A generalised matrix transfer technique for the numerical solution of fractional–in–space partial differential equations

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Abstract

In this paper we present a theoretical basis for the Matrix Transfer Technique for approximating solutions to fractional-in-space partial differential equations. Furthermore, we extend the method to the solution of equations involving complete Bernstein functions of infinitesimal generators of bounded C_0 semigroups. We prove that, under appropriate conditions on the right hand side function, the matrix transfer technique converges with the same order as the underlying spatial discretisation. When we extend the matrix transfer technique to finite volume and finite element methods, we find that the resulting discretisations are no longer symmetric with respect to the standard Euclidean inner product, but are instead self-adjoint with respect to a more general inner product on $\mathbb{R}^n$. We propose an M-Lanczos approximation to $f(A)b$ based on the standard Lanczos algorithm under a different inner product and derive an error bound for this case. A number of case studies are presented to illustrate the theory.

1 Introduction

Classical models of heat and fluid flow rely on strong assumptions regarding the underlying particle-level diffusion process: namely that the underlying process is a Brownian motion. In a number of practical situations, however, experimental results have shown that this assumption is violated and it has been suggested that it is more realistic to model particle diffusions using a distribution with heavier tails. If the waiting time between jumps in the underlying stochastic process is taken to be heavy-tailed, the resulting continuum model typically involves a fractional time derivative. In the case of *Lévy flights*, where the jump-length distribution is assumed to be heavy tailed, fractional spatial derivatives arise in the continuum model [35, 36].

The prototypical fractional–in–space partial differential equation is the Dirich-

let problem for the fractional Poisson equation

$$(-\Delta)^{\alpha/2}\phi(x) = w(x), \qquad x \in \Omega \subset \mathbb{R}^d, \quad \alpha > 1/2, \tag{1a}$$

$$\phi(x) = 0, \qquad x \in \partial\Omega, \tag{1b}$$

where $\Delta = \sum_{i=1}^{d} \partial^2/\partial x_i^2$ is the Laplacian on Ω subject to Dirichlet boundary conditions [29]. The restriction to $\alpha > 1/2$ in (1) is required in order to ensure that we can unambiguously define Dirichlet boundary conditions [4,20,32]. Similar restrictions on α arise when considering other boundary conditions [32].

Numerically, the construction of an approximation to (1) poses an interesting challenge: the fractional Laplacian $(-\Delta)^{\alpha/2}$ is a *non-local* operator and, hence, standard discretisation techniques, such as the finite element method, require the solution of a large *dense* linear system [40]. In this paper, we focus primarily on the Matrix Transfer Technique (MTT) of Ilić et al. [27–29] for solving the fractional Poisson equation. The key advantage of the MTT is that it solves the necessarily dense linear systems *using only sparse matrix operations*.

The MTT for solving (1) proceeds by noting that numerical discretisations of the standard Poisson equation lead to the discrete system

$$A_n u_n = w_n,$$

where A_n is the matrix representation of the Laplacian obtained via a chosen discretisation method, such as the finite difference, finite element or finite volume method, and w_n is the discretised right hand side. The idea of the MTT is that, for large enough n the solution to (1) can be approximated by the solution to the structurally dense linear system

$$A_n^{\alpha/2}\phi_n = w_n.$$

We note that it is never necessary to form the dense matrix $A_n^{\alpha/2}$ and in Section 5 we will show that the MTT approximation to (1) can be computed using only sparse matrix techniques [50]. We note that a similar idea was presented independently in [19,21,22].

The allure of the MTT is in its simplicity however, to the best of our knowledge, there has been no investigation of the convergence of this scheme. There is, however, a great deal of numerical evidence that the approximation $\phi_n = A_n^{-\alpha/2} w_n$ converges [27–29]. In fact, it is not even entirely obvious what is meant by a 'matrix representation of the Laplacian'. It was suggested in [27,28] that the one should consider the convergence of the eigenvalues of A_n to the eigenvalues of $(-\Delta)$, however, it is well known that a linear operator is not fully determined by its spectrum. Regardless, this type of reasoning suggests that a naïve application of the MTT to the finite element and finite volume methods will not lead to a convergent discretisation. In this paper we consider the MTT under the abstract framework of convergence of semigroups and we show in Theorem 1 that, under certain conditions, *the MTT converges and has the same order as the underlying discretisation scheme*. Furthermore, the precise

conditions allow us to construct the correct MTT for finite element and finite volume methods. While resulting matrix representations are non-symmetric, they are self-adjoint with respect to a different inner product on $\mathbb{R}^n$.

A simple extension of (1) to anisoptropic diffusion is given by the equation

$$\mathcal{L}^{\alpha/2}\phi = w,$$

subject to appropriate boundary conditions, where $\mathcal{L}$ is a positive definite elliptic operator. This approach has not been taken in the literature, which focuses mainly on mixing fractional directional derivatives [34]. It can, however, be motivated at the stochastic process level by considering the subordination in the sense of Bochner [45] of an anisotropic diffusion process with infinitesimal generator $\mathcal{L}$. The MTT can be easily extended to this situation. It should be noted that the HKT method presented in [21, 22] does not cover this general case, applying only to separable $\mathcal{L}$.

In this paper, we extend the MTT beyond fractional powers of elliptic operators to cover the more general equation

$$g(A)u = w, \qquad w \in \mathcal{D}(A),$$

where g is a complete Bernstein function and $(A, \mathcal{D}(A))$ is the infinitesimal generator of a bounded C_0 semigroup. In particular, we extend the methods in [22] to cover elliptic PDEs with variable coefficients and non-self-adjoint differential operators. This more abstract formulation suggests the use of a framework similar to that of the Trotter-Kato Theorem [31, 37, 55] for analysing convergence. Furthermore, by varying g, one can investigate related equations that arise in the theory of fractional generalised random fields such as

$$(-\Delta)^{\alpha/2}(I-\Delta)^{\beta/2}u(x) = w(x), \qquad \alpha \in (0,2), \alpha+\beta \in [0,2], x \in \Omega \subseteq \mathbb{R}^d,$$

subject to the appropriate boundary conditions (see [41] for details). Another advantage of this scheme is that A can be defined over a general Banach space, which allows for the simultaneous study of finite difference schemes, which are generally formulated in $C^2(\Omega)$, and finite element/volume schemes, which are usually formulated in $L_2(\Omega)$.

Although this paper shares many similarities with previous work in the literature [19, 21, 22], we feel that the focus is different and our considerations are more general. Firstly, Gavrilyuk et al. [19] focus on a class of operators who's spectra are contained within a given region of the complex plain, whereas our results only assume that the operator generates a bounded C_0 semigroup and has a bounded inverse. It should be noted that a strongly elliptic partial differential operator with strictly positive spectrum is in both classes. Secondly, we do not specify a method for approximating the underlying matrix function. As such, our analysis covers both the HKT approximation of [21,22] and Krylov subspace based approximations to matrix functions [17]. This is especially useful as the HKT method requires that the elliptic operator is separable in order to achieve $\mathcal{O}(d^2n^2\log(n))$ complexity and even stronger assumptions on the underlying

discretisation are required to achieve $\mathcal{O}(d^2 n \log(n))$ complexity. When these assumptions are not met, a slew of efficient methods for approximating $f(A_n)w_n$ for the analytic functions $f = 1/g$ exist: the most popular of these being the Lanczos or Arnoldi approximations [11, 12, 17, 18, 24, 25, 39, 42, 46, 47, 51, 54], restarted and preconditioned Krylov subspace approximations [13, 26, 30, 39] or rational approximations [19, 23, 53]. In this paper, we propose a new variant of the Lanczos approximation, which is built around the inner product in which A_n is self-adjoint.

It should also be noted that, in this paper, we consider a different class of functions to those considered in [19]. Our motivation for focusing on complete Bernstein functions is twofold. Firstly, the class of Bernstein functions preserves both Feller and sub-Markovian properties of semigroups, that is, if $-A$ generates a Feller or a sub-Markovian semigroup, then so too does $-g(-A)$ if g is a Bernstein function. This is important, in particular, as Feller semigroups are positivity preserving, which is usually an important property in practical models [6]. The second reason for the restriction to complete Bernstein functions is that the multiplicative inverses of complete Bernstein function form a convex cone and have a useful integral representation, whereas this is not the case for general Bernstein functions [6].

The remainder of the paper is as follows. In Section 2, we will review the necessary definitions from semigroup theory. These definitions will be used to pose an abstract version of the generalised MTT in Section 3 and an error bound relating the error to that of the underlying discretisation will be presented. In Section 4, the convergence framework is used to construct the matrix representations of the Laplacian corresponding to the finite difference, finite volume and finite element methods that are required for the solution of the fractional Poisson equation. When the MTT is applied to the finite volume and finite element methods, it is necessary to compute functions of a non-symmetic matrix. Hence, in Section 5, we investigate the M–Lanczos approximation, which is the Lanczos approximation formulated in terms of the inner product under which the matrix representation A_n is self-adjoint. Finally, in Section 6, we apply the MTT to the finite difference and finite volume discretisations.

2 Functions of infinitesimal generators

Let $\{T_t\}_{t\geq 0}$ be a bounded C_0 semigroup of operators on a Banach Space $(X, \|\cdot\|)$ with infinitesimal generator $(-A, \mathcal{D}(A))$ [55]. We will further require that

$$\left\|(A+\lambda I)^{-1}\right\| \leq \frac{K}{\lambda+\omega}, \qquad \lambda > -\omega, \tag{2}$$

for some $\omega > 0$ and $K > 0$, i.e. A^{-1} is a bounded operator on $\mathcal{D}(A)$. For $0 < \alpha < 2$, the fractional powers $A^{\alpha/2}$ that are defined by

$$A^{\alpha/2}x = \frac{\sin(\alpha\pi/2)}{\pi}\int_0^\infty \lambda^{\alpha/2-1}(\lambda I + A)^{-1}Ax\, d\lambda, \qquad x \in \mathcal{D}(A) \tag{3}$$

also generate a bounded C_0 semigroup [55]. When A is self-adjoint, this is equivalent to the spectral representation of $A^{\alpha/2}$ [55]. This idea can be generalised to Bernstein functions of infinitesimal generators.

It is well known that there is a one-to-one correspondence between the class of Bernstein functions, $\mathcal{B}$ and vaguely continuous convolution semigroups of subprobability measures supported on $[0,\infty)$, $\{\mu_t\}$, namely that $g \in \mathcal{B}$ iff g is the negative logarithm of the Laplace-Stieltjes transform of a vaguely continuous convolution semigroup [6]. For a given Bernstein function f with corresponding semigroup $\{\mu_t\}$ we define the *subordinate semigroup* by the Bochner integral

$$T_t^g u = \int_0^\infty T_s u \, d\mu_t.$$

It is possible to obtain expressions for the generator $-A^g$ of T_t^g using a Lévy-Khinchin-type representation of g [45]. We are, however, not interested in g, but rather in its multiplicative inverse $f = \frac{1}{g}$. Such functions can be represented as the Laplace transform of a potential kernel κ, however, the cone of potential kernels, and hence the cone $\left\{ \frac{1}{g} | g \in \mathcal{B} \right\}$, is not convex and, therefore, it is useful to consider sub-cones that do have this property [6]. One such sub-cone, which has a particularly convenient structure, is the cone of Stieltjes transforms.

Definition 1. *([7]) A function f is said to be a* Stieltjes transform *if it is of the form*

$$f(x) = a + \int_0^\infty \frac{d\mu(t)}{x+t}, \qquad x \in \mathbb{C}\backslash(-\infty, 0),$$

where $\lim_{x\to\infty} f(x) = a \geq 0$ and μ is a non-negative measure on $[0,\infty)$ satisfying

$$\int_0^\infty \frac{d\mu(t)}{1+t} < \infty.$$

The set of all Stieltjes transforms forms a convex cone, known as the Stieltjes cone*, and this set is denoted $\mathcal{S}$.*

We will denote by $\mathcal{R}$ the convex sub-cone of $\mathcal{B}$ generated by the multiplicative inverses of Stieltjes transforms. The cone $\mathcal{R}$ is known in the literature as the cone of *complete Bernstein functions* or *operator monotone functions* [5, 45]. Important functions in $\mathcal{R}$ include $g(t) = t^\alpha$, $\alpha \in [0,1]$; $g(t) = \log(1+t)$; $g(t) = t^\alpha(1+t)^\beta$, $\alpha \in (0,1]$ and $\alpha + \beta \in [0,1]$. Further information about Stieltjes functions and their relationship with complete Bernstein functions can be found in [5, 6, 45]. Analogously to (3), we can define $f(A)$ for a Stieltjes function f as the closure of the operator

$$f(A)x = \int_0^\infty (tI + A)^{-1} x \, d\mu(t), \qquad x \in \mathcal{D}(A).$$

3 Convergence of the generalised MTT

Throughout this section, g^{-1} will denote the multiplicative inverse of the function g, i.e.

$$g^{-1}(t) = \frac{1}{g(t)}.$$

In this section we will develop an abstract MTT to solve the equation

$$g(A)u = w, \qquad w \in \mathcal{D}(A), \tag{4}$$

for some $g \in \mathcal{R}$. Assuming (2) holds, the solution to (4) is given by

$$u = g^{-1}(A)w, \tag{5}$$

where $g^{-1} \in \mathcal{S}$.

Consider a sequence of approximating Banach spaces $\{X_n, \|\cdot\|^{(n)}\}$ and associate with each of these spaces a 'projection' operator $P_n \in L(X, X_n)$ and an 'interpolation' operator $E_n \in L(X_n, X)$. Following [31, 37], we impose the following conditions of P_n and E_n:

P1. $\exists p \in [0, \infty)$ such that $\|P_n x\|^{(n)} \leq p \|x\|$.

P2. $\exists q \in [0, \infty)$ such that $\|E_n x\| \leq q \|x\|^{(n)}$.

P3. $P_n E_n x = x$ for $n \geq 1$, $x \in X_n$.

Let $\{A_n\}$ be a sequence of bounded linear operators on X_n that, for some $t_0 \geq 0$ and some sequence $\{\epsilon_n\}_{n=1}^{\infty} \searrow 0$, satisfies

P4. $\left\|(A + t_0 I)^{-1} x - E_n (A_n + t_0 I)^{-1} P_n x\right\| \leq \epsilon_n \left\|(A + t_0 I)^{-1} x\right\|, \qquad \forall x \in Y,$

where I is the identity operator and Y is a subspace of $\mathcal{D}(A)$. This implies that the solution of

$$(A_n + t_0 I)u_n = P_n w \tag{6}$$

converges to $u = (A + t_0 I)^{-1} w$. Finally, we need the stability condition

P5. $\left\|(A_n + tI)^{-1}\right\| \leq \frac{K_n}{t + \omega_n}, \qquad \forall t > -\omega_n,$

for some $K_n > 0$ and $\omega_n > 0$.

The following theorem shows that the approximations $u^{(n)} = E_n g^{-1}(A_n) P_n w$ converge to $u = g^{-1}(A)w$ as $n \to \infty$ for $w \in \mathcal{D}(A)$. Furthermore, it shows that, if $a \lim_{t \to \infty} g^{-1}(t) = 0$, the MTT converges at the same rate as the underlying discretisation.

Theorem 1. *Let $w \in \mathcal{D}(A)$ and $(A + t_0 I)^{-1} w \in Y$. Then, under the conditions P1–P5 on A, P_n, E_n and A_n listed above,*

$$\left\|u - E_n g^{-1}(A_n) P_n w\right\| \leq a \operatorname{dist}(X, X_n) + C\epsilon_n \|w\|,$$

where $C = (g^{-1}(\omega) - a)K(1 + K_n pq)\max\left\{1, \frac{t_0}{\omega}\right\}$, $a = \lim_{t\to\infty} g^{-1}(t)$, ω *and* K *are the same as in* (2)*, and*

$$\operatorname{dist}(X, X_n) = \sup_{x\in X} \inf_{x^{(n)}\in X_n} \left\| x - E_n x^{(n)} \right\|.$$

Proof. As $w \in \mathcal{D}(A)$, it follows from the definition of a Stieltjes function that there exists a Borel measure μ such that

$$\begin{aligned} u - u^{(n)} &= g^{-1}(A)w - E_n g^{-1}(A_n)P_n w \\ &= a(w - E_n P_n w) + \int_0^\infty \left[(A + tI)^{-1}w - E_n(A_n + tI)^{-1}P_n w\right] d\mu(t). \end{aligned}$$

If we denote the resolvent of A by $R(t) = (A + tI)^{-1}$ and the resolvent of A_n by $R_n(t) = (A_n + tI)^{-1}$, then

$$R(t) - E_n R_n(t) P_n = (I + (t_0 - t)E_n R_n(t) P_n)(R(t_0) - E_n R_n(t_0) P_n)(A + t_0)R(t), \tag{7}$$

where $t, t_0 \in [0, \infty)$ [37, p. 226]. Therefore, it follows from the estimate (2) and the assumptions on w that

$$\|R(t)w - E_n R_n(t) P_n w\| \leq K\left((1 + K_n pq\left|\frac{t - t_0}{t + \omega_n}\right|\right)\frac{\|w\|}{t + \omega}\epsilon_n. \tag{8}$$

The result follows by noting that $\left|\frac{t-t_0}{t+\omega_n}\right| \leq \max\left\{1, \frac{t_0}{\omega}\right\}$. □

Remark 1. *The requirement that* $w \in \mathcal{D}(A)$ *is very important. In Case Study 5, we apply the MTT to the fractional Poisson equation when* w *does not satisfy the Dirichlet boundary conditions and is, therefore, not in* $\mathcal{D}(A)$*. We find that the convergence is much slower than the rate predicted in Theorem 1.*

4 Matrix representations of the Laplacian

Having presented a general convergence framework for the MTT, the main purpose of this section is to identify the projection and interpolation corresponding to a discretisation and construct the matrix representation A_n for the numerical solution of the fractional Poisson equation. In particular, we will consider the finite difference method on a regular grid, which was the method considered in [29]. We will extend these considerations to the finite volume and finite element methods on unstructured meshes.

4.1 The finite difference method on a regular grid

The finite difference method is usually posed on the Banach space $X = C(\Omega)$, the space of continuous functions on the rectangular region Ω, endowed with the

usual sup-norm. In this case, the Laplacian can be written as the infinitesimal generator A, defined by

$$\mathcal{D}(A) = \{x \in C^2(\Omega) | x = 0 \text{ on } \partial\Omega\}$$
$$Ax = -\Delta x, \qquad x \in \mathcal{D}(A).$$

For simplicity, let us consider the one dimensional Laplacian on $\Omega = [0, 1]$. The discrete operators A_n for the n point finite difference approximation at the points $x_i = \frac{i-1}{n-1}$, $i = 1, \ldots, n$ correspond to the system of linear equations

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = w(x_i), \qquad 2 \leq i \leq n-1,$$

where $u_1 = u_n = 0$. In this case, the 'projection' operators $P_n : \mathcal{D}(A) \to \mathbb{R}^N$ are given by

$$(P_n w)_i = w(x_i) \qquad w \in \mathcal{D}(A),$$

and the 'interpolation' operators $E_n : \mathbb{R}^N \to X$ are the usual linear interpolation operators. Clearly, these operators satisfy conditions P1-P3 with $p = q = 1$. Furthermore, It follows from the standard analysis of the finite difference method that the matrix representations A_n satisfy condition P4 with $\epsilon_n = \mathcal{O}(n^{-2})$ and the stability condition P5 with $K_n = 1$ and $\omega_n = \lambda_{min}^{(n)}$, where $\lambda_{min}^{(n)}$ is the smallest eigenvalue of A_n [52].

4.2 The finite volume method

In this section, we consider the matrix representation of the Laplacian that corresponds to the finite volume approximation to

$$-\Delta\phi = w, \qquad x \in \Omega \subset \mathbb{R}^2 \tag{9}$$

subject to Dirichlet boundary conditions, where $w \in L^2$ and Ω is a convex polygonal domain. The finite volume method proceeds by constructing the tessellation $\mathcal{T}_n$ of Ω and then forming the control volumes by connecting barycenter of each triangle in $\mathcal{T}_n$ with the mid-points of each face. Four typical finite volume meshes are shown in Figure 2.

The finite volume approximation to (9) is constructed by integrating the equation over a single control volume V_i centred at node i and applying the divergence theorem to obtain

$$-\int_{\partial V_i} \nabla\phi \cdot \hat{n}\, ds = \int_{V_i} w\, dV, \tag{10}$$

where ds is the surface measure the boundary of V_i, $\hat{n}$ is the unit outward pointing normal to the surface and dV is the volume measure on V_i. Applying the midpoint quadrature rule to (10), we arrive at the control volume finite element method (CV-FEM) discretisation of (9), namely

$$\sum_{F_j^{(i)} \in \partial V_i} [\nabla\phi(x) \cdot \hat{n}]_{m_j^{(i)}} |F_j^{(i)}| = |V_i| w(x_i)$$

for each control volume V_i, where $F_j^{(i)}$ is the jth face of the ith control volume, $m_j^{(i)}$ is the midpoint of $F_j^{(i)}$ and the flux through the face of the control volume is approximated using piecewise linear shape functions [3,10,16]. Detailed analysis of CV-FEM can be found in Ewing *et al* [15].

In order to assess the applicability of CV-FEM for approximating the solution to the fractional Poisson equation, we need to ensure that the projection and interpolation operators are correctly defined. If, for each control volume V_i, we define the indicator function

$$\chi_i(x) = \begin{cases} 1, & x \in V_i \\ 0, & x \notin V_i \end{cases},$$

the global interpolation operator can be written as

$$(E_n w_n)(x) = \sum_{i=1}^{n} (w_n)_i \chi_i(x),$$

where $(w_n)_i$ is the ith component of $w_n \in \mathbb{R}^n$ and n is the number of nodes [15]. Comparing equations (6) and (10), it is clear that the projection operator should be of the form

$$(P_n w(x))_i = C \int_{V_i} w(x)\, dV.$$

The constant C can be determined by the condition P3 ($P_n E_n w_n = w_n$) and it can be clearly seen that $C = |V_i|^{-1}$, where $|V_i|$ is the Lebesgue measure of V_i. Hence, the form of (10) that is suitable for the MTT is

$$-\frac{1}{|V_i|} \int_{\partial V_i} \nabla\phi \cdot \hat{n}\, ds = \frac{1}{|V_i|} \int_{V_i} w\, dV. \tag{11}$$

The resulting matrix representation of the Laplacian is of the form $A_n = C_n^{-1} H_n$, where $C_n = \mathrm{diag}\{|V_i|\}$ is the finite volume representation of the identity operator and H_n is the usual symmetric matrix obtained from the finite volume approximation to the Poisson equation. When the mesh in not uniform, the operators A_n corresponding to the numerical approximation of (11) will be non-symmetric.

4.3 The finite element method

In the previous section, we observed that the matrix representation of the Laplacian resulting from the finite volume method was of the form $A_n = C_n^{-1} H_n$, where C_n is the finite volume representation of the identity operator. In this section, we will extend these arguments to the finite element approximation to (9). The discussion of the finite element method presented in this section is heavily influenced by Chapter 5 of [9].

The finite element method is constructed from a tessellation $\mathcal{T}_n$ of Ω by defining the usual piecewise linear basis functions $\{\psi_i\}_{i=1}^n$ [2, 9]. These basis

functions span the finite element space $\mathcal{V}_n$. Define the interpolation operator

$$E_n v = \sum_{i=1}^{n} v_i \psi_i(x), \qquad v \in \mathbb{R}^n,$$

and the restriction operator

$$(R_n v)_i = \int_\Omega \psi_i(x) f(x)\, dx.$$

The finite element approximation to the Poisson equation (9) is given by $w \approx E_n w_n$, where ϕ_n is the solution to the linear system

$$R_n A E_n \phi_n = R_n w. \tag{12}$$

Fixing a basis for the finite element space $\mathcal{V}_n$, the matrix representation of $R_n A E_n : \mathcal{V}_n \to \mathbb{R}^n$ is given by [9]

$$(H_n)_{ij} = \int_\Omega \nabla\psi_i \cdot \nabla\psi_j\, dV.$$

The matrix H_n is usually referred to as the *stiffness matrix* [2,9]. The discretised system (12) is still not in the correct form, as R_n does not satisfy condition P3. We note, however, that the operator $P_n = C_n^{-1} R_n$ does satisfy this condition, where $C_n = R_n E_n$ is the finite element representation of the identity [9]. Using the same basis for $\mathcal{V}_n$, it can easily be seen that

$$(C_n)_{ij} = \int_\Omega \psi_i(x)\psi_j(x)\, dx,$$

is the usual finite element *mass matrix* [2,9]. Hence, the matrix representation of the Laplacian corresponding the the finite element method is

$$A_n = C_n^{-1} H_n.$$

Interestingly, not only is A_n non-symmetric, but it is also *dense*. Fortunately, it is possible to form fast matrix-vector products with A_n, which facilitates the use of Krylov subspace methods.

5 Krylov subspace approximations to functions of self-adjoint matrices

In Section 4, we saw that the matrix representations of the Laplacian corresponding to the finite element and finite volume methods were non-symmetric. This is unfortunate as the computation of functions of non-symmetric matrices is a far more delicate problem than the computation of functions of symmetric matrices [24]. In this section, we investigate Krylov subspace approximations

to the matrix-vector product $f(A_n)w_n$, where $f = g^{-1}$ is a Stieltjes function. In particular, we focus on the finite element and finite volume representations of the Laplacian.

The standard Krylov subspace method for approximating the product $f(A_n)w_n$ for non-symmetric A_n is based on the Arnoldi method for computing the partial reduction to upper Hessenberg form

$$A_n V_m = V_m \mathcal{H}_m + \beta_{m+1} v_{m+1} e_m^T, \tag{13}$$

where the columns of V_m form an orthonormal basis for the Krylov subspace $\mathcal{K}_m(A_n, w_n) = \text{span}\{w_n, A_n w_n, \ldots, A_n^{m-1} w_n\}$ and $\mathcal{H}_m = V_m^T A_n V_m \in \mathbb{R}^{m \times m}$ is an upper Hessenberg matrix [43]. Clearly, when A_n is symmetric, $\mathcal{H}_m$ is a symmetric, tridiagonal matrix and the Arnoldi decomposition simplifies to the Lanczos decomposition. The *Arnoldi approximation* [11, 12, 17, 18, 24, 25, 39, 42, 46, 47, 51, 54] constructs the approximate matrix vector product

$$f(A_n)w_n \approx V_m f(\mathcal{H}_m) V_m^T w_n.$$

In Section 4, we saw that, when applying the MTT to the finite difference, finite element or finite volume methods, the matrix representation of the Laplacian is given by

$$A_n = C_n^{-1} H_n,$$

where H_n is the symmetric finite difference/volume/element discretisation of the Laplacian and C_n is the finite difference/volume/element discretisation of the identity operator. When considering the finite difference method on a regular grid, $C_n = h^2 I$ and A_n is symmetric positive definite. However, when considering more general methods, A_n is non-symmetric. We will see in the remainder of the section that we can still exploit the more general symmetries present in A_n. This decomposition into the product of two symmetric positive definite matrices is important as it shows that, while A_n is non-symmetric, it is self-adjoint and positive definite with respect to the inner product

$$\langle x, y \rangle_{C_n} = x^T C_n y.$$

The Arnoldi decomposition (13) is derived by applying the Gram-Schmidt process to the Krylov basis $\{w_n, A_n w_n, A_n^2 w_n, \ldots, A_n^{m-1} w_n\}$ to produce a basis that is orthonormal with respect to the standard Euclidean inner product. However, the discussion in the previous paragraph suggests that a more natural inner product for this problem is the C_n–inner product. Hence, we will consider matrix function approximations based on the Arnoldi decomposition in the C_n-inner product. The C_n–Arnoldi decomposition is well known in the context of solving non-symmetric linear systems [48, Section 13]. Essai [14] showed that the C_n–Arnoldi decomposition has the form

$$A_n U_m = U_m \tilde{\mathcal{H}}_m + \beta_m u_{m+1} e_m^T,$$

where the columns of U_m form a basis for $\mathcal{K}_m(A_n, w_n)$, $U_m^T C_n U_m = I$ and $\tilde{\mathcal{H}}_m = U_m^T C_n A_n U_m$ is an $m \times m$ upper Hessenberg matrix. The advantage of

using the C_n inner product is that, as A_n is C_n–self-adjoint, $\tilde{\mathcal{H}}_m$ is a symmetric tridiagonal matrix and the C_n–Arnoldi decomposition can be replaced with the C_n–Lanczos decomposition

$$A_n U_m = U_m \tilde{T}_m + \beta_m u_{m+1} e_m^T.$$

With the C_n–Lanczos decomposition in place, we can define the C_n–Lanczos approximation to $f(A_n)w_n$ as

$$f(A_n)w_n \approx \|w_n\|_{C_n} U_m f(\tilde{T}_m)e_1,$$

where $\|w_n\|_{C_n} = \sqrt{\langle w_n, w_n \rangle_{C_n}}$.

In general, we will refer the the Lanczos approximation based on the M–inner product $\langle x, y \rangle_M = x^T M y$ as the *M–Lanczos approximation*. The algorithm for the C_n-Lanczos approximation is given in Algorithm 1 for the case $M = C_n$, which is identical to the standard Lanczos approximation with every norm and inner product replaced with the C_n-norm and the C_n-inner product. We note the amount of storage can be reduced in the M–Lanczos approximation by adapting a two–pass strategy, in which $f(\tilde{T}_m)e_1$ is computed using only three vectors of storage and the low-dimensional approximation is projected back to $\mathbb{R}^n$ by recomputing the Lanczos vectors in a second pass of the algorithm [39]. We can also derive an *a posteriori* error bound that is similar in spirit to those found in [30, 54].

Theorem 2. *Let $A_n U_m = U_m \tilde{T}_m + \beta_m u_{m+1} e_m^T$ be the M–Lanczos decomposition. Then, For any $f \in \mathcal{S}$, the error in the M–Lanczos approximation to $f(A)b$ satisfies*

$$\left\| f(A)w_n - \|w_n\|_M U_m f(\tilde{T}_m)e_1 \right\|_2 \leq K_n(f(\omega_n) - a) \|b\|_M \tilde{\beta}_m \|u_{m+1}\|_2 |e_m^T \tilde{T}_m^{-1} e_1|, \tag{14}$$

where K_n and ω_n are the constants in condition P5.

Proof. For convenience, we will set $e_m = f(A_n)w_n - \|w_n\|_M U_m f(\tilde{T}_m)e_1$. Using the integral representation of a Stieltjes function, it follows that

$$\begin{aligned}
e_m &= \int_0^\infty (A_n + tI)^{-1} \left(w_n - \|w_n\|_M (A_n + tI) U_m (\tilde{T}_m + tI)^{-1} e_1 \right) d\mu(t) \\
&= \int_0^\infty (A_n + tI)^{-1} \left(w_n - \|w_n\|_M (U_m(\tilde{T}_m + tI) + \tilde{\beta}_{m+1} u_{m+1} e_m^T)(\tilde{T}_m + tI)^{-1} e_1 \right) d\mu(t) \\
&= -\int_0^\infty (A_n + tI)^{-1} \left(\|w_n\|_M \tilde{\beta}_m u_{m+1} e_m^T (\tilde{T}_m + tI)^{-1} e_1 \right) d\mu(t)
\end{aligned}$$

The result follows by bounding the quantities in the integral. Firstly, condition P5 gives $\left\|(A_n + tI)^{-1}\right\|_2 \leq K_n(\omega_n + t)^{-1}$. Secondly, the crux of Lemma 5 in [54] is that for any SPD tridiagonal matrix T and any $t > 0$, $|e_m^T (T + tI)^{-1} e_1| \leq |e_m^T T^{-1} e_1|$. With these bounds in place, it follows that

$$\|e_m\|_2 \leq K_n(f(\omega_n) - a) \|b\|_M \tilde{\beta}_m \|u_{m+1}\|_2 |e_m^T \tilde{T}_m^{-1} e_1|.$$

□

In order to derive a practical stopping criterion from Theorem 2, we need good estimates for K_n and ω_n. When A_n is symmetric positive definite, and therefore orthogonally diagonalisable, it is easily seen that $K_n = 1$ and ω_n is the smallest eigenvalue of A. As the matrix representations A_n corresponding to the finite element and finite volume methods are M–self-adjoint, for some matrix M, it can be shown that the eigenvectors of A_n form an M–orthogonal basis for $\mathbb{R}^n$ and, therefore,

$$A_n = Y_n \Lambda_n Y_n^{-1},$$

where Λ_n is a diagonal matrix with the eigenvalues of A_n on the diagonal and the columns of Y_n contain the eigenvectors of A_n normalised such that $Y_n^T M Y_n = I$. Furthermore, the eigenvalues of A_n are real and positive. It follows that, when $t \geq 0$,

$$\begin{aligned}\left\|(A + tI)^{-1}\right\|_M &\leq \|Y_n\|_M \left\|Y_n^{-1}\right\|_M \left\|(\Lambda_n + tI)^{-1}\right\|_M \\ &= \kappa_M(Y_n) \left(\lambda_{min}^{(n)} + t\right)^{-1},\end{aligned}$$

where $\lambda_{min}^{(n)}$ is the smallest eigenvalue of A_n and $\kappa_M(Y_n)$ is the M–norm condition number of Y_n. We can convert the above bound to the 2–norm by noting that, if μ_{min} and μ_{max} are, respectively, the smallest and largest eigenvalues of M, then

$$\sqrt{\mu_{min}}\,\|x\|_M \leq \|x\|_2 \leq \sqrt{\mu_{max}}\,\|x\|_M\,, \qquad x \in \mathbb{R}^n. \tag{15}$$

Therefore, noting that A_n has no eigenvalues of the negative real axis,

$$\begin{aligned}\left\|(A_n + tI)^{-1}\right\|_2 &= \sup_{x \neq 0} \frac{\left\|(A_n + tI)^{-1} x\right\|_2}{\|x\|_2} \\ &\leq \frac{\sqrt{\mu_{max}}}{\sqrt{\mu_{min}}} \sup_{x \neq 0} \frac{\left\|(A_n + tI)^{-1} x\right\|_M}{\|x\|_M} \\ &= \sqrt{\kappa_2(M)}\left\|(A_n + tI)^{-1}\right\|_M,\end{aligned}$$

where $\kappa_2(M)$ is the 2–norm condition number of M. Hence, when A_n is M–self-adjoint,

$$\left\|(A_n + tI)^{-1}\right\|_2 \leq \sqrt{\kappa_2(M)}\kappa_M(Y_n) \left(\lambda_{min}^{(n)} + t\right)^{-1}.$$

We can bound $\kappa_M(Y_n)$ by noting that $\|Y_n x\|_M = \|x\|_2$ and, therefore, it follows from (15)

$$\|Y_n\|_M = \sup_{x \neq 0} \frac{\|x\|_2}{\|x\|_M} \leq \sqrt{\mu_{max}}.$$

Similarly,

$$\left\|Y_n^{-1}\right\|_M = \sup_{x \neq 0} \frac{\left\|Y^{-1} x\right\|_M}{\|x\|_M} = \sup_{z \neq 0} \frac{\|z\|_M}{\|Yz\|_M} \leq \frac{1}{\sqrt{\mu_{min}}}.$$

Hence, the bound in Theorem 2 holds with $K_n = \kappa_2(M)$ and $\omega_n = \lambda_{min}^{(n)}$.

Remark 2. *In practice, we can approximate $\lambda_{min}^{(n)}$ with the smallest eigenvalue of $\tilde{T}_m$, which proves to be a good estimator after the first few iterations. This estimate is used in all of the numerical experiments in this section.*

Remark 3. *When considering the finite element MTT, A_n is self–adjoint with respect to the C_n inner product, where C_n is the finite element mass matrix. For a sufficiently regular family of triangularisations, $\kappa_2(C_n)$ is independent of n [2, 9].*

The convergence of the C_n–Lanczos approximation to $A_n^{-1/2} w_n$ is shown in Figure 1 for the finite volume method on the finest mesh in Figure 2. The solid line shows the error in the C_n–Lanczos approximation and the dashed line shows the bound from Theorem 2. The error bound appears to follow the convergence of the C_n–Lanczos approximation quite well, although it is unable to detect the stagnation that occurs for large m. Interestingly, if we replace the bound from Theorem 2 with the equivalent quantity $\kappa_2(M)(f(\omega_n) - a)\,\|r_m\|_2$, where $r_m = w_n - \|w_n\|_{C_n} A_n U_m \tilde{T}_m^{-1} e_1$ is the residual after using m steps of C_n–FOM (the dot-dashed line in Figure 1), then the stagnation is captured, although the bound still predicts slightly better error than is actually achieved. For comparison purposes, the black line in Figure 1 shows the convergence of the Arnoldi approximation. These two approximations are very similar, although not equivalent. In fact, Essai [14] showed that if $U_m = V_m R_m$ is the QR decomposition of U_m, where V_m is the Arnoldi basis for $\mathcal{K}_m(A_n, w_n)$, then the relationship between the upper Hessenberg matrix $\mathcal{H}_m$ obtained from the Arnoldi decomposition and the tridiagonal matrix $\tilde{T}_m$ is $\tilde{T}_m = R_m^{-1} \mathcal{H}_m R_m + E_m$, where $E_m \in \mathbb{R}^{m \times m}$ is zero if and only if m is the degree of the minimal polynomial or v_{m+1} and u_{m+1} are linearly dependent. Hence, as $\tilde{T}_m$ is not, in general, similar to H_m, the approximations are not equivalent. This type of behaviour has been observed when using Krylov methods based on non-standard inner products to solve linear systems [44].

6 Case studies

In this section, we present a number of case studies that demonstrate the theory presented in the previous section. In the first two case studies, the underlying discretisation is taken to be the finite difference method on a regular grid. In this case, the matrix representation of the Laplacian is symmetric positive definite and the corresponding matrix functions are computed using the standard Lanczos approximation [8, 24, 25, 42]. We note, however that the Lanczos approximation can often converge very slowly and a number of other efficient and reliable methods are available [23, 33, 38]. These methods have been compared in the context of solving fractional–in–space partial differential equations by the authors [50].

The third case study investigate the convergence of the FV-MTT for the problems considered in the first two case studies. In the fourth case study, we consider the behaviour of the MTT when the right hand side function does not

Input: The discretised Laplacian H_n, the discretised identity operator C_n and R.H.S. w_n, tolerance τ, α and m.
Output: An approximation to $x = f(A_n)w_n$, where $A_n = C_n^{-1}H_n$.

Set $\rho = \sqrt{w_n^T C_n w_n}$;
Set $u_1 = w_n/\rho$;
for $j = 1 : m$ **do**
  Set $q = H_n u_j$;
  Set $q = C_n^{-1} q$;
  if $j \neq 1$ **then**
    $q = q - \beta_{j-1} u_{j-1}$;
  end
  $\alpha_j = u_j^T C_n q$;
  $q = q - \alpha_j u_j$;
  $\beta_j = \sqrt{q^T C_n q}$;
  $u_{j+1} = q/\beta_j$;
  Calculate $y_m = \left(\sqrt{b^T C_n b}\right) T_m^{-1} e_1$;
  If necessary, re-compute θ_{min}—the smallest eigenvalue of T_m. ;
  if $\kappa_2(M)\rho f(\theta_{min})\beta_j \left\|u_{j+1}\right\|_2 |e_m^T y_m| < \tau$ **then**
    Break;
  end
end
Set $x = \rho V_m T_m^{-\alpha/2} e_1$;

Algorithm 1: The M-Lanczos approximation to $f(C_n^{-1}H_n)w_n$, where f is a Stieljes transform and C_n and H_n are symmetric positive definite matrices.

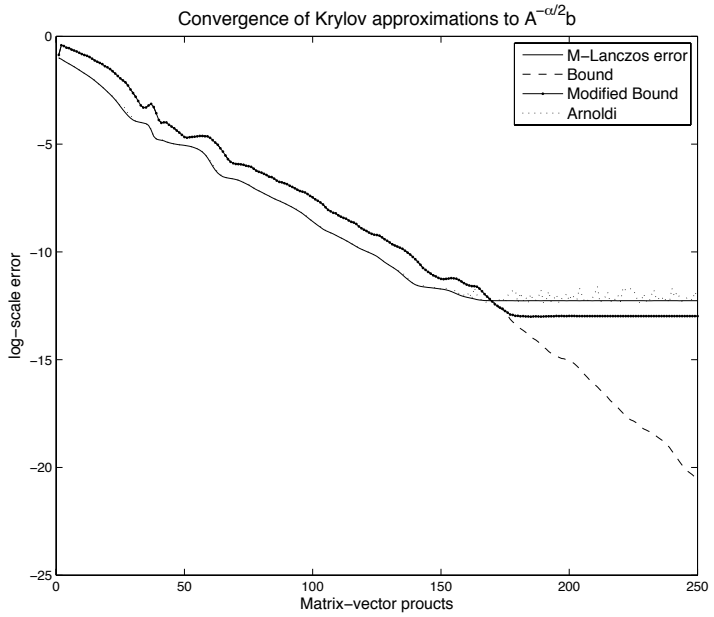

Figure 1: The convergence of the C_n–Lanczos approximation to $A_n^{-1/2}w_n$ for the finest mesh.

satisfy the boundary conditions. In this case, the analytic solution is extremely steep at the boundaries. The MTT does not achieve full accuracy in this case. In both of these case studies, A_n is non-symmetric and we use Algorithm 1 to compute $A_n^{-\alpha/2}w_n$. As is the case when A_n is symmetric, there are a number of alternatives to the M–Lanczos approximation [23, 33, 38]. A preliminary comparison of these methods in the context of solving the fractional Poisson equation is presented in the first author's PhD thesis [49].

6.1 Case study 1: finite difference approximation to the fractional Poisson equation on the unit square

For our first case study we will consider the MTT approximation to the fractional Poisson equation

$$\begin{aligned}(-\Delta)^{\alpha/2}u(x,y) &= xy(1-x)(1-y), && x \in (0,1)^2, \alpha > 0,\\ \phi(x) &= 0, && x \in \partial[0,1]^2,\end{aligned}$$

h^2	$\alpha = 2$	$\alpha = 1.5$	$\alpha = 1$
8.3e-03	2.8e-04	6.4e-04	1.5e-03
3.8e-04	3.7e-05	9.4e-05	2.4e-04
4.4e-05	1.1e-05	2.9e-05	7.6e-05

Table 1: This table shows the relative error in the finite difference approximation to the solution of $(-\Delta)^{\alpha/2}u = xy(1-x)(1-y)$ for various values of h. The error appears to be $\mathcal{O}(h^2)$, which is the rate predicted in Theorem 1.

h^2	$\alpha = 2$	$\alpha = 1.5$	$\alpha = 1$
8.3e-03	2.8e-04	2.7e-04	2.7e-04
3.8e-04	3.7e-05	3.7e-05	3.7e-05
4.4e-05	1.1e-05	1.1e-05	1.1e-05

Table 2: This table shows the relative error in the finite difference approximation to the solution of $(-\Delta)^{\alpha/2}(1-\Delta)^{1-\alpha/2}\phi = xy(1-x)(1-y)$ for various values of h. The error appears to be $\mathcal{O}(h^2)$, which is the rate predicted in Theorem 1.

where the underlying discretisation is a standard finite difference scheme. The exact solution to this equation is

$$u(x,y) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{16(1+(-1)^{n+1}+(-1)^{n+m}+(-1)^{m+1})}{n^3m^3\pi^8(n^2+m^2)(\pi^2(n^2+m^2))^{\alpha/2}} \sin(n\pi x)\sin(m\pi y).$$

Table 1 shows the sup–norm errors $\left\|P_n u - A_n^{-\alpha/2}P_n w\right\|_\infty / \|P_n w\|_\infty$ for different values of α and different mesh sizes h. As was predicted in Theorem 1, the error in the MTT approximation appears to be $\mathcal{O}(h^2)$. It is also worth noting that, while it remains of the correct order, the error appears to increase as α decreases.

6.2 Case study 2: The Riesz-Bessel equation on the unit square

In this section, we will consider the solution to the Riesz-Bessel fractional differential equation on the unit square,

$$\begin{aligned}(-\Delta)^{\alpha/2}(I-\Delta)^{\beta/2}u(x) = h(x), \quad & \alpha \in (0,2), \alpha+\beta \in [0,2] x \in (0,1)^2, \alpha > 0,\\ \phi(x) = 0, \qquad & x \in \partial[0,1]^2.\end{aligned}$$

We will again employ a finite difference approximation to the Laplacian as the basis of the MTT. One again, we expect the errors to be $\mathcal{O}(h^2)$. This prediction is confirmed in Table 2.

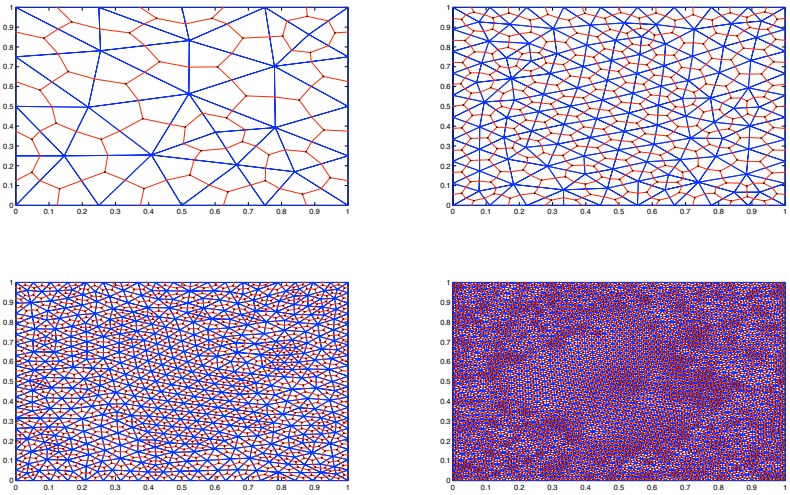

Figure 2: The hierarchy of meshes used to test the FV-MTT. The meshes have 28, 126, 472 and 1863 nodes respectively.

6.3 Case study 3: revisiting the FPE and the Riesz-Bessel equation

In this case study, we applied the finite volume MTT (FV-MTT) to the problems considered in the previous two case studies. The results of this for a sequence of meshes, shown in Figure 2, are given in Table 3. The FV-MTT appears to converge at the same rate as the standard finite volume method in all of these cases. It is interesting to note, however, that as α decreases in the FV-MTT approximation to the fractional Poisson equation, the quality of the solution degrades when compared to larger values of α. The error in the FV-MTT approximation is shown in Figure 3. The error is clearly the largest near the boundaries. This phenomenon will be discussed more thoroughly in the next section.

6.4 Case Study 5: The effect of boundary behaviour

We conclude this section with an example in which the FV-MTT does not behave as expected. We will focus on a variant of Case Study 1

$$\begin{aligned} (-\Delta)^{\alpha/2}u(x,y) &= 10, & x &\in (0,1)^2, \alpha > 0, \\ \phi(x) &= 0, & x &\in \partial[0,1]^2 \end{aligned}$$

The function $w(x) = 10$ is not in $\mathcal{D}(A) = H_0^2((0,1)^2)$ as it does not satisfy the Dirichlet boundary conditions. Therefore, we do not expect the bound in

N	Poisson	Fractional Poisson		Riesz-Bessel	
		$\alpha = 1.5$	$\alpha = 1$	$\alpha = 1.5$	$\alpha = 1$
28	4.18e-2	3.91e-2	4.69e-2	4.12e-2	4.05e-2
126	1.25e-2	1.30e-2	2.18e-2	1.24e-2	1.24e-2
472	2.16e-3	5.00e-3	1.18e-2	2.18e-3	2.19e-3
1863	8.43e-4	1.91e-3	6.71 e-3	8.48e-4	8.53e-4

Table 3: This table shows the relative error in the FV-MTT approximation to the solution of $(-\Delta)^{\alpha/2}(1-\Delta)^{1-\alpha/2}\phi = xy(1-x)(1-y)$, for various values of α and for various mesh sizes. The error appears in all cases appears to decay at the same rate as the standard finite volume approximation to the Poisson equation.

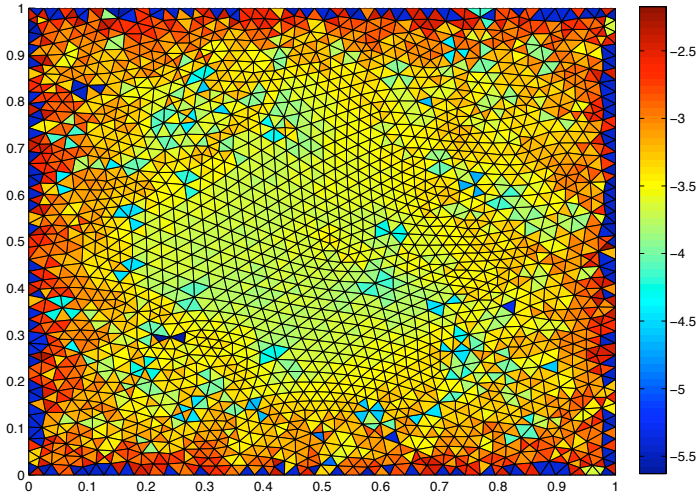

Figure 3: The log scale error of the FV-MTT approximation to the fractional Poisson equation with $\alpha = 1$. It can be clearly seen that the error is worst near the boundaries.

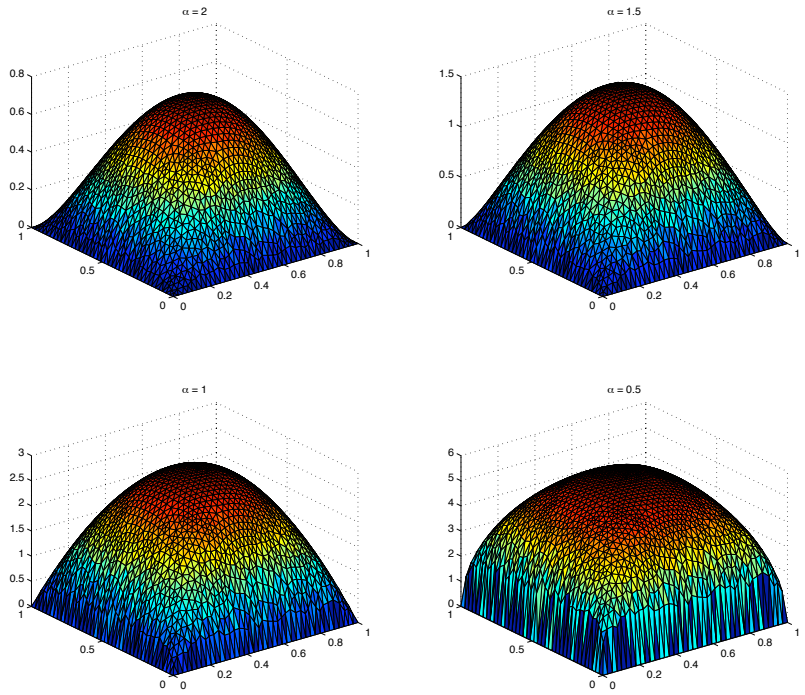

Figure 4: The FV-MTT approximation to the fractional Poisson equation for varying values of α. As α decreases, the solution becomes very steep at the boundaries.

Theorem 1 to hold.

The exact solution to this equation is

$$u(x,y) = \frac{16}{\pi^2} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin((2n+1)\pi x)\sin((2m+1)\pi y)}{(2n+1)(2m+1)(\pi^2((2n+1)^2+(2m+1)^2))^{\alpha/2}}.$$

We note that the exact solution is not differentiable at the boundaries of the unit square. Hence, we expect there to be regions of rapid change on the boundaries. The computed solution on the finest mesh is plotted in Figure 4 for varying values of α. It can be seen that, as α decreases, the solution becomes very steep at the boundaries. The corresponding relative error is shown in Figure 5. The errors, which are reported in Table 4 appear to be of similar order in the interior, however the steep boundary behaviour is not adequately captured for small α.

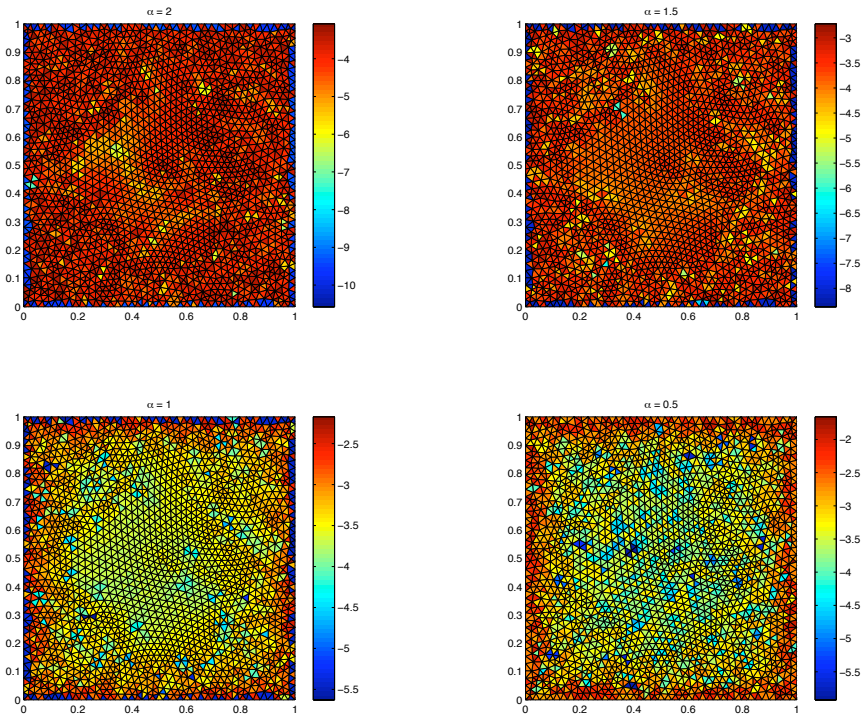

Figure 5: The log scale error of the FV-MTT approximation to the fractional Poisson equation for various values of α. The error is clearly largest near the boundaries and decreasing α appears to exacerbate this effect.

N	$\alpha = 2$	$\alpha = 1.5$	$\alpha = 1$	$\alpha = 1/2$
28	4.18e-2	3.91e-2	4.69e-2	5.02 e-2
126	1.25e-2	1.3e-2	2.18e-2	2.82e-2
472	2.16e-3	5e-3	1.18e-2	2.27e-2
1863	8.43e-4	1.91e-3	6.71e-3	2.19e-2

Table 4: This table shows the relative error in the FV-MTT approximation to the solution of $(-\Delta)^{\alpha/2}\phi = 10$ for various values mesh sizes. The quality of the computed solution clearly deteriorates as α decreases.

7 Conclusion

In this paper, we have considered the matrix transfer technique (MTT) for solving fractional–in–space partial differential equations. We were able to prove, under quite general conditions, that the asymptotic rate of convergence of the MTT is, in theory, the same as the convergence of the underlying discretisation. When considering the finite volume matrix transfer technique (FV-MTT), it was found that the behaviour of the solution at the boundary of the domain may impede the convergence of the method. This suggests that *a posteriori* analysis of the FV-MTT is required in order to build adaptive methods.

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