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A finite volume method for solving the two-sided time-space fractional advection-dispersion equation

Editorial

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Abstract: We present a finite volume method to solve the time-space two-sided fractional advection-dispersion equation on a one-dimensional domain. The spatial discretisation employs fractionally-shifted Grünwald formulas to discretise the Riemann-Liouville fractional derivatives at control volume faces in terms of function values at the nodes. We demonstrate how the finite volume formulation provides a natural, convenient and accurate means of discretising this equation in conservative form, compared to using a conventional finite difference approach. Results of numerical experiments are presented to demonstrate the effectiveness of the approach.

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1. Introduction

In recent times, the use of fractional partial differential equations to model transport processes has become popular among scientists, engineers and mathematicians. This surge in popularity is due to the growing number of real-world applications whose dynamics have been found to be more ably described by fractional models than by traditional integer-order models.

Fractional derivatives are a natural tool for modelling non-Fickian diffusion or dispersion processes, that is, processes exhibiting anomalous diffusion. The theoretical grounding is well established – Metzler and Klafter [7] show how fractional diffusion equations arise from continuous time random walk models with diverging characteristic waiting times and jump length variances. Particle transport in heterogeneous porous media is a well-known application where anomalous diffusion is observed. Zhang et al. [26] review many of the fractional models in this area, and describe several experiments where anomalous diffusion has been observed in the field.

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In this paper, we consider the following two-sided time-space fractional advection-dispersion equation with variable coefficients:

$$D_t^{\gamma}C(x,t) + \frac{\partial}{\partial x}(V(x,t)C(x,t)) = \\ \frac{\partial}{\partial x}\left[K(x,t)\left(\beta\frac{\partial^{\alpha}C}{\partial x^{\alpha}} - (1-\beta)\frac{\partial^{\alpha}C}{\partial(-x)^{\alpha}}\right)\right] + S(x,t) \tag{1}$$

on the interval $[a, b]$, subject to homogeneous Dirichlet boundary conditions. In the context of particle transport, $C(x, t)$ represents the concentration of particles at position x and time t. The symbol $D_t^{\gamma}C(x,t)$ represents the Caputo fractional derivative of order γ.

Definition 1. (Caputo fractional derivative on $[0, \infty)$) [15]

$$D_t^{\gamma}C(x,t) = \begin{cases} \frac{1}{\Gamma(1-\gamma)}\int_0^t \frac{\partial C(x,\eta)}{\partial \eta}(t-\eta)^{-\gamma}d\eta, & 0 < \gamma < 1, \\ \frac{\partial}{\partial t}C(x,t), & \gamma = 1\,. \end{cases}$$

The symbols $\partial^{\alpha}C/\partial x^{\alpha}$ and $\partial^{\alpha}C/\partial(-x)^{\alpha}$ represent the left and right Riemann-Liouville fractional derivatives of order α.

Definition 2. (Riemann-Liouville fractional derivatives on $[a, b]$) [15]

$$\frac{\partial^{\alpha}C(x,t)}{\partial x^{\alpha}} = \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_a^x \frac{C(\xi,t)}{(x-\xi)^{\alpha+1-n}}d\xi, \tag{2}$$

$$\frac{\partial^{\alpha}C(x,t)}{\partial(-x)^{\alpha}} = \frac{(-1)^n}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_x^b \frac{C(\xi,t)}{(\xi-x)^{\alpha+1-n}}d\xi, \tag{3}$$

where n is the smallest integer greater than or equal to α.

In this paper we consider regimes where $0 < \gamma \leq 1$ and $0 < \alpha \leq 1$. The inclusion of the skewness $\beta \in [0, 1]$ in equation (1) allows for modelling of regimes where the forward and backward jump probabilities are different [6]. The remaining components of equation (1) are the velocity $V(x, t)$, the anomalous dispersion coefficient $K(x, t) > 0$ and the source term $S(x, t)$.

The literature on numerical methods for solving fractional differential equations is not as well-developed as for integer-order equations. Finite difference methods have dominated the literature. The L1 scheme [13] and variations thereof have formed the basis for many finite difference discretisations of Caputo time fractional derivatives, such as the widely used method of Lin and Xu [3].

In space too, finite difference methods have proved very popular. The pioneering work of Meerschaert et al. [4–6, 20] laid the groundwork for many of the popular finite difference discretisations for space-fractional derivatives. These are based on the equivalence of Riemann-Liouville and Grünwald-Letnikov fractional derivatives (for sufficiently smooth functions). The Grünwald-Letnikov definition is preferred numerically because it lends itself naturally to discretisation in a finite difference sense. A crucial observation was the necessity of using shifted formulas to ensure stability of these numerical schemes [5].

Many of these methods have since been generalised and extended in various ways, leading to non-standard finite difference schemes [8–10], finite difference schemes for problems of variable fractional order [17–19, 27] and "fast" finite difference schemes [11, 12, 14, 21, 22] to name a few.

Other numerical methods have received less attention in the literature to date. The literature on finite volume methods for fractional partial differential equations in particular is still in early stages of development. A finite volume method for the space fractional advection-dispersion equation was proposed by Zhang et al. [24, 25], who chose to discretise the Riemann-Liouville derivatives directly, rather than use the Grünwald-Letnikov definition.

Previously we have considered a finite volume method for the two-sided space-fractional advection-dispersion equation with constant coefficients [1], based on the Grünwald-Letnikov definition, where we proved the stability and convergence of the method. In this paper, we extend the method to solve the two-sided time-space fractional advection-dispersion equation with variable coefficients. Additionally we derive a new result concerning the relationship between the finite difference method and the finite volume method in the constant coefficient case. We also demonstrate the improvement in accuracy provided by the finite volume method over the finite difference method for a given test problem.

The remainder of the paper is organised as follows. In section 2 we derive equation (1) from conservation principles. In section 3 we derive the new finite volume method for (1) and also make comparisons between it and the finite difference method in the constant coefficient case. In section 4 we illustrate the method's performance on test problems. Finally, we draw our conclusions in section 5.

2. Derivation

The derivation of the advection-dispersion equation, whether standard or fractional, begins with the law of mass conservation which, in conservative form, is

$$\frac{\partial C}{\partial t} = -\frac{\partial Q}{\partial x} + S(x,t) \tag{4}$$

where Q is the flux. The flux comprises two components:

$$Q(x,t) = V(x,t)C(x,t) + q(x,t), \tag{5}$$

the advective component is $V(x,t)C(x,t)$ and the dispersive component is denoted $q(x,t)$. For standard diffusion or dispersion, where Fick's law applies, the form of the dispersive flux $q(x,t)$ is

$$q(x,t) = -K(x,t)\frac{\partial C}{\partial x}$$

where K is the dispersion coefficient. Substituting this form of q into (5) and returning to (4), the standard advection-diffusion equation

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(V(x,t)C(x,t)) = \frac{\partial}{\partial x}\left[K(x,t)\frac{\partial C}{\partial x}\right] + S(x,t) \tag{6}$$

is derived. In the special case of constant velocity and dispersion coefficient, we may write (6) as

$$\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial x} = K\frac{\partial^2 C}{\partial x^2} + S(x,t)\,. \tag{7}$$

2.1. Space-fractional derivatives

Fick's law is equivalent to the assumption of Brownian motion at the particle scale [7]. In complex heterogeneous media this assumption may not be reasonable, and instead an alternative law that allows for diverging jump length variances ("long jumps") and unequal forward and backward jump probabilities at the particle scale is required. The fractional Fick's law [2]

$$q(x,t) = -K(x,t)\left(\beta\frac{\partial^\alpha C(x,t)}{\partial x^\alpha} - (1-\beta)\frac{\partial^\alpha C(x,t)}{\partial(-x)^\alpha}\right)$$

incorporates both of these aspects. Substituting this form of q into (5) and returning to (4) we derive a two-sided space-fractional advection-dispersion equation

$$\begin{aligned}&\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(V(x,t)C(x,t)) = \\ &\quad\frac{\partial}{\partial x}\left[K(x,t)\left(\beta\frac{\partial^\alpha C}{\partial x^\alpha} - (1-\beta)\frac{\partial^\alpha C}{\partial(-x)^\alpha}\right)\right] + S(x,t)\,.\end{aligned} \tag{8}$$

An interesting aspect of this equation is the minus sign in front of the right Riemann-Liouville derivative. To confirm that this sign is appropriate, we consider the case of constant velocity V and dispersion coefficient K and show that the fractional-order model (8) recovers (7) in the integer-order limit $\alpha = 1$.

Applying Definition 2, the first term on the right of (8) may be written as

$$\begin{aligned}\frac{\partial}{\partial x}\Bigg[K\Bigg(&\beta\frac{1}{\Gamma(1-\alpha)}\frac{\partial}{\partial x}\int_a^x \frac{C(\xi,t)}{(x-\xi)^\alpha}d\xi\Bigg) \\ &- (1-\beta)\frac{(-1)}{\Gamma(1-\alpha)}\frac{\partial}{\partial x}\int_x^b \frac{C(\xi,t)}{(\xi-x)^\alpha}d\xi\Bigg)\Bigg]\,.\end{aligned}$$

Combining the derivatives and letting $\nu = \alpha + 1$, we obtain

$$K\left[\beta \frac{1}{\Gamma(2-\nu)} \frac{\partial^2}{\partial x^2} \int_a^x \frac{C(\xi,t)}{(x-\xi)^{\nu-1}} d\xi \right. \\ \left. + (1-\beta) \frac{(-1)^2}{\Gamma(2-\nu)} \frac{\partial^2}{\partial x^2} \int_x^b \frac{C(\xi,t)}{(\xi-x)^{\nu-1}} d\xi \right],$$

which, again with the help of Definition 2, is simply

$$K\left[\beta \frac{\partial^\nu C}{\partial x^\nu} + (1-\beta) \frac{\partial^\nu C}{\partial(-x)^\nu}\right].$$

Hence we have the space-fractional advection-dispersion equation with constant coefficients

$$\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial x} = K\left[\beta \frac{\partial^\nu C}{\partial x^\nu} + (1-\beta) \frac{\partial^\nu C}{\partial(-x)^\nu}\right] + S(x,t)\,. \tag{9}$$

In the integer limit $\nu = 2$ ($\alpha = 1$) both fractional derivatives recover the standard second-order derivative $\partial^2 C/\partial x^2$, and hence we see that (for any value of β) (9) does indeed reduce to (7) in this case.

2.2. Time-fractional derivative

The time-space fractional advection-dispersion equation (1) is obtained from (8) by replacing the first order time derivative $\partial C/\partial t$ with the Caputo time-fractional derivative $D_t^\gamma C(x,t)$ of order γ. This extension allows for the modelling of transport where the characteristic waiting times diverge ("long rests") [7]. Such is the case in strongly heterogeneous media where the trapping times have a broad distribution [26].

3. Numerical method

3.1. Derivation of finite volume method

We consider a transport domain $[a,b]$ that is discretised with $N+1$ uniformly-spaced nodes $x_i = a+ih, i = 0\dots N$, with the spatial step $h = (b-a)/N$. A finite volume discretisation is applied by integrating the governing equation over the ith control volume $[x_{i-1/2}, x_{i+1/2}]$:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial^\gamma C}{\partial t^\gamma}\, dx = -\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial Q}{\partial x}\, dx + \int_{x_{i-1/2}}^{x_{i+1/2}} S(x,t)\, dx \tag{10}$$

where the total flux is $Q = VC - q$ and the dispersive flux component q has the form derived in Section 2

$$q(x,t) = -K(x,t)\left(\beta \frac{\partial^\alpha C(x,t)}{\partial x^\alpha} - (1-\beta)\frac{\partial^\alpha C(x,t)}{\partial(-x)^\alpha}\right). \tag{11}$$

Performing the integration on the first term on the right, and interchanging the order of integration and differentiation on the other terms, we have

$$\frac{\mathrm{d}^\gamma}{\mathrm{d}t^\gamma}\int_{x_{i-1/2}}^{x_{i+1/2}} C\ dx \ = \ -\left\{Q|_{x_{i+1/2}} - Q|_{x_{i-1/2}}\right\} + \int_{x_{i-1/2}}^{x_{i+1/2}} S(x,t)\ dx\,. \tag{12}$$

This leads to the finite volume discretisation

$$\frac{\mathrm{d}^\gamma \bar{C}_i}{\mathrm{d}t^\gamma} = \frac{1}{h}\left\{Q|_{x_{i-1/2}} - Q|_{x_{i+1/2}}\right\} + \bar{S}_i \tag{13}$$

where barred quantities denote control volume averages $\bar{f}_i = 1/h\int_{x_{i-1/2}}^{x_{i+1/2}} f\ dx$.

A standard approximation is to use the nodal value in place of the control volume average. Hence we have

$$\frac{\mathrm{d}^\gamma C_i}{\mathrm{d}t^\gamma} = \frac{1}{h}\left\{Q|_{x_{i-1/2}} - Q|_{x_{i+1/2}}\right\} + S(x_i,t) \tag{14}$$

where the introduction of this approximation means that this is now an equation for the approximate numerical solution $C_i(t) \approx C(x_i,t)$ at node x_i.

To complete the spatial discretisation we require approximations for the total flux $Q|_{x_{i\pm1/2}}$ at the control volume faces. We derive these approximations by utilising the link between the Riemann-Liouville fractional derivative and the Grünwald-Letnikov fractional derivatives. Similarly to the finite difference method of Meerschaert et al. [5], the Grünwald-Letnikov derivatives must be shifted.

We first introduce the standard (non-shifted) definition for the Grünwald-Letnikov fractional derivatives.

Definition 3. (Grünwald-Letnikov fractional derivatives on $[a,b]$) [15]

$$\frac{\partial^\alpha C(x,t)}{\partial x^\alpha} = \lim_{\Delta x\to 0}\frac{1}{\Delta x^\alpha}\sum_{j=0}^{\left[\frac{x-a}{\Delta x}\right]}(-1)^j\binom{\alpha}{j}C(x-j\Delta x,t)\,, \tag{15}$$

$$\frac{\partial^\alpha C(x,t)}{\partial (-x)^\alpha} = \lim_{\Delta x\to 0}\frac{1}{\Delta x^\alpha}\sum_{j=0}^{\left[\frac{b-x}{\Delta x}\right]}(-1)^j\binom{\alpha}{j}C(x+j\Delta x,t)\,. \tag{16}$$

For sufficiently smooth functions C, the Riemann-Liouville derivatives (2), (3) and the Grünwald-Letnikov derivatives (15), (16) coincide [15, p.199]. The standard Grünwald formulas are obtained from (15) and (16) by replacing Δx with the spatial step h, yielding finite sum approximations.

Definition 4. (Grünwald formulas on $[a,b]$) [15]

$$\frac{\partial^\alpha C(x,t)}{\partial x^\alpha} \approx \frac{1}{h^\alpha}\sum_{j=0}^{\left[\frac{x-a}{h}\right]}(-1)^j\binom{\alpha}{j}C(x-jh,t)\,, \tag{17}$$

$$\frac{\partial^\alpha C(x,t)}{\partial (-x)^\alpha} \approx \frac{1}{h^\alpha}\sum_{j=0}^{\left[\frac{b-x}{h}\right]}(-1)^j\binom{\alpha}{j}C(x+jh,t)\,. \tag{18}$$

The *shifted* Grünwald formulas modify these equations by introducing a shift value.

Definition 5. (Shifted Grünwald formulas on $[a, b]$)

$$\frac{\partial^\alpha C(x,t)}{\partial x^\alpha} \approx \frac{1}{h^\alpha} \sum_{j=0}^{\left[\frac{x-a}{h}+p\right]} (-1)^j \binom{\alpha}{j} C(x-(j-p)h,t)\,, \tag{19}$$

$$\frac{\partial^\alpha C(x,t)}{\partial (-x)^\alpha} \approx \frac{1}{h^\alpha} \sum_{j=0}^{\left[\frac{b-x}{h}+p\right]} (-1)^j \binom{\alpha}{j} C(x+(j-p)h,t)\,, \tag{20}$$

where p is the shift value.

If we define weights

$$w_0^\alpha = 1,\ w_{\alpha,j} = (-1)^j \frac{\alpha(\alpha-1)\dots(\alpha-j+1)}{j!},\ j = 1, 2, \dots \tag{21}$$

then we may write (19) and (20) more simply as

$$\frac{\partial^\alpha C(x,t)}{\partial x^\alpha} \approx \frac{1}{h^\alpha} \sum_{j=0}^{\left[\frac{x-a}{h}+p\right]} w_j^\alpha C(x-(j-p)h,t)\,, \tag{22}$$

$$\frac{\partial^\alpha C(x,t)}{\partial (-x)^\alpha} \approx \frac{1}{h^\alpha} \sum_{j=0}^{\left[\frac{b-x}{h}+p\right]} w_j^\alpha C(x+(j-p)h,t)\,. \tag{23}$$

The inclusion of the shift p in the formulas was originally motivated by the fact that the standard (non-shifted) Grünwald formulas lead to unstable methods for certain finite difference discretisations [5, 16, 20, 23], whereas the shifted Grünwald formulas lead to stable methods.

In the present method, the fractional shift $p = 1/2$ is used, allowing us to build approximations of fractional derivatives at control volume *faces* $x_{i\pm 1/2}$ in terms of function values at the *nodes* x_j [1]. Hence we derive the fractionally-shifted Grünwald formulas

$$\frac{\partial^\alpha C(x_{i-1/2},t)}{\partial x^\alpha} \approx \frac{1}{h^\alpha} \sum_{j=0}^{i} w_j^\alpha C(x_{i-j},t)\,, \tag{24}$$

$$\frac{\partial^\alpha C(x_{i-1/2},t)}{\partial (-x)^\alpha} \approx \frac{1}{h^\alpha} \sum_{j=0}^{N-i+1} w_j^\alpha C(x_{i+j-1},t) \tag{25}$$

at the face $x_{i-1/2}$, and

$$\frac{\partial^\alpha C(x_{i+1/2},t)}{\partial x^\alpha} \approx \frac{1}{h^\alpha} \sum_{j=0}^{i+1} w_j^\alpha C(x_{i-j+1},t)\,, \tag{26}$$

$$\frac{\partial^\alpha C(x_{i+1/2},t)}{\partial (-x)^\alpha} \approx \frac{1}{h^\alpha} \sum_{j=0}^{N-i} w_j^\alpha C(x_{i+j},t) \tag{27}$$

at the face $x_{i+1/2}$.

Altogether then, the dispersive flux (11) is approximated at the face $x_{i-1/2}$ by

$$q(x_{i-1/2},t) \approx -K(x_{i-1/2},t) \times \left(\frac{\beta}{h^\alpha}\sum_{j=0}^{i} w_j^\alpha C(x_{i-j},t) - \frac{(1-\beta)}{h^\alpha}\sum_{j=0}^{N-i+1} w_j^\alpha C(x_{i+j-1},t)\right) \tag{28}$$

and at the face $x_{i+1/2}$ by

$$q(x_{i+1/2},t) \approx -K(x_{i+1/2},t) \times \left(\frac{\beta}{h^\alpha}\sum_{j=0}^{i+1} w_j^\alpha C(x_{i-j+1},t) - \frac{(1-\beta)}{h^\alpha}\sum_{j=0}^{N-i} w_j^\alpha C(x_{i+j},t)\right). \tag{29}$$

Previously [1] we have shown this discretisation to be of first order spatial accuracy for the constant coefficient case.

For the advective flux $V(x,t)C(x,t)$ we use a standard averaging scheme

$$V(x_{i\pm1/2},t)C(x_{i\pm1/2},t) \approx \frac{V(x_{i\pm1/2},t)}{2}\left[C(x_i,t) + C(x_{i\pm1},t)\right]. \tag{30}$$

This completes the spatial discretisation. For the temporal discretisation, we define a temporal partition $t_n = n\tau$ for $n = 0, 1, \ldots$ where τ is the timestep, and discretise the Caputo time fractional derivative using the L1-algorithm (see [3])

$$\frac{\mathrm{d}^\gamma C_i(t_{n+1})}{\mathrm{d}t^\gamma} = \frac{\tau^{-\gamma}}{\Gamma(2-\gamma)}\sum_{j=0}^{n} b_j^\gamma [C_i(t_{n+1-j}) - C_i(t_{n-j})] + O(\tau^{2-\gamma}), \tag{31}$$

where $b_j^\gamma = (j+1)^{1-\gamma} - j^{1-\gamma}, j = 0, 1, \ldots, n.$

Letting $C_i^n \approx C_i(t_n)$ denote the approximate numerical solution at node i at time t_n , and using the discretisations just derived, we obtain the fully implicit scheme

$$\begin{aligned}
&\frac{\tau^{-\gamma}}{\Gamma(2-\gamma)}\sum_{j=0}^{n} b_j^\gamma [C_i^{n+1-j} - C_i^{n-j}] \\
&= \frac{V_{i-1/2}^{n+1}}{2h}\left[C_i^{n+1} + C_{i-1}^{n+1}\right] - \frac{V_{i+1/2}^{n+1}}{2h}\left[C_i^{n+1} + C_{i+1}^{n+1}\right] \\
&+ \frac{K_{i-1/2}^{n+1}}{h}\left[\frac{\beta}{h^\alpha}\sum_{j=0}^{i} w_j^\alpha C_{i-j}^{n+1} - \frac{(1-\beta)}{h^\alpha}\sum_{j=0}^{N-i+1} w_j^\alpha C_{i+j-1}^{n+1}\right] \\
&- \frac{K_{i+1/2}^{n+1}}{h}\left[\frac{\beta}{h^\alpha}\sum_{j=0}^{i+1} w_j^\alpha C_{i-j+1}^{n+1} - \frac{(1-\beta)}{h^\alpha}\sum_{j=0}^{N-i} w_j^\alpha C_{i+j}^{n+1}\right] + S_i^{n+1}.
\end{aligned} \tag{32}$$

Collecting like terms, we may write the scheme in the form

$$\frac{\tau^{-\gamma}}{\Gamma(2-\gamma)}\sum_{j=0}^{n} b_j^{\gamma}[C_i^{n+1-j} - C_i^{n-j}] = \frac{1}{h}\sum_{j=0}^{N} g_{ij}C_j^{n+1} + S_i^{n+1} \tag{33}$$

where the coefficients g_{ij} are given by

$$g_{ij} = \begin{cases} \frac{K_{i+1/2}^{n+1}\beta}{h^{\alpha}}\, w_{i-j+1}^{\alpha} - \frac{K_{i-1/2}^{n+1}\beta}{h^{\alpha}}\, w_{i-j}^{\alpha}, & j < i-1; \\ \frac{K_{i+1/2}^{n+1}\beta}{h^{\alpha}}\, w_2^{\alpha} - \frac{K_{i-1/2}^{n+1}\beta}{h^{\alpha}}\, w_1^{\alpha} + \frac{K_{i-1/2}^{n+1}(1-\beta)}{h^{\alpha}}\, w_0^{\alpha} + V_{i-1/2}^{n+1}/2, & j = i-1; \\ \frac{K_{i+1/2}^{n+1}\beta + K_{i-1/2}^{n+1}(1-\beta)}{h^{\alpha}}\, w_1^{\alpha} - \frac{K_{i-1/2}^{n+1}\beta + K_{i+1/2}^{n+1}(1-\beta)}{h^{\alpha}}\, w_0^{\alpha} & \\ + \frac{V_{i-1/2}^{n+1} - V_{i+1/2}^{n+1}}{2}, & j = i; \\ \frac{K_{i-1/2}^{n+1}(1-\beta)}{h^{\alpha}}\, w_2^{\alpha} - \frac{K_{i+1/2}^{n+1}(1-\beta)}{h^{\alpha}}\, w_1^{\alpha} + \frac{K_{i+1/2}^{n+1}\beta}{h^{\alpha}}\, w_0^{\alpha} - V_{i+1/2}^{n+1}/2, & j = i+1; \\ \frac{K_{i-1/2}^{n+1}(1-\beta)}{h^{\alpha}} w_{j-i+1}^{\alpha} - \frac{K_{i+1/2}^{n+1}(1-\beta)}{h^{\alpha}} w_{j-i}^{\alpha}, & j > i+1. \end{cases} \tag{34}$$

As our problem has homogeneous Dirichlet boundary conditions, we solve for just the internal nodes, and set $C_0^n = C_N^n = 0$ for $n = 0, 1, \ldots$. Denoting the numerical solution vector $\mathbf{C}^n = [C_1^n, \ldots, C_{N-1}^n]^{\mathsf{T}}$ and source vector $\mathbf{S}^{n+1} = [S(x_1, t_{n+1}), \ldots, S(x_{N-1}, t_{n+1})]^{\mathsf{T}}$, we have the vector equation

$$\left(\mathbf{I} + \frac{\tau^{\gamma}\Gamma(2-\gamma)}{h}\mathbf{A}\right)\mathbf{C}^{n+1} = b_n^{\gamma}\mathbf{C}^0 + \sum_{j=0}^{n-1}(b_j^{\gamma} - b_{j+1}^{\gamma})\mathbf{C}^{n-j} + \tau^{\gamma}\Gamma(2-\gamma)\mathbf{S}^{n+1} \tag{35}$$

to solve at each timestep, where the matrix $\mathbf{A}$ has elements $a_{ij} = -g_{ij}$.

3.2. Comparison with finite difference scheme

It is instructive to compare the coefficients g_{ij} with those obtained from a finite difference discretisation of the same problem. To do this, we consider the case of constant velocity V and dispersion coefficient K. The problem (1) can then be written

$$D_t^{\gamma}C(x,t) + V\frac{\partial C}{\partial x} = K\left[\beta\frac{\partial^{\alpha+1}C}{\partial x^{\alpha+1}} + (1-\beta)\frac{\partial^{\alpha+1}C}{\partial(-x)^{\alpha+1}}\right] + S(x,t) \tag{36}$$

and both the finite difference and finite volume methods can be used to discretise this problem.

For the finite volume method, the coefficients (34) simplify to

$$g_{ij} = \begin{cases} \frac{K\beta}{h^\alpha}(w^\alpha_{i-j+1} - w^\alpha_{i-j}), & j < i-1; \\ \frac{K\beta}{h^\alpha}(w^\alpha_2 - w^\alpha_1) + \frac{K(1-\beta)}{h^\alpha} w^\alpha_0 + V/2, & j = i-1; \\ \frac{K}{h^\alpha}(w^\alpha_1 - w^\alpha_0), & j = i; \\ \frac{K(1-\beta)}{h^\alpha}(w^\alpha_2 - w^\alpha_1) + \frac{K\beta}{h^\alpha} w^\alpha_0 - V/2, & j = i+1; \\ \frac{K(1-\beta)}{h^\alpha}(w^\alpha_{j-i+1} - w^\alpha_{j-i}), & j > i+1. \end{cases} \tag{37}$$

The finite difference discretisation of [6] applied to (36), combined with a standard second order central difference approximation for the advection term, yields a scheme with coefficients

$$\tilde{g}_{ij} = \begin{cases} \frac{K\beta}{h^\alpha} w^{\alpha+1}_{i-j+1}, & j < i-1; \\ \frac{K\beta}{h^\alpha} w^{\alpha+1}_2 + \frac{K(1-\beta)}{h^\alpha} w^{\alpha+1}_0 + V/2, & j = i-1; \\ \frac{K}{h^\alpha} w^{\alpha+1}_1, & j = i; \\ \frac{K(1-\beta)}{h^\alpha} w^{\alpha+1}_2 + \frac{K\beta}{h^\alpha} w^{\alpha+1}_0 - V/2, & j = i+1; \\ \frac{K(1-\beta)}{h^\alpha} w^{\alpha+1}_{j-i+1}, & j > i+1. \end{cases} \tag{38}$$

For the two schemes to be equivalent, we require the identity $w^\alpha_j - w^\alpha_{j-1} = w^{\alpha+1}_j$ for $j = 1, 2, \ldots$. To prove this result, we will use formula (21) for the Grünwald weights, as well as the recursive formula

$$w^\alpha_0 = 1,\ w^\alpha_j = \left(1 - \frac{\alpha+1}{j}\right) w^\alpha_{j-1},\ j = 1, 2, \ldots \tag{39}$$

which is easily seen to be equivalent to (21).

Proposition 3.1.

The Grünwald weights w^α_j satisfy $w^\alpha_j - w^\alpha_{j-1} = w^{\alpha+1}_j$ for $j = 1, 2, \ldots$.
Proof: From (39) we have, for $j \geq 1$,

$$\begin{aligned} w^\alpha_j - w^\alpha_{j-1} &= \left(1 - \frac{\alpha+1}{j}\right) w^\alpha_{j-1} - w^\alpha_{j-1} \\ &= -\left(\frac{\alpha+1}{j}\right) w^\alpha_{j-1} \end{aligned}$$

and since from (21) we have

$$w^\alpha_{j-1} = (-1)^{j-1} \frac{\alpha(\alpha-1)\ldots(\alpha-(j-1)+1)}{(j-1)!}$$

we see that

$$
\begin{aligned}
w_j^\alpha - w_{j-1}^\alpha &= -\left(\frac{\alpha+1}{j}\right)(-1)^{j-1} \times \\
&\qquad \frac{\alpha(\alpha-1)\dots(\alpha-(j-1)+1)}{(j-1)!} \\
&= (-1)^j \frac{(\alpha+1)(\alpha+1-1)\dots(\alpha+1-j+1)}{j!} \\
&= w_j^{\alpha+1}
\end{aligned}
$$

as required.

Hence we see that for constant V and K, the finite volume and finite difference methods are equivalent for this problem. However, for variable V and K, the finite volume method is preferred, since it applies directly to equation (1) written in conservative form.

4. Numerical Experiments

In order to demonstrate the effectiveness of the finite volume method, we consider two numerical experiments.

Example 1. Consider the following two-sided time-space fractional advection-dispersion equation with variable coefficients and a source term

$$
\begin{aligned}
&D_t^\gamma C(x,t) + \frac{\partial}{\partial x}(V(x,t)C(x,t)) = \\
&\frac{\partial}{\partial x}\left[K(x,t)\left(\beta\frac{\partial^\alpha C}{\partial x^\alpha} - (1-\beta)\frac{\partial^\alpha C}{\partial(-x)^\alpha}\right)\right] + S(x,t)
\end{aligned} \tag{40}
$$

for $(x,t) \in [0,1] \times [0,T]$ together with following boundary and initial conditions

$$
\begin{cases}
C(0,t) = C(1,t) = 0, \quad 0 \le t \le T, \\
C(x,0) = 0, \quad 0 \le x \le 1
\end{cases} \tag{41}
$$

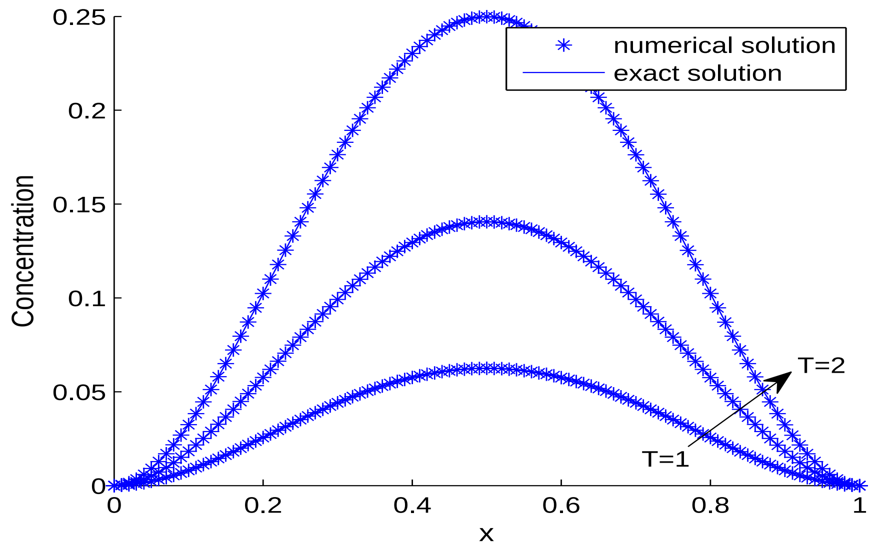

Figure 1. Comparison between exact and numerical solutions with $\gamma = 0.8$, $\alpha = 0.85$ and $\beta = 0.5$, using $h = \tau = 0.01$ at final time $T = 1.0, 1.5, 2.0$, T increases in the direction of the arrow.

with velocity $V(x,t) = 1 + x^2t^2$, dispersion coefficient $K(x,t) = 1 + x + t$ and a source term $S(x,t) = S_1(x,t) - S_2(x,t) - S_3(x,t) - S_4(x,t)$, where

$$
\begin{aligned}
S_1(x,t) &= 2\frac{t^{2-\gamma}}{\Gamma(3-\gamma)}x^2(1-x)^2,\\
S_2(x,t) &= (1+x+t)\left(t^2(\beta-1)g(1-x) - t^2\beta g(x)\right),\\
S_3(x,t) &= t^2\beta f(x) + t^2(\beta-1)f(1-x),\\
S_4(x,t) &= -2t^4x^3(x-1)^2 - 2t^2x(1+x^2t^2)(x-1)^2\\
&\quad -t^2x^2(2x-2)(1+x^2t^2),\\
g(x) &= \frac{\Gamma(3)(\alpha-2)x^{1-\alpha}}{\Gamma(3-\alpha)} - \frac{2\Gamma(4)(\alpha-3)x^{2-\alpha}}{\Gamma(4-\alpha)} + \frac{\Gamma(5)(\alpha-4)x^{3-\alpha}}{\Gamma(5-\alpha)},\\
f(x) &= \frac{\Gamma(3)x^{2-\alpha}}{\Gamma(3-\alpha)} - \frac{2\Gamma(4)x^{3-\alpha}}{\Gamma(4-\alpha)} + \frac{\Gamma(5)x^{4-\alpha}}{\Gamma(5-\alpha)}.
\end{aligned}
$$

The source term is not part of the physical model but is included in the numerical experiment so that the exact solution to this problem is known and is given by $C(x,t) = t^2x^2(1-x)^2$.

Fig. 1 shows the exact and numerical solutions with $\gamma = 0.8$, $\alpha = 0.85$ and $\beta = 0.5$ at different times T, using $h = \tau = 0.01$. It can be seen that the numerical solution is in excellent agreement with the exact solution. In Table 1 we confirm numerically that our solution is accurate to second order in space by computing the error in the numerical solution for a sequence of spatial and temporal steps h and τ. The first two columns list the values of h and τ, the third and fifth columns show two norms for computing errors for the numerical solution at

Table 1. **Maximum error with temporal and spatial step reduction at $T = 1$ for $\gamma = 0.8$, $\alpha = 0.85$, $\beta = 0.5$**

h	$\tau = h^{1/(2-\gamma)}$	E_∞	$Ratio_\infty$	E_2	$Ratio_2$
0.0031	0.0082	7.03×10^{-6}		4.14×10^{-6}	
0.0016	0.0046	3.90×10^{-6}	1.8023	2.30×10^{-6}	1.8028
7.81×10^{-4}	0.0026	2.02×10^{-6}	1.9309	1.19×10^{-6}	1.9285
3.90×10^{-4}	0.0014	1.03×10^{-6}	1.9565	6.10×10^{-7}	1.9548

$T = 1$; $E_\infty = \max_i \mid C_{exact}(i) - C_{numeric}(i) \mid$ and $E_2 = \sqrt{h \sum_i [C_{exact}(i) - C_{numeric}(i)]^2}$. The fourth and sixth columns are the ratios ($Ratio_\infty$ and $Ratio_2$) of the errors (E_∞ and E_2) in the row above to that of the present row respectively. We see that when h is reduced by a factor of two and with the stepsize τ linked to the value of h via the known temporal rate of convergence $O(\tau^{2-\gamma})$, the ratio is approaching the expected value of two.

In this example, we have included fractional orders in both time and space, as well as time- and space-varying velocity and dispersion coefficients. Since the numerical solution agrees well with the exact solution, we conclude that the numerical scheme is performing correctly.

Example 2. Consider the following two-sided space fractional advection-dispersion equation

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[K(x,t)\left(\beta\frac{\partial^\alpha C}{\partial x^\alpha} - (1-\beta)\frac{\partial^\alpha C}{\partial(-x)^\alpha}\right)\right] \tag{42}$$

for $(x,t) \in [-1,1] \times [0,T]$ together with following boundary and initial conditions

$$\begin{cases} C(-1,t) = C(1,t) = 0, & 0 \le t \le T, \\ C(x,0) = \delta(x), & -1 \le x \le 1 \end{cases} \tag{43}$$

with dispersion coefficient $K(x,t) = 2 + \tanh(10x)$. This function effectively partitions the domain $[-1,1]$ into two regions with dispersion coefficients approximately 1 and 3, with a rapid transition between the two around the origin. Figure 2 illustrates the solution to this problem over space and time, illustrating the asymmetric dispersion of the initial pulse.

We use this test problem to highlight the advantage of our finite volume formulation compared to a standard finite difference method. Using finite differences, the product rule is applied to (42), leading to a term involving the derivative $\partial K/\partial x$. The finite volume method deals directly with (42) in its conservative form, and hence involves no such term.

Firstly, we solve (42) using a very fine mesh ($h = 0.0002$) and small time steps ($\tau = 0.0001$) to get a benchmark fine mesh solution. Then we compare finite volume and finite difference numerical solutions against that benchmark solution.

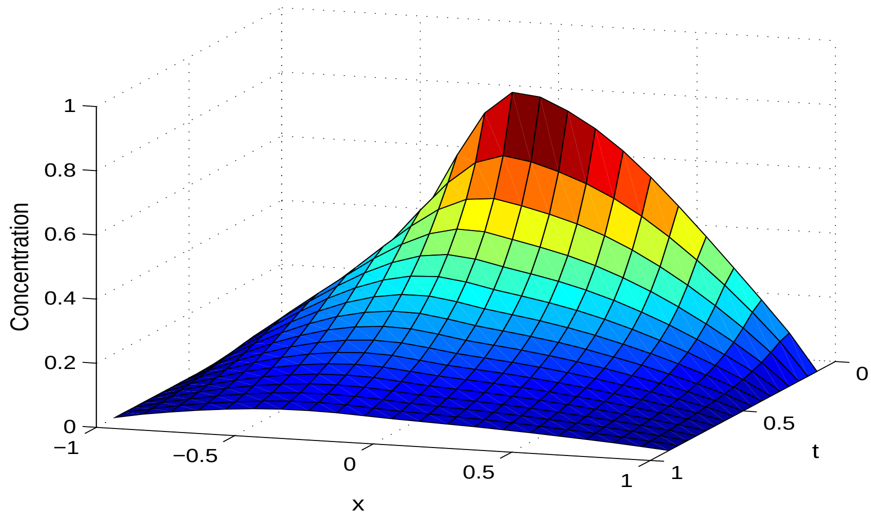

Figure 2. **Illustration of the solution to example 2 showing the asymmetric diffusion profile.**

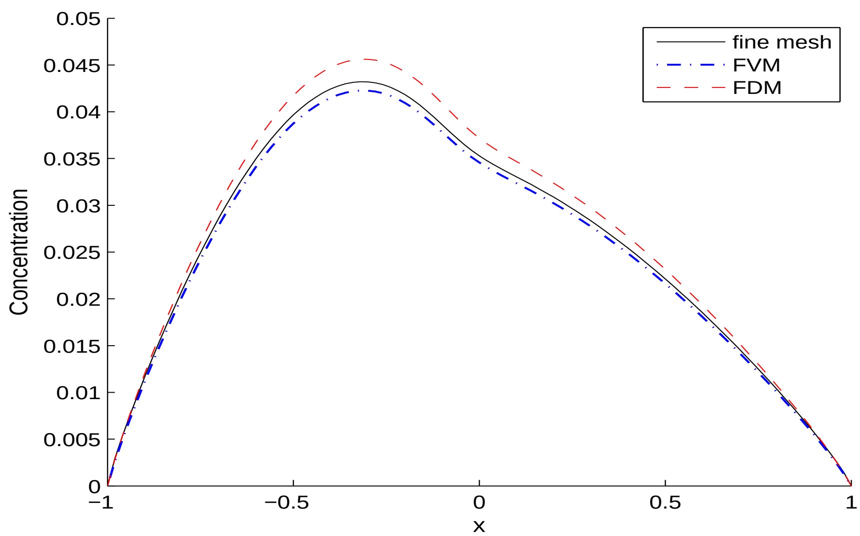

Figure 3. Comparison between fine mesh solution, finite volume and finite difference methods for example 2 with $\alpha = 0.7$ and $\beta = 0.5$, using $h = 0.02$ and $\tau = 0.0001$ at final time $T = 1$.

Figure 3 shows the comparison between fine mesh solution, finite volume and finite difference methods for solving (42) with $\alpha = 0.7$ and $\beta = 0.5$ at final time $T = 1$, using $h = 0.02$ and $\tau = 0.0001$. The small timestep τ has been used to ensure that any differences in the solutions are purely due to the spatial discretisation. From the figure it is evident that the finite volume solution with 100 nodes more accurately represents the correct solution as compared to the finite difference solution with 100 nodes. We conclude that the finite volume method offers a genuine advantage when solving problems such as this with variable dispersion coefficients.

5. Conclusion

In this paper, we presented a finite volume method to solve the time-space two-sided fractional advection-dispersion equation with variable coefficients on a one-dimensional finite domain with homogeneous Dirichlet boundary conditions. The novel spatial discretisation employs fractionally-shifted Grünwald formulas to discretise the Riemann-Liouville fractional derivatives at control volume faces in terms of function values at the nodes, while the L1-algorithm is used to discretise the Caputo time fractional derivative.

We showed that in the constant coefficient case, the scheme is equivalent to the finite difference scheme described by [6]. For the variable coefficient case, the finite volume scheme presented in this work is preferred for solving equation (1), since it deals directly with the equation in conservative form.

Numerical experiments confirm that the scheme recovers the correct solution for test problems with fractional orders in both time and space, as well as time- and space-varying velocity and dispersion coefficients.

Tadjeran et al. [20] have shown how to increase the order of their finite difference scheme by Richardson extrapolation. This too should be possible for the finite volume scheme, and will be the subject of future research.

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