section 2.2), and the finite difference schemes of interest (Section 2.3). In Section 3 we present various numerical results that support the bound obtained from the principle of frozen coefficients for a conservative and non-conservative explicit scheme with discontinuous coefficients. Moreover, in Section 4 we prove that the 1-dimensional (1-D) bound

$$\frac{\Delta t}{\Delta x^2} < \frac{1}{2\max(k)}$$

and the 2-dimensional (2-D) bound

$$\frac{\Delta t}{\Delta x^2} + \frac{\Delta t}{\Delta y^2} < \frac{1}{2\max(k)},$$

where Δx, Δy, and Δt are the size of the FD intervals and k is the diffusivity coefficient, are sufficient conditions for stability in the conservative scheme. Finally, in Section 5 we discuss the implications and future directions of our work.

2 Background

2.1 Notation

In our 1-D FD scheme, we discretize the domain Ω, as seen in Figure 1, into the $n_x + 2$ points $\{x_i \mid i \in [0, n_x + 1]\}$, where x_0 and x_{n_x+1} are the boundary points, $\partial\Omega$. These points are evenly spaced across the domain, and we denote the finite difference $x_{i+1} - x_i = \Delta x$. Similarly, in 2-D, we discretize the domain to $(n_x+2)\cdot(n_y+2)$ points $\{(x_i, y_j) \mid i \in [0, n_x + 1], j \in [0, n_y + 1]\}$, where boundary points $\partial\Omega$ are of the form $(x_0, y_j), (x_{n_x+1}, y_j), (x_i, y_0), (x_i, y_{n_y+1})$. The FD is similarly denoted $\Delta x = x_{i+1} - x_i$ and $\Delta y = y_{j+1} - y_j$, such that the points are evenly spaced parallel to the x-axis and y-axis, but these two spacings need not be the same.

We also evenly discretize the dimension of time into the points $\{t_l\}$, such that t_0 is the initial point in time and define n_t such that $t_{n_t} - t_0$ is 1 unit of time. We also denote the time step $t_{\ell+1} - t_\ell$ by Δt. The Courant number in 1-D, which equals $\frac{\Delta t}{\Delta x^2}$ [1], is denoted by μ. In 2-D, $\mu_x = \frac{\Delta t}{\Delta x^2}$, $\mu_y = \frac{\Delta t}{\Delta y^2}$, and $\mu = \mu_x + \mu_y$.

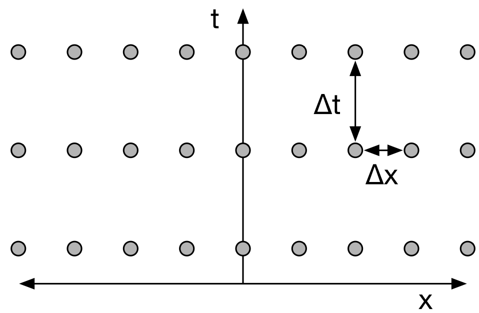


Figure 1: FD discretization of the 1-D domain.

For ease of notation, in our 1-D discretization, we let u_i^ℓ denote the approximated value of $u(x_i, t_\ell)$. Vector $\mathbf{u}^\ell$ represents $(u_1^\ell, u_2^\ell, \dots, u_{n_x}^\ell)^T$. We also denote $k(x_i)$, the diffusivity at x_i, by k_i, and by extension use $k_{i+\frac{1}{2}}$ to denote $k\left(\frac{x_i+x_{i+1}}{2}\right)$. In 2-D, $u_{i,j}^\ell$ denotes the approximated value of $u(x_i, y_j, t_\ell)$. Vector $\mathbf{u}^\ell$ represents $(u_{1,1}^\ell, u_{1,2}^\ell, \dots, u_{n_x,1}^\ell, u_{n_x,2}^\ell, \dots, u_{n_x,n_y}^\ell)^T$. We also denote $k\left(x_i, y_j\right)$, the diffusivity at point (x_i, y_j), by $k_{i,j}$. Similarly, we let $k_{i+\frac{1}{2},j} = k\left(\frac{x_i+x_{i+1}}{2}, y_j\right)$ and $k_{i,j+\frac{1}{2}} = k\left(x_i, \frac{y_j+y_{j+1}}{2}\right)$.

We use $\rho(A)$ to denote the spectral radius of matrix A, the maximum absolute value of its eigenvalues, or $\max|\lambda(A)|$.

2.2 Preliminaries

The FD method approximates partial derivatives in terms of the discretized function values. For example, the partial derivative $\frac{\partial u}{\partial x}$ at $u(x_i, t_\ell)$ is approximated as

$$\frac{\partial u(x_i, t_\ell)}{\partial x} = \frac{u_{i+1}^\ell - u_{i-1}^\ell}{2\Delta x}$$

by a central FD. Using these partial derivative approximations, we can generate a system of simultaneous linear equations which can be solved for the discretized function values. For example, using a central FD in space and forward FD in time, also known as the Forward-Time-Central-Space or FTCS scheme, on Equation (1.1) in 1-D, with constant diffusivity k, produces

$$u_i^{\ell+1} = u_i^\ell + \frac{\Delta t}{\Delta x^2}\left(u_{i+1}^\ell + u_{i-1}^\ell - 2u_i^\ell\right), \quad \forall \ell, i \in \Omega.$$

These linear equations can be compiled into the equation

$$\mathbf{u}^{\ell+1} = A\mathbf{u}^\ell, \quad \forall \ell \in \Omega,$$

forming the matrix A.

An important characteristic of a FD scheme, the way in which the partial derivatives are approximated, is convergence, as it guarantees accuracy for a sufficient discretization.

Definition 1. A FD scheme is *convergent* if, for any $t^* > 0$, $\forall x \in \Omega, t \in [0, t^*]$,

$$\lim_{\Delta x \to 0} \lim_{i \to \frac{x}{\Delta x}} \lim_{\ell \to \frac{t}{\Delta t}} u_i^\ell = u(x,t).$$

Essentially, as the discretization of the domain becomes finer and approaches continuity, the errors approach 0. Unlike for ordinary differential equations, schemes on PDEs can be conditionally convergent; certain criteria, such as the Courant-Friedrichs-Lewy condition for hyperbolic PDEs, describe when explicit FD schemes are convergent. Unfortunately, convergence analysis involves the bounding of limits of errors, which can be complicated [1].

Stability, another characteristic of FD schemes, describes the behavior of a FD scheme as its discretization becomes finer.

Definition 2. A FD scheme is *stable* if, for any $t^* > 0$, there exists a constant $c(t^*) > 0$, such that for $\ell = 0, 1, \ldots, \lfloor \frac{t^*}{\Delta t} \rfloor$, $\Delta x \to 0$,

$$\left(\Delta x \sum_{i \in \Omega} |u_i^\ell|^2 \right)^{\frac{1}{2}} < c(t^*).$$

Simply put, the ratio of $\Delta x^{\frac{1}{2}}$ to the ℓ^2-norm of u^ℓ at every time step less than t^* is bounded by t^*. Von Neumann first introduced methods for stability analysis through the use of Fourier and eigenvalue analysis [1]. For example, Theorem 2.1 relates the eigenvalues of the matrix produced by a FD scheme to its stability; we use similar eigenvalue techniques to study the stability of our explicit FD schemes on the heat equation.

Theorem 2.1 ([1])**.** *Say the matrix A produced by a FD scheme is normal, meaning $AA^T = A^T A$, for every sufficiently small $\Delta x > 0$, and there exists $\nu \geq 0$ such that*

$$\rho(A) \leq e^{\nu \Delta t}.$$

Then the scheme is stable.

Lax, in Theorem 2.1, links stability and convergence, allowing the simpler techniques of stability analysis to provide conclusions about convergence. Thus, Theorem 2.1 is considered one of the most fundamental theorems in the numerical analysis of PDEs.

Theorem 2.1 (Lax Equivalence Theorem [7])**.** *For a well-posed, linear, initial-value PDE, a consistent finite difference scheme is convergent if and only if it is stable.*

We shall prove stability conditions for our explicit FD schemes on the discontinuous coefficient heat diffusion equation, thus providing results about convergence through Theorem 2.1.

2.3 Finite Difference Schemes

We discretize the interval $[0, 1]$ in 1-D and the unit square region formed by (0,0), (0,1), (1,0), (1,1) in 2-D. Our discretized points are equally spaced along each axis, and we use the simple Dirichlet boundary condition $u = 0$ on $\partial\Omega$, which can be lifted up. We will bound $k(x)$ below by a constant $\alpha > 0$ to avoid degenerate cases. In simulation, we use the initial conditions $u(x) = \sin(x)$ and $u(x) = 1 - \sin(x)$ to see how heat diffuses across the surface for different initial conditions; the heat should always converge to 0 after sufficient time due to the absorbing boundary.

For our FD schemes, we refer to the *conservative* and *non-conservative* explicit FTCS schemes [8]. The conservative scheme is named as such due to the fact that the coefficient of point x_i^ℓ in the calculation of $x_j^{\ell+1}$ is the same as the coefficient of the point x_j^ℓ in the calculation of the point $x_i^{\ell+1}$, thus producing a symmetric matrix. The non-conservative scheme does not have this reflexive coefficient property, and thus the produced matrix is not necessarily symmetric. In 1-D, the schemes are derived from the following two equivalent equations, which are both forms of Equation (1.1):

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(k(x)\frac{\partial u}{\partial x}\right) \tag{2.1}$$

and

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x}\frac{\partial k}{\partial x} + k(x)\frac{\partial^2 u}{\partial x^2}. \tag{2.2}$$

From Equation (2.1), we produce the 1-D conservative scheme,

$$\frac{u_i^{l+1} - u_i^l}{\Delta t} = \frac{1}{\Delta x^2}\left(k_{i+\frac{1}{2}}\left(u_{i+1}^l - u_i^l\right) - k_{i-\frac{1}{2}}\left(u_i^l - u_{i-1}^l\right)\right). \tag{2.3}$$

From Equation (2.2), we produce the 1-D non-conservative scheme,

$$\frac{u_i^{l+1} - u_i^l}{\Delta t} = \frac{1}{\Delta x^2}\left(\frac{(k_{i+1} - k_{i-1})}{2}\frac{\left(u_{i+1}^l - u_{i-1}^l\right)}{2} + k_i\left(u_{i+1}^l + u_{i-1}^l - 2u_i^l\right)\right). \tag{2.4}$$

For the 2-dimensional case, we can write analogous forms of Equations (2.1) and (2.2).

For the 2-D conservative scheme, we get

$$\begin{aligned}\frac{u_{i,j}^{l+1}-u_{i,j}^{l}}{\Delta t} &= \frac{1}{\Delta x^2}\left(k_{i+\frac{1}{2},j}(u_{i+1,j}^{l}-u_{i,j}^{l})-k_{i-\frac{1}{2},j}(u_{i,j}^{l}-u_{i-1,j}^{l})\right)\\ &+\frac{1}{\Delta y^2}\left(k_{i,j+\frac{1}{2}}(u_{i,j+1}^{l}-u_{i,j})-k_{i,j-\frac{1}{2}}(u_{i,j}^{l}-u_{i,j-1}^{l})\right).\end{aligned} \tag{2.5}$$

For the 2-D non-conservative scheme, we get

$$\begin{aligned}\frac{u_{i,j}^{l+1}-u_{i,j}^{l}}{\Delta t} &= \frac{1}{\Delta x^2}\left(k_{i,j}(u_{i+1,j}^{l}+u_{i-1,j}^{l}-2u_{i,j})+\frac{(k_{i+1,j}-k_{i-1,j})}{2}\frac{(u_{i+1,j}^{l}-u_{i-1,j}^{l})}{2}\right)\\ &+\frac{1}{\Delta y^2}\left(k_{i,j}(u_{i,j+1}^{l}+u_{i,j-1}^{l}-2u_{i,j}^{l})+\frac{(k_{i,j+1}-k_{i,j-1})}{2}\frac{(u_{i,j+1}^{l}-u_{i,j-1}^{l})}{2}\right).\end{aligned} \tag{2.6}$$

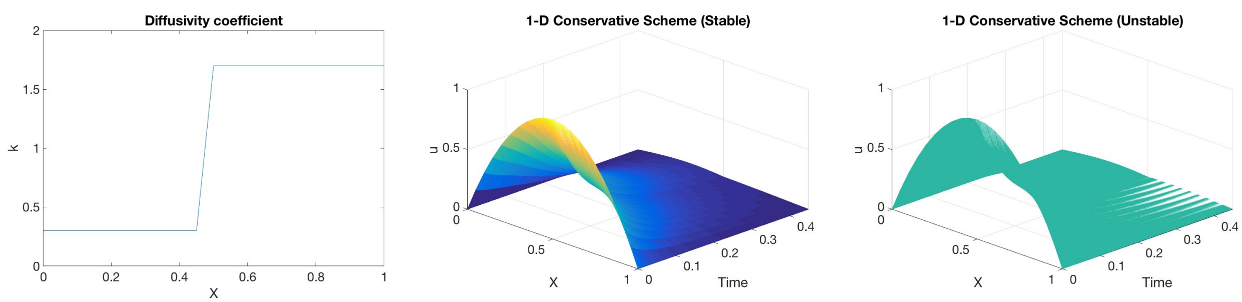
3 Numerical Results

For the heat diffusion equation with constant diffusivity, an explicit FD scheme is stable when $\mu k \leq \frac{1}{2}$. By the principle of frozen coefficients, we expect the stability condition in both 1-D and 2-D to be

$$\mu \max_{x\in\Omega}(k(x)) \leq \frac{1}{2} \tag{3.1}$$

when diffusivity is variable [1]. In Tables 1 to 4, we present numerical evidence suggesting that Equation (3.1) is not necessary for stability, but that it is sufficient, in both the conservative and non-conservative 1-D schemes. In Figures 3, 4, 9 and 10, we see that this condition suffices for stability in both the conservative and non-conservative 2-D schemes, even with randomness and discontinuity in the diffusivity coefficient.

3.1 1-Dimensional Conservative Scheme



(a) The diffusivity coefficient; $k = 0.3$ when $x < 0.5$ and $k = 1.7$ when $x \geq 0.5$.

(b) The conservative scheme stable and converging, with $\mu \max(k) = 0.5$ ($n_x = 20$ and $n_t = 1360$). Converges to 0 within 0.45 seconds.

(c) The conservative scheme unstable, with $\mu \max(k) = 0.513208$ ($n_x = 20$ and $n_t = 1325$). Begins to diverge within 0.45 seconds.

$k_1(x)$	$k_2(x)$	n_x	n_t	$\mu \max(k)$
1.0	1.0	20	796	0.502513
1.0	1.0	30	1796	0.501114
1.0	1.0	40	3196	0.500626
1.0	1.0	50	4996	0.500400
0.9	1.1	20	863	0.509849
0.9	1.1	30	1962	0.504587
0.9	1.1	40	3501	0.502714
0.9	1.1	50	5481	0.501733
0.8	1.2	20	941	0.510096
0.8	1.2	30	2139	0.504909
0.8	1.2	40	3819	0.502749
0.8	1.2	50	6222	0.501639
0.7	1.3	20	1018	0.510806
0.7	1.3	30	2317	0.504963
0.7	1.3	40	4137	0.502708
0.7	1.3	50	6476	0.501853

Table 1: This table lists the minimum n_t achieving stability for the given n_x, k_1, and k_2 in the conservative scheme, where the diffusivity coefficient is the piecewise function $k_1(x)$ for $x < 0.5$ and $k_2(x)$ for $x \geq 0.5$. For fixed k_1, k_2, the bound on $\mu \max(k)$ is observed to decrease as n_x increases. In these examples, the stability condition (3.1) is sufficient for stability.

$k_1(x)$	$k_2(x)$	n_x	n_t	$\mu \max(k)$
1.0	1.0	50	4996	0.500400
0.9	1.0	50	4983	0.501706
0.8	1.0	50	4982	0.501807
0.7	1.0	50	4982	0.501807
0.6	1.0	50	4982	0.501807
0.5	1.0	50	4982	0.501807
0.4	1.0	50	4982	0.501807
0.3	1.0	50	4982	0.501807
0.2	1.0	50	4982	0.501807
0.1	1.0	50	4982	0.501807

Table 2: This table lists the minimum n_t achieving stability for $n_x = 50$ and $k_2(x) = 1$ in the conservative scheme, while varying $k_1(x)$. The diffusivity coefficient is the discontinuous piecewise function $k_1(x)$ for $x < 0.5$ and $k_2(x)$ for $x \geq 0.5$. In these examples, the stability condition (3.1) is sufficient for stability.

3.2 1-Dimensional Non-Conservative Scheme

$k_1(x)$	$k_2(x)$	n_x	n_t	$\mu \max(k)$
1.0	1.0	20	796	0.502513
1.0	1.0	30	1796	0.501114
1.0	1.0	40	3196	0.500626
1.0	1.0	50	4996	0.500400
0.9	1.1	20	865	0.508671
0.9	1.1	30	1963	0.504330
0.9	1.1	40	3502	0.502570
0.9	1.1	50	5482	0.501642
0.8	1.2	20	943	0.509014
0.8	1.2	30	2141	0.420364
0.8	1.2	40	3820	0.502618
0.8	1.2	50	5980	0.501672
0.7	1.3	20	1022	0.508806
0.7	1.3	30	2320	0.504310
0.7	1.3	40	4139	0.502537
0.7	1.3	50	6478	0.501698

Table 3: This table lists the minimum n_t achieving stability for the given n_x, k_1, and k_2 in the non-conservative scheme, where the diffusivity coefficient is the piecewise function $k_1(x)$ for $x < 0.5$ and $k_2(x)$ for $x \geq 0.5$. For fixed k_1, k_2, the bound on $\mu \max(k)$ is observed to decrease as n_x increases. In these examples, the stability condition (3.1) is sufficient for stability.

$k_1(x)$	$k_2(x)$	n_x	n_t	$\mu \max(k)$
1.0	1.0	50	4996	0.500400
0.9	1.0	50	4984	0.501605
0.8	1.0	50	4983	0.501706
0.7	1.0	50	4983	0.501706
0.6	1.0	50	4983	0.501706
0.5	1.0	50	4983	0.501706
0.4	1.0	50	4983	0.501706
0.3	1.0	50	4983	0.501706
0.2	1.0	50	4983	0.501706
0.1	1.0	50	4983	0.501706

Table 4: This table lists the minimum n_t achieving stability for $n_x = 50$ and $k_2(x) = 1$ in the non-conservative scheme, while varying $k_1(x)$. The diffusivity coefficient is the discontinuous piecewise function $k_1(x)$ for $x < 0.5$ and $k_2(x)$ for $x \geq 0.5$. In these examples, the stability condition Equation (3.1) is sufficient for stability.

3.3 2-Dimensional Conservative Scheme

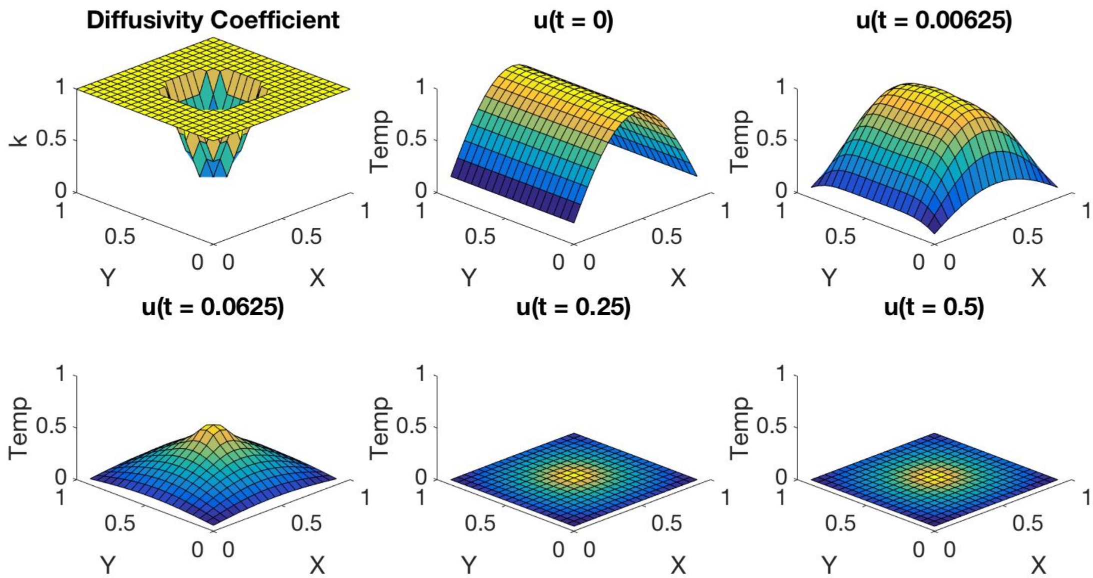


Figure 3: The diffusivity coefficient forms concentric circles, with a minimum value of 0.2 and a maximum value of 1, as depicted in the first frame. The next five frames depict the evolution of the heat function as approximated by the conservative scheme at t_0, t_{10}, t_{100}, t_{400}, and t_{800}. The conservative scheme is stable with $\mu \max(k) = 0.5$ (with $n_x = 20$, $n_y = 20$, $n_t = 1600$).

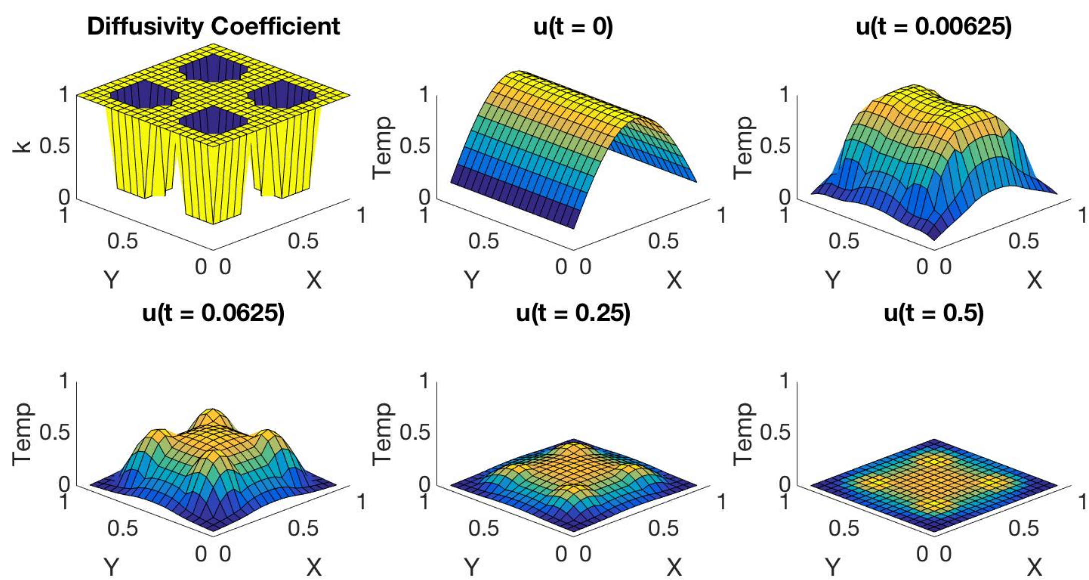


Figure 4: The diffusivity coefficient is 1 everywhere except for four regions which have a value of 0.1, as depicted in the first frame. The next five frames depict the evolution of the heat function as approximated by the conservative scheme at t_0, t_{10}, t_{100}, t_{400}, and t_{800}. The conservative scheme is stable with $\mu \max(k) = 0.5$ (with $n_x = 20$, $n_y = 20$, $n_t = 1600$).

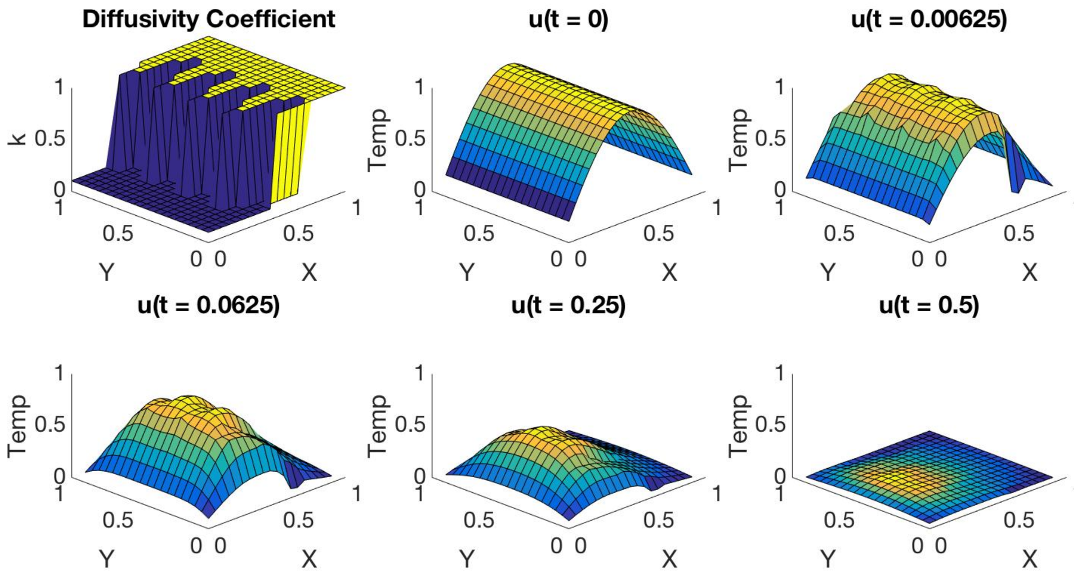


Figure 5: The diffusivity coefficient is 1 for half of the domain and 0.1 for the other half, as depicted in the first frame. The next five frames depict the evolution of the heat function as approximated by the conservative scheme at t_0, t_{10}, t_{100}, t_{400}, and t_{800}. The conservative scheme is stable with $\mu \max(k) = 0.5$ $(n_x = 20, n_y = 20, n_t = 1600)$.

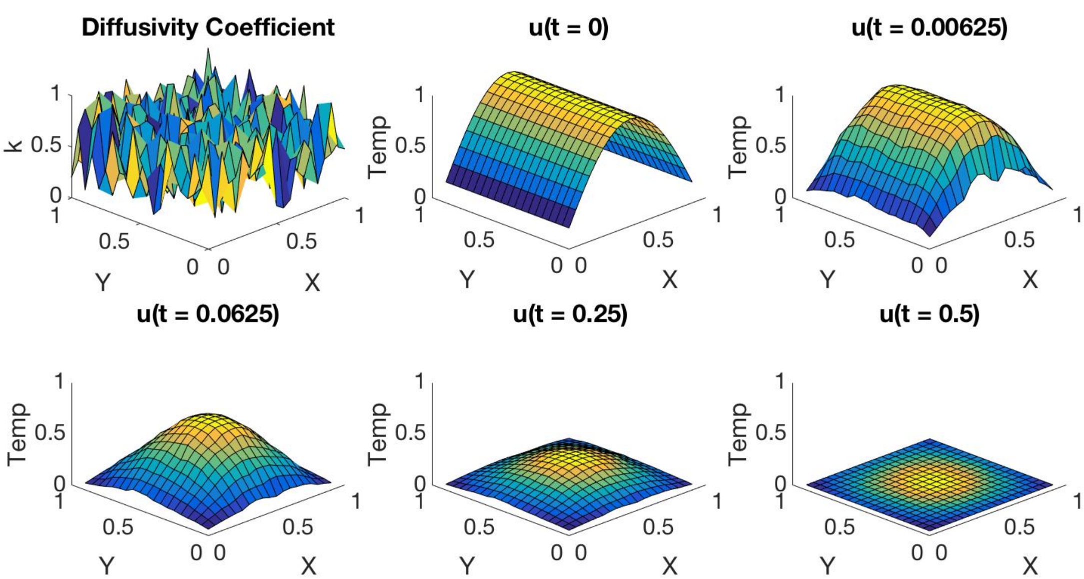


Figure 6: The diffusivity coefficient is random within the bounds 0.2 and 1, as depicted in the first frame. The next five frames depict the evolution of the heat function as approximated by the conservative scheme at t_0, t_{10}, t_{100}, t_{400}, and t_{800}. The conservative scheme is stable with $\mu \max(k) = 0.5$ $(n_x = 20, n_y = 20, n_t = 1600)$.

3.4 2-Dimensional Non-Conservative Scheme

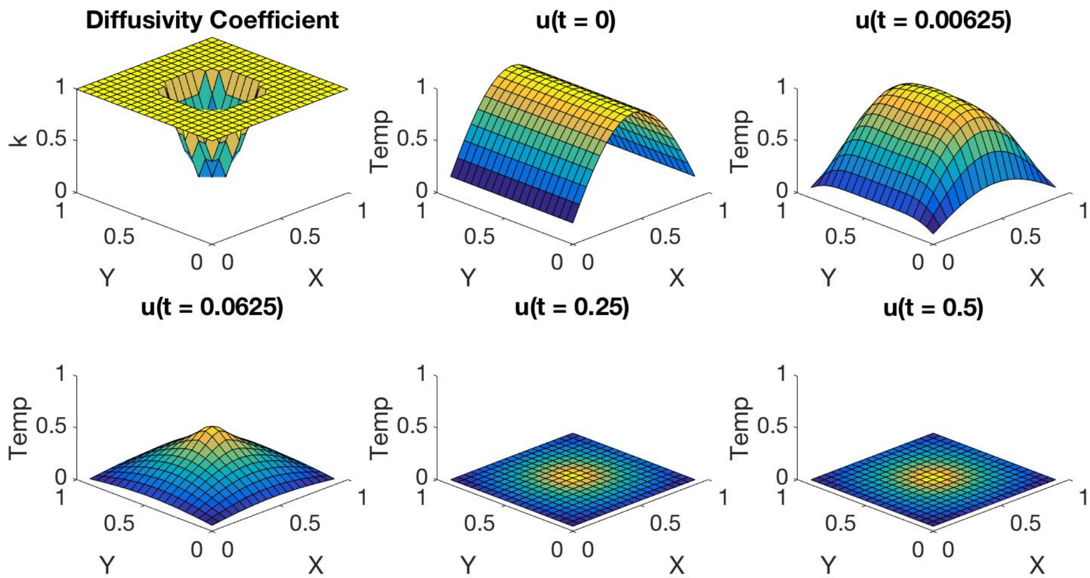


Figure 7: The diffusivity coefficient forms concentric circles, with a minimum value of 0.2 and a maximum value of 1, as depicted in the first frame. The next five frames depict the evolution of the heat function as approximated by the non-conservative scheme at t_0, t_{10}, t_{100}, t_{400}, and t_{800}. The non-conservative scheme is stable with $\mu \max(k) = 0.5$ ($n_x = 20, n_y = 20, n_t = 1600$).

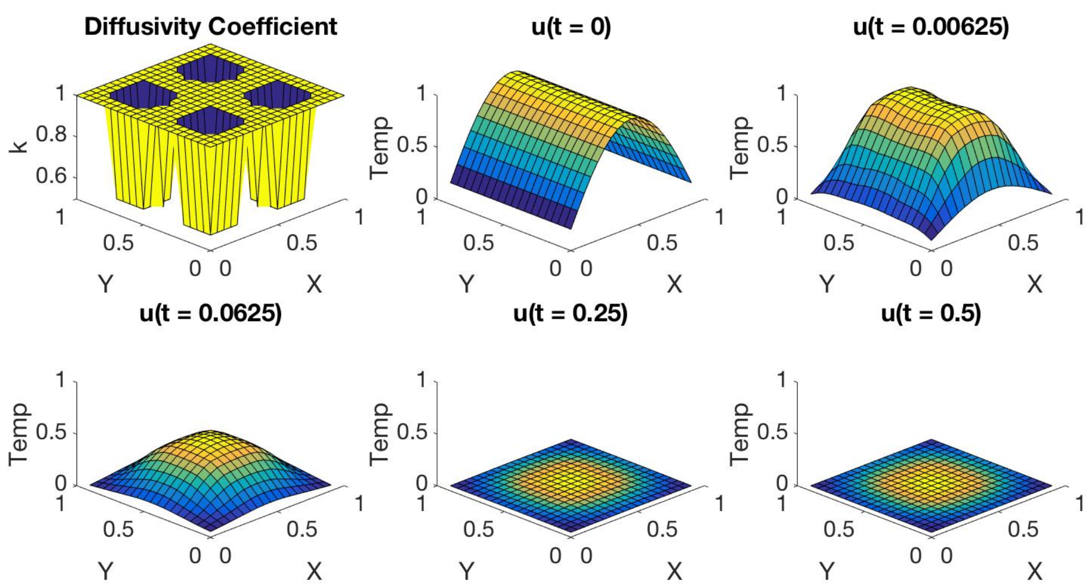


Figure 8: The diffusivity coefficient is 1 everywhere except for four circles which have a value of 0.5, as depicted in the first frame. The next five frames depict the evolution of the heat function as approximated by the non-conservative scheme at t_0, t_{10}, t_{100}, t_{400}, and t_{800}. The non-conservative scheme is stable with $\mu \max(k) = 0.5$ ($n_x = 20, n_y = 20, n_t = 1600$).

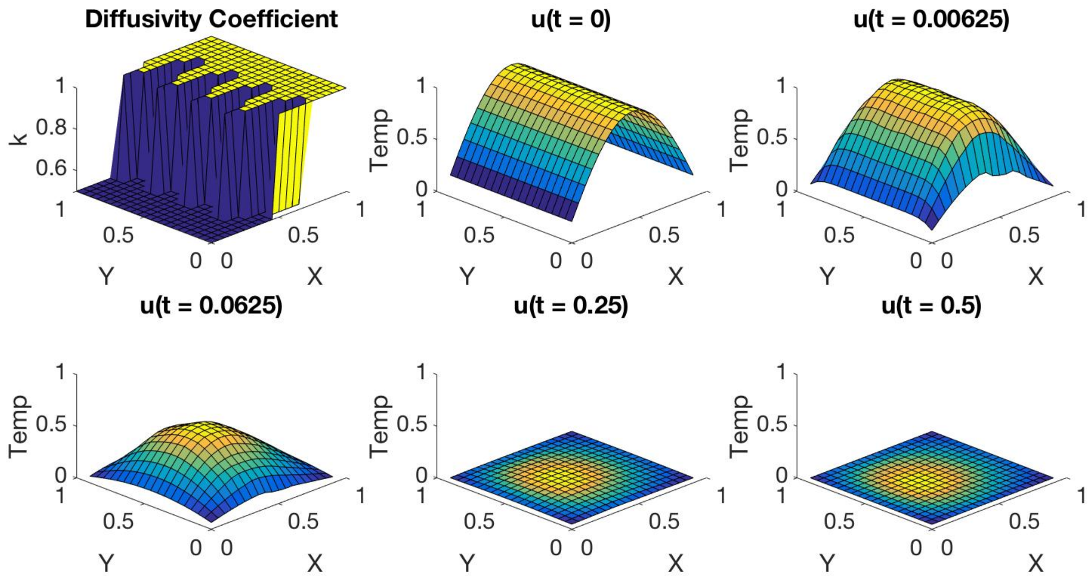


Figure 9: The diffusivity coefficient is 1 for half of the domain and 0.5 for the other half, as depicted in the first frame. The next five frames depict the evolution of the heat function as approximated by the non-conservative scheme at t_0, t_{10}, t_{100}, t_{400}, and t_{800}. The non-conservative scheme is stable with $\mu \max(k) = 0.5$ (with $n_x = 20$, $n_y = 20$, $n_t = 1600$).

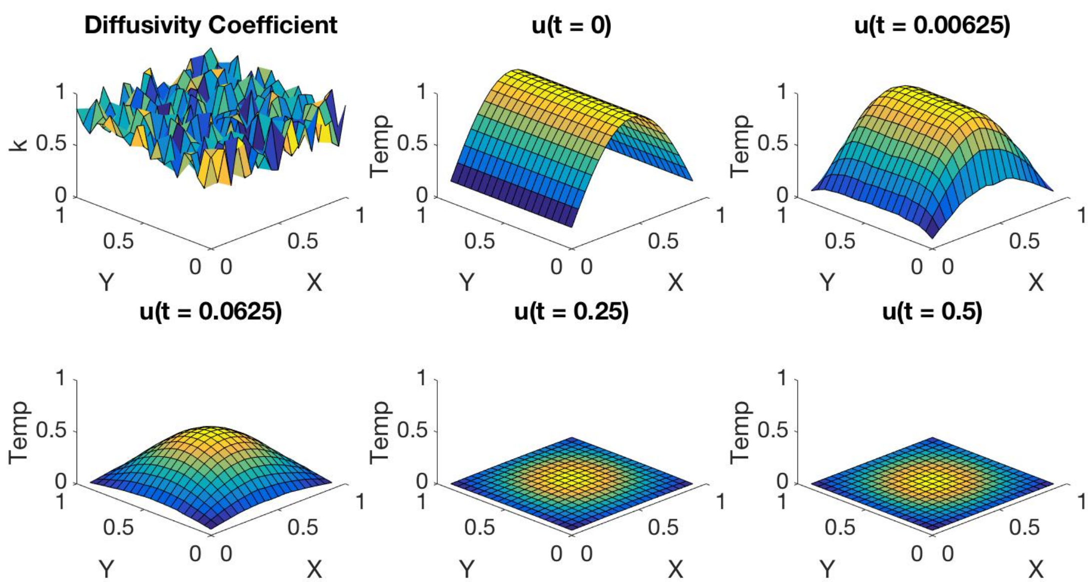


Figure 10: The diffusivity coefficient is random within the bounds 0.5 and 1, as depicted in the first frame. The next five frames depict the evolution of the heat function as approximated by the non-conservative scheme at t_0, t_{10}, t_{100}, t_{400}, and t_{800}. The non-conservative scheme is stable with $\mu \max(k) = 0.5$ (with $n_x = 20$, $n_y = 20$, $n_t = 1600$).

4 Analytical Results

We see numerically that the proposed stability condition (3.1) is sufficient for stability. For the 1-dimensional and 2-dimensional conservative FTCS schemes, we now prove that this condition is sufficient.

The FD schemes each produce a matrix A which describe the evolutionary relation $\mathbf{u^{l+1}} = A\mathbf{u^l}$. Recall Theorem 2.1:

Theorem 2.1 ([1])**.** *Say the matrix A produced by a FD scheme is normal, meaning $AA^T = A^T A$, for every sufficiently small $\Delta x > 0$, and there exists $\nu \geq 0$ such that*

$$\rho(A) \leq e^{\nu \Delta t}.$$

Then the scheme is stable.

So, given A is normal, showing $\rho(A) \leq 1$ implies stability. In order to analyze eigenvalues, we use Theorem 4.1.

Theorem 4.1 (Gershgorin Disc Theorem)**.** *Given an $n \times n$ matrix A, we define $R_i = \sum_{j=1, j\neq i}^{n} |a_{ij}|$, the sum of the off-diagonal entries of i^{th} row. Then every eigenvalue of A is in at least one of the imaginary discs in the set: $\{z : |z - a_{ii}| \leq R_i\}$.*

4.1 1-Dimensional Conservative Scheme

Theorem 4.2 (1-D Stability Condition)**.** *The conservative 1-D scheme given in Equation* (2.3) *is stable when the inequality in* (3.1)*,*

$$\mu \max_{x\in\Omega}(k(x)) \leq \frac{1}{2},$$

is satisfied, where $\mu = \frac{\Delta t}{\Delta x^2}$, Courant's number, and $\max_{x\in\Omega}(k(x))$ is the maximum diffusivity coefficient throughout the domain.

Proof. From the conservative scheme (2.3), we can write the conservative matrix

$$A_c = I + \mu \begin{pmatrix} -(k_{\frac{1}{2}} + k_{\frac{3}{2}}) & k_{\frac{3}{2}} & 0 & \cdots & \cdots \\ k_{\frac{3}{2}} & -(k_{\frac{3}{2}} + k_{\frac{5}{2}}) & k_{\frac{5}{2}} & 0 & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & k_{n_x - \frac{1}{2}} & -(k_{n_x-\frac{1}{2}} + k_{n_x+\frac{1}{2}}) \end{pmatrix}.$$

Recalling Theorem 2.1, we need to show $\rho(A_c) \leq 1$. Note that A_c is symmetric, and thus normal and its eigenvalues are real. By Theorem 4.1, we find bounds for the eigenvalues of A_c. The Gershgorin discs have centers of the form

$$1 - \mu\left(k_{i-\frac{1}{2}} + k_{i+\frac{1}{2}}\right).$$

Additionally, the Gershgorin discs have radii of the form

$$|\mu k_{i-\frac{1}{2}}| + |\mu k_{i+\frac{1}{2}}| = \mu k_{i-\frac{1}{2}} + \mu k_{i+\frac{1}{2}}.$$

Thus, all eigenvalues λ are bounded:

$$1 - 2\mu\left(k_{i-\frac{1}{2}} + k_{i+\frac{1}{2}}\right) \leq \lambda \leq 1.$$

Under the proposed condition (3.1),

$$\begin{aligned} 1 - 2\mu\left(k_{i-\frac{1}{2}} + k_{i+\frac{1}{2}}\right) &\geq 1 - 4\mu \max(k) \\ &\geq 1 - 4 \cdot \frac{1}{2} \\ &= -1. \end{aligned}$$

Thus, $\rho(A_c) \leq 1$ by the stability condition (3.1). □

So the stability condition (3.1) is proven for the 1-D conservative scheme. However, in practice we notice that this condition is not as strict. In Sections 3.1 and 3.2, we notice that the maximum stable value of $\mu \max(k)$ decreases as n_x increases. This is explained by Theorem 4.4.

Lemma 4.3 ([9])**.** *A sequence $\{a_k\}_{k=1}^{n}$ is a chain sequence if and only if*

$$0 < a_k < \frac{1}{4\cos^2\left(\frac{\pi}{n+1}\right)}$$

Theorem 4.4 (Wall-Wetzel Theorem)**.** *A symmetric diagonal matrix with positive entries,*

$$\begin{pmatrix} a_1 & b_1 & & & \\ b_1 & a_2 & b_2 & & \\ & b_2 & \ddots & \ddots & \\ & & \ddots & \ddots & b_{n-1} \\ & & & b_{n-1} & a_n \end{pmatrix},$$

is positive definite if and only if

$$\left\{ \frac{b_i^2}{a_i a_{i+1}} \right\}_{i=1}^{n-1} \tag{4.1}$$

forms a chain sequence.

Note: Theorem 4.4 can be used to prove stability of the 1-D conservative scheme as well (not shown). However, the proof is only applicable to the 1-D conservative scheme, as Theorem 4.4 only applies to tridiagonal matrices. The proof by Theorem 4.4 is different because it provides a more lenient stability condition,

$$(\mu k_{i+\frac{1}{2}})^2 < \frac{\left(2 - \mu\left(k_{i-\frac{1}{2}} + k_{i+\frac{1}{2}}\right)\right)\left(2 - \mu\left(k_{i+\frac{1}{2}} + k_{i+\frac{3}{2}}\right)\right)}{4\cos^2\left(\frac{\pi}{n_x+1}\right)}$$

instead of

$$(\mu k_{i+\frac{1}{2}})^2 < \frac{\left(2 - \mu\left(k_{i-\frac{1}{2}} + k_{i+\frac{1}{2}}\right)\right)\left(2 - \mu\left(k_{i+\frac{1}{2}} + k_{i+\frac{3}{2}}\right)\right)}{4},$$

which is what the stability condition (3.1) provides. Thus, as n_x approaches infinity, the stability condition is necessary.

4.2 2-D Conservative Scheme

Theorem 4.5 (2-D Stability Condition)**.** *The conservative scheme* (2.5) *is stable when the inequality* (3.1)

$$\mu \max_{(x,y)\in\Omega} (k(x,y)) \leq \frac{1}{2}$$

is satisfied, where

$$\mu = \frac{\Delta t}{\Delta x^2} + \frac{\Delta t}{\Delta y^2}.$$

Proof. From scheme (2.5), we can write the matrix produced by the conservative scheme as

$$A_c = I + \mu_x \begin{pmatrix} X_1 & \hat{X}_1 & & & \\ \hat{X}_1 & X_2 & \hat{X}_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \hat{X}_{n_x-2} & X_{m-1} & \hat{X}_{n_x-1} \\ & & & \hat{X}_{n_x-1} & X_{n_x} \end{pmatrix} + \mu_y \begin{pmatrix} Y_1 & & & & \\ & Y_2 & & & \\ & & \ddots & & \\ & & & Y_{n_x-1} & \\ & & & & Y_{n_x} \end{pmatrix},$$

where

$$X_i = \begin{pmatrix} -\left(k_{i-\frac{1}{2},1} + k_{i+\frac{1}{2},1}\right) & & \\ & \ddots & \\ & & -\left(k_{i-\frac{1}{2},n_y} + k_{i+\frac{1}{2},n_y}\right) \end{pmatrix} \text{ and } \hat{X}_i = \begin{pmatrix} k_{i+\frac{1}{2},1} & & \\ & \ddots & \\ & & k_{i+\frac{1}{2},n_y} \end{pmatrix}$$

and

$$Y_i = \begin{pmatrix} -\left(k_{i,\frac{1}{2}} + k_{i,\frac{3}{2}}\right) & k_{i,\frac{3}{2}} & & \\ k_{i,\frac{3}{2}} & \ddots & \ddots & \\ & \ddots & -\left(k_{i,n_y-\frac{3}{2}} + k_{i,n_y-\frac{1}{2}}\right) & k_{i,n_y-\frac{1}{2}} \\ & & k_{i,n_y-\frac{1}{2}} & -\left(k_{i,n_y-\frac{1}{2}} + k_{i,n_y+\frac{1}{2}}\right) \end{pmatrix}.$$

Recall that we would like to show $\rho(A_c) \leq 1$. Also, recall that A_c is symmetric, and thus the eigenvalues are real. Similar to the proof in 1-D, we use Theorem 4.1 to bound the eigenvalues. The Gershgorin discs have centers of the form

$$1 - \mu_x \left(k_{i-\frac{1}{2},j} + k_{i+\frac{1}{2},j}\right) - \mu_y \left(k_{i,j-\frac{1}{2}} + k_{i,j+\frac{1}{2}}\right),$$

and radii of the form

$$\mu_x \left(k_{i-\frac{1}{2},j} + k_{i+\frac{1}{2},j}\right) + \mu_y \left(k_{i,j-\frac{1}{2}} + k_{i,j+\frac{1}{2}}\right).$$

Thus, all eigenvalues λ are bounded:

$$1 - 2\mu_x \left(k_{i-\frac{1}{2},j} + k_{i+\frac{1}{2},j}\right) - 2\mu_y \left(k_{i,j-\frac{1}{2}} + k_{i,j+\frac{1}{2}}\right) \leq \lambda \leq 1.$$

From Equation (3.1),

$$\begin{aligned} 1 - 2\mu_x \left(k_{i-\frac{1}{2},j} + k_{i+\frac{1}{2},j}\right) - 2\mu_y \left(k_{i,j-\frac{1}{2}} + k_{i,j+\frac{1}{2}}\right) &\geq 1 - 4\left(\mu_x + \mu_y\right)\max(k) \\ &\geq 1 - 4 \cdot \frac{1}{2} \\ &= -1. \end{aligned}$$

Thus, when Equation (3.1) is satisfied, $-1 \leq \lambda \leq 1$, and $\rho(A) \leq 1$. □

5 Conclusion

We have provided both numerical and analytic evidence that the condition (3.1) is sufficient for stability of schemes with discontinuous diffusivity. For the non-conservative FD scheme in 1-D and 2-D, we have seen numerical evidence that the condition implies stability. For the conservative FD scheme in 1-D and 2-D, we have seen similar numerical evidence, but we have also proven condition (3.1) to be sufficient for stability by eigenvalue methods, using Theorems 4.1 and 4.4.

These results can be practically applied to ensure stability, and thus convergence, of simulations of the diffusion equation with a discontinuous coefficient. This need arises in many fields such as geophysics [10] and fluid dynamics [11, 12, 13]. One example is the heat transfer in composite porous media [5], where thermal conductivities are discontinuous along the boundaries between two different materials. Other simulation techniques have been proposed to simulate diffusion through discontinuous media [6, 14], but finite difference methods are simpler.

Theorem 4.1 did not work for the explicit non-conservative scheme, and future work could include developing a new technique to prove stability conditions for this scheme. Our use of Theorem 4.1 to analyze the eigenvalues of a FD scheme can be used to study other conservative FD schemes as well. We could also study schemes for other PDEs, including extensions to the more general diffusion equation

$$\frac{\partial u}{\partial t} = \nabla \cdot \left(\begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \nabla u \right),$$

or the diffusion-convection equation

$$\frac{\partial u}{\partial t} = \nabla \cdot (k_1 \nabla u) - \nabla \cdot (k_2 u).$$

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