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A second-order accurate numerical method for the two-dimensional fractional diffusion equation

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Abstract

Spatially fractional order diffusion equations are generalizations of classical diffusion equations which are used in modeling practical superdiffusive problems in fluid flow, finance and others. In this paper, we present an accurate and efficient numerical method to solve a fractional superdiffusive differential equation. This numerical method combines the alternating directions implicit (ADI) approach with a Crank–Nicolson discretization and a Richardson extrapolation to obtain an unconditionally stable second-order accurate finite difference method. The stability and the consistency of the method are established. Numerical solutions for an example super-diffusion equation with a known analytic solution are obtained and the behavior of the errors are analyzed to demonstrate the order of convergence of the method.

Keywords: Two-dimensional fractional partial differential equation; Extrapolated Crank–Nicolson method; Numerical solution for superdiffusion; Alternating direction implicit methods; Second-order accurate method for fractional diffusion

1. Introduction

Fractional diffusion equations are used to model problems in physics (see a comprehensive review by Metzler and Klafter [25]), finance [10,16,28,31,30], and hydrology [2,4,5,32,33]. Fractional space derivatives may be used to formulate anomalous dispersion models, where a particle plume spreads at a rate that is different than the classical Brownian motion model. When a fractional derivative of order $1 < \alpha < 2$ replaces the second derivative in a diffusion or dispersion model, it leads to a superdiffusive flow model. Analytic closed-form solutions for these initial-boundary value problems are elusive. This paper presents a practical second-order accurate numerical method for solving two-dimensional superdiffusion problems on a rectangular region with variable diffusion coefficients, using a variation on the classical alternating-directions implicit (ADI) Crank–Nicolson method which is followed by a Richardson extrapolation. The finite difference methods

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obtained from the classical Grünwald sums have first-order truncation errors but are unstable. Therefore, we use a shifted version of the usual Grünwald finite difference approximation, and we show that this leads to unconditional stability. To improve the first-order accuracy of the solutions that are obtained in this way, we apply a spatial Richardson extrapolation to obtain a solution that is second-order accurate in both the spatial and temporal grid sizes. Similar to the treatment of the classical multi-dimensional diffusion problems, a number of ADI splitting options are possible, but a careful selection of the splitting method is required to maintain consistency and to properly handle the source/sink term in the differential equation. In this paper, we establish the consistency and the unconditional stability (and therefore convergence) of the proposed hybrid method for a superdiffusion equation with variable diffusion coefficients and Dirichlet boundary conditions. We also prove second-order convergence in both time and space, and finally we demonstrate the order of convergence with a numerical example for which the fractional diffusion equation has an exact analytical solution.

Consider a two-dimensional fractional diffusion equation

$$\frac{\partial u(x,y,t)}{\partial t} = d(x,y)\frac{\partial^{\alpha} u(x,y,t)}{\partial x^{\alpha}} + e(x,y)\frac{\partial^{\beta} u(x,y,t)}{\partial y^{\beta}} + q(x,y,t) \tag{1}$$

on a finite rectangular domain $x_L < x < x_H$ and $y_L < y < y_H$, with fractional orders $1 < \alpha \leqslant 2$ and $1 < \beta \leqslant 2$, where the diffusion coefficients $d(x,y) > 0$ and $e(x,y) > 0$. The 'forcing' function $q(x,y,t)$ can be used to represent sources and sinks. We will assume that this fractional diffusion equation has a unique and sufficiently smooth solution under the following initial and boundary conditions (some results on existence and uniqueness are developed in [9]). Assume the initial condition $u(x,y,t=0) = f(x,y)$ for $x_L < x < x_H, y_L < y < y_H$, and Dirichlet boundary conditions $u(x,y,t) = B(x,y,t)$ on the boundary (perimeter) of the rectangular region $x_L \leqslant x \leqslant x_H, y_L \leqslant y \leqslant y_H$, with the additional restriction that $B(x_L,y,t) = B(x,y_L,t) = 0$. For example, in dispersion of solutes in ground water aquifers, this means that the left/lower boundary is set far enough away from an evolving plume that no significant concentrations reach that boundary. The classical dispersion equation in two dimensions is given by $\alpha = \beta = 2$. The values of $1 < \alpha < 2$, or $1 < \beta < 2$ model a super-diffusive process in that coordinate.

Eq. (1) uses a (left) Riemann fractional derivative of order α, defined by

$$\frac{\mathrm{d}^{\alpha} f(x)}{\mathrm{d}x^{\alpha}} = \frac{1}{\Gamma(n-\alpha)}\frac{\mathrm{d}^{n}}{\mathrm{d}x^{n}}\int_{L}^{x}\frac{f(\xi)}{(x-\xi)^{\alpha+1-n}}\mathrm{d}\xi \tag{2}$$

where n is an integer such that $n-1 < \alpha \leqslant n$. Other definitions of the fractional derivative exist. The case $L = 0$ is generally called the Riemann–Liouville form, and the case $L = -\infty$ is the Liouville definition for the fractional derivative. Similar definitions for right fractional derivatives exist. We note that the right and the left fractional derivatives at a point are generally not equal. Fractional derivatives are non-local operators of convolution type [1,6,20]. The value of the left Riemann–Liouville fractional derivative at a point x depends on the function values at all the points in the interval $[L,x]$. With our boundary conditions (and zero-extending the solution functions for $x < x_L$ or $y < y_L$) the Riemann and Liouville fractional derivatives become equivalent. For more details on fractional derivative concepts and definitions, see [26,27,34].

An extrapolated Crank–Nicolson method for a one-dimensional fractional diffusion equation is discussed in [35]. To our knowledge, this is the only published finite difference method to obtain an unconditionally convergent numerical solution that is second-order accurate in temporal and spatial grid sizes for such 1-D problems. A 2-D ADI method for the implicit Euler method is discussed in [24], where we prove that this method yields an unconditionally stable and convergent solution that is first-order accurate in both the temporal and spatial grid sizes. Similar to the numerical schemes for the classical dispersion/diffusion equations, the splitting methods for the fractional diffusion equation have the potential to significantly reduce the computational work in obtaining a numerical solution, while maintaining the underlying convergence order of the numerical method. Additional Refs. [12,13,15,21] treat explicit or implicit finite difference methods for space fractional diffusion equations, and [9,29] examine finite element methods for such problems. Refs. [7,36] address finite differences for time fractional differential equations.

Eq. (1) is a special case of a two-sided fractional diffusion equation

$$\frac{\partial u(x,y,t)}{\partial t} = d(x,y)\left[(1-p_1)\frac{\partial^\alpha u(x,y,t)}{\partial(-x)^\alpha} + p_1\frac{\partial^\alpha u(x,y,t)}{\partial x^\alpha}\right] + e(x,y)\left[(1-p_2)\frac{\partial^\beta u(x,y,t)}{\partial(-y)^\beta} + p_2\frac{\partial^\beta u(x,y,t)}{\partial y^\beta}\right] + q(x,y,t) \tag{3}$$

where $\partial^\alpha u/\partial(-x)^\alpha$ and $\partial^\beta u/\partial(-y)^\beta$ are negative (right) fractional derivatives, and the weights $p_1, p_2 \in [0,1]$. The homogeneous equation (3) with constant coefficients governs the transition densities of an operator stable Lévy process with independent stable components of order α, β and skewness determined by the weights p_1 and p_2. The operator Lévy process is a stochastic model for anomalous diffusion [17,18], the accumulation of independent random jumps in each coordinate. In this model, the probability of a jump larger than $r > 0$ in the xy direction falls off like $r^{-\alpha}$ and $r^{-\beta}$, respectively. The weights p_1 and p_2 are the probabilities of a jump in the positive x, y direction, and hence $1 - p_1$ and $1 - p_2$ are the probabilities of a jump in the negative x, y direction, respectively. To simplify notation, in this paper we restrict our attention to the one-sided version (1), but the extension to the more general form (3) is straightforward. See [23] for the one-dimensional case. The fractional derivatives in (3) decouple because the x and y jumps are assumed independent. A more complicated form that mixes the two orders α and β of fractional differentiation pertains if the diffusing particle makes x and y jumps that are not statistically independent [3,18,19]. See [22] for one possible approach to developing numerical schemes in this more complicated setting. An alternative method based on particle tracking is presented in [38].

2. Numerical preliminaries and notations

For a finite difference approximation to the Riemann–Liouville fractional derivative, we employ a right-shifted Grünwald approximation, since the standard (i.e., unshifted) Grünwald formula generally leads to unstable finite difference approximations regardless of whether the methods are explicit or implicit [21]. We will show that the shifted Grünwald estimate leads to an unconditionally convergent alternating-directions-implicit ADI method in a Crank–Nicolson type discretization of the two-dimensional superdiffusion equation.

The right-shifted Grünwald formula for $1 < \alpha \leqslant 2$ is [21]

$$\frac{\partial^\alpha u(x,y,t)}{\partial x^\alpha} = \frac{1}{\Gamma(-\alpha)}\lim_{N_x\to\infty}\frac{1}{h^\alpha}\sum_{k=0}^{N_x}\frac{\Gamma(k-\alpha)}{\Gamma(k+1)}u[x-(k-1)h,y,t] \tag{4}$$

where N_x is a positive integer, $h = (x - x_L)/N_x$ and $\Gamma(\cdot)$ is the gamma function. We also define the 'normalized' Grünwald weights by

$$g_{\alpha,k} = \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} = (-1)^k(\alpha k) \tag{5}$$

and remark that these normalized weights only depend on the order α and the index k.

For the numerical approximation scheme, define $t_n = n\Delta t$ to be the integration time $0 \leqslant t_n \leqslant T$, $\Delta x = (x_H - x_L)/N_x = h_x > 0$ is the grid size in x-direction, with $x_i = x_L + i\Delta x$ for $i = 0,\ldots,N_x$; $\Delta y = (y_H - y_L)/N_y = h_y > 0$ is the grid size in y-direction, with $y_j = y_L + j\Delta y$ for $j = 0,\ldots,N_y$. Define $u^n_{i,j}$ as the numerical approximation to $u(x_i,y_j,t_n)$. Similarly, define $d_{i,j} = d(x_i,y_j)$, $e_{i,j} = e(x_i,y_j)$, and $q^n_{i,j} = q(x_i,y_j,t_n)$. The initial conditions are set by $u^0_{i,j} = f_{i,j} = f(x_i,y_j)$. The Dirichlet boundary condition on the boundary of this rectangular region are at $x = x_L$, $u^n_{0,j} = B^n_{0,j} = B(x_L,y_j,t_n) = 0$; at $x = x_H$, $u^n_{N_x,j} = B^n_{N_x,j} = B(x_H,y_j,t_n)$; at $y = y_L$, $u^n_{i,0} = B^n_{i,0} = B(x_i,y_L,t_n) = 0$; and at $y = y_H$, $u^n_{i,N_y} = B^n_{i,N_y} = B(x_i,y_H,t_n)$.

The following results on the asymptotic expansion of the error terms assume that the solution function $u(x,y,t)$ is sufficiently smooth and vanishes on the left ($x = x_L$) and the lower ($y = y_L$) boundaries of the rectangular region $\{(x,y)|x_L < x < x_H, y_L < y < y_H\}$. For details on these conditions and the results see Proposition 3.1 in [35]. Define the following (shifted α-fractional) finite difference operator

$$\delta_{\alpha,x}u_{i,j}^{n} = \frac{d_{i,j}}{(\Delta x)^{\alpha}}\sum_{k=0}^{i+1} g_{\alpha,k}u_{i-k+1,j}^{n}$$

which gives an $O(\Delta x)$ estimate to the corresponding αth fractional partial derivative with an asymptotic truncation error expansion of the form $C_1\Delta x + C_2(\Delta x)^2 + O[(\Delta x)^3]$ where the coefficients C_i do not depend on the grid size Δx. Similarly, the (shifted β fractional) finite difference operator

$$\delta_{\beta,y}u_{i,j}^{n} = \frac{e_{i,j}}{(\Delta y)^{\beta}}\sum_{k=0}^{j+1} g_{\beta,k}u_{i,j-k+1}^{n}$$

is an $O(\Delta y)$ approximation to the βth fractional partial derivative term with an asymptotic error expansion of the form $D_1\Delta y + D_2(\Delta y)^2 + O[(\Delta y)^3]$, where the coefficients D_i do not depend on the grid size Δy.

3. Numerical scheme

A Crank–Nicolson type finite difference equation for the two-dimensional superdiffusion equation (1) may be obtained by substituting the shifted Grünwald estimates into the differential equation centered at time $t_{n+1/2} = \frac{1}{2}(t_{n+1} + t_n)$ to obtain

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{\Delta t} = \frac{[\delta_{\alpha,x}u_{i,j}^{n+1} + \delta_{\alpha,x}u_{i,j}^{n} + \delta_{\beta,y}u_{i,j}^{n+1} + \delta_{\beta,y}u_{i,j}^{n}]}{2} + q_{i,j}^{n+1/2} \tag{6}$$

Note that the centering in time implies that Eq. (6) has a truncation error with an $O[(\Delta t)^2]$ temporal error component, but a spatial error component which is $O(\Delta x) + O(\Delta y)$, since the Grünwald estimates are only first-order accurate.

Eq. (6) may be re-arranged and written in the operator notation

$$\left(1 - \frac{\Delta t}{2}\delta_{\alpha,x} - \frac{\Delta t}{2}\delta_{\beta,y}\right)u_{i,j}^{n+1} = \left(1 + \frac{\Delta t}{2}\delta_{\alpha,x} + \frac{\Delta t}{2}\delta_{\beta,y}\right)u_{i,j}^{n} + q_{i,j}^{n+1/2}\Delta t \tag{7}$$

The alternating directions implicit (ADI), locally one-dimensional (LOD), and splitting methods are similar schemes that are used to significantly reduce the computational work in solving classical multi-dimensional diffusion equations [14]. These methods use some 'perturbation' of Eq. (7) to derive schemes that require only implicitness of the numerical solution in a single spatial direction, which are then iterated for each spatial direction with a proportionally reduced time step. For our problem, the relevant perturbation of Eq. (7) is

$$\left(1 - \frac{\Delta t}{2}\delta_{\alpha,x}\right)\left(1 - \frac{\Delta t}{2}\delta_{\beta,y}\right)u_{i,j}^{n+1} = \left(1 + \frac{\Delta t}{2}\delta_{\alpha,x}\right)\left(1 + \frac{\Delta t}{2}\delta_{\beta,y}\right)u_{i,j}^{n} + q_{i,j}^{n+1/2}\Delta t \tag{8}$$

The system of equations defined by (8) can now be solved by the following (Peaceman–Rachford type) set of matrix equations defining the ADI method:

$$\left(1 - \frac{\Delta t}{2}\delta_{\alpha,x}\right)u_{i,j}^{*} = \left(1 + \frac{\Delta t}{2}\delta_{\beta,y}\right)u_{i,j}^{n} + \frac{\Delta t}{2}q_{i,j}^{n+1/2} \tag{9}$$

$$\left(1 - \frac{\Delta t}{2}\delta_{\beta,y}\right)u_{i,j}^{n+1} = \left(1 + \frac{\Delta t}{2}\delta_{\alpha,x}\right)u_{i,j}^{*} + \frac{\Delta t}{2}q_{i,j}^{n+1/2} \tag{10}$$

To see this, multiply (9) by the operator $\left(1 + \frac{\Delta t}{2}\delta_{\alpha,x}\right)$ on both sides, multiply (10) by $\left(1 - \frac{\Delta t}{2}\delta_{\alpha,x}\right)$ on both sides, and add the resulting equations to obtain (8).

Eqs. (9) and (10) define an intermediate solution $u_{i,j}^{*}$ in order to advance the numerical solution $u_{i,j}^{n}$ at time t_n to the numerical solution $u_{i,j}^{n+1}$ at time t_{n+1}. The corresponding algorithm is implemented as follows:

(1) First solve on each fixed horizontal slice $y = y_k$ $(k = 1, \ldots, N_y - 1)$, a set of $N_x - 1$ equations at the points x_i, $i = 1, \ldots, N_x - 1$ defined by (9) to obtain the intermediate solution slice $u_{i,k}^{*}$.
(2) Next, change/alternate the spatial direction, and on each fixed vertical slice $x = x_k$ $(k = 1, \ldots, N_x - 1)$ solve a set of $N_y - 1$ equations at the points y_j, $j = 1, \ldots, N_y - 1$ defined by (10) to obtain the solution slice $u_{k,j}^{n+1}$.

More specifically, a 'sweep' along the horizontal line $y = y_k$ according to the first step (9) gives a system of $(N_x - 1)$ linear equations, where the ith equation, which results from the discretization at the point (x_i, y_k), is of the form

$$\sum_{m=0}^{i+1} A_{i,m} u^*_{m,k} = \sum_{m=0}^{k+1} B_{i,m} u^n_{i,m} + \frac{\Delta t}{2} \quad q^{n+1/2}_{i,k} \quad \text{for } i = 1, \ldots, N_x - 1 \tag{11}$$

where for each y_k, the coefficients $A_{i,m}$ for $i = 1, \ldots, N_x - 1$ and $m = 0, \ldots, i + 1$ are defined by:

$$A_{i,m} = \begin{cases} -D_{i,k} g_{\alpha,i-m+1} & \text{for } m \leqslant i - 1 \\ 1 - D_{i,k} g_{\alpha,1} & \text{for } m = i \\ -D_{i,k} g_{\alpha,0} & \text{for } m = i + 1 \end{cases}$$

and the coefficients $B_{i,m}$ for $i = 1, \ldots, N_x - 1$ and $m = 0, \ldots, k + 1$ are defined by:

$$B_{i,m} = \begin{cases} E_{i,k} g_{\beta,k-m+1} & \text{for } m \leqslant k - 1 \\ 1 + E_{i,k} g_{\beta,1} & \text{for } m = k \\ E_{i,k} g_{\beta,0} & \text{for } m = k + 1 \end{cases}$$

with

$$D_{i,k} = \frac{d_{i,k} \Delta t}{2(\Delta x)^{\alpha}} \tag{12}$$

$$E_{i,k} = \frac{e_{i,k} \Delta t}{2(\Delta y)^{\beta}} \tag{13}$$

For example, at y_2 (that is, $k = 2$) and for $i = 1$ the equation becomes

$$\begin{aligned} &- D_{1,2} g_{\alpha,2} u^*_{0,2} + (1 - D_{1,2} g_{\alpha,1}) u^*_{1,2} - D_{1,2} g_{\alpha,0} u^*_{2,2} \\ &\quad = E_{1,2} g_{\beta,3} u^n_{1,0} + E_{1,2} g_{\beta,2} u^n_{1,1} + (1 + E_{1,2} g_{\beta,1}) u^n_{1,2} + E_{1,2} g_{\beta,0} u^n_{1,3} + \frac{\Delta t}{2} q^{n+1}_{1,2} \end{aligned}$$

and at y_2 for $i = 2$ we have

$$\begin{aligned} &- D_{2,2} g_{\alpha,3} u^*_{0,2} - D_{2,2} g_{\alpha,2} u^*_{1,2} + (1 - D_{2,2} g_{\alpha,1}) u^*_{2,2} - D_{2,2} g_{\alpha,0} u^*_{3,2} \\ &\quad = E_{2,2} g_{\beta,3} u^n_{2,0} + E_{2,2} g_{\beta,2} u^n_{2,1} + (1 + E_{2,2} g_{\beta,1}) u^n_{2,2} + E_{2,2} g_{\beta,0} u^n_{2,3} + \frac{\Delta t}{2} q^{n+1}_{2,2} \end{aligned}$$

and at y_2 for $i = N_x - 1$ we get

$$\begin{aligned} &- D_{N_x-1,2} g_{\alpha,N_x} u^*_{0,2} - D_{N_x-1,2} g_{\alpha,N_x-1} u^*_{1,2} + \cdots + (1 - D_{N_x-1,2} g_{\alpha,1}) u^*_{N_x-1,2} - D_{N_x-1,2} g_{\alpha,0} u^*_{N_x,2} \\ &\quad = E_{N_x-1,2} g_{\beta,3} u^n_{N_x-1,0} + E_{N_x-1,2} g_{\beta,2} u^n_{N_x-1,1} + (1 + E_{N_x-1,2} g_{\beta,1}) u^n_{N_x-1,2} + E_{N_x-1,2} g_{\beta,0} u^n_{N_x-1,3} + \frac{\Delta t}{2} q^{n+1}_{N_x-1,2} \end{aligned}$$

In an analogous manner, when the direction of the sweep is alternated, the equations obtained from the second step (10) on each vertical line $x = x_k$ (that is, $i = k$) lead to a system of $(N_y - 1)$ linear equations, where the jth equation resulting from the discretization at the point (x_k, y_j) is of the form

$$\sum_{m=0}^{j+1} \widehat{B}_{j,m} u^{n+1}_{k,m} = \sum_{m=0}^{k+1} \widehat{A}_{j,m} u^*_{m,j} + \frac{\Delta t}{2} q^{n+1/2}_{k,j} \quad j = 1, \ldots, N_y - 1 \tag{14}$$

where at each x_k, the coefficients $\widehat{A}_{j,m}$ for $j = 1, \ldots, N_y - 1$ and $m = 0, \ldots, k + 1$ are defined by:

$$\widehat{A}_{j,m} = \begin{cases} D_{k,j} g_{\alpha,j-m+1} & \text{for } m \leqslant j - 1 \\ 1 + D_{k,j} g_{\alpha,1} & \text{for } m = j \\ D_{k,j} g_{\alpha,0} & \text{for } m = j + 1 \end{cases}$$

and the coefficients $\widehat{B}_{j,m}$ for $j = 1, \ldots, N_y - 1$ and $m = 0, \ldots, j+1$ are defined by:

$$\widehat{B}_{j,m} = \begin{cases} -E_{k,j} g_{\beta,j-m+1} & \text{for } m \leqslant k-1 \\ 1 - E_{k,j} g_{\beta,1} & \text{for } m = k \\ -E_{k,j} g_{\beta,0} & \text{for } m = k+1 \end{cases}$$

To maintain the consistency of the set of equations defined by (9) and (10) with (8), the intermediate solution $u^*_{i,j}$ should be defined carefully on the boundary, prior to solving the system of equations defined by (11) and (14). Otherwise, the first-order spatial accuracy of the two-step ADI method outlined above will be impacted. This is accomplished by subtracting Eq. (10) from (9) to get the following equation to define $u^*_{i,j}$

$$2u^*_{i,j} = \left(1 - \frac{\Delta t}{2}\delta_{\beta,y}\right) u^{n+1}_{i,j} + \left(1 + \frac{\Delta t}{2}\delta_{\beta,y}\right) u^n_{i,j} \tag{15}$$

Thus, the boundary conditions for $u^*_{i,j}$ (i.e., $i = 0$ or $i = N_x$ for $j = 1, \ldots, N_y - 1$) needed to solve each set of equations in (9) are set from

$$\begin{aligned} u^*_{0,j} &= \frac{1}{2}\left[\left(1 - \frac{\Delta t}{2}\delta_{\beta,y}\right) u^{n+1}_{0,j} + \left(1 + \frac{\Delta t}{2}\delta_{\beta,y}\right) u^n_{0,j}\right] = 0 \\ u^*_{N_x,j} &= \frac{1}{2}\left[\left(1 - \frac{\Delta t}{2}\delta_{\beta,y}\right) u^{n+1}_{N_x,j} + \left(1 + \frac{\Delta t}{2}\delta_{\beta,y}\right) u^n_{N_x,j}\right] \\ &= \frac{1}{2}\left[\left(1 - \frac{\Delta t}{2}\delta_{\beta,y}\right) B^{n+1}_{N_x,j} + \left(1 + \frac{\Delta t}{2}\delta_{\beta,y}\right) B^n_{N_x,j}\right] \end{aligned} \tag{16}$$

In the following section, we establish the consistency and unconditional stability of this method. We emphasize that the method outlined above will only be $O[(\Delta t)^2] + O(\Delta x) + O(\Delta y)$ accurate. An additional extrapolation step, as discussed later in this paper, is needed to achieve $O[(\Delta t)^2] + O[(\Delta x)^2] + O[(\Delta y)^2]$ accuracy.

4. Consistency and stability of the fractional ADI-CN method

In this section, we demonstrate that the ADI applied to the Crank–Nicolson discretization for the fractional initial-boundary value problem (1) is both consistent and unconditionally stable. Together, these results imply (according to Lax's equivalence theorem) that the method is convergent. Proposition 4.1 below shows that if the exact solution of the superdiffusion equation is sufficiently smooth, then the ADI-CN numerical method is consistent and its truncation error has a Taylor's expansion in powers of the spatial grid size (i.e., Δx and Δy).

Proposition 4.1. *Assume that the solution $u(t,x,y)$ to the fractional differential equation (1) is unique, and that its temporal (i.e., t) partial derivatives up to order 2 and spatial (i.e., x and y) partial derivatives up to order r are in $\mathscr{L}^1(\mathbb{R}^3)$, and its spatial partial derivatives up to order $r-1$ vanish at infinity, where $r > \alpha + \beta + 3$. Then ADI-CN discretization for (1) defined by (8) is consistent, with a truncation error of the order $O[(\Delta t)^2] + O(\Delta x) + O(\Delta y)$. Moreover, this truncation error is of the form $O[(\Delta t)^2] + K\Delta x + O[(\Delta x)^2] + M\Delta y + O[(\Delta y)^2]$, where the coefficients K and M do not depend on the grid sizes Δx or Δy.*

Proof. First note that, as in the classical Crank–Nicolson method, the centered divided difference $[u(t_{n+1}, x_i, y_j) - u(t_n, x_i, y_j)]/\Delta t$ provides an $O[(\Delta t)^2]$ accurate estimate for the $\partial u(t_{n+1/2}, x_i, y_j)/\partial t$.

Next as $r > 5$ for the factor values $\alpha > 1$ and $\beta > 1$, we may apply Proposition 3.1 in Ref. [35] to write

$$\begin{aligned} \delta_{\alpha,x} u^n_{i,j} &= d_{i,j} \frac{\partial^\alpha u(x_i, y_j, t_n)}{\partial x^\alpha} + K\Delta x + O[(\Delta x)^2] \\ \delta_{\beta,y} u^n_{i,j} &= e_{i,j} \frac{\partial^\beta u(x_i, y_j, t_n)}{\partial y^\beta} + M\Delta y + O[(\Delta y)^2] \end{aligned}$$

where the coefficients K and M do not depend on the grid sizes Δx or Δy.

Therefore, the centered Crank–Nicolson finite difference equations (6), or equivalently (7) provide an $O[(\Delta t)^2] + K\Delta x + O[(\Delta x)^2] + M\Delta y + O[(\Delta y)^2]$ estimate for the superdiffusion equation (1).

Next, we invoke Theorem 3.1 in Ref. [24] to conclude that the mixed fractional derivative term

$$[\delta_{\alpha,x}\delta_{\beta,y}]u_{i,j}^n$$

is $O(\Delta x) + O(\Delta y)$ uniformly for $(x, y) \in \mathbb{R}^2$. The ADI-CN finite difference equations (8) differs from (7) by a perturbation equal to

$$\frac{(\Delta t)^2}{4}\delta_{\alpha,x}\delta_{\beta,y}[u_{i,j}^{n+1} - u_{i,j}^n] \tag{17}$$

which can be deduced by distributing the operator products in (8). Since the term $(u_{i,j}^{n+1} - u_{i,j}^n)$ is an $O(\Delta t)$ term, it follows that this perturbation contributes an $O[(\Delta t)^2]$ error component to the truncation error of the fractional Crank–Nicolson finite difference method (6).

Therefore, the ADI-CN finite difference equations defined by (8) have a truncation error also of the form $K\Delta x + O[(\Delta x)^2] + M\Delta y + O[(\Delta y)^2] + O[(\Delta t)^2]$, where the coefficients K and M do not depend on the grid sizes Δx or Δy. □

Next, we investigate the stability of the ADI-CN method. Eq. (8) can be written in the matrix form

$$(I - S)(I - T)U^{n+1} = (I + S)(I + T)U^n + R^{n+1} \tag{18}$$

where the matrices S and T represent the operators $\frac{\Delta t}{2}\delta_{\alpha,x}$ and $\frac{\Delta t}{2}\delta_{\beta,y}$, and

$$U^n = [u_{1,1}^n, u_{2,1}^n, \ldots, u_{N_x-1,1}^n, u_{1,2}^n, u_{2,2}^n, \ldots, u_{N_x-1,2}^n, \ldots, u_{1,N_y-1}^n, u_{2,N_y-1}^n, \ldots, u_{N_x-1,N_y-1}^n]^{\mathrm{T}}$$

and the vector R^{n+1} absorbs the forcing terms $q_{i,j}^{n+1/2}$ and the Dirichlet boundary conditions at time $t = t_{n+1}$ in the discretized equation. The matrices S and T are (large) matrices of size $(N_x - 1)(N_y - 1) \times (N_x - 1)(N_y - 1)$.

Under a commutativity assumption for the operators $\left(1 - \frac{\Delta t}{2}\delta_{\alpha,x}\right)$ and $\left(1 - \frac{\Delta t}{2}\delta_{\beta,y}\right)$ in (8), the ADI-CN method will be shown to be unconditionally stable. The commutativity assumption for these two operators is a common practice in establishing stability of the classical ADI methods (i.e., $\alpha = \beta = 2$) for the diffusion equation (see for example [8]). The commutativity of these operators implies that the matrices S and T commute. For example, if the diffusion coefficients are of the form $d = d(x)$ and $e = e(y)$, then these operators commute.

Proposition 4.2. *The ADI-CN method, defined by (8), is unconditionally stable for* $1 < \alpha < 2$, $1 < \beta < 2$ *if the matrices S and T commute.*

Proof. The matrix S is a $(N_y - 1) \times (N_y - 1)$ block diagonal matrix whose blocks are the square $(N_x - 1) \times (N_x - 1)$ super-triangular A_k matrices resulting from Eq. (9), and so one may write $S = \mathrm{diag}(A_1, \ldots, A_2, A_{N_y-1})$. This is easy to see if we write the ADI system of Eq. (18) as the following equivalent form

$$(I - S)U^* = (I + T)U^n + \frac{1}{2}R^{n+1}$$

$$(I - T)U^{n+1} = (I + S)U^* + \frac{1}{2}R^{n+1}$$

with

$$U^* = [u_{1,1}^*, u_{2,1}^*, \ldots, u_{N_x-1,1}^*, u_{1,2}^*, u_{2,2}^*, \ldots, u_{N_x-1,2}^*, \ldots, u_{1,N_y-1}^*, u_{2,N_y-1}^*, \ldots, u_{N_x-1,N_y-1}^*]^{\mathrm{T}}$$

We observe that the matrix S is a diagonally dominant matrix. At row i, $i = 1, 2, \ldots, (N_x - 1)(N_y - 1)$, the diagonal entry $S_{i,i} = Dg_{\alpha,1} = -D\alpha$, where $D = D_{m,k}$ with $k = [\frac{i-1}{N_x-1}] + 1$ and $m = i - (k - 1)(N_x - 1)$, and $D_{m,k}$ is defined in (12). The sum of the absolute value of the off-diagonal entries on this row i of matrix S is given by

$$\sum_{j=0, j\neq 1}^{m} Dg_{\alpha,j} < D\alpha$$

This is because $g_{\alpha,1} = -\alpha$, and for $1 < \alpha < 2$ and $j \neq 1$ we have $g_{\alpha,j} > 0$, as well as $\sum_{j=0}^{\infty} g_{\alpha,j} = 0$, see [35]. Therefore, according to Greschgorin theorem, the eigenvalues of the matrix S have negative real parts. Next, note that λ is an eigenvalue of S if and only if $(1-\lambda)$ is an eigenvalue of the matrix $(I-S)$, if and only if $(1+\lambda)/(1-\lambda)$ is an eigenvalue of the matrix $(I-S)^{-1}(I+S)$. We observe that the first part of this statement implies that all the eigenvalues of the matrix $(I-S)$ have a magnitude larger than 1, and thus this matrix is invertible. This implies that every eigenvalue of the matrix $(I-S)^{-1}(I+S)$ has a modulus less than 1. Therefore, the spectral radius of the matrix $(I-S)^{-1}(I+S)$ is less than 1.

Similarly, the matrix T is a diagonally-dominant block super-triangular matrix of $(N_y-1)\times(N_y-1)$ blocks whose non-zero blocks are the square $(N_x-1)\times(N_x-1)$ diagonal matrices resulting from Eq. (10). At row i, the diagonal entry $T_{i,i} = Eg_{\beta,1} = -E\beta$, where $E = E_{m,k}$ with m and k as defined above for the matrix S, and $E_{m,k}$ defined by (13). For this row i, the sum of the absolute value of the off-diagonal entries is bounded as before

$$\sum_{j=0, j\neq 1}^{m} Eg_{\beta,j} < E\beta$$

Again, the Greschgorin theorem is invoked to conclude that and the matrix $(I-T)$ is invertible, and the spectral radius of the matrix $(I-T)^{-1}(I+T)$ is less than 1.

Note that the linear system of equations imply that an error ϵ^0 in U^0 results in an error ϵ^n at time t_n in U^n given by

$$\epsilon^n = [(I-T)^{-1}(I-S)^{-1}(I+S)(I+T)]^n \epsilon^0$$

As the matrices S and T commute, we may re-write the above as:

$$\epsilon^n = [(I-S)^{-1}(I+S)]^n [(I-T)^{-1}(I+T)]^n \epsilon^0$$

Since the spectral radius of each matrix $[(I-S)^{-1}(I+S)]$ and $[(I-T)^{-1}(I+T)]$ is less than one, it follows that $[(I-S)^{-1}(I+S)]^n \to 0$ and $[(I-T)^{-1}(I+T)]^n \to 0$ as $n \to \infty$, where 0 is the zero (or null) matrix (see Theorem 1.4 in [37]). Therefore, the ADI-CN method is stable. □

The proper application of the ADI-CN method as discussed above, yields a numerical solution that is only $O[(\Delta t)^2] + O(\Delta x) + O(\Delta y)$ accurate. Furthermore, the second-order convergence in Δt will usually be masked in actual computations by the first-order spatial errors.

The asymptotic expansion of the truncation errors, in the form $O[(\Delta t)^2] + K\Delta x + O[(\Delta x)^2] + M\Delta y + O[(\Delta y)^2]$ suggests the application of a Richardson extrapolation step to gain second-order accuracy in the spatial directions.

To improve spatial convergence order for non-integer values of $1 < \alpha < 2$ and $1 < \beta < 2$, we employ an extrapolation method only at the timestep, where the numerical solution is desired in the spatial directions. If the Crank–Nicolson method is applied on a (coarse) grid, with spatial grids of $h_x = \Delta x$, $h_y = \Delta y$, and then again on a (fine) grid with $h_x/2$ and $h_y/2$, the Richardson extrapolation method (see, e.g., [11]) may be used to get a solution with local truncation error $O[(\Delta t)^2] + O[(\Delta x)^2] + O[(\Delta y)^2]$. The refinement of the grid is only in the spatial direction, with the time grid remaining unchanged. In this way, the extrapolated solution is computed from $U_{t_n,x} = 2U_{t_n,x,h_x/2,y,h_y/2} - U_{t_n,x,h_x,y,h_y}$, where (x,y) is a common grid point on both the coarse and the fine meshes, and $U_{t_n,x,h_x,y,h_y}, U_{t_n,x,h_x/2,y,h_y/2}$ denote the Crank–Nicolson solutions at the grid point (x,y) on the coarse grid (h_x, h_y) and the fine grid ($h_x/2$, $h_y/2$), respectively. In other words, $x = x_i$ and $y = y_j$ on the coarse grid, while $x = x_{2i}$ and $y = y_{2J}$ on the fine grid.

We emphasize that the boundary conditions for the intermediate solution u^* should be set according to Eq. (16). Otherwise, the numerical solution will fail to be linearly convergent, and the extrapolation step will not produce a second-order accurate numerical estimate.

Finally, we remark that a similar approach can also be useful for the more general fractional diffusion equation (3), replacing the operators $\delta_{\alpha,x}$ and $\delta_{\beta,y}$ by their two-sided analogues. See [23] for details on the extension to two-sided fractional derivatives in the one-dimensional case. For the full two-sided Eq. (3) in two dimensions with $0 < p_1, p_2 < 1$ we require zero Dirichlet boundary conditions on all four sides of the rectangular domain in order to truncate the Grünwald approximation formula for the negative and positive fractional

derivatives. Extensions to non-zero boundary conditions and more general (mixing) fractional derivatives [18] remain as interesting open problems.

5. A numerical example

The fractional differential equation

$$\frac{\partial u(x,y,t)}{\partial t} = d(x,y)\frac{\partial^{1.8} u(x,y,t)}{\partial x^{1.8}} + e(x,y)\frac{\partial^{1.6} u(x,y,t)}{\partial y^{1.6}} + q(x,y,t)$$

was considered on a finite rectangular domain $0 < x < 1$, $0 < y < 1$, for $0 \leqslant t \leqslant T_{\text{end}}$. The diffusion coefficients are

$$d(x,y) = \Gamma(2.2)x^{2.8}y/6$$

and

$$e(x,y) = 2xy^{2.6}/\Gamma(4.6)$$

and the forcing function is

$$q(x,y,t) = -(1+2xy)e^{-t}x^3y^{3.6}$$

with the initial conditions

$$u(x,y,0) = x^3y^{3.6}$$

and Dirichlet boundary conditions on the rectangle in the form $u(0,y,t) = u(x,0,t) = 0$, $u(1,y,t) = e^{-t}y^{3.6}$, and $u(x,1,t) = e^{-t}x^3$ for all $t \geqslant 0$. The exact solution to this two-dimensional fractional diffusion equation is given by

$$u(x,y,t) = e^{-t}x^3y^{3.6}$$

which may be verified by direct differentiation and substitution in the fractional differential equation, using the formula

$$\frac{\partial^\alpha}{\partial x^\alpha}[x^p] = \frac{\Gamma(p+1)}{\Gamma(p+1-\alpha)}x^{p-\alpha}$$

for this Riemann–Liouville fractional derivative (2) with $L = 0$.

Table 1 shows the magnitude of the largest numerical error, at time $t = 1.0$, between the exact analytical solution and the numerical solution obtained by applying the ADI-CN method discussed in this paper for the non-extrapolated solution and the extrapolated solution. The algorithm was implemented using the Intel Fortran compiler on a Dell Pentium PC. All computations were performed in single precision. The second column shows the maximum error for the un-extrapolated Crank–Nicolson method. As the gridsize is halved, the maximum error in the un-extrapolated Crank–Nicolson numerical solution is also halved (first-order convergence). The third column shows the maximum error for the extrapolated Crank–Nicolson method. The extrapolated solution is obtained by first computing a second numerical solution on a finer spatial grid obtained by keeping the same timestep (Δt) but halving the spatial gridsizes. This fine grid solution is then used to obtain an extrapolated solution on the coarse grid as discussed earlier. The last column in the table

Table 1
Maximum error behavior for the example problem at time $T_{\text{end}} = 1$, contrasting the first-order convergence of the original method with the second-order convergence of the extrapolated method

$\Delta t = \Delta x = \Delta y$	Max error before extrapolation	Max error after extrapolation
1/5	3.98493E − 3	1.05564E − 3
1/10	2.02702E − 3	2.61694E − 4
1/20	1.02996E − 3	6.57067E − 5
1/40	5.14504E − 4	1.55866E − 5

shows that the maximum error in the extrapolated Crank–Nicolson method decreases by (approximately) a factor of 4 as the gridsize is halved.

This problem was previously considered for a first-order ADI-implicit Euler method, see [24]. A comparison of the results in Table 1 in this paper with the corresponding Table 1 in [24] shows that the extrapolated ADI-CN provides significant improvement in the accuracy of the numerical solution.

We also remark that this example problem does not meet the requirement for the commutativity of the operators in (8) which was used to establish the stability of the ADI-CN method. The quadratic order of convergence for the numerical solution for this example suggests that the stability results may be extended beyond the requirement for commutativity.

6. Conclusions

Although second-order finite difference estimates for fractional derivatives have been elusive, higher order accuracy convergent methods for superdiffusion equation are achievable through the application of extrapolation schemes applied to the basic lower order ADI-CN method obtained by the use of shifted Grünwald estimates. We emphasize again that the standard (i.e., non-shifted) Grünwald formula generally leads to unstable methods. Additionally, to maintain proper convergence order, and to successfully apply the Richardson extrapolation to achieve higher order accuracy in the ADI-CN method, the Dirichlet boundary conditions for the intermediate solution should be treated carefully.

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