Finite difference approximation of space-fractional diffusion problems: the matrix transformation method

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Abstract

A mathematical analysis is presented to establish the convergence of the matrix transformation (or matrix transfer) method for the finite difference approximation of space-fractional diffusion problems. Combined this with an implicit Euler time discretization the optimal order convergence is proved with respect to the discrete L_2 and the maximum norm. The analysis is performed on general two and three-dimensional domains with homogeneous boundary conditions. The corresponding error estimates are illustrated with some numerical experiments.

Keywords: fractional-order diffusion, matrix transformation method, finite difference method

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1. Introduction

Numerical solution of space-fractional diffusion problems has been studied extensively in the last decade. The finite difference methods for the conventional diffusion problems were extended in some sense including the development of higher-order methods for the spatial discretization [1], [2] and the time integration [3], generalization of ADI methods [4], [5], construction of appropriate iterative solvers [6] and computing on non-uniform meshes [7]. On the development of the computational efficiency we refer to [5] and [7].

Usually, the first step of the numerical solution is the discretization of the fractional diffusion operator. Initiated by the work [8] many authors contributed to this by developing high-order [9] or compact [10] finite difference approximations. Another possibility is the finite element discretization, which using a dimensional lifting is fully analyzed in [11]. The non-trivial aspect of the finite difference approximations is that we have to use a wide stencil for the approximations due to the non-local nature of the corresponding differential operators. This results in full matrices

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with non-trivial matrix entries. Also, the coefficients of a straightforward approximation have to be shifted to ensure the stability in the time integration [8].

A favorable alternative to bypass this procedure is offered by the so-called matrix transformation method, which was first proposed in [12] and [13]. According to this, we simply have to take the power of the matrix corresponding to the conventional diffusion (negative Laplacian) operator. For the computation of this matrix [14] or immediately solving the linear systems in the time integration efficient techniques have been proposed [15].

But can we establish the convergence of this simple approach? A corresponding analysis is only available in case of finite element discretizations [16] and for cubic domains in case of finite difference approximations.

The aim of this contribution is to prove a general convergence result of the matrix transformation (MTM) method for finite difference approximation of space-fractional diffusion problems in two and three space dimensions.

After the formal problem statement we collect some tools which will be used in the error analysis. The estimates for the Laplacian eigenfunctions and eigenvalues are of central importance. We perform then the error analysis verifying the conditions of the Lax equivalence theorem. The article is closed with some numerical experiments illustrating the convergence results.

2. Mathematical preliminaries

The equation to solve. We investigate the finite difference numerical solution of the space-fractional diffusion problem

$$\begin{cases} \partial_t u(t,\mathbf{x}) = -\mu(-\Delta_{\mathcal{D}})^{\alpha} u(t,\mathbf{x}) & \mathbf{x}\in\Omega,\ t>0 \\ u(0,\mathbf{x}) = u_0(\mathbf{x}) & \mathbf{x}\in\Omega \end{cases} \tag{1}$$

where $\Delta_{\mathcal{D}}$ denotes the Laplacian operator on the computational domain $\Omega\subset\mathbb{R}^d$ with homogeneous Dirichlet boundary conditions, which are implicitly prescribed in this way. Using the compact embedding $H_0^1(\Omega)\hookrightarrow L_2(\Omega)$, we have that $\Delta_{\mathcal{D}}^{-1}: L_2(\Omega)\to L_2(\Omega)$ is positive, compact and self-adjoint, such that the power in (1) makes sense. Here μ is a positive diffusion coefficient, $d=2,3$ is the space dimension and $u_0:\Omega\to\mathbb{R}$ is given. Since we apply a finite difference approach, we assume at this stage that $u_0\in C_0^2(\Omega)$ to have a well-defined classical Laplacian, which is approximated first.

Note that various operators are available for modeling space-fractional diffusion problems. The favor of using the fractional Laplacian on the right-hand side of (1) is that this operator is arising from discrete stochastic models [17], which correspond to real-life observations. Also this can be recognized as a special non-local operator, which satisfies a modified Fick's law with mass conservation [18]. For alternative definitions of fractional order derivatives, we refer to [19] and [20] and a detailed comparison of them can be found in [21].

Eigenfunction expansion, the fractional Laplacian and an imbedding theorem. The Hilbert–Schmidt theory gives that the eigenfunctions $\{\phi_j\}_{j\in\mathbb{Z}^+}$ of -$\Delta_{\mathcal{D}}$ form a complete orthogonal system in $L_2(\Omega)$ with the associated eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \ldots$. With these

$$u = \sum_{j=1}^{\infty} u_j \phi_j \tag{2}$$

denotes the Fourier expansion of u provided that $\|\phi_j\|_{L_2(\Omega)} = 1$.

The fractional Laplacian is defined then on the linear space

$$D_{2\alpha} := \left\{ u \in L_2(\Omega) : \sum_{j=1}^{\infty} u_j^2 \lambda_j^{2\alpha} < \infty \right\}$$

with

$$(-\Delta_{\mathcal{D}})^{\alpha} u := \sum_{j=1}^{\infty} u_j \lambda_j^{\alpha} \phi_j \quad \text{and} \quad |u|_{D_{2\alpha}}^2 := \sum_{j=1}^{\infty} u_j^2 \lambda_j^{2\alpha}. \tag{3}$$

We will make use of a classical Sobolev imbedding theorem $H^6(\Omega) \subset C^4(\Omega)$, which implies that

$$\|u\|_{C^4(\Omega)} \lesssim \|u\|_{H^6(\Omega)}. \tag{4}$$

For the general statement and the proof we refer to [22], Theorem 4.12.

The notation $A \lesssim B$ means that there is a mesh-independent constant c such that $A \leq cB$ for the (usually mesh-dependent) quantities A and B. If both $A \lesssim B$ and $B \lesssim A$ are satisfied then we simply write $A \approx B$.

Estimates for Laplacian eigenvalues and eigenfunctions. The asymptotic behavior of the series $(\lambda_j)_{j\in\mathbb{Z}^+}$ can be given as

$$\lambda_k \approx k^{\frac{2}{d}}, \tag{5}$$

see [23]. For the maximum of $|\phi_m|$ we have the following esimate:

$$\max_{\Omega} |\phi_k| \leq \lambda_k^{\frac{d}{4}}, \tag{6}$$

see [24]. For an exhaustive review of similar results we refer to [25].

We also need a statement on the regularity of the eigenfunctions $\{\phi_j\}_{j\in\mathbb{N}^+}$. We recall a simplified version of Theorem 3.1 in [26].

If Ω is a bounded Lipschitz domain then there is an index j_0 such that for all $j \geq j_0$ and $n \in \mathbb{N}$ we have

$$\|\nabla^{n+2}\phi_j\|_0 \lesssim \lambda_j^{\frac{n}{2}+1}. \tag{7}$$

Matrix powers and their relation to the fractional Laplacian. The power for positive semidefinite matrices is defined using the binomial series expansion: if $K > \|A\|_*$ for any matrix norm, we have

$$A^\alpha = K^\alpha \sum_{k=0}^{\infty} (-1)^k (I - \frac{A}{K})^k. \tag{8}$$

On the finite dimensional subspace $S_M = \text{span } \{\phi_1, \phi_2, \ldots, \phi_M\} \subset L_2(\Omega)$ the following operator is defined for $K > \lambda_M$:

$$A_\alpha \mathbf{u} := K^\alpha \sum_{k=0}^{\infty} \sum_{j=1}^{M} \binom{\alpha}{k} (-1)^k \left(1 - \frac{\lambda_j}{K}\right)^k u_j, \tag{9}$$

where $\mathbf{u} = (u_1, u_2, \ldots, u_M)$. For the application of the binomial series we also note that

$$(-1)^k \binom{\alpha}{k} \le 0 \quad \text{for } 0 \le \alpha \le 1 \quad \text{and } k = 1, 2, \ldots \tag{10}$$

and

$$\sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} = (1-1)^\alpha = 0. \tag{11}$$

We also introduce the Fourier projection $P_M : L_2(\Omega) \to S_M$ with

$$P_M u = P_M \left(\sum_{j=1}^{\infty} u_j \phi_j \right) = \sum_{j=1}^{M} u_j \phi_j. \tag{12}$$

A cornerstone of our analysis is the following observation.

Lemma 1. *For $u \in S_M$ we have the identity $(-\Delta_{\mathcal{D}})^\alpha u = A_\alpha u$.*

Proof: Since $2K > \lambda_M$, we can use the binomial series expansion $(1+x)^\alpha = \sum_{k=0}^{\infty} \binom{\alpha}{k} x^k$ for $x = -(1 - \frac{\lambda_l}{K})$, which gives

$$\lambda_l^\alpha \varphi_l = K^\alpha \sum_{k=0}^{\infty} \binom{\alpha}{k} (-1)^k \left(1 - \frac{\lambda_l}{K}\right)^k \varphi_l.$$

Inserting this identity into the definition of the fractional Laplacian and - due the absolute convergence - changing the order of summation we get (9). $\square$

Discretization. The closure $\bar{\Omega}$ of the computational domain is discretized with an equally spaced rectangular grid Ω_h with the grid cells of size (h_x, h_y) or (h_x, h_y, h_z). The grid points are identified with integer pairs or triplets: the first, second and the third component refers to the first, second and the third coordinate, respectively.

For $d = 2$, we call (i, j) an interior grid point if all of its neighbors $(i-1, j), (i+1, j), (i, j-1)$ and $(i, j+1)$ are in Ω_h. The matrix $A_h \in \mathbb{R}^{N \times N}$ denotes the approximation of the operator $\Delta_{\mathcal{D}}$ with the standard five-star difference scheme such that for each vector $\mathbf{u} \in \mathbb{R}^N$ indexed according to the grid points we have

$$-(A_h \mathbf{u})_{i,j} := \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j} + u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h^2}, \tag{13}$$

whenever (i, j) is an interior grid point. According to the homogeneous boundary conditions, $u_{k,l} = 0$ if (i, j) is not an interior grid point.

For functions on Ω_h we define the "discrete" $\| \cdot \|_{0,h}$-norm for the with

$$\|g\|_{0,h} = \left(h_x h_y \sum_{\mathbf{x} \in \Omega_h} |g(\mathbf{x})|^2 \right)^{\frac{1}{2}}.$$

An obvious modification of this definitions give A_h and the $\| \cdot \|_{0,h}$-norm for the three-dimensional case.

We also use the grid projection operator $P_h : C(\bar{\Omega}) \to \Omega_h$ given by

$$P_h u = \{u(\mathbf{x}) : \mathbf{x} \in \Omega_h\},$$

which maps to a continuous function its grid values. With this we can quantify the approximation property of the matrix A_h: we overall assume that for $u \in C^4(\bar{\Omega})$ we have

$$\|P_h(-\Delta_{\mathcal{D}})u - A_h P_h u\|_{0,h} \lesssim h^2 \|u\|_{C^4},$$

which for $u = \phi_j$ with $P_h(-\Delta_{\mathcal{D}})u = P_h(-\Delta_{\mathcal{D}})\phi_j = \lambda_j P_h \phi_j$ gives

$$\|(\lambda_j I - A) P_h \phi_j\|_{0,h} \lesssim h^2 \|\phi_j\|_{C^4} =: h^2 \sup_{\mathbf{x} \in \Omega, |\beta| = 4} |\partial^\beta \phi_j(\mathbf{x})| \approx h^2 \sup_{\mathbf{x} \in \Omega} |\nabla^4 \phi_j(\mathbf{x})|. \tag{14}$$

This is indeed, an assumption on the domain Ω. Note that the last relation means the equivalence of the corresponding norms: the first one is used as a definition of the $\| \cdot \|_{C^4}$-norm, while we have the regularity estimate with respect to the second one in (7).

3. Results

Well-posedness and smoothness assumptions. In the analysis of the finite difference methods one should use rather strict smoothness assumptions, which manifests in upper estimates for the coefficients in (2). We investigate this connected with the well-posedness of (1).

Proposition 1. *For arbitrary* $u_0 = \sum_{j=1}^{\infty} u_{0j}\phi_j \in L_2(\Omega)$ *the problem in* (1) *is well-posed and for any* $t \in \mathbb{R}^+$ *and* $K \in \mathbb{N}$ *the series* $\sum_{j=1}^{\infty} j^K u_j$ *is convergent with the Fourier coefficients* $\{u_j\}_{j\in\mathbb{N}}$ *of* $u(t,\cdot)$*. Consequently, we also have* $u(t,\cdot) \in C^{\infty}(\Omega)$ *for any* $t \in \mathbb{R}^+$*.*

Proof: According to [27], the solution of (1) can be given as

$$u(t,\cdot) = \sum_{j=1}^{\infty} e^{-\lambda_j^{\alpha} t} u_{0j}\phi_j.$$

such that using also (5) and the boundedness of $\{u_{j0}\}_{j\in\mathbb{N}}$ we have

$$\sum_{j=1}^{\infty} j^K u_j = \sum_{j=1}^{\infty} j^K e^{-\lambda_j^{\alpha} t} u_{0j} \lesssim \sum_{j=1}^{\infty} j^K e^{-j^{\frac{2}{3}\alpha t}} u_{0j} \lesssim \sum_{j=1}^{\infty} j^K e^{-j^{\frac{2}{3}\alpha t}} < \infty$$

by the root test for numerical series.

Also, for arbitrary $k \in \mathbb{N}$ we have

$$(-\Delta)^k u(t,x) = \sum_{j=1}^{\infty} \lambda_j^k e^{-\lambda_j^{\alpha} t} u_{0j}\phi_j(x)$$

where using again (5) and the boundedness of $\{u_{j0}\}_{j\in\mathbb{N}}$ we have for the coefficients

$$\sum_{j=1}^{\infty} \left(\lambda_j^k e^{-\lambda_j^{\alpha} t} u_{0j}\right)^2 \lesssim \sum_{j=1}^{\infty} j^4 e^{-j^{\frac{2}{3}\alpha t}} < \infty.$$

This means that for arbitrary $t > 0$ and $k \in \mathbb{N}$ we have $(-\Delta)^k u(t,\cdot) \in L_2(\Omega)$. By the elliptic regularity (see, *e.g.*, [28], p. 316, Theorem 3) we obtain that $u(t,\cdot) \in C^{\infty}(\Omega)$ as stated. $\square$

To have sufficient smoothness also for the initial function we use the following.

Assumption 1. *The series* $\sum_{j=1}^{\infty} j^{\frac{6}{d}}|u_{0j}|$ *and* $\sum_{j=1}^{\infty} j^{\frac{2\alpha}{d}+1}|u_{0j}|$ *are convergent.*

Remark: For the second order accuracy of the pointwise approximation of the operator $\Delta_{\mathcal{D}}$ we need that $u_0 \in C^4(\Omega)$. In one space dimension for $\Omega = (0,\pi)$ it means that we can differentiate term-by-term the sine series in (2) to obtain

$$\partial^4 u_0(x) = \sum_{j=1}^{\infty} j^4 u_{0j} \sin jx.$$

Accordingly, the smoothness assumption yields that $\sum_{j=1}^{\infty} j^8 u_{0j}^2$ should be convergent.

Consistency. The consistency result is given in the following statement, which is proved in several steps.

Theorem 1. *Using Assumption 1, for arbitrary $\alpha \in \mathbb{R}^+$ and $t \in \mathbb{R}_0^+$ we have the following estimate:*

$$\|P_h(-\Delta_{\mathcal{D}})^\alpha u(t,\cdot) - A_h^\alpha P_h u(t,\cdot)\|_{0,h} \lesssim h^2. \tag{15}$$

Proof: In the consecutive derivations, for the simplicity we use u instead of $u(t,\cdot)$ for a generic $t\mathbb{R}_0^+$. We first decompose the left hand side of (15) as

$$\begin{aligned} &\|P_h(-\Delta_{\mathcal{D}})^\alpha u - A_h^\alpha P_h u\|_{0,h} \\ &\leq \|P_h(-\Delta_{\mathcal{D}})^\alpha u - P_h(-\Delta_{\mathcal{D}})^\alpha P_M u\|_{0,h} + \|P_h(-\Delta_{\mathcal{D}})^\alpha P_M u - A_h^\alpha P_h P_M u\|_{0,h} + \|A_h^\alpha P_h P_M u - A_h^\alpha P_h u\|_{0,h} \end{aligned} \tag{16}$$

so that we use M with

$$M \geq \max\left\{h^{-4}, h^{-\frac{4}{11}(\alpha+1)}\right\}. \tag{17}$$

Step 1: Estimation of the first term. The expansion in (2), the definition in (3), the estimates in (6) and (5) imply the following estimate:

$$\begin{aligned} &\|P_h(-\Delta_{\mathcal{D}})^\alpha u - P_h(-\Delta_{\mathcal{D}})^\alpha P_M u\|_{0,h} = \left\|P_h(-\Delta_{\mathcal{D}})^\alpha \sum_{j=M+1}^{\infty} u_j\phi_j\right\|_{0,h} = \left\|P_h \sum_{j=M+1}^{\infty} \lambda_j^\alpha u_j\phi_j\right\|_{0,h} \\ &\leq \sup_{\mathbf{x}\in\Omega} \sum_{j=M+1}^{\infty} |\lambda_j^\alpha u_j \phi_j(\mathbf{x})| \leq \sum_{j=M+1}^{\infty} \lambda_j^\alpha |u_j| \lambda_j^{\frac{d}{4}} \lesssim \sum_{j=M+1}^{\infty} j^{\frac{2\alpha}{d}} |u_j| j^{\frac{2d}{4d}} \leq \frac{1}{\sqrt{M}} \sum_{j=M+1}^{\infty} j^{\frac{2\alpha}{d}+1}|u_j|. \end{aligned}$$

Therefore, using Assumption 1 and the condition (17) for M we obtain

$$\|P_h(-\Delta_{\mathcal{D}})^\alpha u - P_h(-\Delta_{\mathcal{D}})^\alpha P_M u\|_{0,h} \lesssim \frac{1}{\sqrt{M}} \lesssim h^2. \tag{18}$$

Step 2: Estimation of the second term. We first note that using the notation $K_0 = \min\{\lambda_1, \lambda_{1,h}\}$ we have

$$\max\left\{\left|1 - \frac{\lambda_j}{K}\right|, \left\|I_h - \frac{A_h}{K}\right\|\right\} = 1 - \frac{K_0}{K}.$$

Using this with Lemma 1 and the equality in (8) we obtain that

$$
\begin{aligned}
&\|P_h(-\Delta_{\mathcal{D}})^\alpha P_M u - A_h^\alpha P_h P_M u\|_{0,h} \\
&= \left\| K^\alpha \sum_{k=0}^{\infty} \binom{\alpha}{k} (-1)^k \sum_{j=1}^{M} \big(1 - \frac{\lambda_j}{K}\big)^k u_j P_h \phi_j - K^\alpha \sum_{k=0}^{\infty} \binom{\alpha}{k} (-1)^k \sum_{j=1}^{M} \big(I_h - \frac{A_h}{K}\big)^k u_j P_h \phi_j \right\|_{0,h} \\
&= K^\alpha \left\| \sum_{k=0}^{\infty} \binom{\alpha}{k} (-1)^k \sum_{j=1}^{M} \Big[\big(1 - \frac{\lambda_j}{K}\big)^k I_h - \big(I_h - \frac{A_h}{K}\big)^k\Big] u_j P_h \phi_j \right\|_{0,h} \\
&= K^\alpha \left\| \sum_{k=1}^{\infty} \binom{\alpha}{k} (-1)^k \sum_{j=1}^{M} \Big[\big(1 - \frac{\lambda_j}{K}\big)^{k-1} I_h + ... + \big(I_h - \frac{A_h}{K}\big)^{k-1}\Big] \Big[\big(1 - \frac{\lambda_j}{K}\big) I_h - \big(I_h - \frac{A_h}{K}\big)\Big] P_h u_j \phi_j \right\|_{0,h} \\
&\leq K^{\alpha-1} \sum_{k=1}^{\infty} \binom{\alpha}{k} (-1)^{k-1} \left\| \sum_{j=1}^{M} \Big[\big(1 - \frac{\lambda_j}{K}\big)^{k-1} I_h + ... + \big(I_h - \frac{A_h}{K}\big)^{k-1}\Big] u_j (\lambda_j I - A_h) P_h \phi_j \right\|_{0,h} \qquad (19) \\
&\leq K^{\alpha-1} \sum_{k=1}^{\infty} \binom{\alpha}{k} (-1)^{k-1} \sum_{j=1}^{M} k \cdot \max\left\{ \left|1 - \frac{\lambda_j}{K}\right|^{k-1}, \left\| I_h - \frac{A_h}{K} \right\|^{k-1} \right\} \|u_j (\lambda_j I - A_h) P_h \phi_j\|_{0,h} \\
&= K^{\alpha-1} \alpha \sum_{k=1}^{\infty} \binom{\alpha-1}{k-1} (-1)^{k-1} \sum_{j=1}^{M} \left(1 - \frac{K_0}{K}\right)^{k-1} \|u_j (\lambda_j I - A_h) P_h \phi_j\|_{0,h} \\
&\leq K^{\alpha-1} \alpha \sum_{k=0}^{\infty} \binom{\alpha-1}{k} (-1)^{k} \left(1 - \frac{K_0}{K}\right)^{k} \sum_{j=1}^{M} \|u_j (\lambda_j I - A_h) P_h \phi_j\|_{0,h} \\
&\leq K^{\alpha-1} \alpha \left(\frac{K_0}{K}\right)^{\alpha-1} \sum_{j=1}^{M} \|u_j (\lambda_j I - A_h) P_h \phi_j\|_{0,h} \lesssim \lambda_1^{\alpha-1} \sum_{j=1}^{M} \|u_j (\lambda_j I - A_h) P_h \phi_j\|_{0,h}.
\end{aligned}
$$

To estimate further, we use inequality (14), the embedding theorem in (4), the regularity estimate in (7) and finally (5) to obtain

$$
\begin{aligned}
\sum_{j=1}^{M} \|u_j (\lambda_j I - A_h) P_h \phi_j\|_{0,h} &\leq \sum_{j=1}^{M} u_j h^2 \sup_{\mathbf{x}\in\Omega, |\beta|=4} |\partial^\beta \phi_j(\mathbf{x})| \leq \sum_{j=1}^{M} u_j h^2 \|\phi_j\|_{H^6(\Omega)} \\
&\leq \sum_{j=1}^{M} u_j h^2 \lambda_j^3 \leq h^2 \sum_{j=1}^{M} u_j j^{\frac{6}{d}} \leq h^2 \sum_{j=1}^{\infty} u_j j^{\frac{6}{d}}.
\end{aligned} \qquad (20)
$$

Comparing (19) and (20) and using Assumption 1 we obtain that

$$
\|P_h(-\Delta_{\mathcal{D}})^\alpha P_M u - A_h^\alpha P_h P_M u\|_{0,h} \lesssim h^2. \qquad (21)
$$

Step 3: Estimation of the third term. Using the method in (21) and the condition in (17) for M we have the following inequality:

$$
\begin{aligned}
\|P_h u - P_h P_M u\|_{0,h} &= \left\| P_h \sum_{j=M+1}^{\infty} u_j \phi_j \right\|_{0,h} = \left\| P_h \sum_{j=M+1}^{\infty} u_j \phi_j \right\|_{0,h} \leq \sup \sum_{j=M+1}^{\infty} |\lambda_j^{\alpha} u_j \phi_j| \\
&\leq \sum_{j=M+1}^{\infty} |u_j| \lambda_j^{\frac{d}{4}} \leq C_0 \sum_{j=M+1}^{\infty} |u_j| j^{\frac{1}{2}} \lesssim M^{-5.5} \sum_{j=M+1}^{\infty} |u_j| j^6 \lesssim M^{-5.5}.
\end{aligned}
\tag{22}
$$

The Gershgorin theorem gives an easy upper bound for an arbitrary eigenvalue of A_h:

$$
|\lambda_{N,h}| \leq (2d + 2d)\frac{1}{h^2}
$$

such that the spectral radius of A_h^{α} is at most $(4dh^{-2})^{\alpha}$. Since A_h^{α} is symmetric, this together with (22) and the condition (17) for M gives that

$$
\|A_h^{\alpha} P_h P_M u - A_h^{\alpha} P_h u\|_{0,h} \leq \|A_h^{\alpha}\| \|P_h P_M u - P_h u\|_{0,h} \leq (4dh^{-2})^{\alpha} M^{-5.5} \lesssim h^{-2\alpha} h^{2\alpha+2} = h^2. \tag{23}
$$

Finally, inserting the inequalities in (18), (21) and (23) into (16) implies the error estimate in the theorem:

$$
\|P_h(-\Delta_{\mathcal{D}})^{\alpha} u - A_h^{\alpha} P_h u\|_{0,h} \lesssim h^2. \tag{24}
$$

□

Stability. Using the MTM, the spectral properties of the matrix A_h^{α} corresponding to the spatial discretization coincides with the properties of A_h^{α}. Therefore, the stability analysis can be performed similarly to the case of the conventional diffusion problems. As an example, we discuss here the case of the implicit Euler time discretization with respect to the $\|\cdot\|_{0,h}$ and the max norm.

Theorem 2. *The implicit Euler method* $\mathbf{u}^{n+1} = (I + \delta A_h^{\alpha})^{-1}\mathbf{u}^n$ *is unconditionally stable with respect to the* $\|\cdot\|_{0,h}$*-norm.*

Proof: Since A_h^{α} is positive semidefinite, we have that the spectral radius of the positive semidefinite matrix $(I+\delta A_h^{\alpha})^{-1}$ is at most *one*. This coincides with its l_2-norm, which proves its stability with respect to the $\|\cdot\|_{0,h}$-norm. □

To investigate the convergence with respect to the max-norm, we first verify the following.

Lemma 2. *For any* $\alpha \in (0, 1]$ *the matrix* A_h^{α} *is diagonally dominant.*

Proof: We first rewrite A_h as $A_h = 2d(I+S)$, where S is elementwise non-positive and use (13) to obtain

$$\|S\|_{\max} = \max_k \sum_{j=1}^{N} |[A_h]_{k,j}| \leq 1. \tag{25}$$

Therefore, we can use the binomial series expansion for $0 \leq \alpha \leq 1$ to have

$$(I+S)^\alpha = \sum_{k=0}^{\infty} \binom{\alpha}{k} S^k = I + \sum_{k=1}^{\infty} \binom{\alpha}{k} S^k. \tag{26}$$

To investigate the second term on the right hand side, we use again (25) with (10) and (11) to get

$$\left\| \sum_{k=1}^{\infty} \binom{\alpha}{k} S^k \right\|_{\max} \leq \sum_{k=1}^{\infty} \left| \binom{\alpha}{k} \right| \|S^k\|_{\max} \leq \sum_{k=1}^{\infty} \left| \binom{\alpha}{k} \right| = 1 - \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} = 1.$$

Therefore, using the notation s_{jk} for the matrix entries of $\sum_{k=1}^{\infty} \binom{\alpha}{k} S^k$ we obtain for the jth row of $(I+S)^\alpha$ that

$$-|s_{j1}| - \cdots - |s_{jj-1}| + |1 + s_{jj}| - |s_{jj+1}| - \cdots - |s_{jN}| \geq -|s_{j1}| - \cdots - |s_{jj-1}| + 1 - |s_{jj}| - |s_{jj+1}| - \cdots - |s_{jN}| \geq 0,$$

which means that $(I+S)^\alpha = \frac{1}{(2d)^\alpha} A_h^\alpha$ is diagonally dominant. $\square$

For the stability analysis we also need the following classical result, see [29].

Lemma 3. *For any diagonally dominant matrix B and $\beta = \min_k \left\{ |B_{kk}| - \sum_{j \neq k} |B_{kj}| \right\}$ we have that B is non-singular and $\|B^{-1}\|_\infty \leq \frac{1}{\beta}$.*

We can now state the stability result.

Theorem 3. *For any $\alpha \in (0,1]$ the implicit Euler method $\mathbf{u}^{n+1} = (I + \delta A_h^\alpha)^{-1} \mathbf{u}^n$ is unconditionally stable with respect to the $\|\cdot\|_{\max}$-norm.*

Proof: According to Lemma 2 the matrix A_h^α is diagonally dominant with positive diagonal entries, we have that

$$1 + [A_h^\alpha]_{kk} - \sum_{j \neq k} |[A_h^\alpha]_{kj}| \geq 1$$

such that Lemma 3 can be applied to $I + A_h^\alpha$ and we have $\beta \geq 1$. Therefore, $(I + A_h^\alpha)^{-1} \leq 1$, which proves the stability with respect to the $\|\cdot\|_{\max}$-norm. $\square$

Using the Lax–Richtmyer theorem we obtain the main theorem of the paper.

Theorem 4. *The implicit Euler method $\mathbf{u}^{n+1} = (I + \delta A_h^\alpha)^{-1} \mathbf{u}^n$ obtained from the matrix transformation method is unconditionally convergent with respect to the $\|\cdot\|_{0,h}$-norm for any $\alpha \in \mathbb{R}^+$ and with respect to the $\|\cdot\|_{\max}$-norm for any $\alpha \in (0,1]$ and the corresponding convergence order is $\mathcal{O}(\delta) + \mathcal{O}(h^2)$.*

4. Numerical experiments

The results in Section 3 are demonstrated in numerical experiments using first the model problem

$$\begin{cases} \partial_t u(t,x,y) = -(-\Delta)^\alpha u(t,x,y) \quad (x,y) \in \Omega_{2L},\ t \in (0,T) \\ u(t,x,y) = 0 \quad (x,y) \in \partial\Omega_{2L},\ t \in (0,T) \\ u(0,x,y) = \sin x \sin 2y + \sin 2x \sin y \quad (x,y) \in \Omega_{2L}, \end{cases} \tag{27}$$

where $\Omega_{2L} = (0,2\pi) \times (0,2\pi) \setminus [\pi,2\pi] \times [\pi,2\pi]$ denotes an L-shaped domain, $T = 0.1$ and $\alpha \in \mathbb{R}^+$ is a given parameter. Note that the analytic solution of (27) is given with $u(t,x,y) = \exp(-5^\alpha t)(\sin x \sin 2y + \sin 2x \sin y)$.

As the second model problem we have solved numerically the following 3-dimensional space-fractional diffusion problem :

$$\begin{cases} \partial_t u(t,\mathbf{x}) = -\mu(-\Delta)^\alpha u(t,\mathbf{x}) \quad \mathbf{x} \in \Omega_{3L},\ t \in (0,T) \\ u(t,\mathbf{x}) = 0 \quad \mathbf{x} \in \partial\Omega_{3L},\ t \in (0,T) \\ u(0,\mathbf{x}) = 100\,(\sin 2\pi x \sin 2\pi y \sin 4\pi z + \alpha \sin 2\pi x \sin 4\pi y \sin 2\pi z + 0.1 \sin 4\pi x \sin 2\pi y \sin 2\pi z) \quad \mathbf{x} \in \Omega_{3L}, \end{cases} \tag{28}$$

where $\mathbf{x} = (x,y,z)$, $\Omega_{3L} = (0,1)^3 \setminus [1/2,1]^3$ denotes a Fichera cube, $T = 1$, $\mu = 0.1$ and $\alpha \in \mathbb{R}^+$ is a given parameter. Note that the analytic solution of (27) is given with

$$u(t,\mathbf{x}) = \exp(-\mu\left(24\pi^2\right)^\alpha t)100\,(\sin 2\pi x \sin 2\pi y \sin 4\pi z + \alpha \sin 2\pi x \sin 4\pi y \sin 2\pi z + 0.1 \sin 4\pi x \sin 2\pi y \sin 2\pi z)\,.$$

According to the matrix transformation method in both cases we proceeded as follows.

- The domain was discretized using a uniform square-grid with the grid size h.
- The standard five-point approximation of the operator $-\Delta_{\mathcal{D}}$ was applied to obtain the matrix A_h.
- The matrix power $-(A_h)^\alpha$ was computed to approximate $-(-\Delta_{\mathcal{D}})^\alpha$.
- Implicit Euler time stepping was applied.

The computational results are shown for the first model problem in Table 1 and Table 2 and for the second model problem in Table 3. While in the two-dimensional case the predicted convergence rate is reached shortly, in the three-dimensional computations a remarkable oscillation can be detected. Since the majority of the real measurements is for the subdiffusive case [30] and the computations are lengthy, we have tested (28) only with a single parameter $\alpha = 0.7$.

Table 1: Computational error and estimated convergence rate `r` with respect to the $L_2(\Omega)$-norm for the matrix transformation method applied to the finite difference approximation of (27). N_δ: number of time steps, N_h the number of subintervals on the longest edge $[0, 2\pi]$.

		$\alpha = 0.6$		$\alpha = 0.8$		$\alpha = 1.2$		$\alpha = 1.4$	
N_δ	N_h	L_2-error	`r`	L_2-error	`r`	L_2-error	`r`	L_2-error	`r`
2	8	0.118	–	0.194	–	0.421	–	0.559	–
4	11	0.0635	1.86	0.105	1.85	0.233	1.81	0.311	1.80
8	16	0.0322	1.97	0.0539	1.95	0.121	1.93	0.162	1.92
16	23	0.0164	1.96	0.0265	2.03	0.0621	1.95	0.0805	2.00
32	32	0.00822	1.99	0.0138	1.92	0.0314	1.98	0.0421	1.92
64	45	0.00413	2.00	0.00696	2.06	0.0158	1.99	0.0212	1.99
128	64	0.00207	2.00	0.0349	1.99	0.00793	1.99	0.0106	2.00

According to Theorem 4 we obtain in each case an optimal convergence rate both in the L_2-norm and in the max-norm. The bottleneck of the above approach is the computation of the matrix power. In MATLAB (or Octave) one can use the subroutine `mpower` or compute it using the equality $A^\alpha = \exp(\alpha \cdot \log A)$. More recent algorithms are available in [15] and [14]. There are several other approaches to reduce the computational cost in the numerical solution of space-fractional diffusion problems. A fast numerical treatment of implicit methods can be found in [31], [5], where the authors explore the special structure of the corresponding dense stiffness matrices.

5. Summary

We have verified the convergence of the matrix transformation method applied to the space-fractional diffusion problems. The corresponding computational algorithm is simple: one can completely avoid the computation of a full matrix containing involved finite differences. At the same time, the spatial accuracy exhibits an optimal accuracy (order 2) for any positive power α. Combined with an implicit Euler time stepping, the corresponding method exhibits optimal convergence rate both in the L_2-norm and for $\alpha \in (0, 1]$ in the max-norm.

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Table 2: Computational error and estimated convergence rate r with respect to the max-norm for the matrix transformation method applied to the finite difference approximation of (27). N_δ: number of time steps, N_h the number of subintervals on the longest edge $[0, 2\pi]$.

		$\alpha = 0.6$		$\alpha = 0.8$		$\alpha = 1.2$		$\alpha = 1.4$	
N_δ	N_h	max-error	r	max-error	r	max-error	r	max-error	r
2	8	0.0436	–	0.0715	–	0.155	–	0.206	–
4	11	0.0231	1.89	0.0384	1.86	0.0849	1.83	0.113	1.82
8	16	0.0119	1.94	0.0199	1.93	0.0447	1.90	0.0598	1.89
16	23	0.00637	1.87	0.0103	1.93	0.0241	1.85	0.0314	1.90
32	32	0.00333	1.91	0.0553	1.87	0.0125	1.93	0.0168	1.87
64	45	0.00167	1.99	0.00278	1.98	0.00631	1.98	0.00846	1.99
128	64	0.000825	2.02	0.00139	2.00	0.00316	2.00	0.00424	2.00

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Table 3: Computational error and estimated convergence rate r with respect to the max-norm and to the $L_2(\Omega)$-norm for the matrix transformation method applied to the finite difference approximation of (28). N_δ: number of time steps, N_h the number of subintervals on the longest edge $[0,1]$.

		$\alpha = 0.7$			
N_δ	N_h	L_2-error	r	max-error	r
5	13	1.2940	–	4.1107	–
8	16	0.75153	2.2746	2.6360	1.86
12	20	0.35881	3.3132	1.1587	3.6836
16	23	0.3414	0.4040	1.0918	0.4831
20	25	0.2652	2.3324	0.8550	2.2635
24	28	0.2169	2.1255	0.7002	2.1116
32	32	0.15835	2.0118	0.51105	2.1822

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