

An explicit high order method for fractional advection diffusion equations



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ABSTRACT

We propose a high order explicit finite difference method for fractional advection diffusion equations. These equations can be obtained from the standard advection diffusion equations by replacing the second order spatial derivative by a fractional operator of order α with $1 < \alpha \leq 2$. This operator is defined by a combination of the left and right Riemann–Liouville fractional derivatives. We study the convergence of the numerical method through consistency and stability. The order of convergence varies between two and three and for advection dominated flows is close to three. Although the method is conditionally stable, the restrictions allow wide stability regions. The analysis is confirmed by numerical examples.

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1. Fractional advection diffusion equation

Fractional derivatives have been used to model anomalous dispersion or diffusion and recently the fractional advection diffusion equation has been presented as a more suitable model for many problems that appear in different fields, such as engineering, physics, chemistry and hydrology. The fractional advection diffusion equation involves a parameter $1 < \alpha < 2$ representing the order of the fractional operator in space and when $\alpha = 2$ we obtain the classical advection diffusion equation. Therefore in experiments, an additional parameter α needs to be adjusted, that helps to characterize the flow.

Some of the works that present experimental results with parameter estimation involving fractional advection diffusion (or dispersion) problems are for instance [5,7,8,11,33]. In [7] the most frequently occurring value of α to adjust the experimental results varies in the range of 1.4 to 2.0 as in [8]. In [11] the average estimate of the parameter α is also around 1.7 and 1.8. However, there are some estimates in [5,33], that concern small parameters of α , less than 1.5.

Similar problems to the one presented here have also been studied from different perspectives and not only from the numerical point of view. The study of analytical approaches, namely discussions about the well-posedness of such problems, that is, on the existence, uniqueness and regularity of the solutions are also a very active research field [2,6,15].

Regarding finite difference methods for fractional advection diffusion problems, in the last years many approaches have been appearing, mostly with convergence of first and second order, some for only pure diffusive problems [4,19,20,29,34] and others for the advection–diffusion models [3,12–14,23,26,28]. Many of the second order approaches rely on implicit methods which are inadequate for advection dominated flows. However, advection often dominates the evolution of transport flows.

Our purpose is to introduce a numerical method that is also suitable for primarily advective flows, that is, with small diffusion. We derive a numerical method which is explicit and it has the particularity that for $\alpha = 2$ matches the numerical

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method introduced in [16] and called QUICKEST. Although this method was introduced a long time ago it has been very popular until today, since it has the goal of providing an accurate solution without strong oscillations presented in some higher order methods. It has also been shown to be more efficient than other schemes for highly advective flows, since it makes a reasonable compromise between improved performance and computational cost [1,9,10,25,31,32]. The numerical method we propose keeps these properties but now for more general models, described by the fractional operator.

The fractional advection diffusion equation can be expressed as follows

$$\frac{\partial u}{\partial t} + V \frac{\partial u}{\partial x} = D \left(\frac{1}{2} + \frac{\beta}{2} \right) \frac{\partial^\alpha u}{\partial x^\alpha} + D \left(\frac{1}{2} - \frac{\beta}{2} \right) \frac{\partial^\alpha u}{\partial (-x)^\alpha} + S, \quad (1)$$

where u represents a concentration, V is the velocity, x is the spatial coordinate, t is the time, D is the diffusion (or dispersion) coefficient, α is the order of the fractional differentiation with $1 < \alpha \leq 2$ and S is the source or sink term. The parameter β is a skewness parameter with $-1 \leq \beta \leq 1$.

We define the fractional operator

$$\nabla_\beta^\alpha u = \frac{1}{2}(1 + \beta) \frac{\partial^\alpha u}{\partial x^\alpha} + \frac{1}{2}(1 - \beta) \frac{\partial^\alpha u}{\partial (-x)^\alpha}. \quad (2)$$

Eq. (1) can be rewritten in the simpler form

$$\frac{\partial u}{\partial t} + V \frac{\partial u}{\partial x} = D \nabla_\beta^\alpha u + S. \quad (3)$$

We consider the problem defined in $x \in \mathbb{R}$ with an initial condition

$$u(x, 0) = f(x), \quad x \in \mathbb{R},$$

and boundary conditions

$$\lim_{x \rightarrow -\infty} u(x, t) = 0 \quad \text{and} \quad \lim_{x \rightarrow \infty} u(x, t) = 0.$$

In the analysis of the numerical method that follows, we assume our problem has a unique and sufficiently smooth solution.

Remark 1. The type of problems we are studying includes the cases for which the solution u is non-zero in a bounded interval $[a, b]$, for all t , that can be seen as being zero otherwise, and by assuming the boundary conditions

$$u(a, t) = 0 \quad \text{and} \quad u(b, t) = 0.$$

For the particular cases, $\beta = 1$ and $\beta = -1$, we can assume respectively the more general boundary conditions

$$u(a, t) = 0 \quad \text{and} \quad u(b, t) = g_b(t)$$

and

$$u(a, t) = g_a(t) \quad \text{and} \quad u(b, t) = 0,$$

where $g_a(t)$ and $g_b(t)$ are given functions.

The fractional derivatives can be represented by the Riemann–Liouville formula. The left and right Riemann–Liouville fractional derivatives of order α , for $x \in [a, b]$, $-\infty \leq a < b \leq \infty$, are respectively defined by

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x, t) = \frac{1}{\Gamma(n - \alpha)} \frac{\partial^n}{\partial x^n} \int_a^x u(\xi, t) (x - \xi)^{n - \alpha - 1} d\xi \quad (n - 1 < \alpha < n), \quad (4)$$

$$\frac{\partial^\alpha u}{\partial (-x)^\alpha}(x, t) = \frac{(-1)^n}{\Gamma(n - \alpha)} \frac{\partial^n}{\partial x^n} \int_x^b u(\xi, t) (\xi - x)^{n - \alpha - 1} d\xi \quad (n - 1 < \alpha < n), \quad (5)$$

where $\Gamma(\cdot)$ is the Gamma function and $n = [\alpha] + 1$, with $[\alpha]$ denoting the integer part of α .

Remark 2. For $n - 1 < \alpha < n$, sufficient conditions for the existence of the Riemann–Liouville derivatives is that $u(\cdot, t) \in AC^{(n)}([a, b])$ [22]. This space represents the space of functions u for which the space derivatives are continuous until order $n - 1$ and the derivative of order $n - 1$ is absolutely continuous.

The application of fractional calculus to scientific and engineering problems presents difficulties that arise from the basic calculus properties, such as, the composition property with derivatives. To preserve composition the function and some of its derivatives should be identically zero at the initial point. For the Riemann–Liouville derivatives, we have the following properties, that can be found, for instance, in [17,21,22].

Proposition 1. Let $\alpha > 0$, if the left Riemann–Liouville derivative (4) of order α and $\alpha + m$ exists, for $m = 1, 2, \dots$, we have

$$\frac{\partial^m}{\partial x^m} \left(\frac{\partial^\alpha u}{\partial x^\alpha}(x, t) \right) = \frac{\partial^{\alpha+m} u}{\partial x^{\alpha+m}}(x, t), \tag{6}$$

$$\frac{\partial^\alpha}{\partial x^\alpha} \left(\frac{\partial^m u}{\partial x^m}(x, t) \right) = \frac{\partial^{\alpha+m} u}{\partial x^{\alpha+m}}(x, t) - \sum_{j=0}^{m-1} \frac{\partial^j u}{\partial x^j}(a, t) \frac{(x-a)^{j-\alpha-m}}{\Gamma(1+j-\alpha-m)}. \tag{7}$$

Proposition 2. Let $\alpha > 0$, if the right Riemann–Liouville derivative (5) of order α and $\alpha + m$ exists, for $m = 1, 2, \dots$, we have

$$\frac{\partial^m}{\partial x^m} \left(\frac{\partial^\alpha u}{\partial (-x)^\alpha}(x, t) \right) = (-1)^m \frac{\partial^{\alpha+m} u}{\partial (-x)^{\alpha+m}}(x, t), \tag{8}$$

$$\frac{\partial^\alpha}{\partial (-x)^\alpha} \left(\frac{\partial^m u}{\partial x^m}(x, t) \right) = (-1)^m \frac{\partial^{\alpha+m} u}{\partial (-x)^{\alpha+m}}(x, t) - \sum_{j=0}^{m-1} \frac{\partial^j u}{\partial x^j}(b, t) \frac{(-1)^{j+m}(b-x)^{j-\alpha-m}}{\Gamma(1+j-\alpha-m)}. \tag{9}$$

From the previous properties, we infer that the interchange of the Riemann–Liouville differentiation operators is allowed under certain conditions. Note that, since we are considering homogeneous boundary conditions, similar results to Proposition 1 and Proposition 2, for the real line case, become

$$\frac{\partial}{\partial x} \left(\frac{\partial^\alpha u}{\partial x^\alpha}(x, t) \right) = \frac{\partial^\alpha}{\partial x^\alpha} \left(\frac{\partial u}{\partial x}(x, t) \right) = \frac{\partial^{\alpha+1} u}{\partial x^{\alpha+1}}(x, t) \tag{10}$$

and

$$\frac{\partial}{\partial x} \left(\frac{\partial^\alpha u}{\partial (-x)^\alpha}(x, t) \right) = \frac{\partial^\alpha}{\partial (-x)^\alpha} \left(\frac{\partial u}{\partial x}(x, t) \right) = (-1)^m \frac{\partial^{\alpha+1} u}{\partial (-x)^{\alpha+1}}(x, t). \tag{11}$$

2. Finite difference approximations

In this section we derive the numerical method that determines the approximate solution for the fractional advection diffusion equation. We start to describe how we discretize in time to get an explicit method and then how to discretize the classical spatial derivatives. The last section discusses how we approximate the fractional operators involved.

2.1. Time discretization

We start to derive the finite difference scheme using Taylor expansions, that is, we expand u about time level n , that is, $t_n = n\Delta t$ and where Δt denotes the time step, to obtain

$$u(x, t_{n+1}) - u(x, t_n) = \Delta t \frac{\partial u}{\partial t}(x, t_n) + \frac{\Delta t^2}{2} \frac{\partial^2 u}{\partial t^2}(x, t_n) + \frac{\Delta t^3}{6} \frac{\partial^3 u}{\partial t^3}(x, t_n) + \mathcal{O}(\Delta t^4). \tag{12}$$

Then, from (3), we can write

$$\frac{\partial^2 u}{\partial t^2} = -V \frac{\partial^2 u}{\partial t \partial x} + D \frac{\partial}{\partial t} (\nabla_\beta^\alpha u) + \frac{\partial S}{\partial t}, \tag{13}$$

$$\frac{\partial^2 u}{\partial x \partial t} = -V \frac{\partial^2 u}{\partial x^2} + D \frac{\partial}{\partial x} (\nabla_\beta^\alpha u) + \frac{\partial S}{\partial x}, \tag{14}$$

$$\nabla_\beta^\alpha \left(\frac{\partial u}{\partial t} \right) = -V \nabla_\beta^\alpha \left(\frac{\partial u}{\partial x} \right) + D \nabla_\beta^\alpha (\nabla_\beta^\alpha u) + \nabla_\beta^\alpha S. \tag{15}$$

Let us assume that

$$\frac{\partial}{\partial t} (\nabla_\beta^\alpha u) = \nabla_\beta^\alpha \left(\frac{\partial u}{\partial t} \right).$$

It can be noted that this equality holds, if we assume $\frac{\partial}{\partial t} u(\cdot, t) \in AC^{(2)}(\mathbb{R})$ (see Remark 2). Therefore, from (13)–(15), we get

$$\frac{\partial^2 u}{\partial t^2} = V^2 \frac{\partial^2 u}{\partial x^2} - VD \frac{\partial}{\partial x} (\nabla_\beta^\alpha u) - V \frac{\partial S}{\partial x} - VD \nabla_\beta^\alpha \left(\frac{\partial u}{\partial x} \right) + D^2 \nabla_\beta^\alpha (\nabla_\beta^\alpha u) + D \nabla_\beta^\alpha S + \frac{\partial S}{\partial t}. \tag{16}$$

From Proposition 1 and Proposition 2 and since we assume homogeneous boundary conditions, we obtain

$$\nabla_{\beta}^{\alpha} \left(\frac{\partial u}{\partial x} (x, t) \right) = \nabla_{\beta}^{\alpha+1} u(x, t), \quad (17)$$

$$\frac{\partial}{\partial x} (\nabla_{\beta}^{\alpha} u(x, t)) = \nabla_{\beta}^{\alpha+1} u(x, t), \quad (18)$$

where

$$\nabla_{\beta}^{\alpha+1} u = \frac{1}{2} (1 + \beta) \frac{\partial^{\alpha+1} u}{\partial x^{\alpha+1}} - \frac{1}{2} (1 - \beta) \frac{\partial^{\alpha+1} u}{\partial (-x)^{\alpha+1}}, \quad (19)$$

and hence from (16)–(19) we obtain

$$\frac{\partial^2 u}{\partial t^2} = V^2 \frac{\partial^2 u}{\partial x^2} - 2VD \nabla_{\beta}^{\alpha+1} u + D^2 \nabla_{\beta}^{\alpha} (\nabla_{\beta}^{\alpha} u) + D \nabla_{\beta}^{\alpha} S + \frac{\partial S}{\partial t} - V \frac{\partial S}{\partial x}. \quad (20)$$

From (20), we have

$$\frac{\partial^3 u}{\partial t^3} = V^2 \frac{\partial}{\partial t} \left(\frac{\partial^2 u}{\partial x^2} \right) - 2VD \frac{\partial}{\partial t} (\nabla_{\beta}^{\alpha+1} u) + D^2 \frac{\partial}{\partial t} (\nabla_{\beta}^{\alpha} (\nabla_{\beta}^{\alpha} u)) + D \nabla_{\beta}^{\alpha} \left(\frac{\partial S}{\partial t} \right) + \frac{\partial^2 S}{\partial t^2} - V \frac{\partial^2 S}{\partial t \partial x}. \quad (21)$$

Note that, from (3), we can write

$$\frac{\partial}{\partial t} \left(\frac{\partial^2 u}{\partial x^2} \right) = -V \frac{\partial^3 u}{\partial x^3} + D \nabla_{\beta}^{\alpha} \left(\frac{\partial^2 u}{\partial x^2} \right) + \frac{\partial^2 S}{\partial x^2}. \quad (22)$$

Henceforth, inserting (22) in (21) we obtain

$$\begin{aligned} \frac{\partial^3 u}{\partial t^3} &= -V^3 \frac{\partial^3 u}{\partial x^3} + V^2 D \nabla_{\beta}^{\alpha} \left(\frac{\partial^2 u}{\partial x^2} \right) + V^2 \frac{\partial^2 S}{\partial x^2} - 2VD \frac{\partial}{\partial t} (\nabla_{\beta}^{\alpha+1} u) + D^2 \frac{\partial}{\partial t} (\nabla_{\beta}^{\alpha} (\nabla_{\beta}^{\alpha} u)) \\ &\quad + D \nabla_{\beta}^{\alpha} \left(\frac{\partial S}{\partial t} \right) + \frac{\partial^2 S}{\partial t^2} - V \frac{\partial^2 S}{\partial t \partial x}. \end{aligned} \quad (23)$$

Next, we derive the finite-difference approximations, by dropping higher-spatial-derivative terms from (20) and (23), that is,

$$\frac{\partial^2 u}{\partial t^2} \approx V^2 \frac{\partial^2 u}{\partial x^2} - 2VD \nabla_{\beta}^{\alpha+1} u + D \nabla_{\beta}^{\alpha} S + \frac{\partial S}{\partial t} - V \frac{\partial S}{\partial x}, \quad (24)$$

$$\frac{\partial^3 u}{\partial t^3} \approx -V^3 \frac{\partial^3 u}{\partial x^3} + D \nabla_{\beta}^{\alpha} \left(\frac{\partial S}{\partial t} \right) + \frac{\partial^2 S}{\partial t^2} - V \frac{\partial^2 S}{\partial t \partial x} + V^2 \frac{\partial^2 S}{\partial x^2}. \quad (25)$$

Inserting (3), (24) and (25) into (12) gives

$$\begin{aligned} u(x, t_{n+1}) &\approx u(x, t_n) + \Delta t \left(-V \frac{\partial u}{\partial x} + D \nabla_{\beta}^{\alpha} u \right) (x, t_n) + \frac{1}{2} \Delta t^2 \left(V^2 \frac{\partial^2 u}{\partial x^2} - 2VD \nabla_{\beta}^{\alpha+1} u \right) (x, t_n) \\ &\quad + \frac{1}{6} \Delta t^3 \left(-V^3 \frac{\partial^3 u}{\partial x^3} \right) (x, t_n) + \Delta t S(x, t_n) + \frac{\Delta t^2}{2} \left(D \nabla_{\beta}^{\alpha} S + \frac{\partial S}{\partial t} - V \frac{\partial S}{\partial x} \right) (x, t_n) \\ &\quad + \frac{\Delta t^3}{6} \left(D \nabla_{\beta}^{\alpha} \left(\frac{\partial S}{\partial t} \right) + \frac{\partial^2 S}{\partial t^2} - V \frac{\partial^2 S}{\partial t \partial x} + V^2 \frac{\partial^2 S}{\partial x^2} \right) (x, t_n). \end{aligned} \quad (26)$$

2.2. Spatial discretization

To derive a finite difference scheme we suppose there are approximations $\mathbf{U}^n := \{U_j^n\}$ to the values $u(x_j, t_n)$ at the mesh points

$$x_j = j\Delta x, \quad j \in \mathbb{Z} \quad \text{and} \quad t_n = n\Delta t, \quad n \geq 0,$$

where Δx denotes the uniform space step and Δt the uniform time step. Let

$$\nu = \frac{V \Delta t}{\Delta x} \quad \text{and} \quad \mu_{\alpha} = \frac{D \Delta t}{\Delta x^{\alpha}}.$$

The quantity ν is called the Courant (or CFL) number and μ_{α} is associated with the diffusion coefficient.

Spatial discretization about a grid point j can be accomplished by first fitting a quadratic across grid points $j-1$, j and $j+1$, and then integrating to obtain the average value of u within the j th mesh cell. This average value is determined at time levels n and $n+1$, thus yielding u^n and u^{n+1} . The difference $(u^{n+1} - u^n)$ becomes

$$u(x, t_{n+1}) - u(x, t_n) \approx U_j^{n+1} - U_j^n + \frac{1}{24} [(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) - (U_{j+1}^n - 2U_j^n + U_{j-1}^n)]. \quad (27)$$

The last two terms of (27) can be interpreted as

$$\frac{1}{24} \Delta t \Delta x^2 \frac{\partial^2}{\partial x^2} \left(\frac{\partial u}{\partial t} \right) \approx -\frac{1}{24} V \Delta t \Delta x^2 \frac{\partial^3 u}{\partial x^3} \tag{28}$$

from (3). Hence, taking in consideration (28) we use (27) to approximate the term $u(x, t_{n+1}) - u(x, t_n)$ appearing in (26).

We now describe how we approximate the spatial derivatives appearing in (26) and (28) to finally obtain the numerical method. Let us define the difference operators

$$\begin{aligned} \Delta_0 U_j^n &= \frac{1}{2} (U_{j+1}^n - U_{j-1}^n), & \delta^2 U_j^n &= U_{j+1}^n - 2U_j^n + U_{j-1}^n, \\ \delta^2 \Delta_- U_j^n &= U_{j+1}^n - 3U_j^n + 3U_{j-1}^n - U_{j-2}^n. \end{aligned} \tag{29}$$

A common alternative used to avoid the shortcomings of discretizing the spatial first derivative with upwinding differencing and central differencing is the use of the discretization presented in [16] involved in the derivation of the QUICKEST scheme. The interpolation formula for positive velocity is

$$\frac{\partial u}{\partial x} \approx \frac{\Delta_0 U_j^n}{\Delta x} - \frac{1}{8} \frac{\delta^2 \Delta_- U_j^n}{\Delta x}. \tag{30}$$

Hence, we discretize the spatial first order derivative in (26) in this manner.

We denote the fractional difference operators by $\delta_\beta^\alpha u(x_j, t_n)$ and $\delta_\beta^{\alpha+1} u(x_j, t_n)$ and such that,

$$\Delta_\beta^\alpha u(x_j, t_n) \approx \frac{\delta_\beta^\alpha u(x_j, t_n)}{\Delta x^\alpha}, \quad \Delta_\beta^{\alpha+1} u(x_j, t_n) \approx \frac{\delta_\beta^{\alpha+1} u(x_j, t_n)}{\Delta x^{\alpha+1}}.$$

These operators will be defined in detail in the next section.

If in (26) we discretize the spatial first order derivative as (30), the second order derivative with second order difference operator and the third-order derivative with third-order difference operator, both defined in (29), and the fractional derivatives with the respective fractional difference operators, to be discussed in the next section, we have the numerical method

$$U_j^{n+1} = U_j^n - \nu \Delta_0 U_j^n + \mu_\alpha \delta_\beta^\alpha U_j^n + \frac{1}{2} \nu^2 \delta^2 U_j^n - \nu \mu_\alpha \delta_\beta^{\alpha+1} U_j^n + \frac{1}{6} (\nu - \nu^3) \delta^2 \Delta_- U_j^n + \Delta t \tilde{S}_j^n(x_j, t_n), \tag{31}$$

where $\tilde{S}_j^n = \tilde{S}(x_j, t_n)$ and \tilde{S} is given by

$$\tilde{S} = S + \frac{\Delta t}{2} \left(D \nabla_\beta^\alpha S + \frac{\partial S}{\partial t} - V \frac{\partial S}{\partial x} \right) + \frac{\Delta t^2}{6} \left(D \nabla_\beta^\alpha \left(\frac{\partial S}{\partial t} \right) + \frac{\partial^2 S}{\partial t^2} - V \frac{\partial^2 S}{\partial t \partial x} + V^2 \frac{\partial^2 S}{\partial x^2} \right).$$

2.3. Derivation of the fractional difference operators

In this section we describe how to approximate the fractional operators $\Delta_\beta^\alpha u$ and $\Delta_\beta^{\alpha+1} u$ defined by (2) and (19) respectively. These approximations have been already denoted by $\delta_\beta^\alpha u / \Delta x^\alpha$ and $\delta_\beta^{\alpha+1} u / \Delta x^{\alpha+1}$ respectively, in the previous section, to write the numerical method (31).

We begin by deriving the approximation for the operator $\Delta_\beta^\alpha u$, defined by (2), (4) and (5), which uses the approximations for the left and right fractional derivatives derived in [27,28]. It consists of approximating the function inside the integral by a linear spline in order to obtain a second order approximation for the fractional operator. More details on this discretization can be seen in [27,28] and they will be also given in the next section during the discussion on the truncation error of our numerical method (31). Afterwards, we derive the approximation for the operator $\Delta_\beta^{\alpha+1} u$.

Set

$$a_m = \begin{cases} (m+1)^{3-\alpha} - 2m^{3-\alpha} + (m-1)^{3-\alpha}, & m \geq 1 \\ 1, & m = 0 \end{cases} \tag{32}$$

and

$$q_m = \begin{cases} a_{m-1} - 2a_m + a_{m+1}, & m \geq 1 \\ -2a_0 + a_1, & m = 0 \\ a_0, & m = -1. \end{cases} \tag{33}$$

The approximation of the left and right fractional derivatives, defined in (4) and (5) are respectively given by

$$\frac{\delta_l^\alpha u(x_j, t)}{\Delta x^\alpha}, \quad \frac{\delta_r^\alpha u(x_j, t)}{\Delta x^\alpha},$$

where the discrete operators are defined by

$$\delta_l^\alpha u(x_j, t) = \frac{1}{\Gamma(4-\alpha)} \sum_{m=-1}^{\infty} q_m u(x_{j-m}, t), \quad (34)$$

$$\delta_r^\alpha u(x_j, t) = \frac{1}{\Gamma(4-\alpha)} \sum_{m=-1}^{\infty} q_m u(x_{j+m}, t). \quad (35)$$

Hence, we define the discrete operator $\delta_\beta^\alpha u$, that approximates $\Delta_\beta^\alpha u$ as

$$\delta_\beta^\alpha u(x_j, t) = \frac{1}{2}(1+\beta)\delta_l^\alpha u(x_j, t) + \frac{1}{2}(1-\beta)\delta_r^\alpha u(x_j, t). \quad (36)$$

We now turn to the operator $\nabla_\beta^{\alpha+1} u$, that is, we describe how we approximate this operator. First, note that

$$\nabla_\beta^{\alpha+1} u(x, t) = \frac{\partial}{\partial x} [\nabla_\beta^\alpha u(x, t)].$$

Therefore an approximation to the operator $\nabla_\beta^{\alpha+1} u(x_j, t)$ can be given by

$$\frac{\delta_\beta^{\alpha+1} u(x_j, t)}{\Delta x^{\alpha+1}} = \frac{1}{\Delta x} \left(\frac{\delta_\beta^\alpha u_j^n}{\Delta x^\alpha} - \frac{\delta_\beta^\alpha u_{j-1}^n}{\Delta x^\alpha} \right).$$

Next, we define

$$\delta_l^{\alpha+1} u_j^n = \delta_l^\alpha u_j^n - \delta_l^\alpha u_{j-1}^n, \quad \delta_r^{\alpha+1} u_j^n = \delta_r^\alpha u_j^n - \delta_r^\alpha u_{j-1}^n,$$

in order to rewrite the discrete operator as

$$\frac{\delta_\beta^{\alpha+1} u_j^n}{\Delta x^{\alpha+1}} = \frac{1}{\Delta x^{\alpha+1}} \left[\frac{1}{2}(1+\beta)\delta_l^{\alpha+1} u_j^n + \frac{1}{2}(1-\beta)\delta_r^{\alpha+1} u_j^n \right].$$

Note that the discrete operators $\delta_l^{\alpha+1} u_j^n$ and $\delta_r^{\alpha+1} u_j^n$ are respectively defined by

$$\delta_l^{\alpha+1} u_j^n = \delta_l^\alpha u_j^n - \delta_l^\alpha u_{j-1}^n = \frac{1}{\Gamma(4-\alpha)} \left[q_{-1} u_{j+1}^n + \sum_{m=0}^{\infty} (q_m - q_{m-1}) u_{j-m}^n \right] \quad (37)$$

and

$$\delta_r^{\alpha+1} u_j^n = \delta_r^\alpha u_j^n - \delta_r^\alpha u_{j-1}^n = -\frac{1}{\Gamma(4-\alpha)} \left[q_{-1} u_{j-2}^n + \sum_{m=0}^{\infty} (q_m - q_{m-1}) u_{j-1+m}^n \right]. \quad (38)$$

Moreover, the numerical method (31), with $\alpha = 2$ and without the source term, is the well known QUICKEST scheme presented in [16].

3. Global error

In this section we discuss theoretically the global error of the numerical method (31). The method can be written in the form

$$U_j^{n+1} = \mathcal{P} U_j^n, \quad (39)$$

with \mathcal{P} an operator defined by $\mathcal{P} = \sum_{k=-\infty}^{\infty} c_k \mathcal{S}^k$, where the coefficients c_k depend on ν and μ_α and \mathcal{S} represents the forward and backward shift operators, that is, $\mathcal{S}^k U_j^n = U_{j+k}^n$.

For the exact solution, and denoting $u(j\Delta x, n\Delta t)$ by u_j^n , we have

$$u_j^{n+1} = \mathcal{P} u_j^n + \Delta t T_j^n, \quad (40)$$

where T_j^n is the local truncation error.

Therefore, the global error defined by $E_j^n = u_j^n - U_j^n$ is given by

$$E_j^{n+1} = \mathcal{P} E_j^n + \Delta t T_j^n. \quad (41)$$

Hence, a global bound for the error depends on the truncation error and the boundedness of the operator \mathcal{P} , which will be discussed in the next subsections. We begin by analyzing the truncation error and then discuss the boundedness of the operator, which is related to the stability analysis.

3.1. Leading terms of the truncation error

To derive the truncation error, we consider without loss of generality, the source term zero and use techniques similar to the modified equation [30]. To obtain the results in this section, we assume u is a function with sufficiently many continuous derivatives in time and space. Since our domain is the real line, it is enough to assume the function u and its spatial derivatives vanish at infinity in an appropriate manner, to allow the interchange of differential operators, fractional and integer. We start to present results regarding the leading terms of the truncation error of the fractional difference operators.

Lemma 3. Suppose u is a function with sufficiently many continuous spatial derivatives that vanish at infinity in an appropriate manner. Then $u_j^n = u(x_j, t_n)$ satisfies

$$\frac{\delta_\beta^\alpha u_j^n}{\Delta x^\alpha} = \nabla_\beta^\alpha u_j^n + \epsilon^\alpha(x_j) \quad \text{and} \quad \frac{\delta_\beta^{\alpha+1} u_j^n}{\Delta x^{\alpha+1}} = \nabla_\beta^{\alpha+1} u_j^n + \epsilon^{\alpha+1}(x_j), \tag{42}$$

where $\epsilon^\alpha(x_j)$ and $\epsilon^{\alpha+1}(x_j)$ are local truncation errors approximately given by

$$\epsilon^\alpha(x_j) \approx \left(\frac{\Delta x^2}{12} + C_2 \Delta x^2 \right) \nabla_\beta^{\alpha+2} u_j^n + C_3 \Delta x^3 \nabla_\beta^{\alpha+3} u_j^n + O(\Delta x^4) \tag{43}$$

$$\epsilon^{\alpha+1}(x_j) \approx -\frac{\Delta x}{2} \nabla_\beta^{\alpha+2} u_j^n + \left(\frac{\Delta x^2}{6} - C_2 \Delta x^2 \right) \nabla_\beta^{\alpha+3} u_j^n + O(\Delta x^3), \tag{44}$$

for $C_i, i = 2, 3$ constants.

Proof. During this proof we omit the variable t , for the sake of clarity, and for an arbitrary and fixed t_n we denote $u(x_j) := u(x_j, t_n)$. We derive only the truncation error to the left fractional derivative since for the right derivative it can be obtained in a similar manner. The left derivative can be written as

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x_j) = \frac{\partial^2}{\partial x^2} I^{2-\alpha} u(x_j),$$

where

$$I^{2-\alpha} u(x_j) = \frac{1}{\Gamma(2-\alpha)} \int_{-\infty}^{x_j} u(\xi) (x_j - \xi)^{1-\alpha} d\xi.$$

The approximation under consideration was obtained first by doing a central approximation of the second order derivative, assuming $I^{2-\alpha} u$ is sufficiently smooth. Therefore, we have

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x_j) = \frac{1}{\Delta x^2} [I^{2-\alpha} u(x_{j+1}) - 2I^{2-\alpha} u(x_j) + I^{2-\alpha} u(x_{j-1})] + \epsilon_a(x_j),$$

where

$$\epsilon_a(x_j) = -\frac{\Delta x^2}{12} \frac{\partial^4}{\partial x^4} I^{2-\alpha} u(x_j) + O(\Delta x^4).$$

Then, $I^{2-\alpha} u(x_j)$ is approximated by $\tilde{I}^{2-\alpha} u(x_j)$, obtained by doing a linear spline approximation of $u(\xi)$ (see [27] for more details). We get

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x_j) = \frac{1}{\Delta x^2} [\tilde{I}^{2-\alpha} u(x_{j+1}) - 2\tilde{I}^{2-\alpha} u(x_j) + \tilde{I}^{2-\alpha} u(x_{j-1}) + \epsilon_s(x_j)] + \epsilon_a(x_j), \tag{45}$$

where $\epsilon_s(x_j)$ is the error associated with the spline approximation. We have

$$\begin{aligned} \epsilon_s(x_j) = \frac{1}{\Gamma(2-\alpha)} & \left\{ \sum_{k=-\infty}^{j-1} \int_{x_{k-1}}^{x_k} (u(\xi) - s_{j-1}(\xi))(x_{j-1} - \xi)^{1-\alpha} d\xi - 2 \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} (u(\xi) - s_j(\xi))(x_j - \xi)^{1-\alpha} d\xi \right. \\ & \left. + \sum_{k=-\infty}^{j+1} \int_{x_{k-1}}^{x_k} (u(\xi) - s_{j+1}(\xi))(x_{j+1} - \xi)^{1-\alpha} d\xi \right\} \end{aligned}$$

where $s_j(\xi)$ denotes the spline that interpolates $x_k = k\Delta x, k \leq j$. For $x_{k-1} \leq x \leq x_k$

$$u(\xi) - s(\xi) = -\frac{1}{2}u''(\xi)l_{k,2}(\xi) - \frac{1}{6}u'''(\xi)l_{k,3}(\xi) - \dots,$$

where

$$l_{k,r}(\xi) = \frac{x_k - \xi}{\Delta x} (x_k - \xi - \Delta x)^r - \frac{\xi - x_{k-1}}{\Delta x} (x_k - \xi)^r.$$

We obtain

$$\epsilon_s(x_j) = -\sum_{r=2}^3 \frac{1}{r!} \epsilon_r(x_j) + \dots, \tag{46}$$

with

$$\begin{aligned} \epsilon_r(x_j) = \frac{1}{\Gamma(2-\alpha)} & \left\{ \sum_{k=-\infty}^{j-1} \int_{x_{k-1}}^{x_k} l_{k,r}(\xi) u^{(r)}(\xi) (x_{j-1} - \xi)^{1-\alpha} - 2 \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} l_{k,r}(\xi) u^{(r)}(\xi) (x_j - \xi)^{1-\alpha} d\xi \right. \\ & \left. + \sum_{k=-\infty}^{j+1} \int_{x_{k-1}}^{x_k} l_{k,r}(\xi) u^{(r)}(\xi) (x_{j+1} - \xi)^{1-\alpha} \right\}. \end{aligned}$$

By changing variables, for $r = 2, 3$, we get

$$\epsilon_r(x_j) = \frac{1}{\Gamma(2-\alpha)} \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} l_{k,r}(\xi) [u^{(r)}(\xi + \Delta x) - 2u^{(r)}(\xi) + u^{(r)}(\xi - \Delta x)] (x_j - \xi)^{1-\alpha} d\xi.$$

Now, since $l_{k,r}(\xi) = O(\Delta x^r)$, for $x_{k-1} \leq \xi \leq x_k$, and by Taylor expansions we have

$$u^{(r)}(\xi + \Delta x) - 2u^{(r)}(\xi) + u^{(r)}(\xi - \Delta x) = \Delta x^2 u^{(r+2)}(\xi) + \frac{\Delta x^4}{12} u^{(r+3)}(\xi) + O(\Delta x^6),$$

we can obtain an estimation for the error given by, for $r = 2, 3$,

$$\begin{aligned} \epsilon_r(x_j) & \approx C_r \Delta x^r \frac{1}{\Gamma(2-\alpha)} \sum_{k=-\infty}^j \int_{x_{k-1}}^{x_k} \Delta x^2 u^{(r+2)}(\xi) (x_j - \xi)^{1-\alpha} d\xi + \dots \\ & = C_r \Delta x^{r+2} \frac{1}{\Gamma(2-\alpha)} \int_{-\infty}^{x_j} u^{(r+2)}(\xi) (x_j - \xi)^{1-\alpha} d\xi + \dots \\ & = C_r \Delta x^{r+2} I^{2-\alpha} \frac{\partial^{r+2} u}{\partial x^{r+2}} + \dots \end{aligned} \tag{47}$$

Note that because we are assuming u has sufficiently many continuous derivatives and that they vanish in an appropriate manner at infinity, we have [21]

$$\frac{\partial^{\alpha+r} u}{\partial x^{\alpha+r}}(x_j) = I^{2-\alpha} \frac{\partial^{r+2} u}{\partial x^{r+2}}(x_j) = \frac{\partial^{r+2} u}{\partial x^{r+2}} I^{2-\alpha} u(x_j), \quad r = 2, 3.$$

Then

$$\epsilon_r(x_j) \approx C_r \Delta x^{r+2} \frac{\partial^{\alpha+r} u}{\partial x^{\alpha+r}}(x_j) + O(\Delta x^{4+r}). \tag{48}$$

Therefore, from (46) and (48) we get, for the error $\epsilon_s(x_j)/\Delta x^2$ appearing in (45),

$$\begin{aligned} \frac{1}{\Delta x^2} \epsilon_s(x_j) & \approx -\frac{1}{2} C_2 \frac{\Delta x^4}{\Delta x^2} \frac{\partial^{\alpha+2} u}{\partial x^{\alpha+2}}(x_j) - \frac{1}{6} C_3 \frac{\Delta x^5}{\Delta x^2} \frac{\partial^{\alpha+3} u}{\partial x^{\alpha+3}}(x_j) + \dots \\ & = -\frac{1}{2} C_2 \Delta x^2 \frac{\partial^{\alpha+2} u}{\partial x^{\alpha+2}}(x_j) - \frac{1}{6} C_3 \Delta x^3 \frac{\partial^{\alpha+3} u}{\partial x^{\alpha+3}}(x_j) + O(\Delta x^4). \end{aligned}$$

Now let us turn to the fractional operator of order $\alpha + 1$. The operator $\nabla_\beta^{\alpha+1} u$ is first given by

$$\nabla_\beta^{\alpha+1} u(x_j) = \frac{1}{\Delta x} [\nabla_\beta^\alpha u(x_j) - \nabla_\beta^\alpha u(x_{j-1})] + \epsilon_b(x_j),$$

where

$$\epsilon_b(x_j) = \frac{\Delta x}{2} \frac{\partial^2}{\partial x^2} \nabla_\beta^\alpha u(x_j) - \frac{\Delta x^2}{6} \frac{\partial^3}{\partial x^3} \nabla_\beta^\alpha u(x_j) + O(\Delta x^3).$$

By Proposition 1 and Proposition 2 and under the lemma assumptions, we can write

$$\epsilon_b(x_j) = \frac{\Delta x}{2} \nabla_\beta^{\alpha+2} u(x_j) - \frac{\Delta x^2}{6} \nabla_\beta^{\alpha+3} u(x_j) + O(\Delta x^3), \tag{49}$$

where

$$\nabla_\beta^{\alpha+2} u(x_j) = \frac{1}{2} (1 + \beta) \frac{\partial^{\alpha+2} u}{\partial x^{\alpha+2}}(x_j) + \frac{1}{2} (1 - \beta) \frac{\partial^{\alpha+2} u}{\partial (-x)^{\alpha+2}}(x_j) \tag{50}$$

$$\nabla_\beta^{\alpha+3} u(x_j) = \frac{1}{2} (1 + \beta) \frac{\partial^{\alpha+3} u}{\partial x^{\alpha+3}}(x_j) - \frac{1}{2} (1 - \beta) \frac{\partial^{\alpha+3} u}{\partial (-x)^{\alpha+3}}(x_j). \tag{51}$$

Secondly, the operator $\nabla_\beta^\alpha u$ is approximated as previously and therefore

$$\begin{aligned} \nabla_\beta^{\alpha+1} u(x_j) &= \frac{1}{\Delta x} [\delta_\beta^\alpha u(x_j) + \epsilon^\alpha(x_j) - \delta_\beta^\alpha u(x_{j-1}) - \epsilon^\alpha(x_{j-1})] + \epsilon_b(x_j) \\ &= \delta_\beta^{\alpha+1} u(x_j) + \frac{1}{\Delta x} [\epsilon^\alpha(x_j) - \epsilon^\alpha(x_{j-1})] + \epsilon_b(x_j). \end{aligned}$$

Then, it follows

$$\begin{aligned} \frac{1}{\Delta x} [\epsilon^\alpha(x_j) - \epsilon^\alpha(x_{j-1})] &= \frac{1}{\Delta x} \left[\left(\frac{\Delta x^2}{12} + C_2 \Delta x^2 \right) \nabla_\beta^{\alpha+2} u(x_j) + C_3 \Delta x^3 \nabla_\beta^{\alpha+3} u(x_j) \right. \\ &\quad \left. - \left(\frac{\Delta x^2}{12} + C_2 \Delta x^2 \right) \nabla_\beta^{\alpha+2} u(x_{j-1}) - C_3 \Delta x^3 \nabla_\beta^{\alpha+3} u(x_{j-1}) \right] \\ &= \left(\frac{\Delta x^2}{12} + C_2 \Delta x^2 \right) \frac{\partial}{\partial x} \nabla_\beta^{\alpha+2} u(x_j) + O(\Delta x^3) \\ &= \left(\frac{\Delta x^2}{12} + C_2 \Delta x^2 \right) \nabla_\beta^{\alpha+3} u(x_j) + O(\Delta x^3). \end{aligned}$$

From this equality and (49) we finally obtain (44). □

In the next result, we present the truncation error for the numerical method (31) obtained through the modified equation, which consists of substituting the exact solution in the numerical method and then after Taylor expansions and some additional calculations we get the local truncation error.

Theorem 4. For the numerical method (31), the local truncation error at $u^n(x_j) = u(x_j, t_n)$, appearing in the global error (41), is given by

$$\begin{aligned} \Delta t T_j^n &= \frac{\Delta x^{\alpha+2}}{12} (-\mu_\alpha - 12C_2\mu_\alpha - 6v\mu_\alpha + 6v^2\mu_\alpha) \nabla_\beta^{\alpha+2} u^n(x_j) \\ &\quad + \frac{\Delta x^4}{24} (2v - 2v^3 - v^2 + v^4) \frac{\partial^4 u^n}{\partial x^4}(x_j) + \frac{\Delta x^{2\alpha}}{2} \mu_\alpha^2 \nabla_\beta^\alpha (\nabla_\beta^\alpha u^n)(x_j) \\ &\quad + \frac{\Delta x^{\alpha+3}}{6} (-6C_3\mu_\alpha - 12C_2v\mu_\alpha - 3v^2\mu_\alpha + 2v^3\mu_\alpha) \nabla_\beta^{\alpha+3} u^n(x_j) + \dots, \end{aligned} \tag{52}$$

for $\mu_\alpha = D \Delta t / \Delta x^\alpha$ and $v = V \Delta t / \Delta x$.

Proof. Substituting the exact solution in the numerical method, we obtain

$$\begin{aligned} \frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{V \Delta t}{2 \Delta x} (u_{j+1}^n - u_{j-1}^n) - \frac{1}{2} V^2 \frac{\Delta t}{\Delta x^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n) - D \frac{\delta_\beta^\alpha u_j^n}{\Delta x^\alpha} \\ + V D \Delta t \frac{\delta_\beta^{\alpha+1} u_j^n}{\Delta x^{\alpha+1}} - \frac{1}{6} \left(\frac{V}{\Delta x} - V^3 \frac{\Delta t^2}{\Delta x^3} \right) (u_{j+1}^n - 3u_j^n + 3u_{j-1}^n - u_{j-2}^n) = 0. \end{aligned}$$

After Taylor expansions, the application of the results of Lemma 3 and some additional small simplifications, we can write

$$\begin{aligned} & \frac{\partial u_j^n}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 u_j^n}{\partial t^2} + \frac{\Delta t^2}{6} \frac{\partial^3 u_j^n}{\partial t^3} + \frac{\Delta t^3}{24} \frac{\partial^4 u_j^n}{\partial t^4} + O(\Delta t^4) \\ & + \frac{V}{2\Delta x} \left(2\Delta x \frac{\partial u_j^n}{\partial x} + \frac{1}{3} \Delta x^3 \frac{\partial^3 u_j^n}{\partial x^3} \right) + O(\Delta x^4) \\ & - \frac{V^2 \Delta t}{2\Delta x^2} \left(\Delta x^2 \frac{\partial^2 u_j^n}{\partial x^2} + \frac{\Delta x^4}{12} \frac{\partial^4 u_j^n}{\partial x^4} \right) + O(\Delta x^4 \Delta t) \\ & - D \nabla_\beta^\alpha u_j^n - D \left(\frac{\Delta x^2}{12} + C_2 \Delta x^2 \right) \nabla_\beta^{\alpha+2} u_j^n - DC_3 \Delta x^3 \nabla_\beta^{\alpha+3} u_j^n + O(\Delta x^4) \\ & + VD \Delta t \nabla_\beta^{\alpha+1} u_j^n - VD \Delta t \frac{\Delta x}{2} \nabla_\beta^{\alpha+2} u_j^n + VD \Delta t \left(\frac{\Delta x^2}{6} - C_2 \Delta x^2 \right) \nabla_\beta^{\alpha+3} u_j^n + O(\Delta t \Delta x^3) \\ & - \frac{1}{6} \left(\frac{V}{\Delta x} - V^3 \frac{\Delta t^2}{\Delta x^3} \right) \left(\Delta x^3 \frac{\partial^3 u_j^n}{\partial x^3} - \frac{\Delta x^4}{2} \frac{\partial^4 u_j^n}{\partial x^4} \right) + O(\Delta t^2 \Delta x^2) + O(\Delta x^4) = 0. \end{aligned}$$

Therefore, the modified equation is given by

$$\begin{aligned} & \frac{\partial u_j^n}{\partial t} + V \frac{\partial u_j^n}{\partial x} - D \nabla_\beta^\alpha u_j^n + \frac{\Delta t}{2} \frac{\partial^2 u_j^n}{\partial t^2} - \frac{V^2 \Delta t}{2} \frac{\partial^2 u_j^n}{\partial x^2} + VD \Delta t \nabla_\beta^{\alpha+1} u_j^n \\ & + \frac{\Delta t^2}{6} \frac{\partial^3 u_j^n}{\partial t^3} + \frac{1}{6} V^3 \Delta t^2 \frac{\partial^3 u_j^n}{\partial x^3} - D \left(\frac{\Delta x^2}{12} + C_2 \Delta x^2 + V \Delta t \frac{\Delta x}{2} \right) \nabla_\beta^{\alpha+2} u_j^n \\ & + \frac{\Delta t^3}{24} \frac{\partial^4 u_j^n}{\partial t^4} + \left(\frac{V \Delta x^3}{12} - V^3 \frac{\Delta t^2 \Delta x}{12} - \frac{V^2 \Delta t \Delta x^2}{24} \right) \frac{\partial^4 u_j^n}{\partial x^4} \\ & - DC_3 \Delta x^3 \nabla_\beta^{\alpha+3} u_j^n + VD \Delta t \left(\frac{\Delta x^2}{6} - C_2 \Delta x^2 \right) \nabla_\beta^{\alpha+3} u_j^n + \sum_{p+q=4} O(\Delta x^p \Delta t^q) = 0. \end{aligned}$$

The modified equation presents an expression for the truncation error. However this is not the desired form since we do not want the truncation error in terms of the derivatives in time. Therefore, similarly to what is done in [30], we use the modified equation itself to eliminate the time derivatives. After some extensive and direct calculations we obtain

$$\frac{\partial u_j^n}{\partial t} + V \frac{\partial u_j^n}{\partial x} - D \nabla_\beta^\alpha u_j^n + T_j^n = 0, \tag{53}$$

where the modification T_j^n satisfies

$$\begin{aligned} T_j^n &= \frac{1}{12} (-D \Delta x^2 - 12C_2 D \Delta x^2 - 6VD \Delta t \Delta x + 6V^2 D \Delta t^2 \Delta x) \nabla_\beta^{\alpha+2} u_j^n \\ &+ \frac{1}{24} (2V \Delta x^3 - 2V^3 \Delta x \Delta t^2 - V^2 \Delta t \Delta x^2 + V^4 \Delta t^3) \frac{\partial^4 u}{\partial x^4} u_j^n + \frac{1}{2} D^2 \Delta t \nabla_\beta^\alpha (\nabla_\beta^\alpha u_j^n) \\ &+ \frac{1}{6} (-6DC_3 \Delta x^3 - 12C_2 VD \Delta t \Delta x^2 - 3V^2 D \Delta t^2 \Delta x + 2V^3 D \Delta t^3) \nabla_\beta^{\alpha+3} u_j^n \\ &+ \dots \end{aligned} \tag{54}$$

From the previous equality we can write the expression for $\Delta t T_j^n$ in terms of μ_α and ν ,

$$\begin{aligned} \Delta t T_j^n &= \frac{\Delta x^{\alpha+2}}{12} (-\mu_\alpha - 12C_2 \mu_\alpha - 6\nu \mu_\alpha + 6\nu^2 \mu_\alpha) \nabla_\beta^{\alpha+2} u_j^n \\ &+ \frac{\Delta x^4}{24} (2\nu - 2\nu^3 - \nu^2 + \nu^4) \frac{\partial^4 u}{\partial x^4} u_j^n + \frac{\Delta x^{2\alpha}}{2} \mu_\alpha^2 \nabla_\beta^\alpha (\nabla_\beta^\alpha u_j^n) \\ &+ \frac{\Delta x^{\alpha+3}}{6} (-6C_3 \mu_\alpha - 12C_2 \nu \mu_\alpha - 3\nu^2 \mu_\alpha + 2\nu^3 \mu_\alpha) \nabla_\beta^{\alpha+3} u_j^n + \dots \quad \square \end{aligned} \tag{55}$$

Note that, the leading terms of the truncation error are given by

$$\begin{aligned} \Delta t T_j^n &= \frac{1}{12} \Delta x^{\alpha+2} (6\nu^2 \mu_\alpha - 6\nu \mu_\alpha - \mu_\alpha - 12C_2 \mu_\alpha) \nabla_\beta^{\alpha+2} u^n(x_j) \\ &+ \frac{1}{24} \Delta x^4 \nu (2 - \nu) (1 - \nu^2) \frac{\partial^4 u^n}{\partial x^4}(x_j) + \frac{1}{2} \Delta x^{2\alpha} \mu_\alpha^2 \nabla_\beta^\alpha (\nabla_\beta^\alpha u^n)(x_j) + \dots \end{aligned} \tag{56}$$

Observing the truncation error, over a finite interval of time, these estimates tell us that the order of the truncation error are sensitive to the values of ν and μ_α considered. The values of ν and μ_α vary depending on how we choose Δt depending on Δx . Additionally, for explicit schemes, the time step and the space step need to be related to each other as we refine the mesh, not only for accuracy purposes but also in order to have convergence of the numerical method, since we need to be inside the stability region. In general, we expect the numerical method to behave between $O(\Delta x^2)$ and $O(\Delta x^3)$. For advection-dominated problems we expect to be closer to $O(\Delta x^3)$. This follows from observing that as D goes to zero, μ_α goes to zero. Therefore, the truncation error is dominated by the second term on the right hand side of (56). From this term and for $\Delta t = O(\Delta x)$ we can easily see that we get a behavior closer to $O(\Delta x^3)$.

We also note that for $\alpha = 2$, $C_2 = 0$ and the truncation error (56) matches the one reported for the classical QUICKEST in works such as [18,25] and given by

$$\Delta t T_j^n = \frac{1}{24} \Delta x^4 (12\mu^2 - 2\mu - 12\mu\nu(1-\nu) + \nu(2-\nu)(1-\nu^2)) \frac{\partial^4 u^n}{\partial x^4}(x_j) + \dots, \tag{57}$$

for $\mu = D\Delta t/\Delta x^2$.

3.2. Stability analysis

For a set of discrete values, the global error (41) can be written in the matricial form

$$E^{n+1} = \mathbf{P}E^n + \Delta t T^n, \tag{58}$$

where \mathbf{P} is the matrix containing the coefficients of the difference formulas and T^n the truncation error. By applying this equality recursively, we obtain

$$E^{n+1} = \mathbf{P}^{n+1}E^0 + \Delta t \sum_{k=0}^n \mathbf{P}^k T^{n-k}. \tag{59}$$

Then a global error bound, for any chosen norm $\|\cdot\|$, is given by

$$\|E^{n+1}\| \leq \|\mathbf{P}^{n+1}\| \|E^0\| + \Delta t \sum_{k=0}^n \|\mathbf{P}^k\| \|T^{n-k}\|, \tag{60}$$

that is,

$$\|E^{n+1}\| \leq \|\mathbf{P}^{n+1}\| \|E^0\| + (n+1)\Delta t \max_{0 \leq k \leq n} \|\mathbf{P}^k\| \|T^{n-k}\|. \tag{61}$$

If $\|\mathbf{P}\|$ is a matrix such that $\|\mathbf{P}^n\| \leq K$, for $0 < n\Delta t < T_0$, then we have practical stability and the error bound is given by

$$\|E^n\| \leq K \|E^0\| + n\Delta t K \max_{0 \leq k \leq n-1} \|T^{n-k}\|. \tag{62}$$

In order to derive stability conditions for the finite difference schemes, we apply the von Neumann analysis or Fourier analysis. Note that the numerical method is von Neumann stable if and only if the operator \mathbf{P} is bounded in the l_2 norm [24]. Of course one of the conditions for which the method becomes unstable is if the spectrum of \mathbf{P} is larger than one. For the special cases when \mathbf{P} is a normal matrix, both conditions are equivalent.

Fourier analysis assumes that we have a solution defined in the whole real line. If u_j^n is the exact solution $u(x_j, t_n)$, let U_j^n be a perturbation of u_j^n . The perturbation error

$$e_j^n = U_j^n - u_j^n \tag{63}$$

will be propagated forward in time according to the equation

$$e_j^{n+1} = e_j^n - \nu \Delta_0 e_j^n + \mu_\alpha \delta_\beta^\alpha e_j^n + \frac{1}{2} \nu^2 \delta^2 e_j^n - \nu \mu_\alpha \delta_\beta^{\alpha+1} e_j^n + \frac{1}{6} (\nu - \nu^3) \delta^2 \Delta_- e_j^n. \tag{64}$$

The von Neumann analysis assumes the error e_j^n will be decomposed into a Fourier series with terms given by $\kappa_p^n e^{i\xi_p(j\Delta x)}$, where κ_p^n is the amplitude of the p -th harmonic. The parameter $\theta = \xi_p \Delta x$ is called the phase angle and covers the domain $[-\pi, \pi]$.

Considering a single mode $\kappa^n e^{ij\theta}$, its time evolution is determined by the same numerical scheme as the error e_j^n . Hence inserting a representation of this form into a numerical scheme we obtain stability conditions. The stability conditions will be satisfied if the amplification factor κ does not grow in time, that is, if we have $|\kappa(\theta)| \leq 1$, for all θ .

Theorem 5. A necessary condition for stability of the numerical method (31) is given by

$$0 \leq v^2 + \frac{2}{3}v(1 - v^2) + s_\alpha(1 - 2v) \leq 1, \tag{65}$$

for

$$s_\alpha = -\frac{\mu_\alpha}{2\Gamma(4 - \alpha)} \sum_{m=-1}^{\infty} (-1)^m q_m.$$

Proof. We denote by $\kappa_\beta(\theta; v, \mu_\alpha)$ the amplification factor since it will depend on μ_α and β . If we insert $\kappa_\beta^n e^{ij\theta}$ in (64) we obtain the equality for the amplification factor

$$\begin{aligned} \kappa_\beta(\theta; v, \mu_\alpha) = & 1 - \frac{v}{2}(e^{i\theta} - e^{-i\theta}) \frac{\mu_\alpha}{\Gamma(4 - \alpha)} \left[\frac{1}{2}(1 + \beta) \sum_{m=-1}^{\infty} q_m e^{-im\theta} + \frac{1}{2}(1 - \beta) \sum_{m=-1}^{\infty} q_m e^{im\theta} \right] \\ & + \frac{1}{2}v^2(e^{i\theta} - 2 + e^{-i\theta}) + \frac{1}{6}(v - v^3)(e^{i\theta} - 3 + 3e^{-i\theta} - e^{-i2\theta}) \\ & - \frac{v\mu_\alpha}{\Gamma(4 - \alpha)} \left\{ \frac{1}{2}(1 + \beta) \left[q_{-1}e^{i\theta} + \sum_{m=0}^{\infty} (q_m - q_{m-1})e^{-im\theta} \right] \right. \\ & \left. - \frac{1}{2}(1 - \beta) \left[q_{-1}e^{-i2\theta} + \sum_{m=0}^{\infty} (q_m - q_{m-1})e^{i(m-1)\theta} \right] \right\} \end{aligned} \tag{66}$$

that is,

$$\begin{aligned} \kappa_\beta(\theta; v, \mu_\alpha) = & 1 - iv \sin \theta + \frac{\mu_\alpha}{\Gamma(4 - \alpha)} \left[\sum_{m=-1}^{\infty} q_m \cos(m\theta) - i\beta \sum_{m=-1}^{\infty} q_m \sin(m\theta) \right] \\ & + v^2(\cos \theta - 1) + \frac{1}{6}(v - v^3)(4 \cos \theta - 3 - 2i \sin(\theta) - \cos(2\theta) + i \sin(2\theta)) \\ & - \frac{1}{2} \frac{v\mu_\alpha}{\Gamma(4 - \alpha)} \left\{ q_{-1}(e^{i\theta} - e^{-i2\theta}) + \sum_{m=0}^{\infty} (q_m - q_{m-1})(e^{-im\theta} - e^{-i(m-1)\theta}) \right. \\ & \left. + \beta \left(q_{-1}(e^{i\theta} + e^{-i2\theta}) + \sum_{m=0}^{\infty} (q_m - q_{m-1})(e^{-im\theta} + e^{-i(m-1)\theta}) \right) \right\}. \end{aligned}$$

The amplification factor will not depend on β for $\theta = \pi$. For $\theta = \pi$ we have

$$\begin{aligned} \kappa_\beta(\pi; v, \mu_\alpha) = & 1 + \frac{\mu_\alpha}{\Gamma(4 - \alpha)} \left[\sum_{m=-1}^{\infty} q_m (-1)^m \right] - 2v^2 - \frac{4}{3}(v - v^3) \\ & - \frac{v\mu_\alpha}{\Gamma(4 - \alpha)} \left\{ -q_{-1} + \sum_{m=0}^{\infty} (q_m - q_{m-1})(-1)^m \right\}. \end{aligned}$$

We can write,

$$\kappa_\beta(\pi; v, \mu_\alpha) = 1 + \frac{\mu_\alpha}{\Gamma(4 - \alpha)} \left[\sum_{m=-1}^{\infty} (-1)^m q_m \right] - 2v^2 - \frac{4}{3}(v - v^3) - 2 \frac{v\mu_\alpha}{\Gamma(4 - \alpha)} \sum_{m=-1}^{\infty} (-1)^m q_m.$$

Set

$$s_\alpha = -\frac{\mu_\alpha}{2\Gamma(4 - \alpha)} \sum_{m=-1}^{\infty} (-1)^m q_m.$$

Note that $s_\alpha \geq 0$. Hence,

$$\kappa_\beta(\pi; v, \mu_\alpha) = 1 - 2s_\alpha(1 - 2v) - 2v^2 - \frac{4}{3}v(1 - v^2).$$

For $|\kappa_\beta(\pi; v, \mu_\alpha)| \leq 1$ we have

$$-1 \leq 1 - 2s_\alpha(1 - 2v) - 2v^2 - \frac{4}{3}v(1 - v^2) \leq 1$$

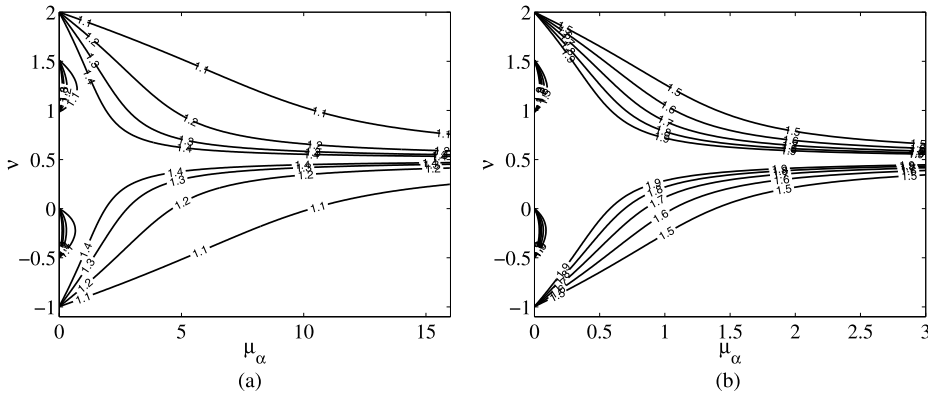


Fig. 1. Theoretical stability condition (65); (a) Contour plots for $\alpha = 1.1, 1.2, 1.3, 1.4$. (b) Contour plots for $\alpha = 1.5, 1.6, 1.7, 1.8, 1.9$.

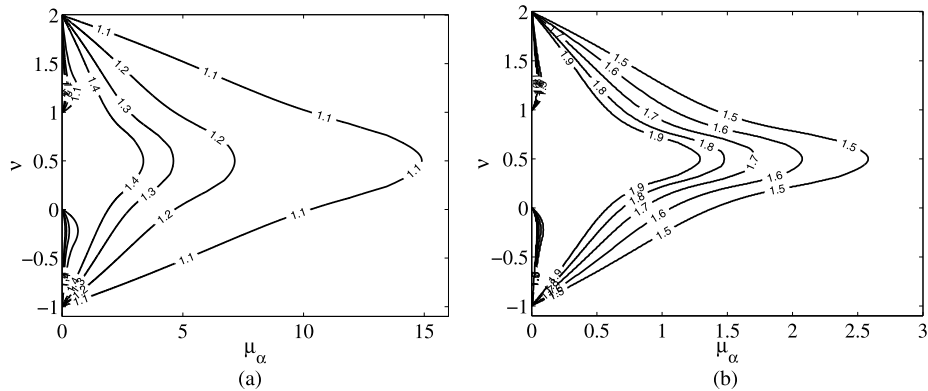


Fig. 2. Stability region for $\beta = 0$; (a) Contour plots for $\alpha = 1.1, 1.2, 1.3, 1.4$. (b) Contour plots for $\alpha = 1.5, 1.6, 1.7, 1.8, 1.9$.

that is,

$$0 \leq v^2 + \frac{2}{3}v(1 - v^2) + s_\alpha(1 - 2v) \leq 1$$

and we have (65). After direct calculations we can also rewrite the previous inequalities as

$$-\frac{2v}{3 - 2v} \leq v^2 + 3s_\alpha \frac{1 - 2v}{3 - 2v} \leq 1. \quad \square$$

We have obtained analytical necessary stability conditions, for all β and α . To obtain necessary and sufficient stability conditions, for all values of β and α , we determine computationally the values v and μ_α , for which the amplification factor verifies

$$|\kappa_\beta(\theta; v, \mu_\alpha)| \leq 1 \quad \text{for all } \theta \in [-\pi, \pi]. \tag{67}$$

We show the results for different values of β and α .

We start to plot in Fig. 1, for some values of α , the analytical necessary stability condition (65) proved in Theorem 5. Note that this condition is necessary for all values of β . In Fig. 2 we show the necessary and sufficient stability conditions for $\beta = 0$ and different values of α by computing numerically condition (67), where the amplification factor $\kappa_\beta(\theta; v, \mu_\alpha)$ is given by (66). Note that for this case, the analytical necessary stability condition (65) plotted in Fig. 1 is very sharp when compared with the necessary and sufficient conditions displayed in Fig. 2.

Similarly in Fig. 3, we present the necessary and sufficient conditions determined numerically for the case when $\beta = 1$, which is the other case that appears very frequently in many applications, where the model only considers the left fractional derivative.

In Fig. 4 we present the case for $\beta = -1$. Comparing with the case $\beta = 1$ we see the two regions, represented in Fig. 3 and Fig. 4 respectively, have some kind of antisymmetry.

We end this section by showing what happens in two more cases, $\beta = 0.5$ and $\beta = -0.5$ presented in Figs. 5 and 6 respectively. We also observe the two stability regions have the same type of asymmetric relation that we have seen between the cases $\beta = 1$ and $\beta = -1$.

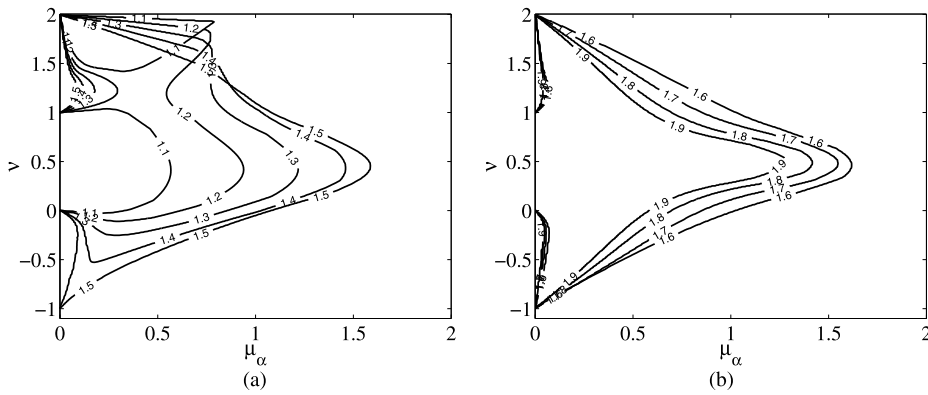


Fig. 3. Stability region for $\beta = 1$; (a) Contour plots for $\alpha = 1.1, 1.2, 1.3, 1.4, 1.5$. (b) Contour plots for $\alpha = 1.6, 1.7, 1.8, 1.9$.

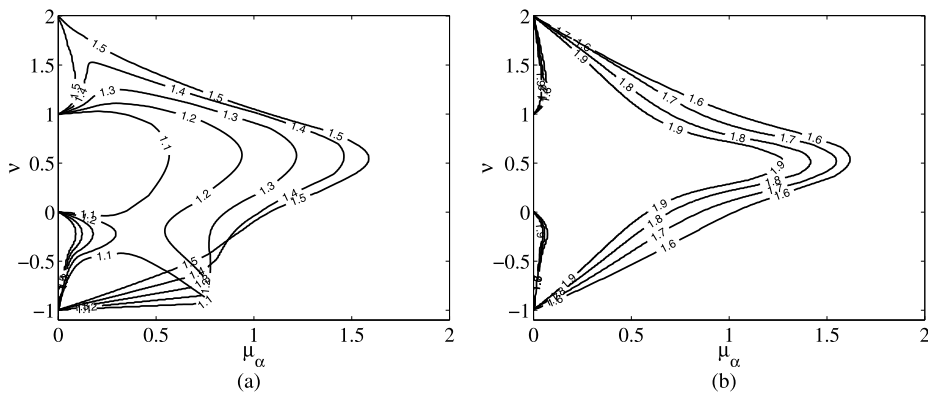


Fig. 4. Stability region for $\beta = -1$; (a) Contour plots for $\alpha = 1.1, 1.2, 1.3, 1.4, 1.5$. (b) Contour plots for $\alpha = 1.6, 1.7, 1.8, 1.9$.

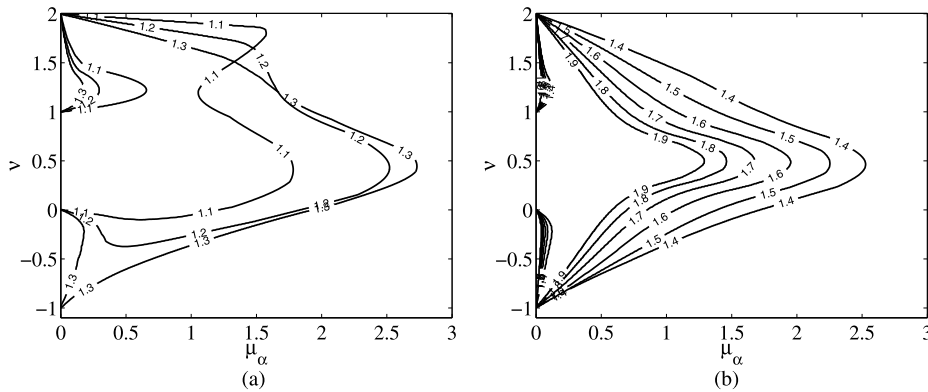


Fig. 5. Stability regions for $\beta = 0.5$; (a) Contour plots for $\alpha = 1.1, 1.2, 1.3$. (b) Contour plots for $\alpha = 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9$.

The results in Figs. 2–6 show that the regions for α larger than 1.4 are similar in shape and the region increases as α decreases. For smaller values of α the stability regions have more irregular shapes. We see the stability regions are quite wide in general for all values of β and α . A region for which the numerical method is in general stable for all values of β and α is the squared region for which $0 \leq \nu \leq 1$ and $0 \leq \mu_\alpha \leq 1/2$.

4. Numerical results

In this section we present some numerical tests to show the convergence order of the numerical method by considering the l_2 error, for an instant of time $t = n\Delta t$, given by

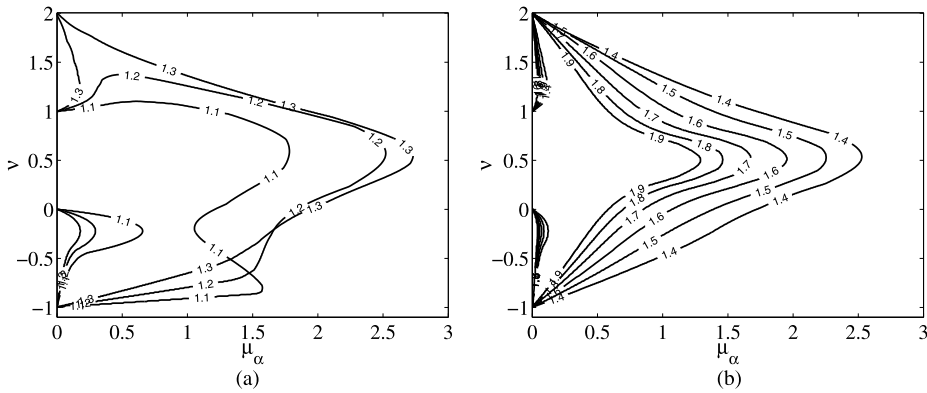


Fig. 6. Stability regions for $\beta = -0.5$; (a) Contour plots for $\alpha = 1.1, 1.2, 1.3$. (b) Contour plots for $\alpha = 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9$.

Table 1
 l_2 error (68) and l_∞ error (69) at $t = 1$, for $\nu = 0.001$ and $V = 5$ and $D = 0.01$.

	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$	$\alpha = 2$
l_2	0.05	5.4701e-5	5.4215e-5	5.3737e-5	5.3480e-5	5.4051e-5
	0.005	3.8768e-8	3.3831e-8	2.8445e-8	2.4457e-8	3.3899e-8
	Rate	3.14	3.20	3.27	3.33	3.20
l_∞	0.05	1.2712e-4	1.2583e-4	1.2438e-4	1.2295e-4	1.2231e-4
	0.005	2.1012e-7	1.9520e-7	1.7163e-7	1.2442e-7	5.9744e-8
	Rate	2.78	2.80	2.86	2.99	3.31

$$\|u - U\|_2 = \left(\Delta x \sum_j |u(x_j, t) - U_j^n|^2 \right)^{1/2}. \tag{68}$$

We also present the l_∞ error given by

$$\|u - U\|_\infty = \max_j |u(x_j, t) - U_j^n|. \tag{69}$$

A large number of applications consider the model problem for $\beta = 0$ and $\beta = 1$ and therefore we give special attention to these cases. We will present examples dominated by advection.

For the first example we assume $\beta = 1$ in Eq. (1), that is, we have the equation

$$\frac{\partial u}{\partial t} + V \frac{\partial u}{\partial x} = D \frac{\partial^\alpha u}{\partial x^\alpha} + S(x, t),$$

in the domain $0 \leq x \leq 1$. We assume the problem has initial condition $u(x, 0) = x^4$ and boundary conditions $u(0, t) = 0, u(1, t) = e^{-t}$. Let

$$S(x, t) = e^{-t} x^3 \left(4V - x - \frac{24D}{\Gamma(5 - \alpha)} x^{1-\alpha} \right).$$

The exact solution is given by $u(x, t) = e^{-t} x^4$.

For this problem, since we only include the left fractional derivative, the numerical method (31) can be written as

$$U_j^{n+1} = U_j^n - \nu \Delta_0 U_j^n + \mu_\alpha \delta_l^\alpha U_j^n + \frac{1}{2} \nu^2 \delta^2 U_j^n - \nu \mu_\alpha \delta_l^{\alpha+1} U_j^n + \frac{1}{6} (\nu - \nu^3) \delta^2 \Delta_- U_j^n + \Delta t \tilde{S}_j^n, \tag{70}$$

with the operators δ_l^α and $\delta_l^{\alpha+1}$ defined respectively by (34) and (37).

In Table 1 and Table 2 we present the l_2 error, for the instant of time $t = 1$, which shows that the numerical method has between second and third order convergence as predicted by the error analysis presented in Section 3. We can also see that the order of convergence is sensitive to the variations of the parameters ν and μ_α involved in the numerical method. The l_∞ error is also shown for additional information.

The results shown in Table 1 and Table 2 are obtained by considering the Courant number $\nu = V \Delta t / \Delta x$ constant and therefore, the time-step is chosen to be $\Delta t = O(\Delta x)$. Since the stability regions are defined by the values of ν and μ_α , we have chosen a value of ν for which we can run the experiments for different values of α, V and D and still be inside the stability region.

Table 2
 l_2 error (68) and l_∞ error (69) at $t = 1$, for $\nu = 0.001$ and $V = 2$ and $D = 0.02$.

	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$	$\alpha = 2$
l_2	0.05	5.2873e-5	5.0118e-5	4.7408e-5	4.6029e-5	4.9564e-5
	0.005	5.8782e-8	8.4323e-7	1.1249e-7	1.3097e-7	8.6496e-8
	Rate	2.95	2.77	2.62	2.54	2.75
l_∞	0.05	1.2392e-4	1.1654e-4	1.0856e-4	1.0179e-4	1.0140e-4
	0.005	2.4250e-7	2.6386e-7	2.5518e-7	4.1236e-7	6.0782e-7
	Rate	2.70	2.64	2.62	2.39	2.22

Table 3
 l_2 error (68) and l_∞ error (69) at $t = 1$, for $\nu = 0.001$ and $V = 2$, $D = 0.001$.

	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$	$\alpha = 2$
l_2	0.05	1.1306e-4	1.1285e-4	1.1263e-4	1.1250e-4	1.1284e-4
	0.005	1.3253e-7	1.7211e-7	2.1050e-7	2.3131e-7	2.4336e-7
	Rate	2.93	2.81	2.72	2.68	2.66
l_∞	0.05	1.4802e-4	1.4772e-4	1.4767e-4	1.4833e-4	1.5047e-4
	0.005	1.7179e-7	2.2956e-7	2.7859e-7	3.0100e-7	2.8221e-7
	Rate	2.93	2.80	2.72	2.69	2.72

Table 4
 l_2 error (68) and l_∞ error (69) at $t = 1$, for $\nu = 0.001$ and $V = 0.2$ $D = 0.0001$.

	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$	$\alpha = 2$
l_2	0.05	1.8897e-4	1.8850e-4	1.8785e-4	1.8719e-4	1.8705e-4
	0.005	2.1113e-7	2.4432e-7	2.9395e-7	3.5927e-7	4.4004e-7
	Rate	2.95	2.88	2.80	2.71	2.62
l_∞	0.05	2.0311e-4	2.0256e-4	2.0182e-4	2.0107e-4	2.0093e-4
	0.005	2.5147e-7	3.0585e-7	3.6768e-7	4.3841e-7	5.2444e-7
	Rate	2.90	2.82	2.73	2.66	2.58

The second example considers Eq. (1) for $\beta = 0$, that is, we have the equation

$$\frac{\partial u}{\partial t} + V \frac{\partial u}{\partial x} = \frac{D}{2} \left(\frac{\partial^\alpha u}{\partial x^\alpha} + \frac{\partial^\alpha u}{\partial (-x)^\alpha} \right) + S(x, t),$$

in the domain $0 \leq x \leq 2$. We assume the initial condition is $u(x, 0) = x^4(2 - x)^4$ and the boundary conditions are $u(0, t) = 0$, $u(2, t) = 0$. Let

$$S(x, t) = e^{-t} \left[-x^4(2 - x)^4 + 8Vx^3(2 - x)^3(1 - x) - \frac{D}{2} \sum_{p=0}^4 (-1)^p 2^{4-p} \binom{4}{p} \frac{\Gamma(p + 5)}{\Gamma(p + 5 - \alpha)} (x^{p+4-\alpha} + (2 - x)^{p+4-\alpha}) \right].$$

The exact solution is given by $u(x, t) = e^{-t}x^4(2 - x)^4$.

For this problem the numerical method includes the left and right fractional derivatives and can be written as

$$U_j^{n+1} = U_j^n - \nu \Delta_0 U_j^n + \frac{1}{2} \mu_\alpha (\delta_l^\alpha U_j^n + \delta_r^\alpha U_j^n) + \frac{1}{2} \nu^2 \delta^2 U_j^n - \frac{1}{2} \nu \mu_\alpha (\delta_l^{\alpha+1} U_j^n + \delta_r^{\alpha+1} U_j^n) + \frac{1}{6} (\nu - \nu^3) \delta^2 \Delta_- U_j^n + \Delta t \tilde{S}_j^n, \tag{71}$$

where the operator δ_l^α , δ_r^α and $\delta_l^{\alpha+1}$, $\delta_r^{\alpha+1}$ are defined respectively by (34), (35) and (37), (38).

In Table 3, Table 4 and Table 5 we present the error values for different values of V and D . In Table 3 we show the results for $V = 2$ and $D = 0.001$ and in Table 4 for $V = 0.2$ and $D = 0.0001$, where V is smaller than the one considered in Table 3, although we have also considered a smaller diffusion term. In Table 5 we present the results for $V = 5$, $D = 0.0001$. In this case the advection term is even more dominant. Note also that the error for different values of α is similar. This is due to the fact that, for this case the parameter D is very small and therefore the value μ_α it will be very small compared with values of ν .

The results shown in Table 3, Table 4 and Table 5 are obtained by considering the Courant number $\nu = V \Delta t / \Delta x$ constant and therefore the time-step is chosen to be $\Delta t = O(\Delta x)$ similarly to what has been done in the previous example.

Table 5 l_2 error (68) and l_∞ error (69) at $t = 1$, for $\nu = 0.001$ and $V = 5$ $D = 0.0001$.

	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$	$\alpha = 2$
l_2	0.05	1.1100e-4	1.1099e-4	1.1098e-4	1.1097e-4	1.1097e-4
	0.005	1.1208e-7	1.1276e-7	1.1366e-7	1.1477e-7	1.1614e-7
	Rate	2.99	2.99	2.98	2.98	2.98
l_∞	0.05	1.2168e-4	1.2167e-4	1.2166e-4	1.2164e-4	1.2163e-4
	0.005	1.2243e-7	1.2447e-7	1.2626e-7	1.2727e-7	1.2777e-7
	Rate	2.99	2.99	2.98	2.98	2.97

We observe that in all the cases, the order of convergence varies between two and three as predicted by the previous error analysis and it is closer to three when the advection term is more dominant.

5. Final remarks

We have derived an explicit numerical method whose order of convergence varies between two and three, depending on the diffusion parameter μ_α and the Courant number ν . This result was predicted using a truncation error analysis and was also corroborated by numerical results. In particular, for advection dominated problems the order of convergence is expected to be more close to three. The stability region of the numerical method depends on the values of α and β , although for all values of α and β there is a common stability region. Finally, note that this numerical method, for $\alpha = 2$, coincides with the popular QUICKEST scheme introduced in [16] for advection diffusion problems.

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