2-1-2019

Diagonalization of 1-D Differential Operators With Piecewise Constant Coefficients Using the Uncertainty Principle

Sarah D. Long
University of Southern Mississippi

Somayyeh Sheikholeslami
Beaumont Health, s.sheikholeslami@usm.edu

James V. Lambers
University of Southern Mississippi, james.lambers@usm.edu

Carley Walker
University of Southern Mississippi

Follow this and additional works at: https://aquila.usm.edu/fac_pubs

Part of the [Mathematics Commons](#)

Recommended Citation

Long, S. D., Sheikholeslami, S., Lambers, J. V., Walker, C. (2019). Diagonalization of 1-D Differential Operators With Piecewise Constant Coefficients Using the Uncertainty Principle. *Mathematics and Computers in Simulation*, 156, 194-226.

Available at: https://aquila.usm.edu/fac_pubs/15542

This Article is brought to you for free and open access by The Aquila Digital Community. It has been accepted for inclusion in Faculty Publications by an authorized administrator of The Aquila Digital Community. For more information, please contact Joshua.Cromwell@usm.edu.

Diagonalization of 1-D Differential Operators with Piecewise Constant Coefficients Using the Uncertainty Principle

Sarah D. Long^a, Somayyeh Sheikholeslami^b, James V. Lambers^a, Carley Walker^a

^a*Department of Mathematics, The University of Southern Mississippi, 118 College Dr #5045, Hattiesburg, MS 39406 USA*

^b*Department of Radiation Oncology, Beaumont Health, Royal Oak, MI 48073 USA*

Abstract

A highly accurate and efficient numerical method is presented for computing the solution of a 1-D time-dependent partial differential equation in which the spatial differential operator features a piecewise constant coefficient defined on n pieces, in either self-adjoint and non-self-adjoint form, on a finite interval with periodic boundary conditions. The Uncertainty Principle is used to estimate the eigenvalues of the operator. Then, these estimates are used to construct a basis of eigenfunctions for use with a spectral method. The solution is presented as a truncated eigenfunction expansion, where each eigenfunction is a wave function that changes frequencies at the interfaces between different materials. Numerical experiments demonstrate the accuracy, efficiency and scalability of the method in comparison to other methods.

Keywords: heat equation, Uncertainty Principle, interface problem, spectral methods, eigenfunction expansion

1. Introduction

Let $\alpha(x)$ be a piecewise constant function on $[0, 2\pi)$, defined on n pieces as follows:

$$\alpha(x) = \begin{cases} \alpha_1 & 0 \leq x < 2\pi\rho_1 \\ \alpha_2 & 2\pi\rho_1 \leq x < 2\pi\rho_2 \\ \vdots & \vdots \\ \alpha_n & 2\pi\rho_{n-1} \leq x < 2\pi \end{cases} \quad (1)$$

where $0 < \rho_1 < \rho_2 < \cdots < \rho_{n-1} < 1$. This function therefore has jump discontinuities at $x_i = 2\pi\rho_i$ for $i = 1, 2, \dots, n-1$. We consider the initial value problems

$$u_t = \alpha^2(x)u_{xx}, \quad (2)$$

or

$$u_t = (\alpha^2(x)u_x)_x \quad (3)$$

on the domain $(0, 2\pi) \times (0, \infty)$, with an initial condition $u(x, 0) = f(x)$ and periodic boundary conditions. Throughout this paper, we use subscripts to denote partial derivatives. That is, $u_t = \partial u / \partial t$ and $u_{xx} = \partial^2 u / \partial x^2$.

Equations (2) and (3) are special cases of the equation for heat transfer in a general medium,

$$u_t = \frac{1}{c(x)^2} (a(x)^2 u_x)_x, \quad (4)$$

where the coefficient $c(x)^2$ is the specific heat, and $a(x)^2$ is the diffusion coefficient that defines the heat flux $J(x) = a(x)^2 u_x$. In equation (2), hereafter referred to as the *non-self-adjoint case*, we assume a constant diffusion coefficient, whereas in (3), hereafter referred to as the *self-adjoint case*, we assume a constant specific heat.

Simulation of phenomena such as diffusion of heat energy or wave propagation through multiple homogeneous media, represented by the piecewise constant coefficient $\alpha(x)$, is challenging for either analytical or numerical methods, because of the discontinuities at the interfaces between different materials. The simple solution method of separation of variables, in the case of a constant coefficient $\alpha(x)$, is no longer practical. Instead, analytical solutions can be found using the classical layer potential [1, 2], though not in closed form. Monte Carlo methods have also been employed [3, 4, 5, 6, 7]. In [8, 9] it is shown how a closed-form representation of the resolvent kernel can be obtained for problems such as those considered in this paper, from which a fundamental solution can be obtained via inversion of a Laplace transform. However, for such problems, this inversion must be carried out numerically.

Numerical methods, such as finite element and finite difference methods [10, 11], have difficulties with PDEs of this form because the discontinuities of the coefficient introduce discontinuities in the first or second derivatives of the solution, which implies slower decay of its Fourier coefficients [12]. As a result, higher spatial resolution is required to represent the solution, and therefore time-stepping methods are susceptible to stiffness. For both implicit and explicit time-stepping methods, stiffness leads to a substantial increase

in computational expense, due to the CFL constraint forcing a smaller time step for explicit methods, or ill-conditioning in systems solved by implicit methods that slows the convergence of iterative methods.

Both (2) and (3) can be written in the form

$$u_t + Lu = 0. \quad (5)$$

The operator L is either $\alpha(x)^2 \partial^2 / \partial x^2$ or $-\partial / \partial x (\alpha(x)^2 \partial / \partial x)$ for (2) or (3), respectively. When the eigenvalues $\{\lambda_j\}_{j=0}^\infty$ and eigenfunctions $\{V_j\}_{j=0}^\infty$ of L are known, separation of variables easily yields a solution of (5) that has the form

$$u(x, t) = \sum_{j=0}^{\infty} V_j(x) e^{-\lambda_j t} \langle W_j, f \rangle / \langle W_j, V_j \rangle, \quad (6)$$

where $u(x, 0) = f(x)$ is the initial condition, and $\langle \cdot, \cdot \rangle$ denotes the standard inner product of square integrable functions on $(0, 2\pi)$,

$$\langle f, g \rangle = \int_0^{2\pi} \overline{f(x)} g(x) dx. \quad (7)$$

The eigenfunction of the adjoint L^* corresponding to λ_j is $W_j(x)$ (for (3), $W_j = V_j$). Not only is a solution of this form readily computed, thus avoiding most of the pitfalls of numerical methods (with the exception of rounding error and discretization error in arising from the inner products), but the form of the solution is far more conducive to qualitative analysis of its behavior than numerical solutions that simply produce a vector of values of the solution at grid points.

Unfortunately, a solution of the form (6) can only be obtained in special cases such as a constant coefficient, for which the eigensystem of L is known. We will still use separation of variables, but because our coefficients are not simply constant, there will be a significant challenge in computing the eigenfunctions and eigenvalues. In this paper, we present a method for accurately and efficiently computing these eigenvalues and eigenfunctions in the case of a piecewise constant coefficient. The resulting algorithm for computing the eigenvalues and coefficients of the eigenfunctions is highly parallelizable, with computational expense independent of spatial resolution. From this algorithm, we can obtain a solution in a much more useful form, and more efficiently, than what is produced by conventional numerical methods. It will also be seen that the proposed solution method is more scalable than such numerical methods.

This work builds on previous work in [13], for the self-adjoint problem (3) in the case of $n = 2$; that is, only a single interface between two materials. The solution of the corresponding eigenvalue problem, for the case of homogeneous Dirichlet boundary conditions, was presented in [14], but without a numerical procedure for practical computation. In this paper, we consider periodic boundary conditions, but the algorithm can readily be modified for the cases of homogeneous Dirichlet and Neumann boundary conditions [13].

The outline of the paper is as follows. In Section 2 we explain how the *SAK* principle can be used to obtain estimates of eigenvalues, which can serve as initial guesses for an iterative method to compute eigenvalues with high accuracy. In Section 3 we derive equations that characterize the eigenvalues, and explain how the eigenfunctions can be constructed. Numerical results are presented in Section 4, and conclusions are given in Section 5.

2. Applying the *SAK* Principle

For the two cases (self-adjoint and non-self adjoint) considered in this paper, with periodic boundary conditions, we will develop a practical algorithm for computing highly accurate approximate eigenvalues and eigenfunctions. This algorithm involves solving a nonlinear equation for each eigenvalue by iteration, which requires an initial guess.

We first discuss how an accurate initial guess can be obtained from the Uncertainty Principle, and its interpretation by Fefferman in [15]. The Uncertainty Principle indicates that the position and momentum of a particle cannot both be measured with arbitrarily high accuracy [16]. This is mathematically equivalent to stating that a function f and its Fourier transform $\hat{f}$ cannot be concentrated within an arbitrarily small box in phase space, which is the Cartesian product of physical space and frequency space [15, 17, 18]. Consider the self-adjoint differential operator

$$A(x, D) = \sum_{|\alpha| \leq m} a_\alpha(x) D^\alpha, \quad D = \frac{1}{i} \frac{\partial}{\partial x},$$

where $i = \sqrt{-1}$ is the imaginary unit. The *symbol* of $A(x, D)$ is defined by

$$A(x, \omega) = e^{-i\omega x} A(x, D) e^{i\omega x} = \sum_{|\alpha| \leq m} a_\alpha(x) \omega^\alpha.$$

The *SAK* principle, due to Fefferman [15], states that the number of eigenvalues of $A(x, D)$ that are less than K is approximately equal to the number of “distorted unit cubes” that can be packed in the set $S(A, K) = \{(x, \omega) | A(x, \omega) < K\}$. By applying $A(x, D)$ to a function $\phi(x)$ which is concentrated within a distorted unit cube in phase space, centered at (x_0, ω_0) , we have

$$A(x, D)\phi(x) \approx A(x_0, \omega_0)\phi(x)$$

where $A(x_0, \omega_0)$ is an approximate eigenvalue, and $\phi(x)$ is an approximate eigenfunction. Intuitively, $\phi(x)$ is a more accurate approximate eigenfunction if $A(x, \omega)$ does not vary much within the region in which $\phi(x)$ is concentrated. Therefore, we seek eigenfunctions concentrated in subsets of phase space that are derived from the level curves of $A(x, \omega)$.

If we define

$$A(x, D) = -\frac{\partial}{\partial x}\alpha^2(x)\frac{\partial}{\partial x} = D\alpha^2(x)D$$

then

$$A(x, \omega) = \begin{cases} \alpha_1^2\omega^2, & 0 \leq x < 2\pi\rho_1, \\ \alpha_2^2\omega^2, & 2\pi\rho_1 \leq x < 2\pi\rho_2, \\ \vdots & \\ \alpha_n^2\omega^2, & 2\pi\rho_{n-1} \leq x < 2\pi. \end{cases}$$

The level curves of this symbol are defined by

$$\{(x, \omega) | \omega = \omega_i, 2\pi\rho_{i-1} \leq x < 2\pi\rho_i, i = 1, 2, \dots, n\}$$

where, for convenience, we define $\rho_0 = 0$ and $\rho_n = 1$, and the values ω_i , $i = 1, \dots, n$, satisfy

$$\alpha_1\omega_1 = \dots = \alpha_n\omega_n. \quad (8)$$

To estimate *which* level curves can be used to define regions of phase in which eigenfunctions are approximately concentrated, we use a heuristic introduced in [19], that the eigenvalues of $A(x, D)$ are approximately characterized by decomposing phase space into regions bounded by level curves of $A(x, \omega)$ such that the area of each region is 2π .

In the following example with $n = 4$ pieces, we will demonstrate how the eigenvalues are estimated. We will choose ω values ($\omega_{11}, \omega_{12}, \omega_{13}, \omega_{14}$) to represent our frequency values of the eigenfunction corresponding to the smallest nonzero eigenvalue λ_1 . By examining the level curves of $A(x, \omega)$, the values of ω are all related by the equations

$$\alpha_1\omega_{11} = \alpha_2\omega_{12} = \alpha_3\omega_{13} = \alpha_4\omega_{14}.$$

Figure 1: The region in phase space for the eigenfunction.

Figure 1 shows the visual representation of how the *SAK* principle can help us approximate the values of ω_{1i} , where $i = 1, 2, 3, 4$. The area of the polygon in the figure is

$$\omega_{11}2\pi\rho_1 + \omega_{12}(2\pi\rho_2 - 2\pi\rho_1) + \omega_{13}(2\pi\rho_3 - 2\pi\rho_2) + \omega_{14}(2\pi - 2\pi\rho_3) = 2\pi.$$

For the case where $\alpha_1 = 1$, $\alpha_2 = 2$, α_3 , $\alpha_4 = 4$, $\rho_1 = \frac{3}{8}$, $\rho_2 = \frac{1}{2}$, and $\rho_3 = \frac{3}{4}$ along with the relationship between the α_i and ω_{ji} values established by the *SAK* Principle, the equation simplifies to

$$2\pi = 4\omega_{14}\frac{3\pi}{4} + 2\omega_{14}\frac{\pi}{4} + \frac{4}{3}\omega_{14}\frac{\pi}{2} + \omega_{14}\frac{\pi}{2}$$

which has the solution

$$\omega_{14} = \frac{3}{7}.$$

We conclude that our initial guess for ω_{j4} , to obtain eigenvalues λ_j , $j = 1, 2, \dots$, should be integer multiples of $\frac{3}{7}$. Heuristically, we expect each pair of exact frequencies that are the closest to ω_{jn} to fall within the interval $(\omega_{(j-1)n}, \omega_{(j+1)n})$, where we define $\omega_{0n} = 0$. Once the frequencies ω_{ji} are obtained, the eigenvalues are given by

$$\lambda_j = (\alpha_n \omega_{jn})^2. \quad (9)$$

Once the eigenvalues are computed, the corresponding eigenfunctions can be constructed, as will be discussed in detail in the next section.

In the case of the general piecewise constant coefficient $\alpha(x)$ defined in (1), we have

$$2\pi = \sum_{i=1}^n \omega_{ji} 2\pi(\rho_i - \rho_{i-1}), \quad \rho_0 = 0, \quad \rho_n = 1. \quad (10)$$

If we define $\tau_i = \frac{\alpha_n}{\alpha_i}$, then we have $\omega_{ji} = \tau_i \omega_{jn}$, and (10) reduces to

$$2\pi = \sum_{i=1}^n \tau_i \omega_{jn} 2\pi(\rho_i - \rho_{i-1}). \quad (11)$$

Then we can solve for the value of the initial guess $\omega_{jn}^{(0)}$ that will be used for iteration:

$$\omega_{jn}^{(0)} = \left\lceil \frac{j}{2} \right\rceil \frac{1}{\sum_{i=1}^n \tau_i(\rho_i - \rho_{i-1})}, \quad (12)$$

where $\lceil x \rceil$ is the “ceiling function” (that is, the smallest integer greater than or equal to x). This is because each integer multiple of $(\sum_{i=1}^n \tau_i(\rho_i - \rho_{i-1}))^{-1}$ is an estimate of a pair of nonzero eigenvalues.

3. Computing Eigenvalues and Eigenfunctions

We seek eigenfunctions of the form

$$V_j(x) = \begin{cases} a_{j1} \cos(\omega_{j1}x) + b_{j1} \sin(\omega_{j1}x) & 0 \leq x < 2\pi\rho_1 \\ a_{j2} \cos(\omega_{j2}x) + b_{j2} \sin(\omega_{j2}x) & 2\pi\rho_1 \leq x < 2\pi\rho_2 \\ \vdots & \\ a_{jn} \cos(\omega_{jn}x) + b_{jn} \sin(\omega_{jn}x) & 2\pi\rho_{n-1} \leq x < 2\pi \end{cases} \quad (13)$$

where $\omega_{j1}, \dots, \omega_{jn}$ are the frequencies, $a_{j1}, \dots, a_{jn}$ and $b_{j1}, \dots, b_{jn}$ represent the unknown amplitudes and phase shifts, ρ_i represents where the interface between materials occurs, and the index value n represents how many pieces are being described.

3.1. Non-Self-adjoint Case

We first consider the non-self-adjoint operator $A(x, D) = \alpha^2(x)D^2$. The eigenfunctions for the piecewise constant coefficient case will be described by equation (13). Our goal is to eliminate all of the parameters except for ω_{jn} so we can solve for it, therefore obtaining the eigenvalues.

The restrictions and conditions of 2π -periodicity and continuity at the interface between materials leads us to the elimination of a_{j1} and b_{j1} . For the two-piece case, we have the following conditions [20]:

$V_j(x)$ and its derivative must be 2π -periodic:

$$V_{j1}(0) = V_{j2}(2\pi) \quad (14)$$

$$V'_{j1}(0) = V'_{j2}(2\pi) \quad (15)$$

In addition, $V_j(x)$ and its derivative must be continuous at the interface:

$$V_{j1}(2\pi\rho_1) = V_{j2}(2\pi\rho_1) \quad (16)$$

$$V'_{j1}(2\pi\rho_1) = V'_{j2}(2\pi\rho_1) \quad (17)$$

From the first periodicity condition (14), it follows that

$$a_{j1} = a_{j2} \cos(2\pi\omega_{j2}) + b_{j2} \sin(2\pi\omega_{j2}). \quad (18)$$

The periodicity of the derivative from (15) yields an equation for b_{j1} :

$$b_{j1} = \frac{-a_{j2}\omega_{j2} \sin(2\pi\omega_{j2}) + b_{j2}\omega_{j2} \cos(2\pi\omega_{j2})}{\omega_{j1}}. \quad (19)$$

The continuity conditions (16), (17) give us the equations

$$\begin{aligned} a_{j1} \cos(2\pi\rho\omega_{j1}) + b_{j1} \sin(2\pi\rho\omega_{j1}) &= a_{j2} \cos(2\pi\rho\omega_{j2}) + \\ & b_{j2} \sin(2\pi\rho\omega_{j2}), \end{aligned} \quad (20)$$

$$\begin{aligned} -a_{j1}\omega_{j1} \sin(2\pi\rho\omega_{j1}) + b_{j1}\omega_{j1} \cos(2\pi\rho\omega_{j1}) &= -a_{j2}\omega_{j2} \sin(2\pi\rho\omega_{j2}) + \\ & b_{j2}\omega_{j2} \cos(2\pi\rho\omega_{j2}). \end{aligned} \quad (21)$$

The equations (18), (19) are substituted into (20) and (21) to eliminate a_{j1} and b_{j1} . Then, we let $\tau_1 = \frac{\alpha_2}{\alpha_1}$ so that $\omega_{j1} = \tau_1\omega_{j2}$, so that ω_{j1} is eliminated from (20) and (21) as well. This yields the homogeneous system of linear equations

$$\left(\begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{bmatrix} + \begin{bmatrix} d_{11} & d_{12} \\ d_{21} & d_{22} \end{bmatrix} \right) \begin{bmatrix} a_{j2} \\ b_{j2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (22)$$

where

$$\begin{aligned}
u_{11} &= c_{22}c_{11} - \frac{1}{\tau_1\omega_{j2}}\omega_{j2}s_{22}s_{11} \\
u_{12} &= s_{22}c_{11} + \frac{1}{\tau_1\omega_{j2}}\omega_{j2}c_{22}s_{11} \\
u_{21} &= -\tau_1\omega_{j2}c_{22}s_{11} - \frac{1}{\tau_1\omega_{j2}}\omega_{j2}s_{22}\tau_1\omega_{j2}c_{11} \\
u_{22} &= -\tau_1\omega_{j2}s_{22}s_{11} + \frac{1}{\tau_1\omega_{j2}}\omega_{j2}c_{22}\tau_1\omega_{j2}c_{11},
\end{aligned}$$

and

$$d_{11} = -c_{12}, \quad d_{12} = -s_{12}, \quad d_{21} = \omega_{j2}s_{12}, \quad d_{22} = -\omega_{j2}c_{12},$$

with $c_{ik} = \cos(2\pi\rho_i\tau_k\omega_{jn})$ and $s_{ik} = \sin(2\pi\rho_i\tau_k\omega_{jn})$. This is the matrix-vector equation for the two-piece case. The basic idea is to extend this to the n -piece case so we can construct a numerical method that will solve the matrix vector equation (22).

The four-piece case can be handled using the same procedure. The conditions based on periodicity and continuity that are similar to Equations (14), (15), (16), and (17) allow us to eliminate parameters and then obtain the system

$$\begin{bmatrix}
-c_{12} & -s_{12} & 0 & 0 & u_{11} & u_{12} \\
\omega_{j2}s_{12} & -\omega_{j2}c_{12} & 0 & 0 & u_{21} & u_{22} \\
c_{22} & s_{22} & -c_{23} & -s_{23} & 0 & 0 \\
-\omega_{j2}s_{12} & \omega_{j2}s_{12} & \omega_{j3}s_{33} & -\omega_{j3}c_{33} & 0 & 0 \\
0 & 0 & c_{33} & s_{33} & -c_{34} & -s_{34} \\
0 & 0 & -\omega_{j3}s_{33} & \omega_{j3}c_{33} & \omega_{j4}s_{34} & -\omega_{j4}c_{34}
\end{bmatrix}
\begin{bmatrix}
a_{j2} \\
b_{j2} \\
a_{j3} \\
b_{j3} \\
a_{j4} \\
b_{j4}
\end{bmatrix}
=
\begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{bmatrix}$$

where

$$\begin{aligned}
u_{11} &= c_{44}c_{11} - \frac{1}{\tau_1\omega_{j4}}\omega_{j4}s_{44}s_{11}, & u_{12} &= s_{44}c_{11} + \frac{1}{\tau_1\omega_{j4}}\omega_{j4}c_{44}s_{11}, \\
u_{21} &= -\tau_1\omega_{j4}c_{44}s_{11} - \frac{1}{\tau_1\omega_{j4}}\tau_1\omega_{j4}^2s_{44}c_{11}, & u_{22} &= -\tau_1\omega_{j4}s_{44}s_{11} + \frac{1}{\tau_1\omega_{j4}}\tau_1\omega_{j4}^2c_{44}c_{11}.
\end{aligned}$$

For the general case of n pieces, we obtain the system

$$M\mathbf{y} = \mathbf{0} \tag{23}$$

which has the form

$$\begin{bmatrix} D_1 & & & & U_0 \\ F_1 & D_2 & & & \\ & F_2 & D_3 & & \\ & & \ddots & \ddots & \\ & & & F_{n-2} & D_{n-1} \end{bmatrix} \begin{bmatrix} a_{j2} \\ b_{j2} \\ \vdots \\ a_{jn} \\ b_{jn} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix}.$$

The matrix M is a block lower triangular matrix plus a rank two-update, with block entries $D_1, \dots, D_{n-1}$, $F_1, \dots, F_{n-2}$ and U_0 defined by

$$D_i = \begin{bmatrix} -c_{i,i+1} & -s_{i,i+1} \\ \omega_{j,i+1} s_{i,i+1} & -\omega_{j,i+1} c_{i,i+1} \end{bmatrix}, \quad (24)$$

$$F_i = \begin{bmatrix} c_{i+1,i+1} & s_{i+1,i+1} \\ -\omega_{j,i+1} s_{i+1,i+1} & \omega_{j,i+1} c_{i+1,i+1} \end{bmatrix}, \quad (25)$$

$$U_0 = \begin{bmatrix} c_{nn}c_{11} - \frac{\omega_{jn}s_{nn}s_{11}}{\tau_1\omega_{jn}} & s_{nn}c_{11} + \frac{\omega_{jn}c_{nn}s_{11}}{\tau_1\omega_{jn}} \\ -\tau_1\omega_{jn}c_{nn}s_{11} - \frac{\tau_1\omega_{jn}^2 s_{nn}c_{11}}{\tau_1\omega_{jn}} & -\tau_1\omega_{jn}s_{nn}s_{11} + \frac{\tau_1\omega_{jn}^2 c_{nn}c_{11}}{\tau_1\omega_{jn}} \end{bmatrix}, \quad (26)$$

where we again use the notation $c_{ik} = \cos(2\pi\rho_i\tau_k\omega_{jn})$ and $s_{ik} = \sin(2\pi\rho_i\tau_k\omega_{jn})$.

The matrix M can be written as

$$M = M_0 + UX^T, \quad U = \begin{bmatrix} U_0 \\ 0 \end{bmatrix}, \quad X = \begin{bmatrix} 0 \\ I_2 \end{bmatrix} \quad (27)$$

where I_2 is a 2×2 identity matrix. The vector $\mathbf{y}$ is made up of the unknown coefficients of our eigenfunctions except the initial a_{j1} and b_{j1} that were found earlier using periodicity conditions:

$$\mathbf{y} = \begin{bmatrix} a_{j2} \\ b_{j2} \\ \vdots \\ a_{jn} \\ b_{jn} \end{bmatrix}. \quad (28)$$

In order to obtain $\mathbf{y} \in \ker(M)$, we need to find values of ω_{jn} that make $\det(M) = 0$.

From the Matrix Determinant Lemma, we have

$$\det(M) = \det(D_1) \det(D_2) \dots \det(D_{n-1}) \det(I_2 + X^T Z), \quad M_0 Z = U. \quad (29)$$

Because M_0 is block lower bidiagonal, with 2×2 blocks, Z is easily computed in $O(n)$ arithmetic operations using block forward substitution. M_0 is invertible, as the determinant of the 2×2 D_i blocks are nonzero; specifically, $\det D_i = \omega_{i+1}$. This allows us to focus on the last determinant, of $I_2 + X^T Z$. This determinant is then passed through the secant method, with initial guesses obtained using the *SAK* principle as described in Section 2, to find the values of ω_{j_n} that make $\det(M) = 0$.

Once M is made singular, the system (23) can be rewritten as

$$M_0 \mathbf{y} + U X^T \mathbf{y} = \mathbf{0}. \quad (30)$$

Then, after multiplying by M_0^{-1} , which is known to exist, we have

$$\mathbf{y} + Z X^T \mathbf{y} = \mathbf{0}$$

and we can multiply both sides by X^T , which yields the equation

$$X^T \mathbf{y} + X^T Z X^T \mathbf{y} = \mathbf{0}.$$

We can then factor out $X^T \mathbf{y}$ to obtain

$$(I_2 + X^T Z)(X^T \mathbf{y}) = \mathbf{0}. \quad (31)$$

If we define $R = I_2 + X^T Z$ and $\mathbf{g} = X^T \mathbf{y}$, the system (31) reduces to

$$R \mathbf{g} = \mathbf{0}. \quad (32)$$

If we let

$$R = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

then we have solutions

$$\mathbf{g}_1 = \begin{bmatrix} b \\ -a \end{bmatrix}, \quad \mathbf{g}_2 = \begin{bmatrix} d \\ -c \end{bmatrix}.$$

We then choose

$$\mathbf{g} = \begin{bmatrix} a_{j_n} \\ b_{j_n} \end{bmatrix}$$

to be the larger of $\mathbf{g}_1$ and $\mathbf{g}_2$ in magnitude, which can be measured using, for example, the ℓ_2 norm on $\mathbb{R}^2$ defined as $\sqrt{(a_{j_n})^2 + (b_{j_n})^2}$, to avoid difficulties

caused by roundoff error. Now that we have a_{jn} and b_{jn} , we can substitute $X^T \mathbf{y} = \mathbf{g}$ into equation (30) to obtain

$$M_0 \mathbf{y} + U \mathbf{g} = \mathbf{0}$$

which has the unique solution

$$\mathbf{y} = -Z \mathbf{g}. \quad (33)$$

From (18) and (19) that came from the periodicity conditions, we obtain a_{j1} and b_{j1} . Now that we have solved for all of the coefficients as well as the frequencies ω_{ji} , $i = 1, 2, \dots, n$, we can construct the eigenfunctions of our differential operator. The following theorem and its proof describe this construction.

Theorem 1. *Let ω_{jn} be such that the matrix M from (23) is singular. Let $\mathbf{y}$ be defined as in (28) and computed as in (33), where Z is as defined in (29) and $\mathbf{g}$ is a nontrivial solution of (32), where $R = I_2 + X^T Z$ and X is as defined in (27). Furthermore, let a_{j1} and b_{j1} be given by*

$$a_{j1} = a_{jn} \cos(2\pi\omega_{jn}) + b_{jn} \sin(2\pi\omega_{jn}), \quad (34)$$

$$b_{j1} = \frac{-a_{jn}\omega_{jn} \sin(2\pi\omega_{jn}) + b_{jn}\omega_{jn} \cos(2\pi\omega_{jn})}{\omega_{j1}}. \quad (35)$$

Finally, let $\omega_{j1}, \dots, \omega_{jn}$ satisfy (8). Then $V_j(x)$, as defined in (13), is a $C^1(\mathbb{R})$ 2π -periodic eigenfunction of the operator $L = -\alpha(x)^2 \partial^2 / \partial x^2$, where $\alpha(x)$ is as defined in (1), with corresponding eigenvalue $\lambda_n = (\alpha_n \omega_{jn})^2$.

Proof: In view of (29), because $\det M = 0$ and the blocks $D_1, \dots, D_{n-1}$ are nonsingular, it follows that R is singular so (32) has a nontrivial solution $\mathbf{g}$. We then have

$$\begin{aligned} M\mathbf{y} &= M_0 \mathbf{y} + U X^T \mathbf{y} \\ &= -M_0 Z \mathbf{g} - U X^T Z \mathbf{g} \\ &= -U \mathbf{g} - U X^T Z \mathbf{g} \\ &= -U(I_2 + X^T Z) \mathbf{g} \\ &= -U R \mathbf{g} \\ &= \mathbf{0}. \end{aligned}$$

We now consider $V_j(x)$ from (13), with its coefficients $a_{j2}, b_{j2}, \dots, a_{jn}, b_{jn}$ taken from the entries of $\mathbf{y}$ and (34), (35). From (34), (35), both $V_j(x)$ and $V'_j(x)$ are 2π -periodic. From the equations

$$F_i \begin{bmatrix} a_{j,i+1} \\ b_{j,i+1} \end{bmatrix} + D_{i+1} \begin{bmatrix} a_{j,i+2} \\ b_{j,i+2} \end{bmatrix} = \mathbf{0}, \quad i = 1, 2, \dots, n-2,$$

and from (24), (25), we obtain, for $i = 1, 2, \dots, n-2$,

$$\begin{aligned} a_{j,i+1} \cos(2\pi\rho_{i+1}\omega_{j,i+1}) + \\ b_{j,i+1} \sin(2\pi\rho_{i+1}\omega_{j,i+1}) &= a_{j,i+2} \cos(2\pi\rho_{i+1}\omega_{j,i+2}) + \\ &\quad b_{j,i+2} \sin(2\pi\rho_{i+1}\omega_{j,i+2}), \\ -a_{j,i+1}\omega_{j,i+1} \sin(2\pi\rho_{i+1}\omega_{j,i+1}) + \\ b_{j,i+1}\omega_{j,i+1} \cos(2\pi\rho_{i+1}\omega_{j,i+1}) &= -a_{j,i+2}\omega_{j,i+2} \sin(2\pi\rho_{i+1}\omega_{j,i+2}) + \\ &\quad b_{j,i+2}\omega_{j,i+2} \cos(2\pi\rho_{i+1}\omega_{j,i+2}), \end{aligned}$$

from which we can conclude that $V_j(x)$ and $V'_j(x)$ are continuous at $x = 2\pi\rho_2, \dots, 2\pi\rho_{n-1}$. Similarly, from

$$D_1 \begin{bmatrix} a_{j2} \\ b_{j2} \end{bmatrix} + u_0 \begin{bmatrix} a_{jn} \\ b_{jn} \end{bmatrix} = \mathbf{0},$$

we can establish continuity of $V_j(x)$ and $V'_j(x)$ at $x = 2\pi\rho_1$ as well. To see this, we note that

$$u_0 \begin{bmatrix} a_{jn} \\ b_{jn} \end{bmatrix} = F_0 \begin{bmatrix} a_{j1} \\ b_{j1} \end{bmatrix},$$

as a consequence of (34), (35). Combined with periodicity, we have that $V_j(x)$ and $V'_j(x)$ are continuous on the entire real line. Finally, to establish that $V_j(x)$ is an eigenfunction, we have, on $[2\pi\rho_{i-1}, 2\pi\rho_i)$,

$$LV_j(x) = \alpha_i^2 \omega_{ji}^2 [a_{ji} \cos(\omega_{ji}x) + b_{ji} \sin(\omega_{ji}x)] = (\alpha_n \omega_{jn})^2 V_j(x),$$

in view of (8). $\square$

3.2. Self-adjoint Case

For the self-adjoint operator $A(x, D) = D\alpha^2(x)D$, we again define each eigenfunction $V_j(x)$, $j = 1, 2, \dots$, as in (13). The frequencies $\{\omega_{ji}\}_{i=1}^n$ are related by

$$\begin{aligned} \alpha_1 \omega_{j1} &= \dots = \alpha_n \omega_{jn} \\ \tau_i &= \frac{\alpha_n}{\alpha_i}, \quad \omega_{ji} = \tau_1 \omega_{in}, \quad i = 1, \dots, n-1. \end{aligned}$$

By substituting $\omega_{ji} = \tau_i \omega_{jn}$ we have

$$\begin{aligned}
a_1 \cos(\tau_1 \omega_{jn} x) + b_1 \sin(\tau_1 \omega_{jn} x) &= V_{j1}(x) \\
a_2 \cos(\tau_2 \omega_{jn} x) + b_2 \sin(\tau_2 \omega_{jn} x) &= V_{j2}(x) \\
&\vdots \\
a_{n-1} \cos(\tau_{n-1} \omega_{jn} x) + b_{n-1} \sin(\tau_{n-1} \omega_{jn} x) &= V_{j,n-1}(x) \\
a_n \cos(\tau_n \omega_{jn} x) + b_n \sin(\tau_n \omega_{jn} x) &= V_{jn}(x)
\end{aligned}$$

By applying the periodicity condition $V_j(0) = V_j(2\pi)$, we can write

$$a_1 = a_n \cos(\tau_n \omega_{jn} 2\pi) + b_n \sin(\tau_n \omega_{jn} 2\pi)$$

Enforcing continuity at the interfaces,

$$V_{ji}(2\pi \rho_i) = V_{j,i+1}(2\pi \rho_i), \quad i = 1, 2, \dots, i-1,$$

yields the conditions

$$\begin{aligned}
a_1 \cos(\tau_1 \omega_{jn} 2\pi \rho_1) + b_1 \sin(\tau_1 \omega_{jn} 2\pi \rho_1) &= a_2 \cos(\tau_2 \omega_{jn} 2\pi \rho_1) + b_2 \sin(\tau_2 \omega_{jn} 2\pi \rho_1) \\
a_2 \cos(\tau_2 \omega_{jn} 2\pi \rho_2) + b_2 \sin(\tau_2 \omega_{jn} 2\pi \rho_2) &= a_3 \cos(\tau_3 \omega_{jn} 2\pi \rho_2) + b_3 \sin(\tau_3 \omega_{jn} 2\pi \rho_2) \\
&\vdots \\
a_{n-2} \cos(\tau_{n-2} \omega_{jn} 2\pi \rho_{n-2}) + & \\
b_{n-2} \sin(\tau_{n-2} \omega_{jn} 2\pi \rho_{n-2}) &= a_{n-1} \cos(\tau_{n-1} \omega_{jn} 2\pi \rho_{n-2}) + \\
&b_{n-1} \sin(\tau_{n-1} \omega_{jn} 2\pi \rho_{n-2}) \\
a_{n-1} \cos(\tau_{n-1} \omega_{jn} 2\pi \rho_{n-1}) + & \\
b_{n-1} \sin(\tau_{n-1} \omega_{jn} 2\pi \rho_{n-1}) &= a_n \cos(\tau_n \omega_{jn} 2\pi \rho_{n-1}) + \\
&b_n \sin(\tau_n \omega_{jn} 2\pi \rho_{n-1}).
\end{aligned}$$

From the matching of conormal derivatives (see [14, 13]),

$$\alpha_i^2 V'_{ji}(2\pi \rho_i) = \alpha_{i+1}^2 V'_{j,i+1}(2\pi \rho_i), \quad i = 1, 2, \dots, n-1,$$

we obtain the conditions

$$\begin{aligned}
-a_1 \sin(\tau_1 \omega_{jn} 2\pi \rho_1) + b_1 \cos(\tau_1 \omega_{jn} 2\pi \rho_1) &= \frac{\tau_1}{\tau_2} (-a_2 \sin(\tau_2 \omega_{jn} 2\pi \rho_1) + b_2 \cos(\tau_2 \omega_{jn} 2\pi \rho_1)) \\
-a_2 \sin(\tau_2 \omega_{jn} 2\pi \rho_2) + b_2 \cos(\tau_2 \omega_{jn} 2\pi \rho_2) &= \frac{\tau_2}{\tau_3} (-a_3 \sin(\tau_3 \omega_{jn} 2\pi \rho_2) + b_3 \cos(\tau_3 \omega_{jn} 2\pi \rho_2)) \\
&\vdots \\
-a_{n-2} \sin(\tau_{n-2} \omega_{jn} 2\pi \rho_{n-2}) + & \\
b_{n-2} \cos(\tau_{n-2} \omega_{jn} 2\pi \rho_{n-2}) &= \frac{\tau_{n-2}}{\tau_{n-1}} (-a_{n-1} \sin(\tau_{n-1} \omega_{jn} 2\pi \rho_{n-2}) + \\
&b_{n-1} \cos(\tau_{n-1} \omega_{jn} 2\pi \rho_{n-2})) \\
-a_{n-1} \sin(\tau_{n-1} \omega_{jn} 2\pi \rho_{n-1}) + & \\
b_{n-1} \cos(\tau_{n-1} \omega_{jn} 2\pi \rho_{n-1}) &= \frac{\tau_{n-1}}{\tau_n} (-a_n \sin(\tau_n \omega_{jn} 2\pi \rho_{n-1}) + \\
&b_n \cos(\tau_n \omega_{jn} 2\pi \rho_{n-1}))
\end{aligned}$$

Let $V_0(x)$ denote the eigenfunction corresponding to $\lambda_0 = 0$, so $V_0(x) \equiv 1$. From the orthogonality of the eigenfunctions, we have $\langle V_j, V_0 \rangle = 0$, or

$$\begin{aligned}
&\int_0^{2\pi \rho_1} [a_1 \cos(\tau_1 \omega_{jn} x) + b_1 \sin(\tau_1 \omega_{jn} x)] dx + \\
&\int_{2\pi \rho_1}^{2\pi \rho_2} [a_2 \cos(\tau_2 \omega_{jn} x) + b_2 \sin(\tau_2 \omega_{jn} x)] dx + \\
&\cdots + \int_{2\pi \rho_{n-2}}^{2\pi \rho_{n-1}} [a_{n-1} \cos(\tau_{n-1} \omega_{jn} x) + b_{n-1} \sin(\tau_{n-1} \omega_{jn} x)] dx + \\
&\int_{2\pi \rho_{n-1}}^{2\pi} [a_n \cos(\tau_n \omega_{jn} x) + b_n \sin(\tau_n \omega_{jn} x)] dx = 0.
\end{aligned}$$

After applying all of the above conditions, we have $2n$ constraints that form the homogeneous system $M\mathbf{y} = \mathbf{0}$, where

$$M = \begin{bmatrix} D_1 & & & & & F_1 \\ F_2 & D_2 & & & & \\ & \ddots & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & \ddots & \ddots & \\ E_1 & \cdots & \cdots & E_{n-2} & F_n & D_n \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} a_2 \\ b_2 \\ \vdots \\ a_n \\ b_n \\ a_1 \\ b_1 \end{bmatrix}. \quad (36)$$

The block entries have the form

$$\begin{aligned}
D_i &= \begin{bmatrix} \frac{-c_{i+1,i}}{\tau_{i+1}} & \frac{-s_{i+1,i}}{\tau_{i+1}} \\ \frac{\tau_i s_{i+1,i}}{\tau_{i+1}} & -\frac{\tau_i c_{i+1,i}}{\tau_{i+1}} \end{bmatrix}, \quad i = 1, \dots, n-1, \\
D_n &= \begin{bmatrix} s_{11} & (-c_{11} + 1) \\ -1 & 0 \end{bmatrix}, \\
F_i &= \begin{bmatrix} c_{i,i} & s_{i,i} \\ -s_{i,i} & c_{i,i} \end{bmatrix}, \quad i = 1, \dots, n-1, \\
F_n &= \begin{bmatrix} \frac{s_{n,n} - s_{n,n-1}}{\omega_{jn}\tau_n} & \frac{-c_{n,n} + c_{n,n-1}}{\omega_{jn}\tau_n} \\ c_{n,n} & s_{n,n} \end{bmatrix}, \\
E_i &= \begin{bmatrix} \frac{s_{n,n} - s_{n,n-1}}{\omega_{jn}\tau_n} & \frac{-c_{n,n} + c_{n,n-1}}{\omega_{jn}\tau_n} \\ 0 & 0 \end{bmatrix}, \quad i = 1, \dots, n-2,
\end{aligned}$$

where, as before, $c_{ik} = \cos(2\pi\rho_i\tau_k\omega_{jn})$ and $s_{ik} = \sin(2\pi\rho_i\tau_k\omega_{jn}) = s_{ik}$.

From the Matrix Determinant Lemma, we have

$$\det(M) = \det(M_0) \det(I_2 + X^T M_0^{-1} U) = \left(\prod_{i=1}^n \det(D_i) \right) \det(I_2 + X^T M_0^{-1} U)$$

where

$$M_0^{-1} U = Z = \begin{bmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_n \end{bmatrix}, \quad U = \begin{bmatrix} F_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad X^T = \begin{bmatrix} 0 & \dots & 0 & I_2 \end{bmatrix},$$

and block forward substitution yields

$$\begin{aligned}
Z_1 &= D_1^{-1} F_1 \\
Z_2 &= -D_2^{-1} F_2 D_1^{-1} F_1 \\
Z_3 &= D_3^{-1} F_3 D_2^{-1} F_2 D_1^{-1} F_1 \\
&\vdots \\
Z_n &= -D_n^{-1} \left(\sum_{i=1}^{n-2} E_i Z_i + F_n Z_{n-1} \right)
\end{aligned}$$

Proceeding as in the non-self-adjoint case, we can solve $M\mathbf{y} = \mathbf{0}$ by first solving

$$(I_2 + X^T Z)\mathbf{g} = \mathbf{0}, \quad \mathbf{g} = X^T \mathbf{y} = \begin{bmatrix} a_1 \\ b_1 \end{bmatrix}$$

and then solving $M_0 \mathbf{y} = -U\mathbf{g}$ which yields

$$\mathbf{y} = -Z\mathbf{g} = \begin{bmatrix} a_2 \\ b_2 \\ \vdots \\ a_n \\ b_n \\ \mathbf{z} \end{bmatrix}$$

We are now able to construct the eigenfunctions. The correctness of these eigenfunctions can be verified in the same way as in the proof of Theorem 1.

3.3. Solving for ω_{jn} by Iteration

Using the estimate of ω_{jn} suggested by the *SAK* principle as described in Section 2, we can solve the equation

$$\det(I_2 + X^T M_0^{-1} U) = 0$$

for ω_{jn} by iteration, using this estimate as an initial guess. For this purpose, we use the secant method, as it is rapidly convergent and does not require the evaluation of derivatives.

Let $\omega_{jn}^{(0)}$ be the estimate obtained via the *SAK* principle. For our second initial guess that is required by the secant method, we simply perturb $\omega_{jn}^{(0)}$. We also “safeguard” the iteration by requiring all iterates to fall within the interval $|\omega - \omega_{jn}^{(0)}| < \omega_{1n}^{(0)}$. We remind the reader that each $\omega_{jn}^{(0)}$ is an integer multiple of $\omega_{1n}^{(0)}$. If an iterate generated by the secant method falls outside this interval, we reject it, and substitute an alternative iterate as follows:

- If there has been at least one positive value and one negative value of the determinant, then we perform one iteration of bisection, and update the search interval accordingly.
- If all iterates produce determinants of the same sign, then we set our new iterate equal to the midpoint of the largest interval between iterates.

Generally, for j odd, $\omega_{jn}^{(0)}$ is near the exact values of ω_{jn} and $\omega_{j+1,n}$, and in most cases, it has been observed to lie between these values. Therefore, after obtaining ω_{jn} by iteration, we adjust the initial guess $\omega_{j+1,n}^{(0)}$ as follows:

$$\omega_{j+1,n}^{(0)} = 2\omega_{jn}^{(0)} - \omega_{jn}.$$

We also reduce the search interval by half, according to whether ω_{jn} is less than or greater than $\omega_{jn}^{(0)}$. For example, in the case $\omega_{jn} < \omega_{jn}^{(0)}$, we search for $\omega_{j+1,n}$ in the interval $(\omega_{jn}^{(0)}, \omega_{jn}^{(0)} + \omega_{1n}^{(0)})$. If the secant iteration fails, then we search in the interval $(\omega_{jn}^{(0)} - \omega_{1n}^{(0)}, \omega_{jn}^{(0)})$.

3.4. Algorithm Description

We now describe, in pseudocode, the algorithms for computing the eigenvalues and eigenfunctions, and from there, the solution of a PDE with given initial data. We first consider the non-self-adjoint case. The following algorithm describes the computation of $\omega_{2j-1,n}$ and $\omega_{2j,n}$ corresponding to a pair of nonzero eigenvalues $\lambda_{2j-1}, \lambda_{2j}$. The vectors $\vec{\tau}$ and $\vec{\rho}$ consist of the values $\tau_1, \dots, \tau_n$ and $\rho_1, \dots, \rho_{n-1}$, respectively.

function $[\omega_{2j-1,n}, \omega_{2j,n}] = \text{getpair}(\vec{\tau}, \vec{\rho}, j)$

Obtain $\omega_{2j-1,n}^{(0)}$ as in (12)

Solve $\det(R) = 0$ for $\omega_{2j-1,n}$ using iteration

$R = I_2 + X^T Z$, defined as in Section 3.1

Use $\omega_{2j-1,n}^{(0)}$ and a small perturbation as initial guesses

$\omega_{2j,n}^{(0)} = 2\omega_{2j-1,n}^{(0)} - \omega_{2j-1,n}$

Solve $\det(R) = 0$ for $\omega_{2j,n}$ using iteration

Use $\omega_{2j,n}^{(0)}$ and a small perturbation as initial guesses

We now describe the overall process, that relies on the **getpair** function. We denote by $\mathbf{x}$ a vector of equally spaced grid points in $[0, 2\pi)$, that is partitioned into vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ such that the elements of $\mathbf{x}_i$ belong to $[2\pi\rho_{i-1}, 2\pi\rho_i)$ for $i = 1, 2, \dots, n$. The initial data $f(x)$ is described by a vector $\mathbf{f}$ consisting of the values of $f(x)$ at the grid points in $\mathbf{x}$. The output of this algorithm is a vector $\mathbf{u}$ that contains an approximation of the solution $u(x, t)$ of (2) on $(0, 2\pi)$, evaluated at the grid points in $\mathbf{x}$, for given t .

$$\mathbf{v}_0 = \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}^T \in \mathbb{R}^n$$

$$\mathbf{w}_0 = 1/\alpha(\mathbf{x})^2$$

```

u =  $\mathbf{v}_0 \mathbf{v}_0^T \mathbf{f} / \mathbf{w}_0^T \mathbf{v}_0$ 
for  $j = 1, 2, \dots$  do
     $[\omega_{2j-1,n}, \omega_{2j,n}] = \text{getpair}(\vec{\tau}, \vec{\rho}, j)$ 
    for  $i = 2j - 1, 2j$  do
         $\lambda_i = \alpha_n^2 \omega_{i,n}^2$ 
        Form  $M_0$ ,  $U$  and  $X$  as in (27)
        Solve  $M_0 Z = U$  using block forward substitution
         $R = I_2 + X^T Z$ 
         $P = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$ 
         $G = P R^T$ 
        Let  $\mathbf{g}$  be the column of  $G$  with largest  $\ell_2$ -norm
        Solve  $M_0 \mathbf{y} = -U \mathbf{g}$  using block forward substitution
        for  $k = 2, \dots, n$  do
             $a_k = y_{2k-3}$ 
             $b_k = y_{2k-2}$ 
        end for
         $a_1 = a_n \cos(2\pi\omega_{in}) + b_n \sin(2\pi\omega_{in})$ 
         $b_1 = (-a_n \omega_{in} \sin(2\pi\omega_{in}) + b_n \omega_{in} \cos(2\pi\omega_{in})) / (\tau_1 \omega_{in})$ 
         $\mathbf{v}_1 = a_1 \cos(\omega_{i1} \mathbf{x}_1) + b_1 \sin(\omega_{i1} \mathbf{x}_1)$ 
        for  $k = 2, \dots, n$  do
             $\mathbf{v}_i = \begin{bmatrix} \mathbf{v}_i \\ a_k \cos(\omega_{ik} \mathbf{x}_k) + b_k \sin(\omega_{ik} \mathbf{x}_k) \end{bmatrix}$ 
        end for
         $\mathbf{w}_j = \mathbf{v}_j / \alpha(\mathbf{x})^2$ 
         $\mathbf{u} = \mathbf{u} + e^{-\lambda_i t} \mathbf{v}_i \mathbf{w}_i^T \mathbf{f} / \mathbf{w}_i^T \mathbf{v}_i$ 
    end for
end for

```

The outermost loop terminates when the terms added to $\mathbf{u}$ are smaller than a chosen tolerance.

We now describe the algorithm for the self-adjoint case, which is similar. In fact, the function **getpair** is no different; it simply works with the equation $\det(M) = 0$, where M is as defined in (36). The overall process for solving (3) with given initial data $f(x)$, represented by the vector $\mathbf{f}$, and time t is as follows.

$\mathbf{u} = \text{mean}(\mathbf{f})$

```

for  $j = 1, 2, \dots$  do
   $[\omega_{2j-1,n}, \omega_{2j,n}] = \text{getpair}(\vec{\tau}, \vec{\rho}, j)$ 
  for  $i = 2j - 1, 2j$  do
     $\lambda_i = \alpha_n^2 \omega_{i,n}^2$ 
    Form  $M = M_0 + UX^T$  as in (36)
    Solve  $M_0 Z = U$  using block forward substitution
     $R = I_2 + X^T Z$ 
     $P = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$ 
     $G = PR^T$ 
    Let  $\mathbf{g}$  be the column of  $G$  with largest  $\ell_2$ -norm
    Solve  $M_0 \mathbf{y} = -U\mathbf{g}$  using block forward substitution
    for  $k = 2, \dots, n$  do
       $a_k = y_{2k-3}$ 
       $b_k = y_{2k-2}$ 
    end for
     $a_1 = y_{2n-1}$ 
     $b_1 = y_{2n}$ 
     $\mathbf{v}_1 = a_1 \cos(\omega_{i1} \mathbf{x}_1) + b_k \sin(\omega_{i1} \mathbf{x}_1)$ 
    for  $k = 2, \dots, n$  do
       $\mathbf{v}_i = \begin{bmatrix} \mathbf{v}_i \\ a_k \cos(\omega_{ik} \mathbf{x}_k) + b_k \sin(\omega_{ik} \mathbf{x}_k) \end{bmatrix}$ 
    end for
     $\mathbf{u} = \mathbf{u} + e^{-\lambda_i t} \mathbf{v}_i \mathbf{v}_i^T \mathbf{f} / \mathbf{v}_i^T \mathbf{v}_i$ 
  end for
end for

```

4. Numerical Results

In this section we demonstrate the effectiveness of our approach for computing eigenvalues and eigenfunctions of the spatial differential operators under consideration, and also using them to solve the diffusion equations (2) and (3). We will compare the computed eigenvalues to those obtained using the MATLAB function `eigs` on a sparse matrix A that discretizes each operator by finite differences in the non-self-adjoint case, and finite elements with piecewise linear basis functions, and elements of equal width, in the self-adjoint case.

When solving PDEs, we compare our approach, labeled “eig-exp” in tables, to the following methods, all of which use the appropriate matrix A :

- Crank-Nicolson (labeled “C-N” in tables),
- Approximating $e^{-At}\mathbf{u}(0)$ using rational Krylov projection, as in [21] (labeled “Krylov” in tables), and
- The MATLAB ODE solver `ode15s` (labeled “`ode15s`” in tables).

We apply these methods with different grid sizes $N = 1024, 2048, 4096$ to examine scalability and spatial convergence. To measure accuracy, solutions are compared to a reference solution computed using `ode15s` with a larger number of grid points, $N_{\text{ref}} = 16,384$, and the smallest allowed time step.

We calculate the error $\mathcal{E}_N$ in each computed solution $\tilde{\mathbf{u}}^N$ with respect to the reference solution $\mathbf{u}^{N_{\text{ref}}}$ by the ℓ_∞ norm of the difference between the computed solution and the restriction of the reference solution to the N -point grid; that is,

$$\mathcal{E}_N = \max_{1 \leq i \leq N} |u_{m(i)}^{N_{\text{ref}}} - \tilde{u}_i^N|,$$

where $m(i) = \frac{N_{\text{ref}}}{N}(i - 1) + 1$ is used to map the values of $\mathbf{u}^N$ on its N -point grid to the N_{ref} -point grid on which the reference solution is computed.

The value of N_{ref} was the largest power of 2 such that MATLAB could compute solutions via `ode15s` for all cases without exceeding storage limits. We note that each reference solution required, at minimum, approximately 30 seconds (for $t_f = 0.01$) to several minutes (for $t_f = 1$) to compute, which, as will be seen in this section, is not competitive with any of the methods featured.

4.1. Non-Self-adjoint Case

4.1.1. Computing Eigenvalues

Tables 1-4 show the smallest ten nonzero eigenvalues of the operator $-\alpha^2(x)\partial_x^2$, as computed using the *SAK* principle with secant iteration, as in Section 3.1, and using the MATLAB function `eigs` with a $N \times N$ matrix obtained via finite-difference discretization. In Tables 1 and 3, $N = 2^{12}$, and in Tables 2 and 4, $N = 2^{23}$. Tables 1 and 2 feature a coefficient with $n = 4$ pieces, while $n = 7$ in Tables 3 and 4.

The number of iterations of the secant method is reported in each table. The relative error shown in these tables is the relative difference between the

two sets of computed eigenvalues. The error in the eigenvalues obtained by secant iteration arises only from roundoff error and the termination of the iteration, which occurs when the absolute difference between iterates is less than 10^{-8} . As such, the error given in the tables is actually indicative of the error in the eigenvalues computed by `eigs`. By comparing the results for the two grid sizes, it can be seen that these eigenvalues are generally converging to the ones obtained via secant iteration.

j	$\lambda_j(SAK)$	$\lambda_j(eig)$	iterations	relative error
1	2.213728201966723	2.214546835371368	8	3.70e-04
2	3.908115974058471	3.911393874896230	6	8.39e-04
3	10.082518215776597	10.094371927238504	8	1.18e-03
4	13.388169744247897	13.388419936929154	5	1.87e-05
5	24.341673078716386	24.282295735999661	8	2.44e-03
6	28.324126848500523	28.372268962285855	6	1.70e-03
7	45.780880112858526	45.788474347323032	8	1.66e-04
8	48.879344768381820	48.851440781676736	7	5.71e-04
9	68.937479644237115	68.960230443978261	7	3.30e-04
10	78.422800516160351	78.488178032528552	5	8.34e-04

Table 1: Eigenvalues computed using the *SAK* principle with secant iteration, and `eigs` on a finite-difference matrix, of the operator $-\alpha^2(x)\partial_x^2$ with $\vec{\alpha} = [1, 2, 3, 4]$, $\vec{\rho} = [3/8, 1/2, 3/4]$ and $N = 4,096$ grid points.

j	$\lambda_j(SAK)$	$\lambda_j(eig)$	iterations	relative error
1	2.213728201966723	2.213728529834787	8	1.48e-07
2	3.908115974058471	3.908111184822544	6	1.23e-06
3	10.082518215776597	10.082519780918508	8	1.55e-07
4	13.388169744247897	13.388165032603471	5	3.52e-07
5	24.341673078716386	24.341667699188690	8	2.21e-07
6	28.324126848500523	28.324127431593521	6	2.06e-08
7	45.780880112858526	45.780880262752021	8	3.27e-09
8	48.879344768381820	48.879180460807362	7	3.36e-06
9	68.937479644237115	68.937529509562850	7	7.23e-07
10	78.422800516160351	78.422819299731756	5	2.40e-07

Table 2: Eigenvalues computed using the *SAK* principle with secant iteration, and `eigs` on a finite-difference matrix, of the operator $-\alpha^2(x)\partial_x^2$ with $\vec{\alpha} = [1, 2, 3, 4]$, $\vec{\rho} = [3/8, 1/2, 3/4]$ and $N = 8,388,608$ grid points.

4.1.2. Solving PDEs

Tables 5-16 compare the performance of the methods listed at the beginning of this section for solving the heat equation (2) at $t = t_f$, in terms of efficiency (odd-numbered tables) and accuracy (even-numbered tables). We use smooth initial data $u(x, 0) = \sin 2x$ or a smoothed characteristic function

j	$\lambda_j(SAK)$	$\lambda_j(eig)$	iterations	relative err
1	2.208768644228804	2.209651291736346	8	4.00e-04
2	3.698554293240147	3.702052427217607	6	9.45e-04
3	9.835635137659720	9.828492009057010	7	7.26e-04
4	12.720325761465526	12.729268908769621	5	7.03e-04
5	22.868339996850548	22.875773648650320	7	3.25e-04
6	27.588004958504420	27.599415204504702	6	4.14e-04
7	43.421531530822222	43.457994198681568	6	8.40e-04
8	46.394983148646915	46.396792705599310	9	3.90e-05
9	66.148542025384060	66.108839948075811	8	6.00e-04
10	78.425134748368009	78.184966066576692	5	3.06e-03

Table 3: Eigenvalues computed using the *SAK* principle with secant iteration, and **eigs** on a finite-difference matrix, of the operator $-\alpha^2(x)\partial_x^2$ with $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$, $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$ and $N = 4,096$ grid points.

j	$\lambda_j(SAK)$	$\lambda_j(eig)$	iterations	relative err
1	2.208768644228804	2.208769184319859	8	2.45e-07
2	3.698554293240147	3.698550379791000	6	1.06e-06
3	9.835635137659720	9.835640922799071	7	5.88e-07
4	12.720325761465526	12.720321404686686	5	3.43e-07
5	22.868339996850548	22.868328754223263	7	4.92e-07
6	27.588004958504420	27.588006625416060	5	6.04e-08
7	43.421531530822222	43.421536596326689	6	1.17e-07
8	46.394983148646915	46.394956202557971	9	5.81e-07
9	66.148542025384060	66.148534991216707	8	1.06e-07
10	78.425134748368009	78.425179055166083	5	5.65e-07

Table 4: Eigenvalues computed using the *SAK* principle with secant iteration, and **eigs** on a finite-difference matrix, of the operator $-\alpha^2(x)\partial_x^2$ with $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$, $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$ and $N = 8,388,608$ grid points.

that still has steep jumps,

$$u(x, 0) = \left(\frac{1}{\pi} \tan^{-1}(d(x - c_1)) + \frac{\pi}{2} \right) - \left(\frac{1}{\pi} \tan^{-1}(d(x - c_2)) + \frac{\pi}{2} \right), \quad (37)$$

with $c_1 = 3\pi/4$, $c_2 = 5\pi/4$ and $d = 40$, the graph of which is shown in Figure 2. The piecewise constant coefficient $\alpha^2(x)$ consists of either four, seven or eight pieces. The three choices of $\alpha(x)$ featured in these experiments are shown in Figure 3.

The various methods used are configured as follows:

- For eigenfunction expansion, we compute eigenvalues $\lambda_0, \lambda_1, \dots, \lambda_m$ and eigenfunctions $V_0(x), V_1(x), \dots, V_m(x)$ using the algorithm described in Section 3.1, where m is chosen so that $e^{-\lambda_j t_f} < \epsilon$ for $j > m$ and $\epsilon = 10^{-4}$. Then, the approximate solution is obtained from the eigen-

Figure 2: Smoothed characteristic function used as initial data $u(x, 0)$

function expansion

$$u(x, t) \approx \sum_{j=0}^m V_j(x) e^{-\lambda_j t} \frac{\langle W_j, u(\cdot, 0) \rangle}{\langle W_j, V_j \rangle}$$

where $W_j(x) = V_j(x)/\alpha^2(x)$ is the eigenfunction of the adjoint operator $-(\alpha^2(x)\partial_x^2)^*$ corresponding to λ_j and $\langle \cdot, \cdot \rangle$ is the standard inner product on $[0, 2\pi]$.

- Crank-Nicolson performs 100 time steps of length $t_f/100$.
- Krylov projection produces iterates $\mathbf{u}_1, \dots, \mathbf{u}_p$, such that $\|\mathbf{u}_p - \mathbf{u}_{p-1}\|_\infty < 10^{-4} \|\mathbf{u}_p\|_\infty$.
- The value Δt_{avg} reported in the tables is the average time step length used by `ode15s` to obtain a solution that satisfies its default error tolerance.

It can be seen that generally, our method computes the solution at time t_f with greater efficiency than the other methods, with rational Krylov projection being the closest competitor. It is worth noting that as the number

Figure 3: Choices of $\alpha(x)$ used in numerical experiments, with four (upper left plot), seven (upper right plot) and eight (lower plot) pieces.

of grid points N increases, the execution time increases more substantially for all of the other methods, compared to eigenfunction expansion. That is, eigenfunction expansion is more scalable. This is shown in Figure 4, which displays the execution times from Table 7 to show that not only is the time taken by our method less, but it also grows at a slower rate as N increases.

Furthermore, our method is much more parallelizable, as all of the eigenpairs can be computed independently of one another, whereas the other methods featured do not lend themselves to parallelism. For our method, such parallelism was not included in the results presented in this paper. Figures 5-10 show the solutions computed by the different methods. We see that, visually, the solutions computed by all four methods match one another, just as the tables indicate that the error in these solutions is generally small.

Regarding accuracy, we see that generally, our approach lags slightly be-

hind the other methods for $t_f = 0.01$, but catches up to or surpasses them as t_f increases. We also note that in most cases, all four methods exhibit roughly first-order convergence in space. An exception is Crank-Nicolson in the case of the initial data (37), because the sharp jumps in the initial data cause deterioration in accuracy of finite differences. This deterioration is not exhibited by Krylov projection or `ode15s`, that also use finite differences, due to adaptivity. For these three methods that use finite differences, second-order accuracy in space is the norm, but not expected in this case due to the eigenfunctions having a discontinuous second derivative. The spatial accuracy of our approach will be discussed further at the end of this section.

Figure 4: Left plot: execution time as a function of grid size N for eigenfunction expansion, Crank-Nicolson, rational Krylov projection, and `ode15s`. Right plot: execution time for all methods normalized to display growth as a function of N .

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.019	25	0.132	0.138	13	0.041	2.703e-04
	2048	0.018	25	0.274	0.065	13	0.091	2.564e-04
	4096	0.028	25	0.987	0.107	13	0.113	2.439e-04
0.1	1024	0.008	11	0.125	0.038	10	0.052	1.538e-03
	2048	0.009	11	0.246	0.049	10	0.101	1.493e-03
	4096	0.012	11	0.597	0.072	10	0.204	1.429e-03
1	1024	0.004	5	0.126	0.018	7	0.084	9.709e-03
	2048	0.004	5	0.254	0.025	7	0.132	9.524e-03
	4096	0.007	5	0.644	0.056	7	0.259	9.259e-03

Table 5: Execution times (in seconds) from Table 7 for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and `ode15s` with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 2, 3, 4]$ and $\vec{\rho} = [1/4, 1/2, 3/4]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	7.5e-05	25	1.5e-03	1.5e-03	13	1.5e-03	2.703e-04
	2048	9.3e-05	25	7.0e-04	6.8e-04	13	6.9e-04	2.564e-04
	4096	9.8e-05	25	3.0e-04	2.9e-04	13	3.0e-04	2.439e-04
0.1	1024	1.5e-04	11	2.4e-03	2.4e-03	10	2.4e-03	1.538e-03
	2048	1.6e-04	11	1.1e-03	1.1e-03	10	1.1e-03	1.493e-03
	4096	1.6e-04	11	4.7e-04	4.8e-04	10	4.8e-04	1.429e-03
1	1024	9.1e-06	5	9.8e-05	9.4e-05	7	1.0e-04	9.709e-03
	2048	5.8e-06	5	4.7e-05	4.3e-05	7	7.7e-05	9.524e-03
	4096	5.7e-06	5	2.3e-05	1.8e-05	7	3.0e-05	9.259e-03

Table 6: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 2, 3, 4]$ and $\vec{\rho} = [1/4, 1/2, 3/4]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.019	29	0.134	0.055	17	0.049	1.852e-04
	2048	0.020	29	0.329	0.082	17	0.097	1.852e-04
	4096	0.033	29	0.623	0.135	17	0.147	1.786e-04
0.1	1024	0.007	11	0.142	0.025	11	0.056	1.266e-03
	2048	0.008	11	0.362	0.069	11	0.135	1.250e-03
	4096	0.012	11	0.526	0.070	11	0.210	1.220e-03
1	1024	0.003	3	0.193	0.021	7	0.087	9.709e-03
	2048	0.003	3	0.288	0.028	7	0.144	9.615e-03
	4096	0.005	3	0.642	0.054	7	0.285	9.434e-03

Table 7: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 2, 3, 4]$ and $\vec{\rho} = [1/4, 1/2, 3/4]$.

4.2. Self-adjoint Case

4.2.1. Computing Eigenvalues

Tables 18-19 show the smallest ten nonzero eigenvalues of the operator $-\partial_x \alpha^2(x) \partial_x$, as computed using the *SAK* principle with secant iteration, as in Section 3.2, and using the MATLAB function **eigs** with a $N \times N$ matrix obtained via finite-element discretization. In Tables 18 and 20, $N = 2^{12}$, and in Tables 17 and 19, $N = 2^{23}$. Tables 18 and 17 feature a coefficient with $n = 4$ pieces, while $n = 8$ in Tables 20 and 19. We observe similar accuracy and convergence behavior as in the non-self-adjoint case, with the exception of the smallest few eigenvalues. On the one hand, with these eigenvalues, we note that the reported error *increases* with N . On the other hand, as will be seen in Tables 29-32, in the case of final time $t_f = 1$, the error in solutions of PDEs using these particular eigenvalues is quite small. This

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	2.8e-03	29	2.5e-04	2.5e-04	17	2.5e-04	1.852e-04
	2048	1.4e-03	29	1.2e-04	1.2e-04	17	1.2e-04	1.852e-04
	4096	6.9e-04	29	4.9e-05	8.9e-05	17	5.4e-05	1.786e-04
0.1	1024	8.7e-04	11	7.7e-04	5.5e-04	11	4.9e-04	1.266e-03
	2048	4.2e-04	11	7.7e-04	2.6e-04	11	2.2e-04	1.250e-03
	4096	1.9e-04	11	7.2e-04	1.1e-04	11	9.0e-05	1.220e-03
1	1024	2.1e-04	3	1.9e-02	2.1e-04	7	2.0e-04	9.709e-03
	2048	9.9e-05	3	1.9e-02	1.0e-04	7	1.0e-04	9.615e-03
	4096	4.3e-05	3	1.9e-02	4.4e-05	7	5.5e-05	9.434e-03

Table 8: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 2, 3, 4]$ and $\vec{\rho} = [1/4, 1/2, 3/4]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.035	31	0.146	0.039	16	0.036	2.326e-04
	2048	0.035	31	0.415	0.084	16	0.087	2.326e-04
	4096	0.047	31	0.601	0.118	16	0.120	2.174e-04
0.1	1024	0.012	11	0.185	0.032	12	0.060	1.351e-03
	2048	0.012	11	0.244	0.039	12	0.086	1.351e-03
	4096	0.017	11	0.530	0.080	12	0.163	1.299e-03
1	1024	0.006	5	0.153	0.018	8	0.073	8.403e-03
	2048	0.006	5	0.339	0.029	8	0.166	8.403e-03
	4096	0.007	5	0.904	0.068	8	0.265	8.197e-03

Table 9: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$ and $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

suggests inaccuracy in the results obtained via **eigs**, which play no role in the computation of the reference solutions of PDEs.

4.2.2. Solving PDEs

Tables 21-32 compare the performance of the methods listed at the beginning of this section for solving the heat equation (3) at $t = t_f$ with the same choices of initial data and coefficient $\alpha(x)$ as in the non-self-adjoint case. We compute eigenvalues $\lambda_0, \lambda_1, \dots, \lambda_m$ and eigenfunctions $V_0(x), V_1(x), \dots, V_m(x)$ using the algorithm described in Section 3.2, where m is chosen so that $e^{-\lambda_j t_f} < \epsilon$ for $j > m$ and $\epsilon = 10^{-4}$. Then, the approximate solution is obtained from the eigenfunction expansion

$$u(x, t) \approx \sum_{j=0}^m V_j(x) e^{-\lambda_j t} \frac{\langle V_j, u(\cdot, 0) \rangle}{\langle V_j, V_j \rangle}$$

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	8.5e-03	31	3.8e-03	3.8e-03	16	3.8e-03	2.326e-04
	2048	4.4e-03	31	1.3e-03	1.3e-03	16	1.3e-03	2.326e-04
	4096	2.0e-03	31	8.9e-04	8.9e-04	16	8.9e-04	2.174e-04
0.1	1024	2.7e-03	11	1.8e-03	1.8e-03	12	1.8e-03	1.351e-03
	2048	1.3e-03	11	1.7e-03	1.7e-03	12	1.7e-03	1.351e-03
	4096	6.4e-04	11	4.2e-04	4.1e-04	12	4.1e-04	1.299e-03
1	1024	1.1e-03	5	1.2e-03	1.2e-03	8	1.2e-03	8.403e-03
	2048	2.9e-04	5	3.9e-04	3.4e-04	8	3.4e-04	8.403e-03
	4096	2.4e-04	5	4.4e-04	2.7e-04	8	2.7e-04	8.197e-03

Table 10: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$ and $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.031	33	0.102	0.034	18	0.031	1.852e-04
	2048	0.034	33	0.209	0.061	18	0.062	1.852e-04
	4096	0.052	33	0.457	0.139	18	0.154	1.786e-04
0.1	1024	0.013	11	0.136	0.024	12	0.049	1.266e-03
	2048	0.013	11	0.288	0.054	12	0.117	1.266e-03
	4096	0.019	11	0.598	0.113	12	0.213	1.220e-03
1	1024	0.006	5	0.136	0.018	8	0.072	9.709e-03
	2048	0.006	5	0.417	0.037	8	0.232	9.615e-03
	4096	0.008	5	0.571	0.060	8	0.254	9.434e-03

Table 11: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$ and $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

where $\langle \cdot, \cdot \rangle$ is the standard inner product on $[0, 2\pi]$.

We observe some very similar patterns in the results as in the non-self-adjoint case. That is, our approach exhibits efficiency and scalability that is superior to that of Crank-Nicolson, Krylov projection or **ode15s**, while its accuracy again lags slightly behind that of the other methods for $t_f = 0.01$ but catches up to and often surpasses the other methods as t_f increases.

Substantially different behavior is observed regarding spatial accuracy. The seven-piece coefficient presents difficulty for all methods; convergence is first-order in space for our method, while sublinear convergence is shown by Krylov projection and **ode15s** and Crank-Nicolson does not show convergence at all. For the other choices of $\alpha(x)$, with four or eight pieces, our method and Krylov projection show second-order convergence in space, while convergence is slower or nonexistent for Crank-Nicolson and **ode15s**.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	4.1e-03	33	9.9e-04	9.9e-04	18	9.9e-04	1.852e-04
	2048	2.3e-03	33	4.9e-04	5.0e-04	18	4.8e-04	1.852e-04
	4096	9.5e-04	33	2.2e-04	2.3e-04	18	2.1e-04	1.786e-04
0.1	1024	1.8e-03	11	1.0e-03	1.0e-03	12	9.7e-04	1.266e-03
	2048	1.1e-03	11	1.0e-03	5.0e-04	12	4.6e-04	1.266e-03
	4096	3.8e-04	11	7.3e-04	1.9e-04	12	1.7e-04	1.220e-03
1	1024	5.9e-04	5	1.9e-02	5.9e-04	8	5.7e-04	9.709e-03
	2048	3.1e-04	5	1.9e-02	3.0e-04	8	2.8e-04	9.615e-03
	4096	1.2e-04	5	1.9e-02	1.2e-04	8	1.0e-04	9.434e-03

Table 12: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$ and $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.020	21	0.112	0.027	13	0.034	1.887e-04
	2048	0.022	21	0.218	0.043	13	0.081	1.818e-04
	4096	0.027	19	0.446	0.082	13	0.119	1.754e-04
0.1	1024	0.008	7	0.119	0.015	8	0.055	1.176e-03
	2048	0.008	7	0.435	0.034	8	0.113	1.163e-03
	4096	0.009	7	0.531	0.054	8	0.171	1.124e-03
1	1024	0.004	3	0.104	0.009	6	0.054	9.259e-03
	2048	0.004	3	0.260	0.022	6	0.106	9.174e-03
	4096	0.006	3	0.621	0.044	6	0.227	8.929e-03

Table 13: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$ and $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

We normally expect second-order accuracy from finite elements with piecewise linear basis functions. It makes sense that this accuracy is only observed in Krylov projection, and not in Crank-Nicolson or **ode15s**, due to the larger temporal error incurred by the latter two methods. The spatial accuracy of our approach is discussed further at the end of this section.

Figures 11-16 show the solutions computed by the different methods. As in the non-self-adjoint case, we see that, visually, the solutions match, except in the case of Crank-Nicolson with the smoothed characteristic function as initial data, where, in some cases, high-frequency oscillations can occur at the jumps in the initial data.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	1.4e-02	21	3.5e-03	3.6e-03	13	3.5e-03	1.887e-04
	2048	6.7e-03	21	1.7e-03	1.7e-03	13	1.7e-03	1.818e-04
	4096	3.2e-03	19	7.1e-04	7.2e-04	13	7.1e-04	1.754e-04
0.1	1024	3.9e-03	7	3.4e-03	3.4e-03	8	3.4e-03	1.176e-03
	2048	1.8e-03	7	1.6e-03	1.6e-03	8	1.6e-03	1.163e-03
	4096	8.3e-04	7	6.8e-04	6.9e-04	8	6.7e-04	1.124e-03
1	1024	2.7e-03	3	3.1e-03	2.7e-03	6	2.7e-03	9.259e-03
	2048	1.3e-03	3	1.6e-03	1.3e-03	6	1.3e-03	9.174e-03
	4096	5.4e-04	3	8.9e-04	5.5e-04	6	5.6e-04	8.929e-03

Table 14: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$ and $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.020	21	0.123	0.048	15	0.044	1.351e-04
	2048	0.025	21	0.281	0.059	15	0.109	1.333e-04
	4096	0.032	21	0.622	0.117	15	0.186	1.316e-04
0.1	1024	0.008	7	0.123	0.020	9	0.056	1.010e-03
	2048	0.009	7	0.235	0.030	9	0.116	1.010e-03
	4096	0.011	7	0.477	0.057	9	0.257	1.000e-03
1	1024	0.004	3	0.108	0.012	6	0.063	8.403e-03
	2048	0.004	3	0.251	0.019	6	0.146	8.333e-03
	4096	0.006	3	0.461	0.039	6	0.232	8.264e-03

Table 15: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$ and $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

4.3. Discussion

While the accuracy and efficiency of our method (for both self-adjoint and non-self-adjoint cases) do not compare favorably to those of the other methods featured in this section, our method is generally much faster, and accuracy does improve as t_f approaches 1. Regarding cases where our method may be slower, it is worth noting that this method is parallelizable, meaning each computation of an eigenfunction is independent of others. Therefore, future work allows this method to be easily improved upon for even greater speed.

In cases where our method is not sufficiently accurate, a different approach to numerical integration to obtain the coefficients in the eigenfunction expansion may be chosen. Currently, our method uses the composite trape-

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	3.9e-03	21	1.7e-03	1.3e-03	15	1.3e-03	1.351e-04
	2048	1.9e-03	21	8.6e-04	6.3e-04	15	6.2e-04	1.333e-04
	4096	9.5e-04	21	4.0e-04	2.7e-04	15	2.7e-04	1.316e-04
0.1	1024	4.7e-04	7	7.3e-03	9.0e-04	9	9.5e-04	1.010e-03
	2048	2.2e-04	7	8.0e-03	4.3e-04	9	4.6e-04	1.010e-03
	4096	9.0e-05	7	8.3e-03	1.9e-04	9	2.1e-04	1.000e-03
1	1024	1.1e-04	3	7.2e-02	1.3e-04	6	2.2e-04	8.403e-03
	2048	5.4e-05	3	7.1e-02	6.1e-05	6	1.4e-04	8.333e-03
	4096	2.4e-05	3	7.1e-02	2.6e-05	6	1.1e-04	8.264e-03

Table 16: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (2) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$ and $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

Figure 5: Solutions of (2), $u(x, 0) = \sin 2x$, computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 2, 3, 4]$, $\vec{\rho} = [1/4, 1/2, 3/4]$.

zoidal method of approximate integration, because of its known effectiveness with periodic functions, which applies to both the eigenfunctions and initial data. However, the error formula in the composite trapezoidal rule assumes a continuous second derivative, which the eigenfunctions do not have.

With smaller values of t_f , more terms are needed in the eigenfunction expansion, due to the slower decay of $e^{-\lambda_j t_f}$. For larger eigenvalues, the eigenfunctions are more oscillatory, thus making numerical integration more difficult. Future work for this method may involve applying Gaussian or adaptive quadrature methods corresponding to each piece of the piecewise constant coefficient instead, so as to improve accuracy. Therefore, while this method may not always perform as well as hoped based on the results presented in this paper, it can be effectively revised and enhanced in order

Figure 6: Solutions of (2), $u(x, 0) = \sin(2x)$, computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$, $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

Figure 7: Solutions of (2), $u(x, 0) = \sin(2x)$, computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$, $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

to deliver even faster and more accurate results than other methods.

5. Conclusion

We have developed an accurate, efficient, scalable, and parallelizable algorithm for computing eigenvalues and eigenfunctions of a second-order differential operator of the form $\alpha^2(x)\partial_{xx}$ or $\partial_x\alpha^2(x)\partial_x$, where $\alpha(x)$ is a piecewise constant coefficient with n pieces, generalizing the work of [13] on the case $n = 2$.

Here, we have used this eigensystem to solve diffusion equations, but it can also be used with other PDEs such as the wave equation by computing functions of eigenvalues such as $\cos(\sqrt{\lambda_j}t)$ rather than $e^{-\lambda_j t}$. We have also

Figure 8: Solutions of (2), $u(x, 0)$ from (37), computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 2, 3, 4]$, $\vec{\rho} = [1/4, 1/2, 3/4]$.

Figure 9: Solutions of (2), $u(x, 0)$ from (37), computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$, $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

used periodic boundary conditions, but the same idea can be applied with homogeneous Dirichlet or Neumann boundary conditions by replacing the periodicity conditions. The resulting matrix M still has the same structure.

Ongoing work considers generalization to higher spatial dimensions, as the *SAK* principle is not limited to 1-D operators. This generalization is complicated by the need to include eigenfunctions of other forms, involving hyperbolic functions [22]. It is also of interest to consider the limit as $n \rightarrow \infty$, in which case approximate eigenfunctions for operators with smoothly varying coefficients could be obtained.

Another future direction of interest would be the case in which the PDE includes an advection term, with a coefficient that is also piecewise constant.

Figure 10: Solutions of (2), $u(x, 0)$ from (37), computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$, $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

j	$\lambda_j(SAK)$	$\lambda_j(eig)$	iterations	relative err
1	3.097941505033577	3.097940432538863	5	3.46e-07
2	4.251422728928484	4.251420921975639	6	4.25e-07
3	13.537755713873489	13.537739478497940	5	1.20e-06
4	15.668508094554506	15.668473921612334	6	2.18e-06
5	31.902087233265412	31.901978395077720	5	3.41e-06
6	35.425319948808259	35.425181211006119	7	3.92e-06
7	56.411139858260810	56.410868559504088	6	4.81e-06
8	61.429391470973243	61.428874641328655	6	8.41e-06
9	89.272086669374303	89.271357580715517	6	8.17e-06
10	95.183229810726530	95.182094519308265	6	1.19e-05

Table 17: Eigenvalues computed using the *SAK* principle with secant iteration, and *eigs* on a finite-difference matrix, of the operator $-\alpha^2(x)\partial_x^2$ with $\vec{\alpha} = [1, 2, 3, 4]$, $\vec{\rho} = [1/4, 1/2, 3/4]$ and $N = 4,096$ grid points.

The case of a piecewise constant advection coefficient, but with a constant diffusion coefficient, was considered in [23]. However, this is a particularly challenging problem, as the approach used in this paper cannot be modified in a straightforward manner to handle this case. In particular, it has been observed that the eigenfunctions do not have a constant amplitude on each piece.

Acknowledgment

The first author was partially supported by a grant from the Center for Undergraduate Research at The University of Southern Mississippi.

- [1] G. B. Folland, Introduction to Partial Differential Equations, 2nd Edition, Princeton University Press, 1995.

j	$\lambda_j(SAK)$	$\lambda_j(eig)$	iterations	relative err
1	3.097941505033577	3.097926927925785	5	4.71e-06
2	4.251422728928484	4.251418333598331	6	1.03e-06
3	13.537755713873489	13.537737194958565	5	1.37e-06
4	15.668508094554506	15.668507008875586	6	6.93e-08
5	31.902087233265412	31.902078078045157	5	2.87e-07
6	35.425319948808259	35.425313532758977	7	1.81e-07
7	56.411139858260810	56.411119659042910	6	3.58e-07
8	61.429391470973243	61.429390833928522	6	1.04e-08
9	89.272086669374303	89.272071303807280	6	1.72e-07
10	95.183229810726530	95.183228514110098	6	1.36e-08

Table 18: Eigenvalues computed using the *SAK* principle with secant iteration, and **eigs** on a finite-difference matrix, of the operator $-\partial_x \alpha^2(x) \partial_x$ with $\vec{\alpha} = [1, 2, 3, 4]$, $\vec{\rho} = [1/4, 1/2, 3/4]$ and $N = 8, 388, 608$ grid points.

j	$\lambda_j(SAK)$	$\lambda_j(eig)$	iterations	relative err
1	3.9679747239207	3.9679723630579	5	5.95e-07
2	12.6253580194816	12.6253454562482	5	9.95e-07
3	24.2171296638348	24.2170508527271	7	3.25e-06
4	46.0526204562029	46.0525391780218	5	1.76e-06
5	68.5575768148243	68.5568461105957	5	1.07e-05
6	82.7275880706043	82.7273505060318	6	2.87e-06
7	121.7888914858721	121.7881800573054	5	5.84e-06
8	145.2960020397981	145.2925406014834	7	2.38e-05
9	209.7194743032816	209.7176162644602	6	8.86e-06
10	242.6942814147148	242.6866432428965	7	3.15e-05

Table 19: Eigenvalues computed using the *SAK* principle with secant iteration, and **eigs** on a finite-difference matrix, of the operator $-\partial_x \alpha^2(x) \partial_x$ with $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$, $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$ and $N = 4, 096$ grid points.

- [2] N. I. Portenko, Generalized diffusion processes, Vol. 83 of Translations of Mathematical Monographs, American Mathematical Society, 1990.
- [3] P. Étoré, On random walk simulation of one-dimensional diffusion processes with discontinuous coefficients, Electron. J. Probab. 11 (9) (2006) 249–275.
- [4] H. Hoteit, R. Mose, A. Younes, F. Lehmann, P. Ackerer, Three-dimensional modeling of mass transfer in porous media using the mixed hybrid finite elements and the random-walk methods, Mathematical Geology 34 (4) (2002) 435–456.
- [5] E. M. LaBolle, G. E. Fogg, A. F. B. Thompson, Random-walk simulation of transport in heterogeneous porous media: Local mass-conservation problem and implementation methods, Water Resources Research 32 (3) (1996) 583–593.

j	$\lambda_j(SAK)$	$\lambda_j(eig)$	iterations	relative err
1	3.9679747239207	3.9679069688242	5	1.71e-05
2	12.6253580194816	12.6253598638896	5	1.46e-07
3	24.2171296638348	24.2171398039054	7	4.19e-07
4	46.0526204562029	46.0525491383453	5	1.55e-06
5	68.5575768148243	68.5575675147394	5	1.36e-07
6	82.7275880706043	82.7274934271921	6	1.14e-06
7	121.7888914858721	121.7888797739920	5	9.62e-08
8	145.2960020397981	145.2959943106795	7	5.32e-08
9	209.7194743032816	209.7194536976682	6	9.83e-08
10	242.6942814147148	242.6942602525224	7	8.72e-08

Table 20: Eigenvalues computed using the *SAK* principle with secant iteration, and **eigs** on a finite-difference matrix, of the operator $-\partial_x \alpha^2(x) \partial_x$ with $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$, $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$ and $N = 8, 388, 608$ grid points.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.033	39	0.061	0.070	26	0.074	1.064e-04
	2048	0.033	39	0.113	0.238	26	0.300	9.091e-05
	4096	0.048	39	0.187	0.118	26	0.298	8.130e-05
0.1	1024	0.011	13	0.043	0.019	15	0.074	7.519e-04
	2048	0.013	13	0.084	0.033	15	0.169	6.623e-04
	4096	0.016	13	0.184	0.063	15	0.723	5.988e-04
1	1024	0.005	5	0.045	0.010	9	0.091	5.495e-03
	2048	0.006	5	0.078	0.016	9	0.206	4.975e-03
	4096	0.007	5	0.167	0.039	9	0.400	4.545e-03

Table 21: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 2, 3, 4]$ and $\vec{\rho} = [1/4, 1/2, 3/4]$.

- [6] A. Lejay, G. Pichot, Simulating diffusion processes in discontinuous media: A numerical scheme with constant time steps, *Journal of Computational Physics* 231 (21) (2012) 7299–7314.
- [7] G. J. M. Uffink, A random walk method for the simulation of macrodispersion in a stratified aquifer, *Relation of Groundwater Quantity and Quality* 146 (1985) 103–114.
- [8] B. Gaveau, M. Okada, T. Okada, Second order differential operators and dirichlet integrals with singular coefficients, *Tohoku Math. Journ.* 39 (1987) 465–504.
- [9] A. Lejay, L. Lenôtre, G. Pichot, Analytic expressions of the solutions of advection-diffusion problems in 1d with discontinuous coefficients, preprint (2017).

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	5.6e-06	39	4.3e-05	2.7e-05	26	3.2e-05	1.064e-04
	2048	1.4e-06	39	4.0e-04	6.7e-06	26	9.6e-06	9.091e-05
	4096	3.4e-07	39	1.0e-03	1.5e-06	26	6.7e-06	8.130e-05
0.1	1024	5.2e-07	13	2.6e-03	5.4e-06	15	5.0e-06	7.519e-04
	2048	1.4e-07	13	4.3e-03	1.4e-06	15	1.5e-06	6.623e-04
	4096	4.6e-08	13	5.1e-03	4.1e-07	15	2.1e-06	5.988e-04
1	1024	6.8e-09	5	1.5e-02	6.8e-07	9	1.1e-06	5.495e-03
	2048	3.1e-09	5	1.7e-02	1.7e-07	9	4.7e-07	4.975e-03
	4096	2.7e-09	5	1.7e-02	3.8e-08	9	1.4e-06	4.545e-03

Table 22: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 2, 3, 4]$ and $\vec{\rho} = [1/4, 1/2, 3/4]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.031	37	0.052	0.046	26	0.042	1.786e-04
	2048	0.034	37	0.086	0.059	26	0.074	1.754e-04
	4096	0.049	37	0.153	0.096	26	0.144	1.695e-04
0.1	1024	0.012	13	0.046	0.018	15	0.057	1.220e-03
	2048	0.012	13	0.097	0.029	15	0.096	1.205e-03
	4096	0.016	13	0.175	0.058	15	0.227	1.176e-03
1	1024	0.005	5	0.039	0.011	9	0.058	9.434e-03
	2048	0.006	5	0.081	0.018	9	0.121	9.259e-03
	4096	0.009	5	0.236	0.038	9	0.359	9.091e-03

Table 23: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 2, 3, 4]$ and $\vec{\rho} = [1/4, 1/2, 3/4]$.

- [10] L. Gerardo-Giorda, P. Le Tallec, F. Nataf, A robin-robin preconditioner for advection-diffusion equations with discontinuous coefficients, *Computer Methods in Applied Mechanics and Engineering* 193 (9-11) (2004) 745–764.
- [11] P. Zunino, Iterative substructuring methods for advection-diffusion problems in heterogeneous media, in: E. Bänsch (Ed.), *Challenges in Scientific Computing - CISC 2002*, Vol. 35 of *Lecture Notes in Computational Science and Engineering*, Springer, 2003, pp. 184–210.
- [12] B. Gustafsson, H. O. Kreiss, J. Oliger, *Time Dependent Problems And Difference Methods*, John Wiley & Sons, Inc., 1995.
- [13] E. M. Garon, J. V. Lambers, *Modeling the diffusion of heat energy*

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	6.2e-06	37	7.3e-06	9.2e-06	26	2.2e-05	1.786e-04
	2048	1.5e-06	37	1.2e-06	2.3e-06	26	2.0e-05	1.754e-04
	4096	3.8e-07	37	1.9e-06	6.2e-07	26	1.4e-05	1.695e-04
0.1	1024	5.5e-07	13	5.3e-04	3.2e-06	15	2.5e-05	1.220e-03
	2048	1.4e-07	13	6.6e-04	7.7e-07	15	2.8e-05	1.205e-03
	4096	3.6e-08	13	6.8e-04	2.0e-07	15	2.8e-05	1.176e-03
1	1024	2.9e-08	5	1.9e-02	2.6e-07	9	8.6e-05	9.434e-03
	2048	7.1e-09	5	1.9e-02	6.5e-08	9	9.2e-05	9.259e-03
	4096	1.8e-09	5	1.9e-02	1.7e-08	9	6.8e-05	9.091e-03

Table 24: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 2, 3, 4]$ and $\vec{\rho} = [1/4, 1/2, 3/4]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.081	43	0.054	0.041	25	0.086	1.031e-04
	2048	0.079	43	0.109	0.092	25	0.179	8.929e-05
	4096	0.105	43	0.266	0.166	25	0.510	7.874e-05
0.1	1024	0.042	15	0.062	0.032	16	0.125	7.519e-04
	2048	0.045	15	0.162	0.071	16	0.299	6.623e-04
	4096	0.043	15	0.630	0.225	16	1.952	6.061e-04
1	1024	0.011	5	0.093	0.027	9	0.266	5.495e-03
	2048	0.011	5	0.207	0.053	9	0.700	5.000e-03
	4096	0.012	5	0.360	0.090	9	2.429	4.630e-03

Table 25: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$ and $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

within composites of homogeneous materials using the uncertainty principle, Computational and Applied Mathematics (2017) In press.

- [14] M. Filoche, S. Mayaboroda, B. Patterson, Localization of eigenfunctions of a one-dimensional elliptic operator, Contemporary Mathematics 581 (2012) 99–116.
- [15] C. Fefferman, The uncertainty principle, Bulletin of the American Mathematical Society 9 (1983) 129–206.
- [16] W. Heisenberg, Über den anschaulichen inhalt der quantentheoretischen kinematik und mechanik, Zeitschrift für Physik 43 (3-4) (1927) 172–198.
- [17] W. O. Amrein, A. M. Berthier, On support properties of lp-functions

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	1.0e-02	43	2.1e-03	2.1e-03	25	2.1e-03	1.031e-04
	2048	1.0e-02	43	1.3e-03	1.1e-03	25	1.1e-03	8.929e-05
	4096	1.0e-02	43	1.1e-03	3.8e-04	25	3.8e-04	7.874e-05
0.1	1024	4.9e-04	15	2.8e-03	4.5e-04	16	4.5e-04	7.519e-04
	2048	3.1e-04	15	3.8e-03	5.7e-04	16	5.7e-04	6.623e-04
	4096	1.1e-04	15	5.2e-03	1.9e-04	16	1.9e-04	6.061e-04
1	1024	2.5e-05	5	1.5e-02	1.7e-05	9	1.7e-05	5.495e-03
	2048	1.3e-05	5	1.7e-02	2.3e-05	9	2.3e-05	5.000e-03
	4096	5.7e-06	5	1.7e-02	7.7e-06	9	7.8e-06	4.630e-03

Table 26: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$ and $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.077	45	0.047	0.037	28	0.047	1.724e-04
	2048	0.067	45	0.322	0.322	28	0.198	1.587e-04
	4096	0.099	45	0.194	0.129	28	0.333	1.493e-04
0.1	1024	0.017	13	0.041	0.016	16	0.065	1.190e-03
	2048	0.018	13	0.081	0.027	16	0.091	1.124e-03
	4096	0.023	13	0.159	0.051	16	0.198	1.075e-03
1	1024	0.008	5	0.069	0.022	10	0.103	9.174e-03
	2048	0.008	5	0.156	0.031	10	0.187	8.772e-03
	4096	0.010	5	0.159	0.035	10	0.258	8.475e-03

Table 27: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$ and $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

and their fourier transforms., Journal of Functional Analysis 24(3), 258-267.

- [18] M. Benedicks, On fourier transforms of functions supported on sets of finite lebesgue measure., J. Math. Anal. Appl. 106(1), 180-183.
- [19] J. V. Lambers, Approximate diagonalization of variable-coefficient differential operators through similarity transformations, Computers and Mathematics with Applications 64 (8) (2012) 2575–2593.
- [20] M. S. Min, D. Gottlieb, On the convergence of the fourier approximation for eigenvalues and eigenfunctions of discontinuous problems, SIAM J. Numer. Anal. 40 (6) (2003) 2254–2269.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	1.7e-02	45	6.6e-05	6.5e-05	28	6.6e-05	1.724e-04
	2048	1.7e-02	45	1.5e-04	5.7e-05	28	5.8e-05	1.587e-04
	4096	1.7e-02	45	1.2e-03	2.0e-05	28	2.0e-05	1.493e-04
0.1	1024	6.7e-04	13	2.4e-03	5.5e-04	16	5.5e-04	1.190e-03
	2048	4.0e-04	13	7.5e-03	3.5e-04	16	3.4e-04	1.124e-03
	4096	1.4e-04	13	1.0e-02	1.2e-04	16	1.3e-04	1.075e-03
1	1024	2.2e-05	5	3.3e-02	2.2e-05	10	5.2e-05	9.174e-03
	2048	1.1e-05	5	3.7e-02	4.2e-05	10	1.0e-04	8.772e-03
	4096	4.9e-06	5	3.8e-02	1.4e-05	10	3.6e-05	8.475e-03

Table 28: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$ and $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.043	27	0.106	0.047	21	0.112	9.009e-05
	2048	0.044	27	0.092	0.044	22	0.166	7.692e-05
	4096	0.055	27	0.178	0.390	22	0.414	6.897e-05
0.1	1024	0.014	9	0.042	0.030	13	0.146	6.410e-04
	2048	0.015	9	0.087	0.028	13	0.188	5.682e-04
	4096	0.018	9	0.159	0.045	13	0.395	5.263e-04
1	1024	0.006	3	0.044	0.014	10	0.113	4.808e-03
	2048	0.006	3	0.106	0.016	8	0.240	4.329e-03
	4096	0.006	3	0.226	0.055	8	0.542	4.115e-03

Table 29: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$ and $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

- [21] I. Moret, P. Novati, Rd-rational approximation of the matrix exponential operator, BIT 44 (2004) 595–615.
- [22] A. Aurko, J. V. Lambers, Computing eigenvalues of 2-d differential operators with piecewise constant coefficients, In preparation.
- [23] D. Dereudre, S. Mazzonetto, S. Roelly, Exact simulation of brownian diffusions with drift admitting jumps, SIAM J. Sci. Comput. 39 (3) (2017) A711–A740.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	3.8e-05	27	7.9e-04	3.4e-05	21	3.9e-05	9.009e-05
	2048	9.2e-06	27	2.1e-03	8.4e-06	22	1.5e-05	7.692e-05
	4096	2.2e-06	27	3.1e-03	2.0e-06	22	6.4e-06	6.897e-05
0.1	1024	2.4e-06	9	9.0e-03	8.9e-06	13	8.6e-06	6.410e-04
	2048	6.2e-07	9	1.1e-02	2.2e-06	13	3.4e-06	5.682e-04
	4096	1.8e-07	9	1.2e-02	5.4e-07	13	1.3e-06	5.263e-04
1	1024	1.3e-09	3	3.8e-02	5.1e-08	10	1.7e-07	4.808e-03
	2048	4.8e-10	3	3.9e-02	1.3e-08	8	1.5e-07	4.329e-03
	4096	2.7e-10	3	4.0e-02	3.4e-09	8	1.2e-07	4.115e-03

Table 30: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0) = \sin 2x$, $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$ and $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	time	m	time	time	p	time	Δt_{avg}
0.01	1024	0.042	27	0.039	0.027	21	0.048	1.250e-04
	2048	0.052	27	0.088	0.053	21	0.142	1.176e-04
	4096	0.059	27	0.360	0.128	21	0.230	1.124e-04
0.1	1024	0.014	9	0.052	0.018	13	0.081	9.434e-04
	2048	0.015	9	0.085	0.028	13	0.129	9.009e-04
	4096	0.019	9	0.200	0.075	13	0.586	8.696e-04
1	1024	0.006	3	0.050	0.013	8	0.079	7.752e-03
	2048	0.006	3	0.183	0.063	8	0.250	7.463e-03
	4096	0.007	3	0.211	0.043	8	0.646	7.246e-03

Table 31: Execution times (in seconds) for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$ and $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

		eig-exp		C-N	Krylov		ode15s	
t_f	N	error	m	error	error	p	error	Δt_{avg}
0.01	1024	1.9e-05	27	3.5e-03	1.3e-05	21	4.0e-05	1.250e-04
	2048	4.6e-06	27	1.1e-02	3.2e-06	21	2.9e-05	1.176e-04
	4096	1.3e-06	27	1.6e-02	8.9e-07	21	2.5e-05	1.124e-04
0.1	1024	3.0e-06	9	4.9e-02	1.5e-06	13	7.0e-05	9.434e-04
	2048	7.6e-07	9	5.7e-02	3.8e-07	13	5.9e-05	9.009e-04
	4096	1.9e-07	9	5.9e-02	9.1e-08	13	5.1e-05	8.696e-04
1	1024	1.1e-08	3	1.4e-01	6.6e-08	8	1.6e-05	7.752e-03
	2048	2.9e-09	3	1.4e-01	1.6e-08	8	1.6e-05	7.463e-03
	4096	9.0e-10	3	1.4e-01	4.0e-09	8	1.8e-05	7.246e-03

Table 32: Absolute ℓ_∞ errors for methods listed from left to right: eigenfunction expansion with m terms, Crank-Nicolson, rational Krylov projection with p projection steps, and **ode15s** with average time step Δt_{avg} , for solving (3) to time t_f on a N -point uniform grid with $u(x, 0)$ from (37), $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$ and $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

Figure 11: Solutions of (3), $u(x, 0) = \sin 2x$, computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 2, 3, 4]$, $\vec{\rho} = [1/4, 1/2, 3/4]$.

Figure 12: Solutions of (3), $u(x, 0) = \sin 2x$, computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$, $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

Figure 13: Solutions of (3), $u(x, 0) = \sin 2x$, computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$, $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.

Figure 14: Solutions of (3), $u(x, 0)$ from (37), computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 2, 3, 4]$, $\vec{\rho} = [1/4, 1/2, 3/4]$.

Figure 15: Solutions of (3), $u(x, 0)$ from (37), computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 2, 3, 4, 2, 6, 4]$, $\vec{\rho} = [3/8, 1/2, 3/4, 4/5, 5/6, 6/7]$.

Figure 16: Solutions of (3), $u(x, 0)$ from (37), computed at $t_f = 0.01, 0.1$ on a uniform grid with $N = 1,024$ points. The coefficient $\alpha^2(x)$ is defined by (1) with $\vec{\alpha} = [1, 5, 3, 4, 2, 7, 6, 8]$, $\vec{\rho} = [1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 7/8]$.