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Collocation-Based Approximation for a Time-Fractional Sub-Diffusion Model

Kaido Lätt, Arvet Pedas *, Hanna Britt Soots and Mikk Vikerpuur

Institute of Mathematics and Statistics, University of Tartu, 51009 Tartu, Estonia; kaido.latt@ut.ee (K.L.); hanna.britt.soots@ut.ee (H.B.S.); mikk.vikerpuur@ut.ee (M.V.)
* Correspondence: arvet.pedas@ut.ee

Abstract: We consider the numerical solution of a one-dimensional time-fractional diffusion problem, where the order of the Caputo time derivative belongs to (0, 1). Using the technique of the method of lines, we first develop from the original problem a system of fractional ordinary differential equations. Using an integral equation reformulation of this system, we study the regularity properties of the exact solution of the system of fractional differential equations and construct a piecewise polynomial collocation method to solve it numerically. We also investigate the convergence and the convergence order of the proposed method. To conclude, we present the results of some numerical experiments.

Keywords: fractional differential equation; Caputo derivative; collocation method; graded grid; method of lines; sub-diffusion

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1. Introduction

Diffusion processes hold a position of utmost significance in science. These processes, ranging from the spread of heat through materials to the dispersion of molecules in fluids, play a pivotal role in understanding various phenomena across diverse scientific disciplines. Traditionally, diffusion has been effectively described using classical, integer-order differential equations, such as Fick's second law or the heat equation. However, these conventional models fail to capture the intricacies observed in systems characterized by anomalous behavior. For example, different aspects such as interactions between particles and memory effects have limited the classical approach in describing a large variety of experimental problems [1].

One way to overcome the shortcomings of the classical approach involving integer-order differential equations is to instead use time-fractional diffusion equations, which have been found useful in many real-life processes where anomalous diffusion occurs [1–5]. In the current paper, we consider the numerical solution of time-fractional diffusion equations corresponding to sub-diffusive models, where the order of the time-fractional differential operator belongs to $(0, 1)$. Sub-diffusion refers to situations where particles spread more slowly than predicted by classical models [1].

Since finding an exact solution to a time-fractional diffusion equation is not usually feasible in practice, the development of effective numerical methods is crucial for solving real-world diffusion problems. One of the more popular approaches is to use finite difference methods for the numerical solution of time-fractional diffusion equations (see [6–15] and the references therein). These methods usually discretize the spatial and temporal domains and approximate the derivatives using appropriate difference formulas. On the other hand, in the numerical solution of ordinary fractional differential equations, an often-used approach is to convert the fractional differential equation to a weakly singular integral equation and to solve the transformed equation using a collocation-type method (see, for example [16–20]). However, only a few researchers have considered the numerical solution of time-fractional diffusion equations by collocation methods [21–24] (see also [25]). In collocation methods one looks for an approximate solution in a finite-dimensional space and determines the approximate solution by requiring that it satisfies the equation on an appropriate finite set of points (on the so-called collocation points). If initial or boundary conditions are present, then the collocation solution will usually be required to fulfill these conditions, too. In particular, collocation methods that use polynomial splines and special non-uniform grids take into account the possible singular behavior of the exact solution of weakly singular integral equations. Moreover, these methods usually enable us to obtain a stable and high-order procedure with uniform convergence on the whole interval of integration. Therefore, in the present article, we are interested in developing a numerical scheme for time-fractional diffusion equations that combines space variable discretization and the classical piecewise polynomial collocation method on a non-uniform grid, where the grid points reflect the possible singular behavior of the underlying solution.

The space variable discretization (sometimes also called the method of lines [26]) is a technique that involves discretizing with respect to the spatial variables and treating the resulting system as a set of coupled fractional ordinary differential equations. For our problem, this allows us to remodel the time-fractional diffusion equation into a system of ordinary fractional differential equations. To solve the obtained system of fractional differential equations, we reformulate it as a system of weakly singular Volterra integral equations of the second kind and employ a suitable collocation method for finding approximate solutions. Our approach enables us to construct a high-order numerical method for solving the sub-diffusion problem, despite the fact (see [12,27,28]) that the temporal partial derivatives of solutions of time-fractional diffusion equations have, in general, weak singularities at the initial time $t = 0$. It is worth mentioning that we can achieve a sufficiently high convergence order even when using polynomials of low degree.

The rest of the paper is organized as follows: In Section 2, we present the underlying problem and necessary notations. Next, in Section 3, we use the method of lines to create a system of ordinary fractional differential equations. In Section 4, we reformulate this system as a system of integral equations and study the regularity properties of its exact solution. Then, we introduce a collocation-based method for finding approximate solutions in Section 5 and study the convergence and convergence order of the proposed method in Section 6. In Section 7, we test our theoretical error estimates using some numerical experiments.

2. Time-Fractional Sub-Diffusion Model

Consider the time-fractional sub-diffusion equation

$$(D_t^\alpha u)(x,t) - p\frac{\partial^2 u(x,t)}{\partial x^2} + \theta(x)u(x,t) = f(x,t), \quad (x,t) \in Q := (0,L) \times (0,b], \tag{1}$$

subject to the following boundary and initial conditions:

$$u(0,t) = 0, \quad t \in [0,b], \tag{2}$$

$$u(L,t) = 0, \quad t \in [0,b], \tag{3}$$

$$u(x,0) = \phi(x), \quad x \in [0,L]. \tag{4}$$

Here, $u = u(x,t)$ is the unknown function, $0 < \alpha < 1$, p is a positive constant (sometimes called the general diffusion coefficient), $\theta \in C[0,L]$ with $\theta \geq 0$, $\phi \in C[0,L]$ and $f \in C(\overline{Q})$, where $\overline{Q} = [0,L] \times [0,b]$. Furthermore, $(D_t^\alpha u)(x,t)$ denotes the α-order Caputo fractional derivative of $u(x,t)$ with respect to the variable t, which, for $\alpha \in (0,1)$, is defined [29,30] by

$$(D_t^\alpha u)(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\partial u(x,s)}{\partial s} ds, \quad (x,t) \in Q,$$

where Γ is the Euler gamma function: $\Gamma(\eta) = \int\limits_0^\infty s^{\eta-1}e^{-s}ds, \quad \eta > 0$. For one-dimensional absolutely continuous functions, y, on $[0, b]$, we will use the simplified notation, $D^\alpha y$, for the Caputo fractional derivative of y:

$$(D^\alpha y)(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} y'(s) ds, \quad t \in (0, b], \quad \alpha \in (0, 1). \tag{5}$$

Using $C^m[a, b]$ and $C^m(\overline{Q})$, with $m \in \mathbb{N}_0 := \{0\} \cup \mathbb{N}$, $\mathbb{N} := \{1, 2, \dots\}$, we denote the sets of m times continuously differentiable functions on $[a, b]$ and $\overline{Q}$, respectively; for $m = 0$, we set $C^0[a, b] = C[a, b]$ and $C^0(\overline{Q}) = C(\overline{Q})$. In particular, $C[a, b]$ denotes the Banach space of continuous functions, w: $[a, b] \to \mathbb{R} := (-\infty, \infty)$, with the usual norm, $\|w\|_\infty = \max\{|w(t)|: a \le t \le b\}$. Below, we will also use the following notations. For

$$\vec{w}(t) = (w_1(t), \dots w_n(t))^T := \begin{pmatrix} w_1(t) \\ \vdots \\ w_n(t) \end{pmatrix}, \quad 0 \le t \le b, \quad n \in \mathbb{N},$$

the writing $\vec{w} \in C_n^m[0, b]$ $(m \in \mathbb{N}_0$; for $m = 0$, we set $C_n^0[0, b] = C_n[0, b])$ means that $w_i \in C^m[0, b]$, $i = 1, \dots, n$; note that $C_n^m[0, b]$ is a Banach space with respect to the norm

$$\|\vec{w}\|_{C_n^m[0,b]} := \max_{1\le i\le n} \max_{0\le j\le m} \max_{0\le t\le b} |w_i^{(j)}(t)|, \quad \vec{w} \in C_n^m[0, b].$$

Using $L^\infty(0, b)$, we denote the space of all essentially bounded measurable functions $w : (0, b) \to \mathbb{R}$, such that

$$\|w\|_{L^\infty(0,b)} := \inf_{\mathbf{meas}(\Omega)=0} \sup_{t\in(0,b)\setminus\Omega} |w(t)| < \infty,$$

where $\mathbf{meas}(\Omega) = 0$ means that the Lebesgue measure of the set $\Omega \subset (0, b)$ is equal to zero. For $\vec{w} = (w_1, \dots w_n)^T$, the writing $\vec{w} \in L_n^\infty(0, b)$ means that $w_i \in L^\infty(0, b)$, $i = 1, \dots, n$, and $L_n^\infty(0, b)$ is a Banach space with respect to the norm

$$\|\vec{w}\|_{L_n^\infty(0,b)} := \max_{1\le i\le n} \|w_i\|_{L^\infty(0,b)}, \quad \vec{w} \in L_n^\infty(0, b).$$

Finally, let X and Y be some linear spaces, and let $B : X \to Y$ be a given operator. Then, for a fixed $n \in \mathbb{N}$ and vector $\vec{w} = (w_1, ..., w_n)^T$ with $w_1, \dots, w_n \in X$, by $\boldsymbol{B}\vec{w}$ we denote the vector $(Bw_1, \dots, Bw_n)^T$, with $Bw_1, \dots, Bw_n \in Y$.

Note that without the loss of generality, we can consider Equation (1) only with homogeneous boundary conditions (2) and (3) since, in the case of more general boundary conditions

$$u(0, t) = \phi_0(t), \quad u(L, t) = \phi_L(t), \quad t \in [0, b], \tag{6}$$

where ϕ_0 and ϕ_L are some sufficiently smooth functions on $[0, b]$, Problem {(1), (4), (6)} is easily transformed to a problem with homogeneous boundary conditions. Indeed, introducing (see, e.g., [31]) an auxiliary function $v = v(x, t)$ by

$$v(x, t) = u(x, t) + \frac{x}{L}(\phi_0(t) - \phi_L(t)) - \phi_0(t),$$

the inhomogeneous boundary conditions (6) for u are transformed to the homogeneous boundary conditions for v: $v(0, t) = v(L, t) = 0$, $t \in [0, b]$. Moreover, we see that both Equation (1) and the initial condition (4) maintain their original form with respect to the new unknown function v:

$$(D_t^\alpha v)(x, t) - p\frac{\partial^2 v(x, t)}{\partial x^2} + \theta(x)v(x, t) = \widehat{f}(x, t), \quad (x, t) \in Q,$$

where

$$\widehat{f}(x,t) = f(x,t) + (D^\alpha \phi_L)(t) + \frac{x-L}{L}(D^\alpha \phi_0)(t) + \theta(x)\Big(\frac{x}{L}(\phi_0(t) - \phi_L(t)) - \phi_0(t)\Big)$$

and

$$v(x,0) = \widehat{\phi}(x), \quad x \in [0,L],$$

where

$$\widehat{\phi}(x) = \phi(x) + \frac{x}{L}(\phi_0(0) - \phi_L(0)) - \phi_0(0).$$

For the existence and uniqueness of a classical solution u to (1)–(4) (that is, $D_t^\alpha u$ and $\frac{\partial^2 u}{\partial x^2}$ both exist in Q and u satisfies (1)–(4) pointwise), we refer the reader to [31]. The regularity properties of solutions u to (1)–(4) are described in [12] (see also [14,28,31,32]). In particular, the smoothness of all the data of (1)–(4) does not imply the smoothness of the solution u in the closed domain $\overline{Q}$, and the essential feature of all typical solutions to (1)–(4) is that the first-order derivative, $\frac{\partial u(x,t)}{\partial t}$, in general, blows up as $t \to 0$ (see [12]). This is a significant obstacle for constructing high-order methods for the numerical solutions to (1)–(4).

On the other hand, in [12], it is shown that when the data of Problem (1)–(4) has sufficient regularity, there exists a constant $C > 0$ such that for the spatial derivatives of the exact solution, $u(x,t)$, to (1)–(4), we have

$$\left|\frac{\partial^k u(x,t)}{\partial x^k}\right| \le C, \quad k = 0,1,2,3,4, \quad (x,t) \in [0,L] \times (0,b]. \tag{7}$$

In our approach below, we assume that the solution, u, to (1)–(4) satisfies the derivative bounds (7). In particular, we will use this assumption already in the space variable discretization described in the next section.

3. Space Variable Discretization

We begin by developing a system of fractional differential equations from Problem (1)–(4) by space variable discretization using the idea of the method of lines. Let $n \in \mathbb{N}$, $n \ge 2$. We introduce a uniform mesh on the interval $[0,L]$ defined by $n+1$ gridpoints

$$x_i = ih, \quad i = 0,\dots,n, \quad h = \frac{L}{n}. \tag{8}$$

Using (8) and a standard second-order difference formula

$$\frac{\partial^2 u(x_i,t)}{\partial x^2} = \frac{u(x_{i+1},t) - 2u(x_i,t) + u(x_{i-1},t)}{h^2} + \mathcal{O}(h^2), \quad t \in (0,b], \quad i = 1,\dots,n-1, \tag{9}$$

we approximate (1)–(4) using a system of equations

$$(D^\alpha y_i)(t) - p\frac{y_{i+1}(t) - 2y_i(t) + y_{i-1}(t)}{h^2} + \theta(x_i)y_i(t) = f(x_i,t), \quad i = 1,\dots,n-1. \tag{10}$$

Here,

$$y_i = y_i(t) \approx u(x_i,t), \quad t \in (0,b], \quad i = 1,\dots,n-1,$$

are the unknown functions, and y_0 and y_n are defined by

$$y_0(t) := u(0,t) = 0, \quad t \in [0,b],$$
$$y_n(t) := u(L,t) = 0, \quad t \in [0,b].$$

Thus, we have for finding $y_1(t), \ldots, y_{n-1}(t)$ a system of fractional differential equations in the form

$$(D^\alpha y_i)(t) + \sum_{j=1}^{n-1} a_{ij} y_j(t) = v_i(t), \quad 0 < t \leq b, \quad \alpha \in (0,1), \quad i = 1, \ldots, n-1, \tag{11}$$

subject to the initial conditions

$$y_i(0) = \phi(x_i), \quad i = 1, \ldots, n-1, \tag{12}$$

where the function ϕ is given by (4), the functions $v_i \in C[0,b]$ are defined by

$$v_i(t) = f(x_i, t), \quad i = 1, \ldots, n-1, \tag{13}$$

and the constants a_{ij} $(i, j = 1, \ldots, n-1)$ are determined by

$$a_{ij} = \begin{cases} \dfrac{2p}{h^2} + \theta(x_i) & \text{if } i = j, \\ -\dfrac{p}{h^2} & \text{if } |i-j| = 1, \\ 0 & \text{otherwise.} \end{cases}$$

For simplicity of presentation, we rewrite (11) and (12) in vector form

$$(\boldsymbol{D}^{\boldsymbol{\alpha}} \vec{y})(t) + A\vec{y}(t) = \vec{v}(t), \quad t \in (0,b], \tag{14}$$
$$\vec{y}(0) = \vec{\beta}, \tag{15}$$

where $\vec{y}(t) = (y_1(t), \ldots, y_{n-1}(t))^T$ is unknown, its Caputo fractional derivative is defined componentwise by $(\boldsymbol{D}^{\boldsymbol{\alpha}} \vec{y})(t) = ((D^\alpha y_1)(t), \ldots, (D^\alpha y_{n-1})(t))^T$, and

$$\vec{v}(t) = \begin{pmatrix} v_1(t) \\ \vdots \\ v_{n-1}(t) \end{pmatrix}, \quad \vec{\beta} = \begin{pmatrix} \phi(x_1) \\ \vdots \\ \phi(x_{n-1}) \end{pmatrix}, \quad A = \begin{pmatrix} a_{1,1} & \ldots & a_{1,n-1} \\ \vdots & \ddots & \vdots \\ a_{n-1,1} & \ldots & a_{n-1,n-1} \end{pmatrix}.$$

Below, we will also need the Riemann–Liouville integral operator, J^δ, of order $\delta \in [0, \infty)$, defined by

$$(J^\delta y)(x) = \frac{1}{\Gamma(\delta)} \int_0^x (x-t)^{\delta-1} y(t) dt, \quad x \in [0,b], \; y \in L^\infty(0,b), \; \delta > 0; \; J^0 = I,$$

where I is the identity mapping and Γ is the Euler gamma function. Note that the operator J^δ is linear, bounded, and compact as an operator from $L^\infty(0,b)$ to $C[0,b]$ (see, e.g., [33]). Moreover, we have for any $y \in L^\infty(0,b)$ that (see, e.g., [34])

$$(J^\delta y)(0) = 0, \quad \delta > 0, \tag{16}$$
$$D^{\delta_1} J^{\delta_2} y = J^{\delta_2 - \delta_1} y, \quad 0 < \delta_1 \leq \delta_2. \tag{17}$$

4. Integral Equation Reformulation

Let $\vec{y} = (y_1, \ldots, y_{n-1})^T \in C_{n-1}[0,b]$ be an arbitrary continuous vector function, such that $\vec{z} := \boldsymbol{D}^{\boldsymbol{\alpha}} \vec{y} \in C_{n-1}[0,b]$. Then, with the help of (5) and (17), we obtain

$$\vec{y}(t) = (\boldsymbol{J}^{\boldsymbol{\alpha}} \vec{z})(t) + \vec{c}, \quad t \in [0,b], \tag{18}$$

where $\vec{c} = (c_1, \ldots, c_{n-1})^T$ is a constant vector and

$$(\boldsymbol{J}^{\boldsymbol{\alpha}}\vec{z})(t) = \begin{pmatrix} (J^{\alpha}z_1)(t) \\ \vdots \\ (J^{\alpha}z_{n-1})(t) \end{pmatrix}, \quad t \in [0,b].$$

It follows from (16) that $\vec{y}$ in the form of (18) satisfies the initial condition (15) if and only if

$$\vec{c} = \vec{\beta}. \tag{19}$$

Let now $\vec{y}$ be a solution to (14) and (15) such that $\vec{y} \in C_{n-1}[0,b]$ and $\vec{z} = \boldsymbol{D}^{\boldsymbol{\alpha}}\vec{y} \in C_{n-1}[0,b]$. Then, due to (18) and (19), we can rewrite Problem (14)–(15) in the form

$$\vec{z} = \boldsymbol{T}\vec{z} + \vec{g}, \tag{20}$$

where

$$(\boldsymbol{T}\vec{z})(t) = -A[(\boldsymbol{J}^{\boldsymbol{\alpha}}\vec{z})(t)], \quad t \in [0,b], \tag{21}$$

$$\vec{g}(t) = \vec{v}(t) - A\vec{\beta}, \quad t \in [0,b]. \tag{22}$$

Conversely, it is easy to see that if $\vec{z} \in C_{n-1}[0,b]$ is a solution to (20), then $\vec{y}$ defined by (18) with $\vec{c} = \vec{\beta}$ is a solution to (14) and (15) and belongs to $C_{n-1}[0,b]$. In this sense, Equation (20) is equivalent to Problem (14)–(15).

In order to describe the existence, uniqueness, and regularity properties of the solution to Problem (14)–(15), we introduce weighted spaces, $C^{q,\kappa}(0,b]$ and $C_n^{q,\kappa}(0,b]$, adaptions of a more general weighted space of functions introduced in [35] (see also [33]). For $t > 0$, we define the weight function

$$\omega_\kappa(t) = \begin{cases} 1 & \text{if } \kappa < 0, \\ \dfrac{1}{1 + |\log t|} & \text{if } \kappa = 0, \\ t^\kappa & \text{if } \kappa > 0, \end{cases}$$

and for given $b \in \mathbb{R}$, $b > 0$, $q \in \mathbb{N}$, $\kappa \in \mathbb{R}$, $\kappa < 1$, by $C^{q,\kappa}(0,b]$, we denote the Banach space of continuous functions, $y : [0,b] \to \mathbb{R}$, which are q times continuously differentiable in $(0,b]$, such that

$$\|y\|_{C^{q,\kappa}(0,b]} := \max_{0 \le t \le b} |y(t)| + \sum_{i=1}^{q} \sup_{0<t\le b} \omega_{i-1+\kappa}(t)|y^{(i)}(t)| < \infty.$$

We see that if $y \in C^{q,\kappa}(0,b]$, then for all $t \in (0,b]$ and $i = 1, \ldots, q$, the following estimation holds:

$$|y^{(i)}(t)| \le c \begin{cases} 1 & \text{if } i < 1 - \kappa, \\ 1 + |\log t| & \text{if } i = 1 - \kappa, \\ t^{1-\kappa-i} & \text{if } i > 1 - \kappa, \end{cases}$$

where $c = c(y)$ is a positive constant.

Further, given $b \in \mathbb{R}$, $b > 0$, $q, n \in \mathbb{N}$ and $\kappa \in \mathbb{R}$, $\kappa < 1$, notation $\vec{y} \in C_n^{q,\kappa}(0,b]$ means that $y_i \in C^{q,\kappa}(0,b]$ for $i = 1, \ldots, n$. The set $C_n^{q,\kappa}(0,b]$ becomes a Banach space if it is equipped with the norm

$$\|\vec{y}\|_{C_n^{q,\kappa}(0,b]} = \max_{1 \le i \le n} \|y_i\|_{C^{q,\kappa}(0,b]}, \quad \vec{y} \in C_n^{q,\kappa}(0,b].$$

Note that

$$C^q_n[0,b] \subset C^{q,\kappa}_n(0,b] \subset C^{m,\eta}_n(0,b] \subset C_n[0,b], \quad q \geq m \geq 1, \quad \kappa \leq \eta < 1, \ n \in \mathbb{N}.$$

Following the proof of Lemma 2.2, in [33], we can prove the following result.

Lemma 1. *Let $\eta \in (-\infty, 1)$ and $n \in \mathbb{N}$. Then operator $\boldsymbol{S}$, defined by*

$$(\boldsymbol{S}\vec{y})(t) = \int_0^t (t-s)^{-\eta}\vec{y}(s)ds, \quad t \in [0,b],$$

is compact as an operator from $L^\infty_n(0,b)$ to $C_n[0,b]$, thus also from $C_n[0,b]$ to $C_n[0,b]$ and from $L^\infty_n(0,b)$ to $L^\infty_n(0,b)$. Furthermore, $\boldsymbol{S}$ is compact as an operator from $C^{q,\kappa}_n(0,b]$ into $C^{q,\kappa}_n(0,b]$, where $\eta \leq \kappa < 1$.

Theorem 1. *Let $0 < \alpha < 1$ and let $\theta \in C[0,L]$, where $\theta \geq 0$, $\phi \in C[0,L]$, $f \in C([0,L] \times [0,b])$. Let $n \in \mathbb{N}$, $n \geq 2$. Then, the following statements are fulfilled.*

(i) *Problem (14)–(15) possesses a unique solution, $\vec{y} = (y_1, \ldots, y_{n-1})^T$, such that it and its Caputo derivative, $\vec{z} = \boldsymbol{D}^{\boldsymbol{\alpha}}\vec{y}$, belong to $C_{n-1}[0,b]$.*

(ii) *Let $\vec{v} = (v_1, \ldots, v_{n-1})^T \in C^{q,\mu}_{n-1}(0,b]$, $q \in \mathbb{N}$, $\mu < 1$, with $v_1, \ldots, v_{n-1}$, given by (13). Then $\vec{y}$, the solution to Problem (14)–(15) and its Caputo derivative, $\vec{z} = \boldsymbol{D}^{\boldsymbol{\alpha}}\vec{y}$, belong to $C^{q,\kappa}_{n-1}(0,b]$, where*

$$\kappa = \max\{1-\alpha, \mu\}. \tag{23}$$

Proof. *(i)* We observe that $\vec{g} = \vec{v} - A\vec{\beta} \in C_{n-1}[0,b]$ since $\vec{v} \in C_{n-1}[0,b]$ and $A\vec{\beta} \in C_{n-1}[0,b]$. Further, $\boldsymbol{T} = -A\boldsymbol{J}^{\boldsymbol{\alpha}}$ is a compact operator from $C_{n-1}[0,b]$ to $C_{n-1}[0,b]$ since $\boldsymbol{J}^{\boldsymbol{\alpha}} : C_{n-1}[0,b] \to C_{n-1}[0,b]$ is compact. Note that the homogeneous equation, $\vec{z} = \boldsymbol{T}\vec{z}$, has in $C_{n-1}[0,b]$ only a trivial solution, $\vec{z} = (0, \ldots, 0)^T$. Therefore, using the Fredholm alternative, we obtain that the equation $\vec{z} = \boldsymbol{T}\vec{z} + \vec{g}$ possesses in $C_{n-1}[0,b]$ a unique solution $\vec{z} \in C_{n-1}[0,b]$. Thus, Problem (14)–(15) has a unique solution $\vec{y} = \boldsymbol{J}^{\boldsymbol{\alpha}}\vec{z} + \vec{\beta} \in C_{n-1}[0,b]$.

(ii) Let $\vec{v} \in C^{q,\mu}_{n-1}(0,b]$, $q \in \mathbb{N}$, $\mu < 1$. Then, clearly $\vec{g} = \vec{v} - A\vec{\beta} \in C^{q,\mu}_{n-1}(0,b] \subset C^{q,\kappa}_{n-1}(0,b]$. Since $1-\alpha \leq \kappa$, it follows from Lemma 1 that $\boldsymbol{J}^{\boldsymbol{\alpha}}$ is a compact operator from $C^{q,\kappa}_{n-1}(0,b]$ to $C^{q,\kappa}_{n-1}(0,b]$. Therefore, $\boldsymbol{T} = -A\boldsymbol{J}^{\boldsymbol{\alpha}}$ is also a compact operator from $C^{q,\kappa}_{n-1}(0,b]$ to $C^{q,\kappa}_{n-1}(0,b]$. Since the homogeneous equation $\vec{z} = \boldsymbol{T}\vec{z}$ has in $C^{q,\kappa}_{n-1}(0,b] \subset C_{n-1}[0,b]$ only a trivial solution, it follows from the Fredholm alternative that equation $\vec{z} = \boldsymbol{T}\vec{z} + \vec{g}$ has a unique solution $\vec{z} \in C^{q,\kappa}_{n-1}(0,b]$. Thus, Problem (14)–(15) possesses a unique solution $\vec{y} = \boldsymbol{J}^{\boldsymbol{\alpha}}\vec{z} + \vec{\beta} \in C^{q,\kappa}_{n-1}(0,b]$. □

5. Approximate Solutions for (14)–(15)

We construct an approximation $\vec{y_N}$ to $\vec{y}$, the exact solution to Problem (14)–(15), as follows. First, we find an approximation $\vec{z_N}$ for $\vec{z}$, the exact solution to (20). Let $N \in \mathbb{N}$. We introduce on the interval $[0,b]$ a graded grid, $\Pi_N = \{t_0, \ldots, t_N\}$, with the grid points

$$t_j = b\left(\frac{j}{N}\right)^r, \quad j = 0, 1, \ldots, N, \tag{24}$$

where $r \in [1, \infty)$ is the so-called grading exponent. We see that for $r = 1$, the points (24) are distributed uniformly, but for $r > 1$ they are more densely clustered near the left endpoint of the interval $[0,b]$.

For a given integer $k \in \mathbb{N}_0$, let π_k denote the set of polynomials of a degree not exceeding k. We introduce the space of piecewise polynomial functions

$$S^{(-1)}_k(\Pi_N) = \{\omega : \quad \omega|_{[t_{j-1},t_j]} \in \pi_k, \ j = 1, \ldots, N\},$$

where $\omega|_{[t_{j-1},t_j]}$ is the restriction of function $\omega : [0,b] \to \mathbb{R}$ to the subinterval $[t_{j-1}, t_j] \subset [0,b]$. Observe that the elements of the space $S_k^{(-1)}(\Pi_N)$ may have jump discontinuities at the interior points $t_1, \dots, t_{N-1}$ of Π_N.

Let $m \in \mathbb{N}$. Let $\eta_1, \dots, \eta_m$ be a fixed system of collocation parameters satisfying

$$0 \leq \eta_1 < \eta_2 < \ldots < \eta_m \leq 1.$$

Using these collocation parameters, we introduce m collocation points in each subinterval $[t_{j-1}, t_j] \subset [0,b]$ by the formula

$$t_{jk} = t_{j-1} + \eta_k(t_j - t_{j-1}), \quad k = 1, \dots, m, \quad j = 1, \dots, N. \tag{25}$$

We find the approximation $\vec{z_N} = (z_{1,N}, \dots, z_{n-1,N})^T$ for the exact solution $\vec{z}$ of equation $\vec{z} = \boldsymbol{T}\vec{z} + \vec{g}$ using collocation conditions

$$\vec{z_N}(t_{jk}) = \boldsymbol{T}\vec{z_N}(t_{jk}) + \vec{g}(t_{jk}), \quad k = 1, \dots, m, \quad j = 1, \dots, N, \tag{26}$$

where $\{t_{jk}\}$ is defined by (25) and $z_{1,N}, \dots, z_{n-1,N} \in S_{m-1}^{(-1)}(\Pi_N)$ $(m, N \in \mathbb{N})$. If $\eta_1 = 0$, then, by $\vec{z_N}(t_{j1})$, we denote the right limit $\lim_{t \to t_{j-1}, t > t_{j-1}} \vec{z_N}(t)$. If $\eta_m = 1$, then, by $\vec{z_N}(t_{jm})$, we denote the left limit $\lim_{t \to t_j, t < t_j} \vec{z_N}(t)$.

The collocation conditions (26) with respect to $\vec{z_N} = (z_{1,N}, \dots, z_{n-1,N})^T$ lead to a system of linear algebraic equations to find $z_{iN} \in S_{m-1}^{(-1)}(\Pi_N)$, $i = 1, \dots, n-1$, the exact form of which is determined by the choice of a basis in the space $S_{m-1}^{(-1)}(\Pi_N)$. We can use Lagrange fundamental polynomial representation

$$z_{iN}(t) = \sum_{\lambda=1}^{N} \sum_{\mu=1}^{m} c_{i\lambda\mu} l_{\lambda\mu}(t), \quad t \in [0,b], \quad i = 1, \dots, n-1, \tag{27}$$

where, for $\lambda = 1, \dots, N$, and $\mu = 1, \dots, m$, we set $l_{\lambda\mu}(t) = 0$ if $t \notin [t_{\lambda-1}, t_\lambda]$ and

$$l_{\lambda\mu}(t) = \begin{Bmatrix} 1, & m = 1 \\ \prod_{\nu=1,\nu\neq\mu}^{m} \frac{t - t_{\lambda\nu}}{t_{\lambda\mu} - t_{\lambda\nu}}, & m > 1 \end{Bmatrix} \quad \text{if } t \in [t_{\lambda-1}, t_\lambda].$$

Then, $z_{iN} \in S_{m-1}^{(-1)}(\Pi_N)$ and $z_{iN}(t_{jk}) = c_{ijk}$ for every $k = 1, \dots, m$, $j = 1, \dots, N$, $i = 1, \dots, n-1$. Thus, we obtain a system of linear algebraic equations with respect to the coefficients $\{c_{ijk}\}$:

$$c_{ijk} = -\sum_{\gamma=1}^{n-1} a_{i\gamma} \left(\sum_{\lambda=1}^{N} \sum_{\mu=1}^{m} (J^\alpha l_{\lambda\mu})(t_{jk}) c_{\gamma\lambda\mu} \right) + v_i(t_{jk}) - \sum_{\gamma=1}^{n-1} a_{i\gamma}\beta_\gamma, \tag{28}$$

for $i = 1, \dots, n-1$, $j = 1, \dots, N$, $k = 1, \dots, m$.

Having found $\{c_{ijk}\}$ by the system (28), we can determine $\vec{z_N} = (z_{1,N}, \dots, z_{n-1,N})^T$ with the help of (27). Thus, we obtain the approximation $\vec{y_N} = (y_{1,N}, \dots, y_{n-1,N})^T$ to $\vec{y}$, the solution to Problem (14)–(15), as follows:

$$\vec{y_N}(t) = (\boldsymbol{J}^{\boldsymbol{\alpha}} \vec{z_N})(t) + \vec{\beta}, \quad t \in [0,b]. \tag{29}$$

6. Convergence Analysis

In this section, we study the convergence and convergence order of our method.

For given $N, m \in \mathbb{N}$, we define the interpolation operator, $\mathcal{P}_N = \mathcal{P}_{N,m} : C[0,b] \to S_{m-1}^{(-1)}(\Pi_N)$, by

$$\mathcal{P}_N\omega \in S_{m-1}^{(-1)}(\Pi_N), \quad (\mathcal{P}_N\omega)(t_{jk}) = \omega(t_{jk}), \quad j = 1, \ldots, N, \quad k = 1, \ldots, m,$$

for any continuous function $\omega \in C[0,b]$. If $\eta_1 = 0$, then, by $(\mathcal{P}_N\omega)(t_{j1})$, we denote the right limit $\lim_{t\to t_{j-1}, t>t_{j-1}}(\mathcal{P}_N\omega)(t)$. If $\eta_m = 1$, then $(\mathcal{P}_N\omega)(t_{jm})$ denotes the left limit $\lim_{t\to t_j, t<t_j}(\mathcal{P}_N\omega)(t)$. Using operator $\mathcal{P}_N$, the conditions (26) for finding $\vec{z_N} = (z_{1,N}, \ldots, z_{n-1,N})$ with $z_{iN} \in S_{m-1}^{(-1)}(\Pi_N)$, $i = 1, \ldots, n-1$, take the form

$$\vec{z}_N = \boldsymbol{\mathcal{P}_N T}\vec{z}_N + \boldsymbol{\mathcal{P}_N}\vec{g}. \tag{30}$$

In order to prove Theorem 2 below, we need Lemmas 2–4. Lemmas 2 and 3 follow from the results of [33,35] and Lemma 4 follows from [16].

Lemma 2. *The operators, $\mathcal{P}_N$, $N \in \mathbb{N}$, belong to the space $\mathcal{L}(C[0,b], L^\infty(0,b))$ and*

$$\|\mathcal{P}_N\|_{\mathcal{L}(C[0,b],L^\infty(0,b))} \le c,$$

with a positive constant c, which is independent of N. Moreover, for every $u \in C[0,b]$, we have

$$\|u - \mathcal{P}_N u\|_{L^\infty(0,b)} \to 0 \quad as \quad N \to \infty.$$

Lemma 3. *Let $\mathcal{A} : L^\infty(0,b) \to C[0,b]$ be a linear compact operator. Then,*

$$\|\mathcal{A} - \mathcal{P}_N\mathcal{A}\|_{\mathcal{L}(L^\infty(0,b),L^\infty(0,b))} \to 0 \quad as \quad N \to \infty.$$

Lemma 4. *Let $u \in C^{m+1,\kappa}(0,b]$, $m \in \mathbb{N}$, $\kappa \in (-\infty, 1)$, $N \in \mathbb{N}$, and $r \in [1,\infty)$. Let J^α $(0 < \alpha < 1)$ be the Riemann–Liouville integral operator of order α. Assume that the collocation points (25) with grid points (24) and parameters $\eta_1, \ldots, \eta_m$ satisfying $0 \le \eta_1 < \ldots < \eta_m \le 1$ are used. Moreover, assume that $\eta_1, \ldots, \eta_m$ are such that a quadrature approximation*

$$\int_0^1 F(x)dx \approx \sum_{k=1}^m w_k F(\eta_k), \quad 0 \le \eta_1 < \ldots < \eta_m \le 1, \tag{31}$$

with appropriate weights $\{w_k\}$ is exact for all polynomials F of degree m.

Then

$$\|J^\alpha(\mathcal{P}_N u - u)\|_{C[0,b]} \le cE_N(m,\kappa,r,\alpha),$$

where c is a positive constant independent of N and

$$E_N(m,\kappa,r,\alpha) = \begin{cases} N^{-m-\alpha} & for \quad m < 1+\alpha-\kappa, & r \ge 1, \\ N^{-m-\alpha}(1+\log N) & for \quad m = 1+\alpha-\kappa, & r = 1, \\ N^{-m-\alpha} & for \quad m = 1+\alpha-\kappa, & r > 1, \\ N^{-r(1+\alpha-\kappa)} & for \quad m > 1+\alpha-\kappa, & 1 \le r < \dfrac{m+\alpha}{1+\alpha-\kappa}, \\ N^{-m-\alpha} & for \quad m > 1+\alpha-\kappa, & r \ge \dfrac{m+\alpha}{1+\alpha-\kappa}. \end{cases} \tag{32}$$

Theorem 2. *Let the assumptions of Theorem 1 be fulfilled. Let $n, m, N \in \mathbb{N}$, $n \ge 2$, and assume that the collocation points (25) with parameters $\eta_1, \ldots, \eta_m$ satisfying $0 \le \eta_1 < \ldots < \eta_m \le 1$ and grid points (24) are used. Moreover, assume that parameters $\{\eta_i\}$ are chosen so that quadrature approximation (31) with appropriate weights is exact for all polynomials F of degree m. Then, the following statements are fulfilled.*

(i) *Problem (14)–(15) possesses a unique solution, $\vec{y} \in C_{n-1}[0,b]$, such that $\vec{z} = \boldsymbol{D}^{\alpha}\vec{y} \in C_{n-1}[0,b]$. There exists an integer $N_0 > 0$, such that for $N \geq N_0$, Equation (30) possesses a unique solution $\vec{z_N} = (z_{1,N}, \ldots, z_{n-1,N})^T$, where $z_{i,N} \in S_{m-1}^{(-1)}(\Pi_N)$ for $i = 1, \ldots, n-1$, determining by (29) a unique approximation $\vec{y}_N \in C_{n-1}[0,b]$ to $\vec{y}$, the solution to (14) and (15), and*

$$\|\vec{y} - \vec{y}_N\|_{C_{n-1}[0,b]} \to 0 \text{ as } N \to \infty. \tag{33}$$

(ii) *If $\vec{v} = (v_1, \ldots, v_{n-1})^T \in C_{n-1}^{m+1,\mu}(0,b]$, with $v_1, \ldots, v_{n-1}$ given by (13), then Problem (14)–(15) has a unique solution $\vec{y} \in C_{n-1}[0,b]$, such that $\vec{y}$ and its Caputo derivative $\vec{z}$ belong to $C_{n-1}^{m+1,\kappa}(0,b]$ and the following error estimate holds:*

$$\|\vec{y} - \vec{y}_N\|_{C_{n-1}[0,b]} \leq cE_N(m,\kappa,r,\alpha). \tag{34}$$

Here, κ is given by Formula (23), r is a grading exponent given in (24), and E_N is defined by (32).

Proof. *(i)* Existence and uniqueness are already proven in Theorem 1; thus, we only need to prove the convergence (33). We note that $\boldsymbol{T}$ is a compact operator from $L_{n-1}^{\infty}(0,b)$ to $C_{n-1}[0,b]$ (see Lemma 1), thus also from $L_{n-1}^{\infty}(0,b)$ to $L_{n-1}^{\infty}(0,b)$. Using the same proof idea as in Theorem 1, we can show that equation $\vec{z} = \boldsymbol{T}\vec{z} + \vec{g}$ possesses a unique solution $\vec{z} \in L_{n-1}^{\infty}(0,b)$. In other words, operator $\boldsymbol{I} - \boldsymbol{T}$ is invertible in $L_{n-1}^{\infty}(0,b)$ and its inverse is bounded: $(\boldsymbol{I} - \boldsymbol{T})^{-1} \in \mathcal{L}(L_{n-1}^{\infty}(0,b), L_{n-1}^{\infty}(0,b))$. From this and Lemma 3, we obtain that for all sufficiently large N, we can say that

$$\left\|(\boldsymbol{I} - \boldsymbol{T})^{-1}\right\|_{\mathcal{L}(L_{n-1}^{\infty}(0,b), L_{n-1}^{\infty}(0,b))} \|\boldsymbol{T} - \boldsymbol{\mathcal{P}_N T}\|_{\mathcal{L}(L_{n-1}^{\infty}(0,b), L_{n-1}^{\infty}(0,b))} < 1.$$

Therefore, operator $\boldsymbol{I} - \boldsymbol{\mathcal{P}_N T}$ is invertible in $L_{n-1}^{\infty}(0,b)$ for sufficiently large N and

$$\left\|(\boldsymbol{I} - \boldsymbol{\mathcal{P}_N T})^{-1}\right\|_{\mathcal{L}(L_{n-1}^{\infty}(0,b), L_{n-1}^{\infty}(0,b))} \leq c, \quad N \geq N_0, \tag{35}$$

where c is a constant independent of N. Thus, for $N \geq N_0$, Equation (30) has a unique solution, $\vec{z}_N$, where $z_{iN} \in S_{m-1}^{(-1)}(\Pi_N)$ for every $i = 1, \ldots, n-1$. For $\vec{z}_N$ and $\vec{z}$, the solution to equation $\vec{z} = \boldsymbol{T}\vec{z} + \vec{g}$, we see that

$$\begin{aligned}(\boldsymbol{I} - \boldsymbol{\mathcal{P}_N T})(\vec{z} - \vec{z}_N) &= \vec{z} - \vec{z}_N - \boldsymbol{\mathcal{P}_N T}\vec{z} + \boldsymbol{\mathcal{P}_N T}\vec{z}_N \\ &= \vec{z} - \boldsymbol{\mathcal{P}_N}(\boldsymbol{T}\vec{z} + \vec{g}) = \vec{z} - \boldsymbol{\mathcal{P}_N}\vec{z}.\end{aligned}$$

Therefore, by (35),

$$\|\vec{z} - \vec{z}_N\|_{L_{n-1}^{\infty}(0,b)} \leq c\|\vec{z} - \boldsymbol{\mathcal{P}_N}\vec{z}\|_{L_{n-1}^{\infty}(0,b)}, \quad N \geq N_0, \tag{36}$$

where c is a positive constant independent of N. It follows from (18), (29), (36), and Lemma 1 that

$$\|\vec{y} - \vec{y}_N\|_{C_{n-1}[0,b]} \leq c_1\|\vec{z} - \boldsymbol{\mathcal{P}_N}\vec{z}\|_{C_{n-1}[0,b]},$$

where c_1 is a positive constant independent of N. Using Lemma 2, we see that convergence (33) holds.

(ii) It follows from Theorem 1 part *(ii)* (with $q = m+1$) that Problem (14)–(15) has a unique solution, such that $\vec{y}, \vec{z} \in C_{n-1}^{q,\kappa}(0,b]$. From the proof of part *(i)*, we know that there exists an integer N_0, such that for $N \geq N_0$, Equation (30) has a unique solution $\vec{z_N} = (z_{1,N}, \ldots, z_{n-1,N})^T$, where for every $i = 1, \ldots, n-1$, $z_{iN} \in S_{m-1}^{(-1)}(\Pi_N)$. Denote

$$\hat{\vec{z}}_N = \boldsymbol{T}\vec{z}_N + \vec{g}, \quad N \geq N_0. \tag{37}$$

With the help of (30), we see that $\mathcal{P}_N\hat{\vec{z}}_N = \vec{z}_N$, and therefore we obtain from (37) the following equation with respect to $\hat{\vec{z}}_N$:

$$\hat{\vec{z}}_N = T\mathcal{P}_N\hat{\vec{z}}_N + \vec{g}, \quad N \geq N_0. \tag{38}$$

Since $\vec{z} = T\vec{z} + \vec{g}$, it follows from (38) for every $N \geq N_0$ that

$$(I - T\mathcal{P}_N)(\hat{\vec{z}}_N - \vec{z}) = T(\mathcal{P}_N\vec{z} - \vec{z}). \tag{39}$$

We know from the proof of part (i) that $(I - \mathcal{P}_N T)$ is invertible in $\mathcal{L}(L^\infty_{n-1}(0,b), L^\infty_{n-1}(0,b))$ for sufficiently large N and $(I - \mathcal{P}_N T)^{-1} \in \mathcal{L}(L^\infty_{n-1}(0,b), L^\infty_{n-1}(0,b))$ for all $N \geq N_0$. Thus, there exists also the inverse of $(I - T\mathcal{P}_N)$ in $\mathcal{L}(L^\infty_{n-1}(0,b), L^\infty_{n-1}(0,b))$ for $N \geq N_0$ and

$$(I - T\mathcal{P}_N)^{-1} = I + T(I - \mathcal{P}_N T)^{-1}\mathcal{P}_N, \quad N \geq N_0. \tag{40}$$

Using (39), (40), (35), and Lemma 2, we obtain

$$\begin{aligned}\|\hat{\vec{z}}_N - \vec{z}\|_{L^\infty_{n-1}(0,b)} &= \left\|(I - T\mathcal{P}_N)^{-1}T(\mathcal{P}_N\vec{z} - \vec{z})\right\|_{L^\infty_{n-1}(0,b)} \\ &\leq c\|T(\mathcal{P}_N\vec{z} - \vec{z})\|_{L^\infty_{n-1}(0,b)}, \quad N \geq N_0,\end{aligned}$$

where c is a positive constant independent of N. From the definition of the operator T we see that

$$\|T(\mathcal{P}_N\vec{z} - \vec{z})\|_{L^\infty_{n-1}(0,b)} \leq c_1\|J^\alpha(\mathcal{P}_N\vec{z} - \vec{z})\|_{L^\infty_{n-1}(0,b)}, \quad N \geq N_0$$

and therefore,

$$\|\hat{\vec{z}}_N - \vec{z}\|_{L^\infty_{n-1}(0,b)} \leq c_2\|J^\alpha(\mathcal{P}_N\vec{z} - \vec{z})\|_{L^\infty_{n-1}(0,b)}, \quad N \geq N_0,$$

where c_1 and c_2 are some positive constants independent of N. Due to $\vec{z}_N = \mathcal{P}_N\hat{\vec{z}}_N$, we obtain

$$\vec{z}_N - \vec{z} = \mathcal{P}_N(\hat{\vec{z}}_N - \vec{z}) + \mathcal{P}_N\vec{z} - \vec{z}.$$

This leads to the estimate

$$\|\vec{y}_N - \vec{y}\|_{C_{n-1}[0,b]} \leq c_3\|J^\alpha(\mathcal{P}_N\vec{z} - \vec{z}))\|_{C_{n-1}[0,b]},$$

where $c_3 > 0$ is a constant that is independent of N and where $\vec{y_N}$ and $\vec{y}$ are defined with the help of (29) and (18), respectively. Using Lemma 4, we see that the error estimate (34) holds. □

In Theorem 3 below, we present the error estimate of our numerical method for solving Problem (1)–(4). We assume that the data of Problem (1)–(4) satisfies the conditions laid out in Theorem 2.1 in [12]. Under these assumptions, it follows from [12] that Problem (1)–(4) has a unique solution u that satisfies (1)–(4) pointwise, and there exists a constant C, such that

$$\left|\frac{\partial^k u(x,t)}{\partial x^k}\right| \leq C, \quad (x,t) \in [0,L] \times (0,b], \quad k = 0,1,2,3,4, \tag{41}$$

$$\left|\frac{\partial^l u(x,t)}{\partial t^l}\right| \leq C(1 + t^{\alpha - l}), \quad (x,t) \in [0,L] \times (0,b], \quad l = 0,1,2. \tag{42}$$

Theorem 3. *Let the solution u to (1)–(4) satisfy the estimates (41) and (42). Let the assumptions of Theorem 2 be fulfilled. Then, the following error estimate holds:*

$$\max_{(x_i,t)\in\bar{Q}} |u(x_i,t) - y_{i,N}(t)| \leq c(h^2 + E_N(m,\kappa,r,\alpha)), \quad i = 1,\ldots,n-1.$$

Here, $h = \frac{L}{n}$ *(*$n \geq 2$*),* $E_N(m, \kappa, r, \alpha)$ *is defined by (32),* $N, m \in \mathbb{N}$*,* κ *is given by formula (23),* r *is a grading exponent given in (25),* $\vec{y_N} = (y_{1,N}, \ldots, y_{n-1,N})^T$ *is given by (29), and* c *is a positive constant that is independent of* n *and* N*.*

Proof. It follows from (9) and Theorem 2 that for $i = 1, \ldots, n-1$, we have

$$\max_{(x_i,t)\in\bar{Q}} |u(x_i,t) - y_{i,N}(t)| \leq \max_{(x_i,t)\in\bar{Q}} |u(x_i,t) - y_i(t)| + \max_{t\in[0,b]} |y_i(t) - y_{i,N}(t)|$$
$$\leq c(h^2 + E_N(m,\kappa,r,\alpha)).$$

Note that x_i are fixed points defined by our numerical method, but t belongs to $[0, b]$. □

7. Numerical Experiments

7.1. Example 1

Consider the equation

$$(D_t^{0.2}u)(x,t) - \frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\Gamma(1.5)}{\Gamma(1.3)} t^{0.3} \sin x + t^{0.5} \sin x \tag{43}$$

for $(x,t) \in Q := (0,\pi) \times (0,1]$ with

$$u(0,t) = 0, \quad t \in [0,1], \tag{44}$$
$$u(\pi,t) = 0, \quad t \in [0,1], \tag{45}$$
$$u(x,0) = 0, \quad x \in [0,\pi]. \tag{46}$$

We see that (43)–(46) is a problem of the form (1)–(4), where $\alpha = 0.2$, $L = \pi$, $b = 1$, $\theta = \phi = 0$, and $f(x,t) = \frac{\Gamma(1.5)}{\Gamma(1.3)} t^{0.3} \sin x + t^{0.5} \sin x$ for $(x,t) \in Q$. The exact solution to (43)–(46) is given by

$$u(x,t) = t^{0.5} \sin x, \quad (x,t) \in \overline{Q}.$$

Let $n \in \mathbb{N}$, $n \geq 2$. We introduce a uniform mesh on the interval $[0,\pi]$ with gridpoints $x_i = ih$, $i = 0, \ldots, n$, where $h = \frac{\pi}{n}$. Using the space-variable discretization described in Section 3, we obtain a system of fractional differential equations in the form (11) with initial conditions (12) and functions

$$v_i(t) = \frac{\Gamma(1.5)}{\Gamma(1.3)} t^{0.3} \sin x_i + t^{0.5} \sin x_i, \quad t \in [0,1], \quad i = 1, \ldots, n-1.$$

It is easy to see that functions v_i belong to $C^{q,\mu}(0,1]$, with $\mu = 0.7$ and arbitrary $q \in \mathbb{N}$. Therefore, by (23),

$$\kappa = \max\{\mu, 1-\alpha\} = 0.8.$$

Approximations $z_{i,N} \in S_{m-1}^{(-1)}(\Pi_N)$ $(N \in \mathbb{N})$ for $i = 1, \ldots, n-1$ for the solution $\vec{z} = (z_1, \ldots, z_{n-1})$ to Equation (20) are found using grid points (24) and collocation points (25), where

$$\eta_1 = \frac{1}{2} \quad (\text{if } m = 1) \tag{47}$$

and

$$\eta_1 = \frac{3-\sqrt{3}}{6}, \quad \eta_2 = 1 - \eta_1 \quad (\text{if } m = 2) \tag{48}$$

are collocation parameters. Note that (47) and (48) are actually the knots of the m-point Gaussian quadrature approximation for $m = 1$ and $m = 2$, respectively (see, e.g., [36]). Finally, based on z_{iN}, the approximate solutions, y_{iN}, to (11) and (12) are found.

We present, in the tables below, some results of numerical experiments for different values of parameters n, m, N, and r. The errors, $\varepsilon_{n,N}$, are calculated as follows:

$$\varepsilon_{n,N} = \max_{i=1,\dots,n-1} \max_{j=1,\dots,N} \max_{k=0,\dots,10} |u(x_i,\tau_{jk}) - y_{i,N}(\tau_{jk})|, \tag{49}$$

where u is the exact solution to (43)–(46) and

$$\tau_{jk} = t_{j-1} + k(t_j - t_{j-1})/10, \quad k = 0,\dots,10, \quad j = 1,\dots,N,$$

with the gridpoints, t_j, defined by (24). In Tables 1 and 2, the ratios

$$\Theta = \frac{\varepsilon_{n,N}}{\varepsilon_{2n,2N}}, \tag{50}$$

characterizing the observed convergence rate, are presented. Using (32), we see that for $m = 1$,

$$E_N(m,\kappa,r,\alpha) = \begin{cases} N^{-0.4r} & \text{if } r < 3, \\ N^{-1.2} & \text{if } r \geq 3. \end{cases} \tag{51}$$

Based on Theorem 3 and (51), ratios Θ for $m = 1$ and for $r = 1$, $r = 2$, and $r = 3$ ought to be $2^{0.4} \approx 1.32$, $2^{0.8} \approx 1.74$, and $2^{1.2} \approx 2.30$, respectively. These values are given in the last row of Table 1. The numerical results in Table 1 indicate that the order of convergence of the method for $m = 1$ is based on $E_N(m,\kappa,r,\alpha)$, which dominates the h^2 component of the error in Theorem 3.

Table 1. Numerical results for Problem (43)–(46) using $m = 1$ and $n = N$.

n	N	$r = 1$	Θ	$r = 2$	Θ	$r = 3$	Θ
2	2	1.89×10^{-1}		1.57×10^{-1}		1.96×10^{-1}	
4	4	1.15×10^{-1}	1.64	5.78×10^{-2}	2.71	7.04×10^{-2}	2.78
8	8	7.87×10^{-2}	1.46	2.82×10^{-2}	2.05	2.71×10^{-2}	2.60
16	16	5.55×10^{-2}	1.42	1.41×10^{-2}	2.00	1.36×10^{-2}	1.99
32	32	3.94×10^{-2}	1.41	7.11×10^{-3}	1.99	6.40×10^{-3}	2.13
64	64	2.80×10^{-2}	1.41	3.58×10^{-3}	1.99	2.91×10^{-3}	2.20
128	128	1.99×10^{-2}	1.41	1.80×10^{-3}	1.99	1.29×10^{-3}	2.25
			1.32		1.74		2.30

Using (32), we see that for $m = 2$,

$$E_N(m,\kappa,r,\alpha) = \begin{cases} N^{-0.4r} & \text{if } r < 5.5, \\ N^{-2.2} & \text{if } r \geq 5.5. \end{cases} \tag{52}$$

Based on Theorem 3 and (52), ratios Θ for $m = 2$ and for $r = 1$ and $r = 2$ ought to be $2^{0.4} \approx 1.32$ and $2^{0.8} \approx 1.74$, respectively. The numerical results in Table 2 indicate that the order of convergence of the method for $r = 1$ and $r = 2$ is based on $E_N(m,\kappa,r,\alpha)$, which dominates the h^2 component of the error in Theorem 3. For $r = 5.5$, the h^2 component dominates the $E_N(m,\kappa,r,\alpha)$ component of the error in Theorem 3 and therefore the ratio ought to be $2^2 = 4.00$. The obtained values for the ratios are given in the last row of Table 2.

Table 2. Numerical results for Problem (43)–(46) using $m = 2$ and $n = N$.

n	N	$r = 1$	Θ	$r = 2$	Θ	$r = 5.5$	Θ
2	2	1.03×10^{-1}		1.04×10^{-1}		1.11×10^{-1}	
4	4	3.11×10^{-2}	3.30	2.61×10^{-2}	4.00	3.01×10^{-2}	3.68
8	8	2.04×10^{-2}	1.52	7.41×10^{-3}	3.52	7.79×10^{-3}	3.86
16	16	1.43×10^{-2}	1.43	3.71×10^{-3}	1.99	2.24×10^{-3}	3.48
32	32	1.02×10^{-2}	1.41	1.88×10^{-3}	1.98	5.83×10^{-4}	3.84
64	64	7.27×10^{-3}	1.40	9.51×10^{-4}	1.98	1.45×10^{-4}	4.02
128	128	5.19×10^{-3}	1.40	4.80×10^{-4}	1.98	3.53×10^{-5}	4.10
			1.32		1.74		4.00

7.2. Example 2

Consider the equation

$$(D_t^{0.25}u)(x,t) - \frac{\partial^2 u(x,t)}{\partial x^2} + xu(x,t) = x(x-0.25)\frac{\Gamma(1.45)}{\Gamma(1.2)}t^{0.2} - 2t^{0.45} + x^2(x-0.25)t^{0.45} \tag{53}$$

for $(x,t) \in Q := (0, 0.25) \times (0, 3]$ with

$$u(0,t) = 0, \quad t \in [0,3], \tag{54}$$

$$u(0.25,t) = 0, \quad t \in [0,3], \tag{55}$$

$$u(x,0) = 0, \quad x \in [0, 0.25]. \tag{56}$$

We see that (53)–(56) is a problem of the form (1)–(4), where $\alpha = 0.25$, $L = 0.25$, $b = 3$, $\phi = 0$, $\theta(x) = x$ for $x \in (0, 0.25)$, $f(x,t) = x(x-0.25)\frac{\Gamma(1.45)}{\Gamma(1.2)}t^{0.2} - 2t^{0.45} + x^2(x-0.25)t^{0.45}$ for $(x,t) \in Q$. The exact solution to (53)–(56) is given by

$$u(x,t) = x(x-0.25)t^{0.45}, \quad (x,t) \in \overline{Q}. \tag{57}$$

To find the numerical solution to (53)–(56), we use the same approach as described in Example 1. For any uniform mesh on the interval $[0, 0.25]$ with gridpoints $x_i = ih$, $i = 0, \ldots, n$, where $h = \frac{0.25}{n}$, functions

$$v_i(t) = x_i(x_i - 0.25)\frac{\Gamma(1.45)}{\Gamma(1.2)}t^{0.2} - 2t^{0.45} + x_i^2(x_i - 0.25)t^{0.45}, \quad t \in [0,1], \quad i = 1, \ldots, n-1,$$

belong to $C^{q,\mu}(0,3]$, with $\mu = 0.8$ and arbitrary $q \in \mathbb{N}$. Therefore, by (23),

$$\kappa = \max\{\mu, 1-\alpha\} = 0.8.$$

We present, in the tables below, some results of numerical experiments for different values of parameters n, m, N, and r. The errors, $\varepsilon_{n,N}$, are calculated by (49), where u is the exact solution to (53)–(56). For Tables 3 and 4, the ratios, Θ, are defined by (50). Using (32), we see that for $m = 1$,

$$E_N(m,\kappa,r,\alpha) = \begin{cases} N^{-0.45r} & \text{if } r < \frac{25}{9}, \\ N^{-1.25} & \text{if } r \geq \frac{25}{9}. \end{cases} \tag{58}$$

Based on Theorem 3 and (58), ratios Θ for $m = 1$ and for $r = 1$, $r = 2$, and $r = \frac{25}{8}$ ought to be $2^{0.45} \approx 1.37$, $2^{0.9} \approx 1.87$, and $2^{1.25} \approx 2.38$, respectively. These values are given in the last row of Table 3. The numerical results in Table 3 indicate that the order of convergence of the method for $m = 1$ is based on $E_N(m,\kappa,r,\alpha)$, which dominates the h^2 component of the error in Theorem 3.

Table 3. Numerical results for Problem (53)–(56) using $m = 1$ and $n = N$.

n	N	$r = 1$	Θ	$r = 2$	Θ	$r = 2.78$	Θ
2	2	2.53×10^{-3}		1.93×10^{-3}		2.43×10^{-3}	
4	4	1.85×10^{-3}	1.37	1.03×10^{-3}	1.87	1.18×10^{-3}	2.06
8	8	1.36×10^{-3}	1.37	5.53×10^{-4}	1.87	5.19×10^{-4}	2.27
16	16	9.94×10^{-4}	1.37	2.96×10^{-4}	1.87	2.23×10^{-4}	2.33
32	32	7.28×10^{-4}	1.37	1.58×10^{-4}	1.87	9.45×10^{-5}	2.36
64	64	5.33×10^{-4}	1.37	8.46×10^{-5}	1.87	3.99×10^{-5}	2.37
128	128	3.90×10^{-4}	1.37	4.52×10^{-5}	1.87	1.68×10^{-5}	2.37
			1.37		1.87		2.38

Using (32), we see that for $m = 2$,

$$E_N(m, \kappa, r, \alpha) = \begin{cases} N^{-0.45r} & \text{if } r < 5 \\ N^{-2.25} & \text{if } r \geq 5 \end{cases}. \tag{59}$$

Note that for Equation (53), we have $\mathcal{O}(h^2) = 0$ in (9). Based on Theorem 3 and (59), ratios Θ for $m = 2$ and for $r = 1$, $r = 2$, and $r = 5$ ought to be $2^{0.45} \approx 1.37$, $2^{0.9} \approx 1.87$, and $2^{2.25} \approx 4.76$, respectively. These values are given in the last row of Table 4.

The numerical results in Table 4 indicate that the order of convergence of the method is based on $E_N(m, \kappa, r, \alpha)$.

Table 4. Numerical results for Problem (53)–(56) using $m = 2$ and $n = N$.

n	N	$r = 1$	Θ	$r = 2$	Θ	$r = 5$	Θ
2	2	6.42×10^{-4}		4.69×10^{-4}		7.39×10^{-4}	
4	4	4.70×10^{-4}	1.37	2.51×10^{-4}	1.87	2.94×10^{-4}	2.51
8	8	3.44×10^{-4}	1.37	1.34×10^{-4}	1.87	7.79×10^{-5}	3.78
16	16	2.51×10^{-4}	1.37	7.15×10^{-5}	1.88	1.79×10^{-5}	4.34
32	32	1.84×10^{-4}	1.37	3.85×10^{-5}	1.86	3.93×10^{-6}	4.57
64	64	1.34×10^{-4}	1.37	2.08×10^{-5}	1.85	8.40×10^{-7}	4.67
128	128	9.80×10^{-5}	1.37	1.13×10^{-5}	1.85	1.79×10^{-7}	4.69
			1.37		1.87		4.76

Finally, we consider what happens when $m = 2$, n is equal to 128, and $N \in \{2, 4, 8, 16, 32, 64, 128\}$. The ratios, Θ, in Table 5,

$$\Theta = \frac{\varepsilon_{128,N}}{\varepsilon_{128,2N}},$$

characterizing the observed convergence rate, are also presented. Based on Theorem 3 and (59), ratios Θ for $m = 2$ and for $r = 1$, $r = 2$, and $r = 5$ ought to be $2^{0.45} \approx 1.37$, $2^{0.9} \approx 1.87$, and $2^{2.25} \approx 4.76$, respectively. These values are given in the last row of Table 5.

Table 5. Numerical results for Problem (53)–(56) using $m = 2$ and $n = 128$.

n	N	$r = 1$	Θ	$r = 2$	Θ	$r = 5$	Θ
128	2	6.43×10^{-4}		4.70×10^{-4}		7.40×10^{-4}	
128	4	4.70×10^{-4}	1.37	2.51×10^{-4}	1.87	2.94×10^{-4}	2.51
128	8	3.44×10^{-4}	1.37	1.34×10^{-4}	1.87	7.79×10^{-5}	3.78
128	16	2.51×10^{-4}	1.37	7.15×10^{-5}	1.88	1.79×10^{-5}	4.34
128	32	1.84×10^{-4}	1.37	3.85×10^{-5}	1.86	3.93×10^{-6}	4.57
128	64	1.34×10^{-4}	1.37	2.08×10^{-5}	1.85	8.40×10^{-7}	4.67
128	128	9.80×10^{-5}	1.37	1.13×10^{-5}	1.85	1.79×10^{-7}	4.69
			1.37		1.87		4.76

We see that all of the performed numerical experiments are in good accordance with the theoretical results. The numerical experiments were performed by writing the code in Python.

8. Conclusions

In the present paper, we have introduced and analyzed a high-order numerical method for solving time-fractional diffusion equations containing Caputo fractional derivatives. By using the technique of the method of lines, we have developed from the original problem a system of fractional ordinary differential equations, which we have reformulated as a system of weakly singular integral equations. We have proven a result concerning the existence, uniqueness, and regularity of the solution to this system of integral equations (Theorem 1). On the basis of these results, we have constructed and analyzed an effective numerical method with the help of specially graded grids and spline collocation techniques (Theorems 2 and 3) and have confirmed the validity of the theoretical error estimates with several numerical experiments.

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