Journal of Computational and Applied Mathematics 273 (2015) 103–115

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Central difference approximation of convection in Caputo fractional derivative two-point boundary value problems

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ARTICLE INFO

Article history:
Received 31 December 2013
Received in revised form 14 May 2014

Keywords:
Fractional differential equation
Caputo fractional derivative
Convective term
Boundary value problem
Finite difference method
Convergence proof

ABSTRACT

A rigorous numerical analysis is given for a fractional derivative two-point boundary value problem. The highest-order term of the differential operator is a Caputo fractional derivative of order $\delta \in (1, 2)$. The second and higher-order derivatives of the solution of the problem are in general unbounded at one end of the interval, which creates difficulties for the analysis. The problem is discretized on an equidistant mesh of diameter h using a standard central difference approximation of the convection term, and nodal convergence of order $O(h^{\delta-1})$ is proved provided that h satisfies a stability condition that depends on δ and the convective coefficient. This condition may be restrictive when δ is near 1; when it is violated the solution may exhibit small oscillations, but these can be removed by a simple and inexpensive postprocessing technique. Numerical results are given to display the performance of the method.

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1. Introduction

The numerical analysis of problems whose differential operators involve fractional derivatives is currently of great interest, owing to the use of these non-classical derivatives in the modelling of many physical processes; see [1] for an extensive list of recent applications and mathematical developments in this area. To carry out rigorously this analysis for any given fractional derivative problem, one must take into account the true behaviour of its solution, which may be singular (in some sense) near certain domain boundaries. In particular, solutions of Caputo fractional derivative two-point boundary value problems can behave badly near one endpoint of their domains [2,3], and this must be taken into account in the analysis of any numerical method.

In this paper we consider the two-point boundary value problem

$$Lu(x) := -D_*^\delta u(x) + b(x)u'(x) + c(x)u(x) = f(x) \quad \text{for } x \in (0, 1), \tag{1a}$$

$$u(0) - \alpha_0 u'(0) = \gamma_0, \qquad u(1) + \alpha_1 u'(1) = \gamma_1, \tag{1b}$$

where D_*^δ is the Caputo fractional derivative of order δ with $1 < \delta < 2$. For $g \in C^1[0, 1]$ with g' absolutely continuous on $[0, 1]$, one has

$$D_*^\delta g(x) := \frac{1}{\Gamma(2-\delta)} \int_{t=0}^{x} (x-t)^{1-\delta} g''(t)\, dt \quad \text{for } 0 < x \leq 1;$$

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http://dx.doi.org/10.1016/j.cam.2014.05.025
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see [2–4]. The constants α_0, α_1, γ_0, γ_1 and the functions b, c and f are given. We assume that $c \geq 0$ in $[0, 1]$, $\alpha_1 \geq 0$ and

$$\alpha_0 \geq \frac{1}{\delta - 1}. \tag{2}$$

Condition (2) guarantees that (1) satisfies a comparison/maximum principle [3].

Problem (1) is a member of the general class of boundary value problems that is analysed in [2]. It is also discussed in [5] and is a steady-state version of the time-dependent problems discussed in [6–9]. The problem models superdiffusion of particle motion when convection is present; see the discussion and references in [10, Section 1].

Existence and uniqueness of a solution to (1) is established in [2,3] by using the space $C^{q,\nu}(0, 1]$ (for $q \geq 1$ an integer and $\nu \in (-\infty, 1)$) of functions $y \in C[0, 1]$ that are q times continuously differentiable in $(0, 1]$ and satisfy the bounds

$$|y^{(i)}(x)| \leq \begin{cases} C & \text{if } i < 1 - \nu, \\ C(1 + |\ln x|) & \text{if } i = 1 - \nu, \\ Cx^{1-\nu-i} & \text{if } i > 1 - \nu, \end{cases} \tag{3}$$

for $0 < x \leq 1$ and $i = 1, 2, \ldots, q$, where C is some constant. In [2,3] it is proved that if $b, c, f \in C^{q,\nu}(0, 1]$ for some integer $q \geq 2$ and $\nu \leq 2 - \delta$, then (1) has a unique solution u with $u \in C^1[0, 1] \cap C^{q+1}(0, 1]$, and for some constant C one has

$$|u^{(i)}(x)| \leq \begin{cases} C & \text{if } i = 0, 1, \\ Cx^{\delta-i} & \text{if } i = 2, 3, \ldots, q + 1, \end{cases} \tag{4}$$

for all $x \in (0, 1]$. These bounds are sharp and show that the second and higher-order derivatives of the solution u may blow up at the end point $x = 0$. This singular behaviour complicates the analysis of the convergence of any numerical method used to approximate the solution of problem (1).

In [3] a finite difference scheme on a uniform mesh, with an upwinded discretization of the convective term bu' in (1a), is used to approximate the two-point boundary value problem (1). This scheme is proved to yield $O(h^{\delta-1})$ convergence at the mesh points without any restriction on the mesh. But in numerical experiments with (1), the central difference discretization of the convective term often produces more accurate solutions than the upwind discretization. To be precise, our numerical experiments indicate that both methods have the same order of convergence but the errors of the central difference scheme are smaller than those of the upwind scheme. These results show that when one discretizes differential operators whose highest-order term is a fractional derivative, the way in which the lower-order terms are discretized can affect significantly the behaviour of computed solutions. This phenomenon contrasts with the situation for integer-order differential operators, where typically the highest-order term dominates the other terms.

In the present paper we analyse the convergence properties of a finite difference scheme based on central differencing and we are able to show that, like upwinding, central differencing is $O(h^{\delta-1})$ convergent at all mesh points. This result is proved under a stability condition on the mesh diameter which – depending on the magnitude of the convective coefficient b – may be restrictive when δ is near 1, though it is usually mild when for example $\delta \in [1.5, 2)$. We have observed in our numerical experiments that the method remains convergent if this mesh condition is violated but the solution can then exhibit small oscillations near the endpoint $x = 1$ when $b > 0$, and very small oscillations near the endpoint $x = 0$ when $b < 0$. To remove these oscillations without disturbing the accuracy of the method, we describe a simple inexpensive postprocessing technique.

The paper has the following structure. In Section 2 the difference scheme is described and its monotonicity is established. Section 3 deals with the error analysis of the scheme. Numerical experiments are presented in Section 4; these lead on naturally to the postprocessing technique of Section 5 that is used to remove oscillations from the computed solution if they appear.

Notation. For each $g \in C[0, 1]$, set $\|g\|_\infty = \max_{x\in[0,1]} |g(x)|$. In several inequalities C denotes a generic constant that depends on the data of the boundary value problem (1) but is independent of the mesh used to solve (1) numerically. Note that C can take different values in different places.

2. Central differencing approximation

2.1. The discretization of the boundary value problem

Let N be a positive integer. Set $h = 1/N$ and $x_j = jh$ for $j = 0, \ldots, N$. To discretize u' in (1a), our scheme uses the *central difference approximation* $u'(x_j) \approx [u(x_{j+1}) - u(x_{j-1})]/(2h)$. The fractional order derivative D_*^δ is approximated by a widely-used first-order finite difference formula; see, e.g., [3,8,11]. In detail, the finite difference discretization of (1a) is

$$-\frac{1}{h^\delta\, \Gamma(3 - \delta)} \sum_{k=0}^{j-1} d_{j-k}\, (u_{k+2} - 2u_{k+1} + u_k) + b_j \frac{u_{j+1} - u_{j-1}}{2h} + c_j u_j = f_j, \tag{5}$$

for $j = 1, 2, \ldots, N-1$, where u_k denotes the computed approximation to $u(x_k)$ and $b_j = b(x_j)$ for each mesh point x_j, with similar definitions for c_j and f_j. The coefficients d_r are defined by

$$d_r = r_+^{2-\delta} - (r-1)_+^{2-\delta} \quad \text{for all integers } r, \tag{6}$$

with

$$s_+ = \begin{cases} s & \text{if } s \geq 0, \\ 0 & \text{if } s < 0. \end{cases}$$

The derivatives in the boundary conditions (1b) are discretized by $u'(0) \approx (u_1 - u_0)/h$ and $u'(1) \approx (u_N - u_{N-1})/h$.

The unknowns $\vec{u} := (u_0\ u_1 \ldots u_N)^T$ are the solution of the linear system $A\vec{u} = \vec{f}$ where $\vec{f} := (\gamma_0\ f_1\ f_2 \ldots f_{N-1}\ \gamma_1)^T$ and $A = (a_{jk})_{j,k=0}^N$ denote the $(N+1) \times (N+1)$ matrix corresponding to the discretization (5): The 0th row of A is $((1+\alpha_0 h^{-1}) - \alpha_0 h^{-1}\ 0\ 0\ \ldots\ 0)$ and its Nth row is $(0\ 0\ \ldots\ 0\ -\alpha_1 h^{-1}\ (1+\alpha_1 h^{-1}))$. For $j = 1, 2, \ldots, N-1$, the entries of the jth row of A satisfy

$$a_{j0} = \frac{-d_j}{h^\delta\, \Gamma(3-\delta)} - \delta_{j1}\frac{b_1}{2h}, \tag{7a}$$

$$a_{j1} = \frac{-d_{j-1} + 2d_j}{h^\delta\, \Gamma(3-\delta)} - \delta_{j2}\frac{b_2}{2h} + \delta_{j1}c_1, \tag{7b}$$

$$a_{jk} = \frac{-d_{j-k} + 2d_{j-k+1} - d_{j-k+2}}{h^\delta\, \Gamma(3-\delta)} + \frac{b_j}{2h}(\delta_{j,k-1} - \delta_{j,k+1}) + \delta_{jk}c_j \tag{7c}$$

for $k = 2, 3, \ldots, N$, where we set

$$\delta_{jk} = \begin{cases} 1 & \text{if } j = k, \\ 0 & \text{otherwise.} \end{cases}$$

In [3] the central difference approximation of $b_j u'(x_j)$ in (5) was replaced by the upwind approximation $b_j D^{\nwarrow} u_j$, where

$$b_j D^{\nwarrow} u_j := \begin{cases} b_j(u_{j+1} - u_j)/h & \text{if } b_j < 0, \\ b_j(u_j - u_{j-1})/h & \text{if } b_j \geq 0. \end{cases} \tag{8}$$

Upwinding moves a positive term to the main diagonal of the matrix A, which gives a more stable scheme, but it can be less accurate than central differencing, as we described in Section 1. Much of the analysis developed in [3] is still applicable to A because the upwind and central difference schemes differ only in the entries a_{ij} with $|i-j| \leq 1$ and $0 < i < N$. Thus from [3, Section 4.1] we know that

$$\begin{aligned} &a_{00} > 0, \qquad a_{01} < 0, \qquad a_{N,N-1} \leq 0, \qquad a_{NN} > 0, \\ &a_{j0} < 0 \quad \text{for } j = 2, 3, \ldots, N-1, \qquad a_{j1} > 0 \quad \text{for } j = 3, 4, \ldots, N-1, \\ &a_{jk} < 0 \quad \text{for } j = 4, 5, \ldots, N-1 \text{ and } k = 2, 3, \ldots, j-2. \end{aligned} \tag{9}$$

We shall give various inequalities for the remaining entries of the matrix A, in order to show that – under a certain condition on the mesh diameter – the matrix A is monotone and consequently our difference scheme is stable. Clearly $a_{jj} > 0$ for $j = 1, 2, \ldots, N-1$ by (7), (6) and $c \geq 0$. If

$$h \leq \left[\frac{2}{\|b\|_\infty \Gamma(3-\delta)}\right]^{1/(\delta-1)} \tag{10}$$

one has $a_{10} \leq 0$ and $a_{j,j+1} \leq 0$ for $j = 1, 2, \ldots, N-1$ from (7a) and (7c), respectively.

By (7b),

$$a_{21} = \frac{2^{3-\delta} - 3}{h^\delta\, \Gamma(3-\delta)} - \frac{b_2}{2h}, \tag{11}$$

so the sign of a_{21} depends on δ, h and b.

The only coefficients remaining are

$$a_{j,j-1} = \frac{-d_1 + 2d_2 - d_3}{h^\delta\, \Gamma(3-\delta)} - \frac{b_j}{2h}, \quad \text{for } j = 3, 4, \ldots, N-1.$$

The concavity of the function $x \mapsto x^{2-\delta} - (x-1)^{2-\delta}$ on the interval $[1, 3]$ implies that $-d_1 + 2d_2 - d_3 = -2[(1/2)d_1 - d_2 + (1/2)d_3] < 0$; then if h satisfies the mesh condition

$$h \leq \left[\frac{2(d_1 - 2d_2 + d_3)}{\|b\|_\infty \Gamma(3-\delta)}\right]^{1/(\delta-1)}, \tag{12}$$

it follows that the coefficients $a_{j,j-1} \leq 0$ for $j = 3, 4, \ldots, N-1$.

Remark 1. Observe that $d_1-2d_2+d_3 < 1$ or equivalently $d_3-2d_2 < 0$, which is true since the function $x \mapsto x^{2-\delta}-(x-1)^{2-\delta}$ is strictly decreasing for $x \geq 1$. Thus the mesh condition (12) is more restrictive than the mesh condition (10).

Remark 2. If $b \geq 0$ on $[0, 1]$, then (7) implies that $a_{j,j-1} \leq 0$ for $j = 1, 3, 4, \ldots, N-1$ so condition (12) need not be imposed.

This completes the description of the entries a_{jk} of A.

2.2. Monotonicity of the discretization matrix A

The positive off-diagonal entries in column 1 of A – see (9) – are an obstacle to proving that $A^{-1} \geq 0$. As in [3], we multiply A by elementary matrices $E^{(k)} := (e_{ij}^{(k)})_{i,j=0}^{N}$ with

$$e_{ij}^{(k)} := \delta_{ij} - \frac{a_{k0}}{a_{00}}\,\delta_{ik}\delta_{j0}.$$

This multiplication by elementary matrices adds a positive multiple of row 0 of A to each lower row to reduce to zero the off-diagonal entries of column 0 and, as we shall see, it also changes the sign of the off-diagonal entries in column 1. Set

$$A' = E^{(N-1)}E^{(N-2)}\ldots E^{(1)}A \tag{13}$$

and write $A' = (a'_{jk})_{j,k=0}^{N}$.

Row 0 of A' is $(a_{00}\ a_{01}\ 0\ 0\ldots 0)$, where we recall that $a_{00} = 1+\alpha_0 h^{-1}$ and $a_{01} = -\alpha_0 h^{-1}$. By construction $a'_{j0} = 0$ for $j = 1, 2, \ldots, N$. For $k > 1$ and all j, clearly $a'_{jk} = a_{jk}$.

The remaining entries of column 1 of A' will be examined in the next lemma.

Lemma 1. *Assume that h satisfies*

$$h \leq \min\left\{\left[\frac{d_2(2^{\delta-1}-1)}{\|b\|_\infty \Gamma(3-\delta)}\right]^{1/(\delta-1)},\ \frac{\alpha_0}{2}\left(2^{\delta-1}-1\right)\right\}. \tag{14}$$

Then the entries of column 1 of the matrix A' satisfy

$$a'_{11} > 0 \quad \textit{and} \quad a'_{j1} < 0 \quad \textit{for } j = 2, 3, \ldots, N-1.$$

Proof. For $j = 1, 2, \ldots, N-1$, from (7) one has

$$\begin{aligned} a'_{j1} &= a_{j1} + \frac{\alpha_0 h^{-1}}{1+\alpha_0 h^{-1}}\,a_{j0} \\ &= \frac{1}{h^\delta\,\Gamma(3-\delta)}\left[-d_{j-1}+2d_j-\frac{\alpha_0 h^{-1}}{1+\alpha_0 h^{-1}}d_j\right] - \delta_{j2}\frac{b_2}{2h} + \delta_{j1}\left(c_1 - \frac{\alpha_0 h^{-1}}{1+\alpha_0 h^{-1}}\frac{b_1}{2h}\right) \\ &= \frac{1}{h^\delta\,\Gamma(3-\delta)}\left[d_j\left(1+\frac{h}{h+\alpha_0}\right)-d_{j-1}\right] - \delta_{j2}\frac{b_2}{2h} + \delta_{j1}\left(c_1 - \frac{\alpha_0}{h+\alpha_0}\frac{b_1}{2h}\right). \end{aligned} \tag{15}$$

It is easy to see that the mesh condition (14) is more restrictive than (10). From condition (10), $d_1 = 1$, $d_0 = 0$ and $c \geq 0$, it follows that $a'_{11} > 0$. In [3, Lemma 4.3] it was proved that $a'_{j1} < 0$ for $j = 3, \ldots, N-1$. Thus, the only case remaining is $j = 2$. The formula (15) yields

$$a'_{21} = \frac{1}{h^\delta\,\Gamma(3-\delta)}\left[d_2\left(1+\frac{h}{h+\alpha_0}\right)-d_1\right] - \frac{b_2}{2h}. \tag{16}$$

Some calculations using (14) show that

$$\frac{h}{h+\alpha_0} = \frac{1}{1+\frac{\alpha_0}{h}} \leq \frac{2^{\delta-1}-1}{2^{\delta-1}+1}$$

so

$$d_2\left(1+\frac{h}{h+\alpha_0}\right)-d_1 \leq d_2\left(1+\frac{2^{\delta-1}-1}{2^{\delta-1}+1}\right)-d_1 = \frac{3(1-2^{\delta-1})}{2^{\delta-1}+1} < 1-2^{\delta-1},$$

and this can be combined with the first condition in (14) to show from (16) that $a'_{21} < 0$. □

Remark 3. By elementary techniques one can show that $\alpha_0(2^{\delta-1}-1)/2 \geq (\ln 2)/2$ using (2), so the second condition in (14) is only a mild restriction on h.

The following technical result proves that the stability condition (14) is more restrictive than the mesh condition (12). It will be used in Theorem 1.

Lemma 2. *One has*

$$d_2(2^{\delta-1}-1) < 2(d_1 - 2d_2 + d_3) \quad \text{for } \delta \in (1,2). \tag{17}$$

Proof. Define the function

$$g(\delta) = 2(d_1 - 2d_2 + d_3) - d_2(2^{\delta-1}-1) = 2(3)^{2-\delta} - 6(2)^{2-\delta} + 6 - (2^{2-\delta}-1)(2^{\delta-1}-1).$$

Then

$$g'(\delta) = (5)2^{2-\delta}\ln 2 - (2)3^{2-\delta}\ln 3 + 2^{\delta-1}\ln 2 > (5)2^{2-\delta}\ln 2 - (2)3^{2-\delta}\ln 3 > 0$$

because $5\ln 2 > 3\ln 3$. Thus g is a strictly increasing function with $g(1) = 0$, which implies that $g(\delta) > 0$ for $1 < \delta < 2$. □

In Theorem 1 we prove that A^{-1} exists and $A^{-1} \geq 0$, i.e., the matrix A is monotone. This property will be used in the error analysis of the finite difference method (7).

Theorem 1. *Assume that h satisfies the stability condition (14). Then A' is an M-matrix. Furthermore, A is invertible and $A^{-1} \geq 0$.*

Proof. By Lemma 2 and Remark 1, the mesh condition (14) implies that (10) and (12) hold true. Thus the properties of A, the construction of A', and Lemma 1 imply that the entries of the $(N+1)\times(N+1)$ matrix A' are positive on its main diagonal and non-positive otherwise. In addition, we have $\sum_{k=0}^{N} a'_{0k} = \sum_{k=0}^{N} a'_{Nk} = 1$, and for $j = 1, 2, \ldots, N-1$ one sees that

$$\begin{aligned}\sum_{k=0}^{N} a'_{jk} &= 0 + \left(a_{j1} + \frac{\alpha_0 h^{-1}}{1+\alpha_0 h^{-1}}\, a_{j0}\right) + \sum_{k=2}^{N} a_{jk} \\ &= \left(\frac{\alpha_0 h^{-1}}{1+\alpha_0 h^{-1}} - 1\right) a_{j0} + \sum_{k=0}^{N} a_{jk} = -\frac{a_{j0}}{1+\alpha_0 h^{-1}} + c_j > 0\end{aligned} \tag{18}$$

using $\sum_{k=0}^{N} a_{jk} = c_j$ from (5) and $a_{j0} < 0$ from (9) for $j = 2, 3, \ldots, N-1$ with $a_{10} < 0$ by virtue of condition (14). Thus $A'(1, 1, \ldots, 1)^T > \vec{0}$ and consequently (see, e.g., [12]) A' is an M-matrix and $(A')^{-1}$ exists with $(A')^{-1} \geq 0$. Then (13) implies that $A^{-1} = (A')^{-1}E^{(N-1)}E^{(N-2)}\ldots E^{(1)}$ exists, and $A^{-1} \geq 0$ since each matrix in this product has non-negative entries. □

Remark 4. The mesh condition (14) may be restrictive when δ is close to 1, but is much less so when $\delta \in [1.5, 2)$. For example, if $b = -2$ then (14) is equivalent to $h \leq 1.2421\times 10^{-15}$, $h \leq 2.1544\times 10^{-4}$ and $h \leq 0.0094$ when $\delta = 1.1, 1.3, 1.5$, respectively.

Remark 5. If $b \geq 0$ on $[0, 1]$, then only the mesh condition (10) is needed to guarantee that A is monotone, by Remark 2 and inspection of the proof of Lemma 1. Furthermore, if $0 \leq b \leq 2/\Gamma(3-\delta)$ on $[0, 1]$, then condition (10) holds true for any value of the discretization parameter N.

3. Error analysis

In this section we examine the accuracy of the difference scheme (7).

Theorem 2. *Let $b, c, f \in C^{q,\nu}(0, 1]$ for some integer $q \geq 2$ and $\nu \leq 2-\delta$. Assume that $c \geq 0$, $\alpha_1 \geq 0$ and the condition (2) is satisfied. Assume also that the mesh width h satisfies condition (14). Then there exists a constant C such that the error in the discretization $A\vec{u} = \vec{f}$ of (1) satisfies*

$$\max_{j=0,1,\ldots,N} |u(x_j) - u_j| \leq Ch^{\delta-1}.$$

Proof. The truncation error, denoted by $\vec{\tau} := (\tau_0\ \tau_1 \ldots \tau_N)^T$, satisfies $A(u - \vec{u}) = \vec{\tau}$, where "$Au$" means that one restricts $u(\cdot)$ to the mesh to form a vector then multiplies this vector by A. Thus

$$\tau_0 = (Au)_0 - \gamma_0 = \alpha_0 u'(x_0) - \frac{\alpha_0}{h}\left[u(x_1) - u(x_0)\right], \tag{19}$$

$$\tau_N = (Au)_N - \gamma_1 = -\alpha_1 u'(x_N) + \frac{\alpha_1}{h}\left[u(x_N) - u(x_{N-1})\right], \tag{20}$$

and for $j = 1, 2, \ldots, N-1$,

$$\tau_j = (Au)_j - f(x_j) = (Au)_j + D_*^{\delta}u(x_j) - b(x_j)u'(x_j) - c(x_j)u(x_j). \tag{21}$$

Similarly to [3], one can use the derivative bounds (4) to show that

$$|\tau_j| \le \begin{cases} Ch^{\delta-1} & \text{if } j=0, \\ C & \text{if } j=1, \\ C(j-1)^{1-\delta} & \text{if } j=2,\dots,N-1, \\ C\alpha_1 h & \text{if } j=N. \end{cases} \tag{22}$$

Define $\tau' := (\tau_0\ \tau_1'\ \tau_2'\dots\tau_{N-1}'\ \tau_N)^T$ by

$$A'(u-\vec{u}) = \vec{\tau}'. \tag{23}$$

From (13) and (7a) it follows that

$$\tau_j' := \tau_j + \frac{\tau_0}{1+\alpha_0 h^{-1}}\left[\frac{d_j}{h^\delta\,\Gamma(3-\delta)} + \delta_{j1}\frac{b_1}{2h}\right] \quad \text{for } j=1,2,\dots,N-1. \tag{24}$$

By Theorem 1 the matrix A' is an M-matrix and its entries satisfy

$$\sum_{k=0}^{N} a_{jk}' = \frac{1}{1+\alpha_0 h^{-1}}\left[\frac{d_j}{h^\delta\,\Gamma(3-\delta)} + \delta_{j1}\frac{b_1}{2h}\right] + c_j, \quad \text{for } j=1,2,\dots,N-1, \tag{25}$$

by (18) and (7a).

Rescale the system (23) by multiplying the jth equation by

$$\frac{(1+\alpha_0 h^{-1})h^\delta\,\Gamma(3-\delta)}{d_j}, \quad \text{for } j=1,2,\dots,N-1.$$

Denote the rescaled matrix and the new right-hand side by $\tilde{A} = (\tilde{a}_{jk})_{j,k=0}^{N}$ and $\vec{\tilde{\tau}} := (\tau_0\ \tilde{\tau}_1\ \tilde{\tau}_2\dots\tilde{\tau}_{N-1}\ \tau_N)^T$ respectively, so that $\tilde{A}(u-\vec{u}) = \vec{\tilde{\tau}}$.

The entries of A' and $\tilde{A}$ have the same sign and by (25) each row sum is now $\sum_{k=0}^{N}\tilde{a}_{jk} \ge 1$ for $j=0,2,3,\dots,N$. If $j=1$, the stability condition (14) yields

$$\begin{aligned}\sum_{k=0}^{N}\tilde{a}_{1k} &\ge 1 - \frac{\|b\|_\infty \Gamma(3-\delta)}{2}h^{\delta-1} \ge 1 - d_2(2^{\delta-1}-1) \\ &= 2^{2-\delta} + 2^{\delta-1} - 2 \ge 2(\sqrt{2}-1).\end{aligned}$$

Hence $\tilde{A}$ is an M-matrix and $\|(\tilde{A})^{-1}\|_\infty \le (\sqrt{2}+1)/2$ (see, e.g., [13, Lemma 2.1]) where $\|\cdot\|_\infty$ is the standard matrix norm notation.

On the other hand, the right-hand side $\vec{\tilde{\tau}}$ satisfies $|\tau_0| \le Ch^{\delta-1}$, $|\tau_N| \le C\alpha_1 h$ and for $j=1,2,\dots,N-1$ one has

$$|\tilde{\tau}_j| = \left|\frac{(1+\alpha_0 h^{-1})h^\delta\,\Gamma(3-\delta)}{d_j}\tau_j + \left[1+\delta_{j1}\frac{b_1}{2h}\cdot\frac{h^\delta\,\Gamma(3-\delta)}{d_j}\right]\tau_0\right| \le Ch^{\delta-1},$$

by (22). The desired result now follows from $\|(\tilde{A})^{-1}\|_\infty \le (\sqrt{2}+1)/2$. □

Remark 6. In [3, Theorem 4.2] it is shown that for the upwind scheme one obtains the same convergence result as Theorem 2, but the numerical experiments of Section 4 will demonstrate that in practice central differencing is often more accurate than upwinding.

4. Numerical experiments

In this section we consider two test problems and compare the numerical results obtained by the central difference and upwind schemes. In Test Problem I the exact solution is used to compute the errors, whereas in Test Problem II the errors are approximated using the two-mesh principle.

In the tables that follow we have used bold font to highlight cases where a numerical check showed that the matrix A is not monotone.

4.1. Test Problem I

We first consider the problem

$$-D_*^\delta u(x) + b(x)u'(x) = f(x) \quad \text{on } (0,1), \tag{26a}$$

$$u(0) - \frac{1}{\delta-1}u'(0) = \gamma_0 \quad \text{and} \quad u(1) + u'(1) = \gamma_1, \tag{26b}$$

Table 1
Test Problem I with $b(x) = -(2x+6)$: maximum errors e_N^δ and their orders of convergence p_N^δ using central differencing.

	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$	$N = 2048$	$N = 4096$
$\delta = 1.1$	**2.042E−001** **1.004**	**1.018E−1** **1.004**	**5.077E−2** **1.004**	**2.532E−2** **1.003**	**1.263E−2** **1.003**	**6.304E−3** **1.003**	**3.146E−3**
$\delta = 1.2$	**2.035E−1** **1.001**	**1.017E−1** **1.000**	**5.085E−2** **1.000**	**2.542E−2** **1.000**	**1.271E−2** **1.000**	**6.356E−3** **1.000**	**3.178E−3**
$\delta = 1.3$	**2.088E−1** **1.000**	**1.044E−1** **0.999**	**5.223E−2** **1.000**	**2.612E−2** **1.000**	**1.306E−2** **1.000**	6.533E−3 1.000	3.267E−3
$\delta = 1.4$	**2.151E−1** **0.998**	**1.077E−1** **0.998**	5.392E−2 0.999	2.699E−2 0.999	1.350E−2 0.999	6.754E−3 1.000	3.378E−3
$\delta = 1.5$	2.225E−1 0.996	1.116E−1 0.997	5.592E−2 0.997	2.801E−2 0.998	1.402E−2 0.999	7.019E−3 0.999	3.512E−3
$\delta = 1.6$	2.304E−1 0.993	1.158E−1 0.994	5.813E−2 0.995	2.916E−2 0.996	1.462E−2 0.997	7.325E−3 0.998	3.668E−3
$\delta = 1.7$	2.381E−1 0.989	1.200E−1 0.991	6.038E−2 0.992	3.036E−2 0.993	1.525E−2 0.994	7.654E−3 0.995	3.839E−3
$\delta = 1.8$	2.440E−1 0.986	1.232E−1 0.987	6.215E−2 0.988	3.133E−2 0.990	1.578E−2 0.991	7.939E−3 0.992	3.991E−3
$\delta = 1.9$	2.447E−1 0.987	1.235E−1 0.987	6.231E−2 0.987	3.143E−2 0.988	1.585E−2 0.989	7.988E−3 0.989	4.024E−3

where the function f and the constants γ_0 and γ_1 are chosen such that $u(x) = x^\delta + x^{2\delta-1} + 1 + 3x - 7x^2 + 4x^3 + x^4$ is the exact solution of the Test Problem I. This solution u attains the bounds on derivatives stated in (4). The two choices $b(x) = -(2x+6)$ and $b(x) = 2x+6$ will be considered separately.

For each value of N and δ, we denote the maximum pointwise error by

$$e_N^\delta := \max_{0\le j\le N} |u(x_j) - u_j|,$$

and the orders of convergence are computed in the standard way:

$$p_N^\delta = \log_2\left(\frac{e_N^\delta}{e_{2N}^\delta}\right).$$

4.1.1. Test Problem I with $b(x) = -(2x+6)$

Numerical results for Test Problem I with $b(x) = -(2x+6)$ are given in Tables 1 and 2 for the central difference and upwind schemes respectively.

The results show that the central difference scheme is more accurate than the upwind scheme for all the values of N and δ considered in this example. In addition, they show that both methods are first-order convergent for all values of δ. Thus the central difference scheme is more accurate in this example than was predicted by Theorem 2.

In Fig. 1 we display the exact solution and the numerical solutions obtained with the central difference and upwind schemes for $\delta = 1.1$ and $N = 128$. For these values the mesh condition (14) is violated, yet the central difference solution is accurate. In Fig. 2 the central differencing solution has small oscillations near $x = 0$, so the matrix A is not monotone, but one should note that the central differencing errors are nevertheless smaller than the upwinding errors (and the $O(h^{\delta-1})$ accuracy of the upwinding solution is guaranteed by the theory of [3]). Furthermore, we have observed experimentally that the amplitude of these oscillations decreases as N grows.

4.1.2. Test Problem I with $b(x) = 2x+6$

The numerical results for the central difference and upwind computed solutions to Test Problem I with $b(x) = 2x+6$ are given in Tables 3 and 4, respectively. Once again the central difference scheme is more accurate than the upwind scheme.

In this example the orders of convergence deteriorate and the largest errors occur when δ is close to 1, for both the central difference and upwind schemes. The numerical results indicated in bold in Table 3 are not covered by Theorem 2 because the matrix A is not monotone for these values of the parameters N and δ.

4.2. Test Problem II

Consider now the problem

$$-D_*^\delta u(x) + 6.7u'(x) = 3.25 \quad \text{on } (0,1), \tag{27a}$$

$$u(0) - \frac{1}{\delta-1}u'(0) = 0.4 \quad \text{and} \quad u(1) + u'(1) = 1.7. \tag{27b}$$

Table 2
Test Problem I with $b(x) = -(2x+6)$: maximum errors e_N^δ and their orders of convergence p_N^δ using upwinding.

	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$	$N = 2048$	$N = 4096$
$\delta = 1.1$	3.817E−1 0.988	1.924E−1 0.994	9.661E−2 0.997	4.840E−2 0.999	2.423E−2 0.999	1.212E−2 1.000	6.061E−3
$\delta = 1.2$	3.853E−1 0.988	1.942E−1 0.994	9.751E−2 0.997	4.886E−2 0.998	2.446E−2 0.999	1.223E−2 1.000	6.119E−3
$\delta = 1.3$	3.911E−1 0.988	1.972E−1 0.994	9.903E−2 0.997	4.962E−2 0.998	2.484E−2 0.999	1.243E−2 1.000	6.216E−3
$\delta = 1.4$	3.991E−1 0.987	2.013E−1 0.993	1.011E−1 0.996	5.070E−2 0.998	2.538E−2 0.999	1.270E−2 0.999	6.353E−3
$\delta = 1.5$	4.093E−1 0.986	2.066E−1 0.992	1.038E−1 0.996	5.208E−2 0.997	2.608E−2 0.998	1.306E−2 0.999	6.532E−3
$\delta = 1.6$	4.211E−1 0.985	2.128E−1 0.991	1.071E−1 0.995	5.374E−2 0.997	2.693E−2 0.998	1.349E−2 0.998	6.751E−3
$\delta = 1.7$	4.339E−1 0.983	2.196E−1 0.989	1.106E−1 0.993	5.558E−2 0.995	2.789E−2 0.996	1.398E−2 0.997	7.003E−3
$\delta = 1.8$	4.460E−1 0.981	2.260E−1 0.987	1.140E−1 0.991	5.737E−2 0.993	2.882E−2 0.994	1.447E−2 0.995	7.258E−3
$\delta = 1.9$	4.544E−1 0.981	2.302E−1 0.987	1.162E−1 0.990	5.847E−2 0.992	2.940E−2 0.993	1.477E−2 0.994	7.416E−3

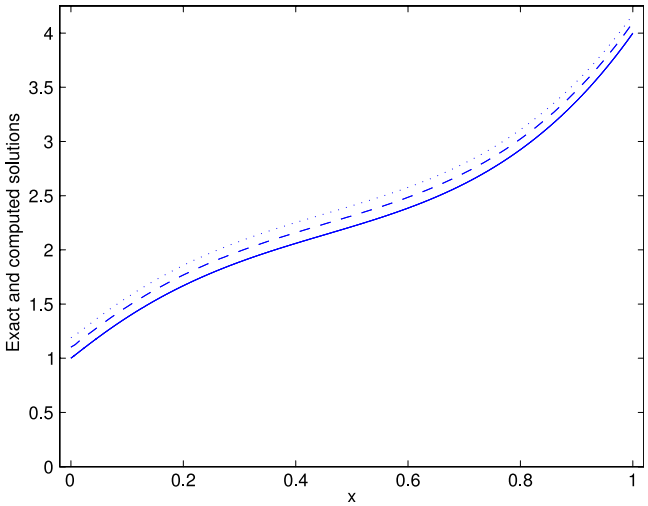


Fig. 1. Exact (solid) and computed solutions for central difference (dashed) and upwind (dotted) schemes of Test Problem I with $b = -(2x+6)$, $\delta = 1.1$ and $N = 128$.

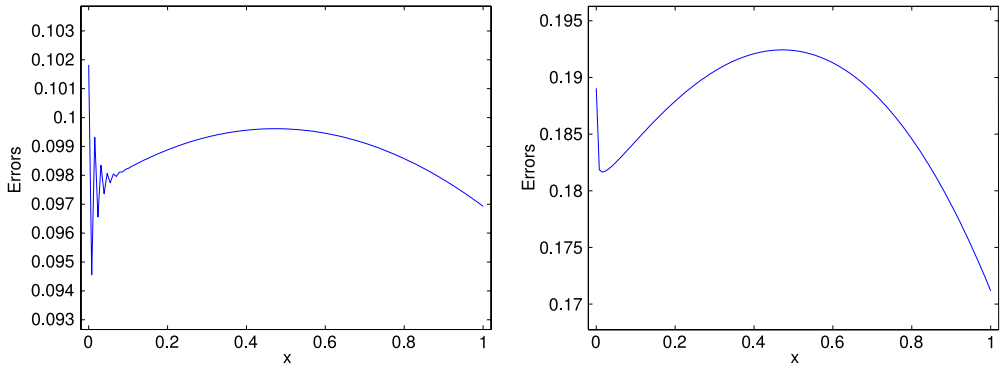


Fig. 2. Errors for Test Problem I with $b(x) = -(2x+6)$, $\delta = 1.1$ and $N = 128$ using central differencing (left figure) and upwinding (right figure).

Table 3
Test Problem I with $b(x) = 2x + 6$: maximum errors e_N^δ and their orders of convergence p_N^δ using central differencing.

	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$	$N = 2048$	$N = 4096$
$\delta = 1.1$	**7.961E+0** **0.087**	**7.493E+0** **0.127**	**6.863E+0** **0.148**	**6.192E+0** **0.161**	**5.537E+0** **0.170**	**4.923E+0** **0.176**	**4.357E+0**
$\delta = 1.2$	**1.892E+0** **0.208**	**1.638E+0** **0.280**	**1.349E+0** **0.330**	**1.074E+0** **0.373**	8.291E−1 0.416	6.215E−1 0.465	4.503E−1
$\delta = 1.3$	**5.238E−1** **0.298**	4.262E−1 0.436	3.150E−1 0.544	2.160E−1 0.641	1.385E−1 0.732	8.339E−2 0.811	4.753E−2
$\delta = 1.4$	1.160E−1 0.265	9.657E−2 0.499	6.833E−2 0.670	4.293E−2 0.785	2.492E−2 0.862	1.371E−2 0.912	7.288E−3
$\delta = 1.5$	2.449E−2 1.240	1.037E−2 0.105	9.641E−3 0.556	6.559E−3 0.744	3.916E−3 0.843	2.183E−3 0.900	1.169E−3
$\delta = 1.6$	6.495E−2 1.202	2.823E−2 1.192	1.236E−2 1.171	5.489E−3 1.145	2.482E−3 1.119	1.143E−3 1.096	5.347E−4
$\delta = 1.7$	7.671E−2 1.092	3.599E−2 1.085	1.696E−2 1.076	8.043E−3 1.066	3.841E−3 1.057	1.846E−3 1.048	8.929E−4
$\delta = 1.8$	8.041E−2 1.064	3.847E−2 1.062	1.842E−2 1.059	8.841E−3 1.055	4.256E−3 1.050	2.055E−3 1.046	9.957E−4
$\delta = 1.9$	8.438E−2 1.041	4.101E−2 1.042	1.992E−2 1.042	9.675E−3 1.041	4.702E−3 1.040	2.287E−3 1.038	1.114E−3

Table 4
Test Problem I with $b(x) = 2x + 6$: maximum errors e_N^δ and their orders of convergence p_N^δ using upwinding.

	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$	$N = 2048$	$N = 4096$
$\delta = 1.1$	7.709E+0 0.008	7.668E+0 0.085	7.228E+0 0.125	6.626E+0 0.148	5.981E+0 0.161	5.349E+0 0.170	4.755E+0
$\delta = 1.2$	1.844E+0 0.074	1.752E+0 0.203	1.522E+0 0.278	1.255E+0 0.332	9.971E−1 0.378	7.675E−1 0.424	5.720E−1
$\delta = 1.3$	4.853E−1 0.098	4.534E−1 0.288	3.713E−1 0.439	2.738E−1 0.558	1.860E−1 0.663	1.174E−1 0.759	6.939E−2
$\delta = 1.4$	8.745E−2 −0.187	9.959E−2 0.321	7.971E−2 0.568	5.378E−2 0.724	3.256E−2 0.828	1.834E−2 0.896	9.853E−3
$\delta = 1.5$	1.278E−1 1.400	4.845E−2 1.501	1.712E−2 1.477	6.149E−3 0.602	4.052E−3 0.783	2.355E−3 0.874	1.285E−3
$\delta = 1.6$	1.624E−1 1.074	7.714E−2 1.074	3.664E−2 1.064	1.753E−2 1.050	8.463E−3 1.038	4.122E−3 1.028	2.021E−3
$\delta = 1.7$	1.628E−1 1.019	8.036E−2 1.027	3.943E−2 1.028	1.934E−2 1.025	9.500E−3 1.022	4.678E−3 1.019	2.309E−3
$\delta = 1.8$	1.540E−1 1.006	7.665E−2 1.018	3.785E−2 1.022	1.863E−2 1.023	9.168E−3 1.022	4.514E−3 1.020	2.225E−3
$\delta = 1.9$	1.464E−1 0.999	7.324E−2 1.012	3.632E−2 1.018	1.794E−2 1.020	8.845E−3 1.021	4.360E−3 1.021	2.149E−3

Using Laplace transforms, the exact solution of this constant coefficient problem can be given in closed form in terms of Mittag-Leffler functions. It is a particular example of the general closed-form solution given in [14]. Nevertheless, in practice this representation of the solution is of limited use because the values of the Mittag-Leffler functions are exponentially large when δ is near 1, making it troublesome to evaluate the exact solution accurately; cf. [15].

For this reason, to estimate the errors of the solution $\{u_j\}_{j=0}^N$ computed on a uniform mesh of width $h = 1/N$ by the finite difference methods, we use the two-mesh principle [16, Section 5.6]: on a uniform mesh of width $h/2$, compute the numerical solution $\{z_j\}_{j=0}^{2N}$ with the same method and hence the two-mesh differences

$$d_N^\delta := \max_{0\le j\le N} |u_j - z_{2j}|;$$

from these values we estimate the orders of convergence by

$$q_N^\delta = \log_2 \left(\frac{d_N^\delta}{d_{2N}^\delta} \right).$$

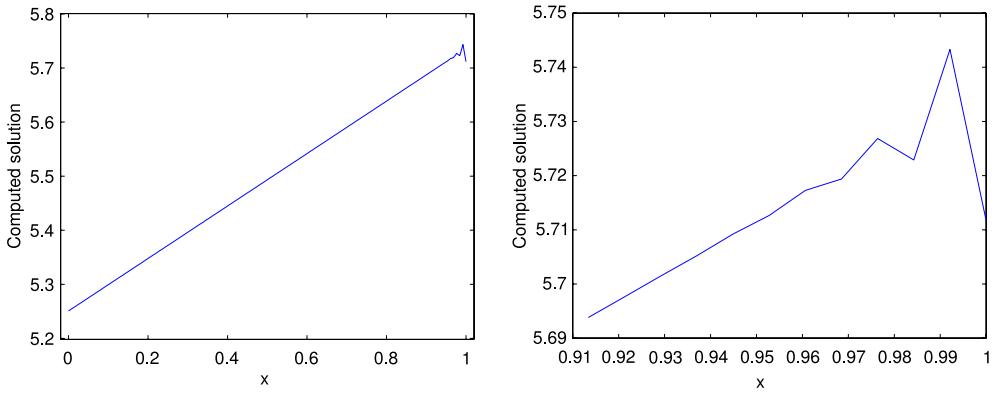


Fig. 3. Computed solution of Test Problem II for $\delta = 1.1$ and $N = 127$ using central differencing. A zoom near $x = 1$ is given in the right figure.

Table 5
Test Problem II: maximum two-mesh differences d_N^δ and their orders of convergence q_N^δ using central differencing.

	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$	$N = 2048$
$\delta = 1.1$	**2.861E−2** **1.084**	**1.349E−2** **1.101**	**6.292E−3** **1.037**	**3.066E−3** **0.960**	**1.576E−3** **0.957**	**8.118E−4**
$\delta = 1.2$	**1.200E−2** **0.896**	**6.450E−3** **0.887**	**3.488E−3** **0.873**	1.904E−3 0.856	1.052E−3 0.836	5.897E−4
$\delta = 1.3$	8.509E−3 0.820	4.818E−3 0.806	2.756E−3 0.796	1.587E−3 0.800	9.114E−4 0.822	5.157E−4
$\delta = 1.4$	6.376E−3 0.797	3.669E−3 0.812	2.090E−3 0.842	1.166E−3 0.880	6.337E−4 0.917	3.356E−4
$\delta = 1.5$	4.593E−3 0.826	2.591E−3 0.860	1.428E−3 0.896	7.674E−4 0.927	4.037E−4 0.950	2.089E−4
$\delta = 1.6$	3.154E−3 0.860	1.738E−3 0.892	9.364E−4 0.920	4.948E−4 0.942	2.575E−4 0.959	1.325E−4
$\delta = 1.7$	2.092E−3 0.885	1.133E−3 0.909	6.032E−4 0.930	3.166E−4 0.946	1.644E−4 0.958	8.461E−5
$\delta = 1.8$	1.343E−3 0.905	7.169E−4 0.922	3.784E−4 0.935	1.979E−4 0.946	1.027E−4 0.955	5.297E−5
$\delta = 1.9$	8.225E−4 0.933	4.309E−4 0.941	2.244E−4 0.948	1.164E−4 0.953	6.011E−5 0.958	3.095E−5

In Fig. 3 we show the computed solution for $\delta = 1.1$ using central differencing with $N = 127$. Small oscillations appear in the numerical solution near $x = 1$. We have observed that the amplitude of these oscillations becomes smaller as N grows.

Table 5 displays the numerical results obtained with central differencing. They show that the method is first-order convergent for all the values of δ considered in this table. Further numerical results (not presented here) show that the central differencing solution is more accurate than the upwinding solution.

5. Postprocessing of oscillatory solutions

Fig. 3 showed that solutions computed by the central difference scheme can exhibit some oscillations in the neighbourhood of $x = 1$ when δ is near 1. In this section we describe a simple postprocessing that removes these oscillations by discarding certain mesh points without affecting the convergence behaviour of the scheme.

A similar procedure was used in [17] to remove oscillations from computed solutions to singularly perturbed boundary value problems, but it is necessary to modify slightly that approach for our fractional two-point boundary problem (1).

Postprocessing to remove oscillations:
Assume that the discretization parameter N is odd. From the solution $\{u_j\}_{j=0}^N$ computed on the mesh $\{x_j\}_{j=0}^N$ by the central difference scheme of Section 2, retain the computed values only at the points $\{x_0, x_1, x_3, x_5, \ldots, x_{N-2}, x_N\}$.

The additional cost of this postprocessing procedure is obviously negligible. Fig. 4 shows the numerical solution obtained when postprocessing is applied to the solution of Fig. 3. Oscillations are no longer visible. Fig. 5 displays simultaneously these original and postprocessed solutions near $x = 1$.

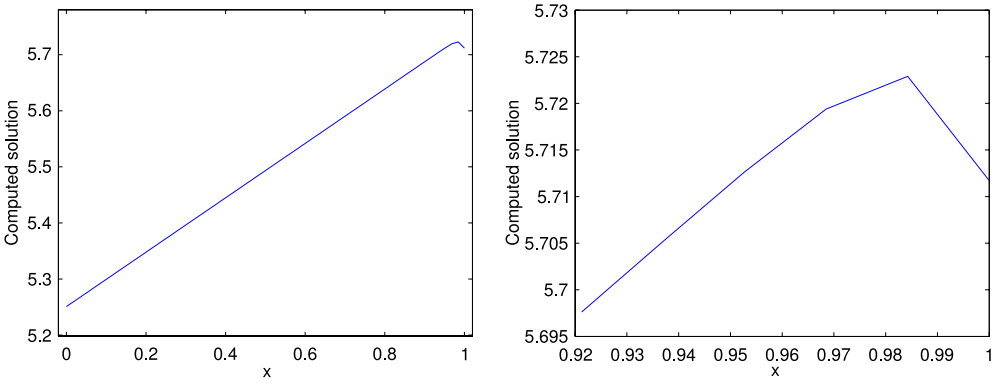


Fig. 4. Postprocessed computed solution of Test Problem II for $\delta = 1.1$ and $N = 127$. A zoom near $x = 1$ is given in the right figure.

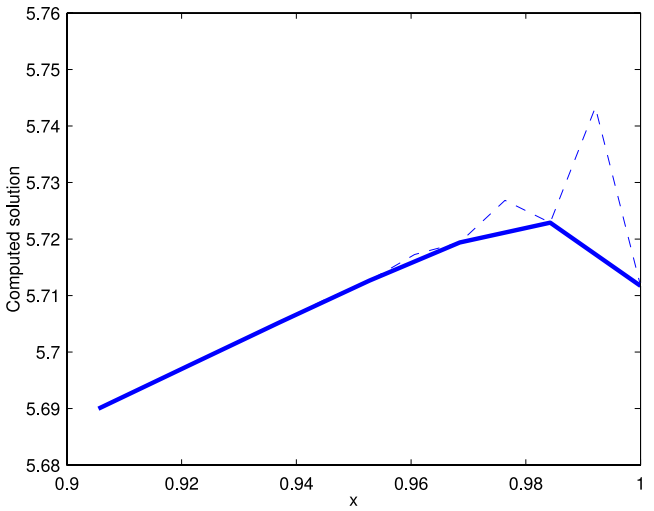


Fig. 5. Original solution $\vec{u}$ (dashed line) and postprocessed solution $\vec{u}_o$ (solid line) for Test Problem II with $\delta = 1.1$ and $N = 127$, near $x = 1$.

This postprocessing also removes any small oscillations near $x = 0$ that appear when $b < 0$ (see Fig. 2); we do not give a figure to illustrate this as these oscillations are smaller than the oscillations of Fig. 5.

In Table 6 we show the maximum two-mesh differences and the orders of convergence after applying the postprocessing procedure to the computed solution with central differencing. Comparing Tables 5 and 6, one sees that the postprocessed solution is more accurate for almost all values of δ and N; in general, if the central difference solution has oscillations, one then observes an improvement in accuracy after postprocessing. The orders of convergence in Table 6 are not as regular as in Table 5 but they do show the convergence of the postprocessing procedure. The negative rates observed in part of the row $\delta = 1.2$ are due to the exceptional accuracy of the postprocessed solution when $N = 256$ and $N = 512$ (for $\delta = 1.2$, compare the two-mesh difference for each of $N = 256$ and $N = 512$ with its neighbouring two-mesh differences in the same column); we believe that the unusual accuracy obtained here is merely fortuitous.

To describe the theory behind this procedure, reorder the unknowns $\vec{u} = (u_0, u_1, u_2, \ldots, u_N)^T$ into the "odd" and "even" vectors

$$\vec{u}_o = (u_0, u_1, u_3, u_5, \ldots, u_{N-2}, u_N)^T \quad \text{and} \quad \vec{u}_e = (u_2, u_4, u_6, \ldots, u_{N-3}, u_{N-1})^T.$$

Define the vectors

$$\vec{f}_o = (\gamma_0, f_1, f_3, f_5, \ldots, f_{N-2}, \gamma_1)^T \quad \text{and} \quad \vec{f}_e = (f_2, f_4, f_6, \ldots, f_{N-3}, f_{N-1})^T,$$

where γ_0 and γ_1 are given in the boundary conditions (1b). The system $A'\vec{u} = \vec{f}$ can be written as

$$\begin{pmatrix} B_{oo} & B_{oe} \\ B_{eo} & B_{ee} \end{pmatrix} \begin{pmatrix} \vec{u}_o \\ \vec{u}_e \end{pmatrix} = \begin{pmatrix} \vec{f}_0 \\ \vec{f}_e \end{pmatrix}$$

where B_{oo}, B_{oe}, B_{eo} and B_{ee} are respectively $(N+3)/2 \times (N+3)/2$, $(N+3)/2 \times (N-1)/2$, $(N-1)/2 \times (N+3)/2$ and $(N-1)/2 \times (N-1)/2$ matrices.

Table 6
Test Problem II: maximum two-mesh differences d_N^δ and their orders of convergence q_N^δ after postprocessing the computed solution with central differences.

	$N = 64$	$N = 128$	$N = 256$	$N = 512$	$N = 1024$	$N = 2048$
$\delta = 1.1$	2.861E−2 1.084	1.349E−2 1.101	6.292E−3 1.120	2.896E−3 1.142	1.312E−3 1.172	5.822E−4
$\delta = 1.2$	6.139E−3 1.739	1.840E−3 3.082	2.173E−4 −0.414	2.895E−4 −0.352	3.696E−4 0.246	3.115E−4
$\delta = 1.3$	1.283E−3 −0.617	1.968E−3 0.210	1.702E−3 0.475	1.224E−3 0.621	7.961E−4 0.725	4.816E−4
$\delta = 1.4$	3.568E−3 0.380	2.743E−3 0.601	1.808E−3 0.735	1.086E−3 0.827	6.121E−4 0.891	3.300E−4
$\delta = 1.5$	3.463E−3 0.615	2.262E−3 0.758	1.338E−3 0.847	7.437E−4 0.903	3.976E−4 0.939	2.074E−4
$\delta = 1.6$	2.652E−3 0.728	1.601E−3 0.830	9.006E−4 0.891	4.856E−4 0.928	2.552E−4 0.952	1.319E−4
$\delta = 1.7$	1.844E−3 0.788	1.068E−3 0.864	5.866E−4 0.909	3.124E−4 0.936	1.633E−4 0.953	8.435E−5
$\delta = 1.8$	1.209E−3 0.825	6.824E−4 0.884	3.697E−4 0.918	1.957E−4 0.938	1.021E−4 0.951	5.283E−5
$\delta = 1.9$	7.456E−4 0.858	4.113E−4 0.906	2.195E−4 0.931	1.151E−4 0.945	5.980E−5 0.954	3.087E−5

Eliminating the variables $\vec{u}_e$ (i.e., discarding them from our computed solution, as was done in Fig. 4) is equivalent to solving the system of equations

$$(B_{oo} - B_{oe}B_{ee}^{-1}B_{eo})\vec{u}_o = (\vec{f}_o - B_{oe}B_{ee}^{-1}\vec{f}_e), \tag{28}$$

whose coefficient matrix is the Schur complement of the matrix B_{ee}.

The structure of the non-sparse matrices B_{oo}, B_{oe}, B_{eo} and B_{ee} is much more complicated than the corresponding matrices in [17] and the analysis of (28) is not easy. Our numerical experiments indicate that if $b(x)$ is a positive constant then the Schur complement of B_{ee} is an M-matrix and therefore monotone; on the other hand, we have observed numerically that the Schur complement of B_{ee} sometimes fails to be monotone although oscillations in the solution of (28) are not apparent, i.e., our postprocessing procedure seems to work in all cases although we cannot yet prove that it always works.

6. Conclusions

In this paper we gave a rigorous error analysis for a finite difference scheme applied on an equidistant mesh to a two-point boundary value problem where the leading term in the differential operator is a Caputo fractional derivative of order $\delta \in (1, 2)$. The scheme uses a central differencing approximation of the convective term, which gives improved accuracy in our numerical experiments compared with the approximation used in [3]. The proof that the scheme converges uses a stability condition on the mesh diameter that may be restrictive when δ is near 1. When this stability condition is violated, the computed solutions may have small oscillations near $x = 1$ and very small oscillations near $x = 0$ but we describe a simple postprocessing that removes these oscillations.

Acknowledgements

This research was partly supported by the Instituto Universitario de Matemáticas y Aplicaciones (IUMA), the Ministerio de Educación, Cultura y Deporte (Programa Nacional de Movilidad de Recursos Humanos del Plan Nacional de I+D+i 2008–2011), project MEC/FEDER MTM 2010-16917 and the Diputación General de Aragón.

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