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The accuracy and stability of an implicit solution method for the fractional diffusion equation

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Abstract

We have investigated the accuracy and stability of an implicit numerical scheme for solving the fractional diffusion equation. This model equation governs the evolution for the probability density function that describes anomalously diffusing particles. Anomalous diffusion is ubiquitous in physical and biological systems where trapping and binding of particles can occur. The implicit numerical scheme that we have investigated is based on finite difference approximations and is straightforward to implement. The accuracy of the scheme is $O(\Delta x^2)$ in the spatial grid size and $O(\Delta t^{1+\gamma})$ in the fractional time step, where $0 \leqslant 1-\gamma < 1$ is the order of the fractional derivative and $\gamma = 1$ is standard diffusion. We have provided algebraic and numerical evidence that the scheme is unconditionally stable for $0 < \gamma \leqslant 1$.

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1. Introduction

In this paper we consider the accuracy and stability of an implicit numerical solution scheme for the fractional diffusion equation (see for example [1,2])

$$\frac{\partial y}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \frac{\partial^2 y}{\partial x^2} \tag{1}$$

with $0 < \gamma \leqslant 1$. In this equation the expression

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$$\frac{\partial^{-\gamma} f}{\partial t^{-\gamma}} = \frac{1}{\Gamma(\gamma)} \int_0^t \frac{f(s)}{(t-s)^{1-\gamma}} \, \mathrm{d}s \tag{2}$$

denotes the Riemann–Liouville fractional integral of order γ of the function $f(t)$ and

$$\frac{\partial^{1-\gamma} f}{\partial t^{1-\gamma}} = \frac{\mathrm{d}}{\mathrm{d}t} \frac{1}{\Gamma(\gamma)} \int_0^t \frac{f(s)}{(t-s)^{1-\gamma}} \, \mathrm{d}s \tag{3}$$

denotes the Riemann–Liouville fractional derivative of order $1-\gamma$ of the function $f(t)$. The fractional diffusion equation, Eq. (1), which has been derived from continuous time random walks (see for example [1], and references therein) is the evolution equation for the probability density function that describes particles diffusing with mean square displacement

$$\langle x^2(t) \rangle \sim t^{\gamma}. \tag{4}$$

Standard diffusion corresponds to $\gamma = 1$ and the parameter range $0 < \gamma < 1$ corresponds to anomalous sub-diffusion. Related equations of importance are the fractional Fokker–Planck equation [3] for anomalous diffusion in an external field, and the fractional reaction–diffusion equation [4,5] for anomalous diffusion with sources and sinks. The theoretical justification for the fractional diffusion equation, for modelling systems with anomalous diffusion, together with the abundance of physical and biological experiments demonstrating the prevalence of anomalous sub-diffusion (see for example [6–10]) has led to an intensive effort in recent years to find accurate and stable methods of solution that are also straightforward to implement.

Numerous numerical methods have been employed to solve fractional order ordinary differential equations [11–19] but relatively few have been developed for fractional order partial differential equations. In this paper we have considered a numerical method for the fractional diffusion equation, and related equations. A centred difference approximation is used to discretize the spatial Laplacian, the backwards Euler approximation is used to discretize the first order time derivative and a standard discretization (known as the L1 scheme [20]) is used to approximate the fractional order time derivative. This leads to a fully implicit finite difference scheme.

An explicit method for solving the fractional diffusion equation was developed recently by Yuste and Acedo [21]. Their method employs the Grünwald–Letnikov definition for the fractional derivative in contrast to the Riemann–Liouville definition we use. An explicit method involving the Riemann–Liouville definition would have difficulties at $t = 0$ because the Riemann–Liouville fractional derivative of a function which is non-zero at $t = 0$ is unbounded [22]. This behaviour is reproduced in the L1 scheme. An advantage of the implicit method is that it is unconditionally stable. The explicit method of Yuste and Acedo [21] is conditionally stable.

Other finite difference methods that have been developed for fractional partial differential equations include; explicit and semi-implicit methods for solving partial differential equations with fractional order spatial derivatives [23]; and an implicit numerical method for solving the fractional wave equation [24,25]

$$\frac{\partial y}{\partial t} = \frac{\partial^{-\gamma}}{\partial t^{-\gamma}} \frac{\partial^2 y}{\partial x^2}. \tag{5}$$

Fractional order partial differential equations can also be solved numerically after first re-writing them as integro-differential equations. For example

$$\frac{\partial u}{\partial t} + \int_0^t \beta(t-s) A u(s) \, \mathrm{d}s = f(t) \tag{6}$$

reduces to the fractional wave equation if:

$$Au = -\frac{\partial^2 u}{\partial x^2}, \tag{7}$$

$$\beta(t) = \frac{t^{\gamma-1}}{\Gamma(\gamma)} \tag{8}$$

and $f(t) = 0$. In this formulation finite element methods have been used to discretize the spatial derivatives and the time derivative has been discretized using either the standard Euler backward difference [26–28], second order backward difference [28,29] or Crank–Nicolson methods [27,28]. The integrals in these schemes are evaluated using numerical quadrature such as the right-handed rectangle rule [28,29], trapezoidal rule [28], mid-point rule [29], or convolution quadrature [27,30]. It is interesting to note that the quadrature weights of the convolution quadrature scheme are similar to the weights of the Grünwald–Letnikov definition of the fractional derivative [22]. More recently, a numerical scheme that employs a Laplace transform to remove the need to evaluate the convolution integral has been developed [31]. This method is rapidly convergent for linear equations involving fractional derivatives or integrals but not for nonlinear problems, such as fractional reaction–diffusion equations, to which our implicit method can also be applied [32].

The plan of the remainder of this paper is as follows. In the following section we develop the governing equations for the implicit method. The accuracy of the method is determined in Section 3. The stability of the method is determined in Section 4 and the paper concludes with a summary in Section 5.

2. Numerical method

In this section we introduce our implicit numerical method for solving the fractional diffusion equation

$$\frac{\partial y}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \frac{\partial^2 y}{\partial x^2}, \quad 0 \leqslant x \leqslant L \tag{9}$$

with the zero flux boundary conditions:

$$\left.\frac{\partial y}{\partial x}\right|_{x=0} = 0, \quad t \geqslant 0, \tag{10}$$

$$\left.\frac{\partial y}{\partial x}\right|_{x=L} = 0, \quad t \geqslant 0 \tag{11}$$

and the initial condition

$$y(x, 0) = g(x), \quad 0 \leqslant x \leqslant L. \tag{12}$$

In the following we take an equally spaced 1-D mesh of N points for the spatial domain, $0 \leqslant x \leqslant L$, and M time steps for the temporal domain. We shall denote the spatial grid points by

$$x_i = (i-1)\Delta x, \quad 1 \leqslant i \leqslant N, \tag{13}$$

and the temporal grid points by

$$t_k = (k-1)\Delta t, \quad 1 \leqslant k \leqslant M, \tag{14}$$

where the grid spacing is simply $\Delta x = L/(N-1)$ in the spatial domain and Δt in the temporal domain.

To approximate the fractional diffusion equation we use the Euler backward difference for the first order time derivative

$$\frac{\partial y(x_i,t_{k+1})}{\partial t} \sim \frac{y_i^{k+1}-y_i^k}{\Delta t} + \mathrm{O}(\Delta t), \tag{15}$$

where we have denoted $y(x_i,t_k) \approx y_i^k$. The second order spatial derivative is approximated using the second order centred difference scheme evaluated at the next time step

$$\frac{\partial^2 y(x_i,t_{k+1})}{\partial x^2} \sim \frac{y_{i+1}^{k+1}-2y_i^{k+1}+y_{i-1}^{k+1}}{\Delta x^2} + \mathrm{O}(\Delta x^2). \tag{16}$$

The fractional derivative was approximated using the L1 scheme (Oldham and Spanier [20]) which is valid for $0 < \gamma \leqslant 1$. Explicitly, the L1 approximation for the fractional derivative of order $1-\gamma$ with respect to time at $t = t_{k+1}$ is given by [20]

$$\frac{\partial^{1-\gamma} y(x_i,t_{k+1})}{\partial t^{1-\gamma}} \approx \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\frac{\gamma y_i^1}{k^{1-\gamma}} + \sum_{l=1}^{k}\left(y_i^{l+1}-y_i^l\right)\left((k-l+1)^\gamma-(k-l)^\gamma\right)\right\}, \tag{17}$$

where Δt is the step length in time and $\Gamma(x)$ is the Gamma function. Note the L1 scheme assumes equally spaced time steps, i.e.

$$y(t_k) = y((k-1)\Delta t), \quad k = 1,2,\ldots \tag{18}$$

but it could be applied to variable time steps.

Our implicit numerical method for the fractional diffusion equation is determined by the finite difference equations ($1 < i < N$)

$$\begin{aligned} y_i^{k+1}(1+2\rho) - \rho y_{i+1}^{k+1} - \rho y_{i-1}^{k+1} &= y_i^k(1+2\rho) - \rho y_{i+1}^k - \rho y_{i-1}^k + \rho\frac{\gamma}{k^{1-\gamma}}\nabla y_i^1 \\ &\quad + \rho\sum_{l=1}^{k-1}\left(\nabla y_i^{l+1}-\nabla y_i^l\right)\left((k-l+1)^\gamma-(k-l)^\gamma\right), \end{aligned} \tag{19}$$

where $\rho = \Delta t^\gamma/\Delta x^2\Gamma(1+\gamma)$ and

$$\nabla y_i^k = y_{i+1}^k - 2y_i^k + y_{i-1}^k. \tag{20}$$

The zero flux boundary conditions are implemented after using a second order difference scheme for the spatial derivative

$$\frac{\partial y_i}{\partial x} = \frac{y_{i+1}^k - y_{i-1}^k}{2\Delta x}, \tag{21}$$

so that $y_0^k = y_2^k$ and $y_{N+1}^k = y_{N-1}^k$. Thus we have a system of N equations in N unknowns to be solved at each time step. Note we need to store the value ∇y_i^k for all k. The finite difference equations can be written in the form

$$\mathbf{A}\underset{\sim}{y}^{k+1} = \mathbf{A}\underset{\sim}{y}^k + \underset{\sim}{f}, \tag{22}$$

where $\mathbf{A}$ is a constant tridiagonal matrix and

$$f_i = \rho\frac{\gamma}{k^{1-\gamma}}\nabla y_i^1 + \rho\sum_{l=1}^{k-1}\left(\nabla y_i^{l+1}-\nabla y_i^l\right)\left((k-l+1)^\gamma-(k-l)^\gamma\right). \tag{23}$$

To update the solution we require only to solve

$$\mathbf{A}\,\Delta\underset{\sim}{y} = \underset{\sim}{f} \tag{24}$$

and use the updating formula

$$\underset{\sim}{y}^{k+1} = \underset{\sim}{y}^{k} + \Delta\underset{\sim}{y}. \tag{25}$$

Since **A** is constant with respect to time its decomposition is only required once.

Most of the computation and storage required in the above method is the evaluation of the fractional derivative. The approximations of the second derivative, ∇y_i^k, need to be stored for each grid point, i, and time step, k, to be available for the summation in the evaluation in Eq. (23). The summation itself requires considerable computational effort which increases with each time step. The number of time steps becomes a significant problem when the duration of the numerical simulation becomes large but a small time step is required for accuracy. This is not a serious problem for the linear fractional diffusion equation where the solution quickly decays to zero however it does present problems for simulations involving systems of nonlinear fractional reaction–diffusion equations where the solutions may not decay quickly to zero but may instead display Turing patterns [5,32]. These problems become even more severe in higher dimensions than the 1-D case considered in this paper.

3. Accuracy

In this section we evaluate the accuracy of our implicit numerical scheme. First we determine the accuracy of the L1 scheme [20]

$$\frac{\mathrm{d}^{1-\gamma}y(t_{k+1})}{\mathrm{d}t^{1-\gamma}} \approx \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\left\{\frac{\gamma y^1}{k^{1-\gamma}} + \sum_{l=1}^{k}\left(y^{l+1}-y^l\right)\left((k-l+1)^\gamma-(k-l)^\gamma\right)\right\}, \tag{26}$$

where $y^k = y((k-1)\Delta t)$ and $0 < \gamma \leqslant 1$ and we assume that $y(t)$ can be expanded in a Taylor series around $t = 0$ with an integral remainder term, i.e.

$$y(t) = y(0) + ty'(0) + \int_0^t y''(s)(t-s)\,\mathrm{d}s. \tag{27}$$

If we apply the fractional differential operator to this expression we find

$$\frac{\mathrm{d}^{1-\gamma}y}{\mathrm{d}t^{1-\gamma}} = y(0)\frac{\mathrm{d}^{1-\gamma}(1)}{\mathrm{d}t^{1-\gamma}} + y'(0)\frac{\mathrm{d}^{1-\gamma}(t)}{\mathrm{d}t^{1-\gamma}} + \frac{\mathrm{d}^{1-\gamma}}{\mathrm{d}t^{1-\gamma}}\int_0^t y''(s)(t-s)\,\mathrm{d}s, \tag{28}$$

where

$$\frac{\mathrm{d}^{1-\gamma}(1)}{\mathrm{d}t^{1-\gamma}} = \frac{t^{\gamma-1}}{\Gamma(\gamma)} \tag{29}$$

and

$$\frac{\mathrm{d}^{1-\gamma}(t)}{\mathrm{d}t^{1-\gamma}} = \frac{t^{\gamma}}{\Gamma(1+\gamma)}. \tag{30}$$

To evaluate the fractional derivative of the convolution

$$\int_0^t y''(s)(t-s)\,\mathrm{d}s, \tag{31}$$

we use the general result [22]

$$\frac{\mathrm{d}^{1-\gamma}}{\mathrm{d}t^{1-\gamma}}\int_0^t f(s)K(t-s)\,\mathrm{d}s=\int_0^t \frac{\mathrm{d}^{1-\gamma}(K)}{\mathrm{d}s^{1-\gamma}}(s)f(t-s)\,\mathrm{d}s+\lim_{s\to+0}f(t-s)\frac{\mathrm{d}^{-\gamma}(K)}{\mathrm{d}s^{-\gamma}}(s) \tag{32}$$

and so we find

$$\frac{\mathrm{d}^{1-\gamma}}{\mathrm{d}t^{1-\gamma}}\int_0^t y''(s)(t-s)\,\mathrm{d}s=\int_0^t \frac{\mathrm{d}^{1-\gamma}(s)}{\mathrm{d}s^{1-\gamma}}(s)y''(t-s)\,\mathrm{d}s+\lim_{s\to+0}y''(t-s)\frac{\mathrm{d}^{-\gamma}(s)}{\mathrm{d}s^{-\gamma}}(s), \tag{33}$$

which simplifies to

$$\frac{\mathrm{d}^{1-\gamma}}{\mathrm{d}t^{1-\gamma}}\int_0^t y''(s)(t-s)\,\mathrm{d}s=\int_0^t y''(s)\frac{(t-s)^{\gamma}}{\Gamma(1+\gamma)}\,\mathrm{d}s. \tag{34}$$

Eq. (28) can then be expressed as

$$\frac{\mathrm{d}^{1-\gamma}(y)}{\mathrm{d}t^{1-\gamma}}=\frac{t^{\gamma-1}}{\Gamma(\gamma)}y(0)+\frac{t^{\gamma}}{\Gamma(1+\gamma)}y'(0)+\frac{1}{\Gamma(1+\gamma)}\int_0^t (t-s)^{\gamma}y''(s)\,\mathrm{d}s. \tag{35}$$

The accuracy of the L1 scheme can be determined by comparing the above result with the result obtained by applying the L1 scheme approximation of the fractional derivative to Eq. (27). Thus we need to evaluate the L1 approximations operating on the functions 1, t and the convolution. To simplify the algebra we rewrite the L1 scheme as

$$\left.\frac{\mathrm{d}^{1-\gamma}(y)}{\mathrm{d}t^{1-\gamma}}\right|_{\mathrm{L1}}=\frac{y(0)t_{k+1}^{\gamma-1}}{\Gamma(\gamma)}+\frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{l=0}^{k}w_l y((k-l)\Delta t), \tag{36}$$

where

$$w_l=\begin{cases}1, & l=0,\\ -k^{\gamma}+(k-1)^{\gamma}, & l=k,\\ (l+1)^{\gamma}-2l^{\gamma}+(l-1)^{\gamma}, & 1\leqslant l<k.\end{cases} \tag{37}$$

The application of the L1 scheme operating on $y(t) = 1$ evaluated at $t_{k+1} = k\Delta t$ is thus

$$\left.\frac{\mathrm{d}^{1-\gamma}(1)}{\mathrm{d}t^{1-\gamma}}\right|_{\mathrm{L1}}=\frac{t_{k+1}^{\gamma-1}}{\Gamma(\gamma)}+\frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{l=0}^{k}w_l \tag{38}$$

which simplifies, with the identity

$$\sum_{l=0}^{k}w_l=0 \tag{39}$$

to give

$$\left.\frac{\mathrm{d}^{1-\gamma}(1)}{\mathrm{d}t^{1-\gamma}}\right|_{\mathrm{L1}}=\frac{t_{k+1}^{\gamma-1}}{\Gamma(\gamma)}. \tag{40}$$

We now consider the application of the L1 scheme operating on t

$$\left.\frac{\mathrm{d}^{1-\gamma}(t)}{\mathrm{d}t^{1-\gamma}}\right|_{\mathrm{L1}}=\frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{l=0}^{k}w_l(k-l)\Delta t. \tag{41}$$

This simplifies using the identities

$$\sum_{l=0}^{k-1} l w_l = k^\gamma (k-1) - (k-1)^\gamma k \tag{42}$$

and

$$\sum_{l=0}^{k-1} w_l = k^\gamma - (k-1)^\gamma \tag{43}$$

to give

$$\left.\frac{\mathrm{d}^{1-\gamma}(t)}{\mathrm{d}t^{1-\gamma}}\right|_{\mathrm{L1}} = \frac{t_{k+1}^{\gamma}}{\Gamma(1+\gamma)}. \tag{44}$$

Note both of these results are identical to the results of the corresponding fractional derivatives of 1 and t at $t = t_{k+1}$. Hence any error in the L1 scheme must arise from the error in the application of the L1 scheme to the convolution term

$$\int_0^t y''(s)(t-s)\,\mathrm{d}s. \tag{45}$$

Applying the L1 scheme to this term we find

$$\left.\frac{\mathrm{d}^{1-\gamma}}{\mathrm{d}t^{1-\gamma}}\left(\int_0^t y''(s)(t-s)\,\mathrm{d}s\right)\right|_{\mathrm{L1}} = \frac{t_{k+1}^{\gamma-1}}{\Gamma(\gamma)} \lim_{t\to 0}\int_0^t y''(s)(t-s)\,\mathrm{d}s + \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{l=0}^{k} w_l \int_0^{(k-l)\Delta t} y''(s)((k-l)\Delta t - s)\,\mathrm{d}s. \tag{46}$$

By noting that the limit and the term $l = k$ of the sum are both zero and by breaking the interval of integration into Δt steps the previous equation can be rewritten as

$$\left.\frac{\mathrm{d}^{1-\gamma}}{\mathrm{d}t^{1-\gamma}}\left(\int_0^t y''(s)(t-s)\mathrm{d}s\right)\right|_{\mathrm{L1}} = \frac{\Delta t^{\gamma-1}}{\Gamma(\gamma+1)}\sum_{l=0}^{k-1} w_l \sum_{n=0}^{k-l-1}\int_{n\Delta t}^{(n+1)\Delta t} y''(s)((k-l)\Delta t - s)\mathrm{d}s. \tag{47}$$

Changing the order of summation we find

$$\left.\frac{\mathrm{d}^{1-\gamma}}{\mathrm{d}t^{1-\gamma}}\left(\int_0^t y''(s)(t-s)\mathrm{d}s\right)\right|_{\mathrm{L1}} = \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{n=0}^{k-1}\int_{n\Delta t}^{(n+1)\Delta t} y''(s)\sum_{l=0}^{k-n-1} w_l((k-l)\Delta t - s)\mathrm{d}s. \tag{48}$$

Now using the identities

$$\sum_{l=0}^{k-n-1} w_l = (k-n)^\gamma - (k-n-1)^\gamma \tag{49}$$

and

$$\sum_{l=0}^{k-n-1} l w_l = (k-n)^\gamma (k-n-1) - (k-n-1)^\gamma (k-n). \tag{50}$$

Eq. (48) simplifies to

$$\left.\frac{\mathrm{d}^{1-\gamma}}{\mathrm{d}t^{1-\gamma}}\left(\int_0^t y''(s)(t-s)\mathrm{d}s\right)\right|_{\mathrm{L1}} = \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{n=0}^{k-1}\int_{n\Delta t}^{(n+1)\Delta t} y''(s)\{(k-n)^\gamma[(n+1)\Delta t - s] - (k-n-1)^\gamma[n\Delta t - s]\}\mathrm{d}s. \tag{51}$$

The error in using the L1 scheme on Eq. (27) compared with the exact value of the fractional derivative given in Eq. (35) can now be evaluated

$$\left|\frac{d^{1-\gamma}(y)}{dt^{1-\gamma}} - \frac{d^{1-\gamma}(y)}{dt^{1-\gamma}}\bigg|_{L1}\right| = \left|\int_0^{k\Delta t} y''(s)\frac{(t-s)^{\gamma}}{\Gamma(1+\gamma)}ds - \frac{\Delta t^{\gamma-1}}{\Gamma(1+\gamma)}\sum_{n=0}^{k-1}\int_{n\Delta t}^{(n+1)\Delta t} y''(s)\{(k-n)^{\gamma}[(n+1)\Delta t - s] - (k-n-1)^{\gamma}[n\Delta t - s]\}ds\right|, \tag{52}$$

or equivalently

$$\left|\frac{d^{1-\gamma}(y)}{dt^{1-\gamma}} - \frac{d^{1-\gamma}(y)}{dt^{1-\gamma}}\bigg|_{L1}\right| = \left|\sum_{n=0}^{k-1}\int_{n\Delta t}^{(n+1)\Delta t}\frac{y''(s)}{\Gamma(1+\gamma)}\left[(t-s)^{\gamma} - \Delta t^{\gamma-1}\{(k-n)^{\gamma}[(n+1)\Delta t - s] - (k-n-1)^{\gamma}[n\Delta t - s]\}\right]ds\right|. \tag{53}$$

Now denoting the maximum absolute value of the second derivative by

$$M_n = \max_{n\Delta t \leqslant s \leqslant (n+1)\Delta t} |y''(s)|, \tag{54}$$

the error becomes

$$\left|\frac{d^{1-\gamma}(y)}{dt^{1-\gamma}} - \frac{d^{1-\gamma}(y)}{dt^{1-\gamma}}\bigg|_{L1}\right| \leqslant \sum_{n=0}^{k-1}\frac{M_n}{\Gamma(1+\gamma)}\left|\int_{n\Delta t}^{(n+1)\Delta t}\left[(t-s)^{\gamma} - \Delta t^{\gamma-1}\{(k-n)^{\gamma}[(n+1)\Delta t - s] - (k-n-1)^{\gamma}[n\Delta t - s]\}\right]ds\right|. \tag{55}$$

The remaining integrals are straightforward so that

$$\left|\frac{d^{1-\gamma}(y)}{dt^{1-\gamma}} - \frac{d^{1-\gamma}(y)}{dt^{1-\gamma}}\bigg|_{L1}\right| \leqslant \sum_{n=0}^{k-1}\frac{M_n\Delta t^{1+\gamma}}{2\Gamma(2+\gamma)}[(k-n)^{\gamma}(2(k-n-1)+1-\gamma) - (k-n-1)^{\gamma}(2(k-n)-1+\gamma)]. \tag{56}$$

If we now denote the maximum value of M_n by M and simplify the summation we arrive at

$$\left|\frac{d^{1-\gamma}(y)}{dt^{1-\gamma}} - \frac{d^{1-\gamma}(y)}{dt^{1-\gamma}}\bigg|_{L1}\right| \leqslant \frac{M\Delta t^{1+\gamma}}{2\Gamma(2+\gamma)}\xi(k,\gamma), \tag{57}$$

where

$$\xi(k,\gamma) = k^{\gamma}[2(k-1)+1-\gamma] - 2(1+\gamma)\sum_{n=1}^{k-1} n^{\gamma}. \tag{58}$$

It immediately follows from Eq. (58) that $\xi(k,0) = 1$ and $\xi(k,1) = 0$ so the error in taking the first order derivative ($\gamma = 0$) is of order Δt and the L1 scheme is the identity operator for $\gamma = 1$. Note the function $\xi(k,\gamma)$ can be rewritten in terms of the Riemann Zeta function $\zeta(-\gamma)$ for large k and $\gamma < 1$

$$\xi(k,\gamma) \sim -2(1+\gamma)\zeta(-\gamma) - \frac{(1+\gamma)\gamma}{6}k^{\gamma-1} + O(k^{\gamma-3}). \tag{59}$$

The function $\xi(k,\gamma)$ is then bounded by

$$\xi(k,\gamma) \leqslant -2(1+\gamma)\zeta(-\gamma) \leqslant \frac{3-2\gamma}{3} \tag{60}$$

for $0 \leqslant \gamma \leqslant 1$ which shows the L1 scheme approximation is $O(\Delta t^{1+\gamma})$ for functions that can be expressed as a Taylor series. The error in evaluating the fractional derivative of the second spatial derivative is then

$$\left|\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{\partial^2 y}{\partial x^2} - \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{\delta^2 y_j}{\Delta x^2}\bigg|_{\mathrm{L1}}\right| \leqslant \left|\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{\partial^2 y}{\partial x^2} - \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{\partial^2 y}{\partial x^2}\bigg|_{\mathrm{L1}}\right| + \left|\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{\partial^2 y}{\partial x^2}\bigg|_{\mathrm{L1}} - \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\frac{\nabla y_i}{\Delta x^2}\bigg|_{\mathrm{L1}}\right|$$
$$\leqslant \frac{M\Delta t^{1+\gamma}}{2\Gamma(2+\gamma)}\xi(k,\gamma) + \left|\frac{\mathrm{d}^{1-\gamma}(M^*)}{\mathrm{d}t^{1-\gamma}}\bigg|_{\mathrm{L1}}\right|\Delta x^2, \tag{61}$$

where:

$$\nabla y_i = y_{i+1} - 2y_i + y_{i-1}, \tag{62}$$

$$M = \max_{0\leqslant t\leqslant k\Delta t}\left|\frac{\partial^4 y}{\partial x^2 \partial t^2}\right| \tag{63}$$

and

$$M^* = \frac{1}{12}\max\left|\frac{\partial^4 y}{\partial x^4}\right|. \tag{64}$$

As a simple test of the above error estimates for the accuracy of the L1 scheme we have compared results from a numerical implementation of the L1 scheme with the exact fractional calculus results for the test function $y(t) = t^{\nu}$. The difference between these results at $t = 1$ is plotted as a function of Δt on a log–log plot in Fig. 1. The left figure shows the error in the case $\nu = 2$ for various values of γ. The straight lines in this figure have slopes of $1 + \gamma$ in agreement with the theoretical analysis. The right figure shows the error in the case $\gamma = 0.5$ for different values of $\nu \geqslant 0.5$. The straight lines all have a slope of $1 + 1/2$ so that we again recover the theoretical result that the error is $O(\Delta t^{1+\gamma})$ even though for values of $\nu < 1$ the Taylor

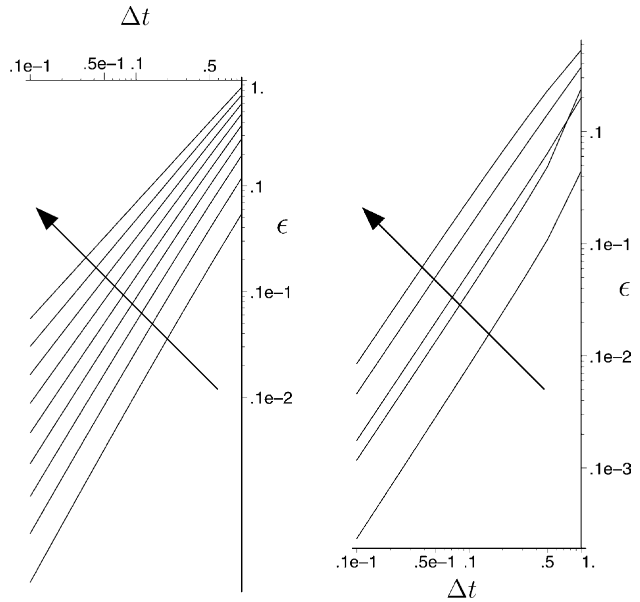

Fig. 1. Comparison of the absolute error, ε, in using the L1 scheme to evaluate the fractional derivative of order $1 - \gamma$ of t^{ν} at $t = 1$. (a) Error in calculation for $\nu = 2.0$ and $\gamma = 0.1(0.1)0.9$ where γ decreases in the direction of the arrow. (b) Error in calculation for $\gamma = 0.5$ where the direction of the arrow indicates the order of $\nu = 0.9, 0.5, 1.5, 2.0, 2.5$. For small Δt the error is of $O(\Delta t^{1+\gamma})$.

expansion in Eq. (27) does not hold and thus the theoretical error estimate does not necessarily hold in this case.

In summary, the overall accuracy of our implicit numerical method is $O(\Delta x^2)$ in space and $O(\Delta t^{1+\gamma})$ in the fractional time derivative.

We have further investigated the accuracy of our numerical scheme by making direct comparisons between numerical simulations and algebraic solutions for the fractional diffusion equation on a fixed domain. These comparisons provide estimates of the global error as a function of Δt.

The solution to the fractional diffusion equation on a fixed domain can be evaluated using separation of variables in terms of the Mittag–Leffler function, $E_\gamma(z)$, defined as (see [22])

$$E_\gamma(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\gamma k + 1)}. \tag{65}$$

In the case of zero flux boundary conditions the solution is given by

$$y(x,t) = \sum_{n=0}^{\infty} c_n^* \cos\left(\frac{n\pi}{L}x\right) E_\gamma\left(-\frac{n^2\pi^2}{L^2}t^\gamma\right), \tag{66}$$

where:

$$c_0^* = \frac{1}{L}\int_0^L g(s)\mathrm{d}s, \tag{67}$$

$$c_n^* = \frac{2}{L}\int_0^L g(s)\cos\left(\frac{n\pi}{L}s\right)\mathrm{d}s \tag{68}$$

and

$$g(x) = y(x,0). \tag{69}$$

To further investigate the accuracy of our numerical scheme we tested it on the fractional diffusion equation with the initial condition

$$y(x,0) = \cos(2\pi x), \quad 0 \leqslant x \leqslant 1 \tag{70}$$

and zero flux boundary conditions

$$\left.\frac{\partial y}{\partial x}\right|_{x=0} = \left.\frac{\partial y}{\partial x}\right|_{x=1} = 0, \quad t \geqslant 0. \tag{71}$$

The algebraic solution in this case simplifies to (see also [1])

$$y(x,t) = \cos(2\pi x)E_\gamma\left(-4\pi^2 t^\gamma\right). \tag{72}$$

For the special cases $\gamma = 1/2$ and $\gamma = 1$ the Mittag–Leffler function simplifies further and the solution given in Eq. (72) can be written as follows:

(i) For $\gamma = 1/2$:

$$y(x,t) = \cos(2\pi x)\mathrm{e}^{16\pi^4 t}\mathrm{erfc}\left(4\pi^2\sqrt{t}\right), \tag{73}$$

$$y(x,t) \approx \cos(2\pi x)(1 - 8\pi^{3/2}\sqrt{t} + 16\pi^4 t - \frac{256}{3}\pi^{11/2}t^{3/2} + O(t^2)), \tag{74}$$

where $\mathrm{erfc}(z)$ is the complementary error function.

(ii) For $\gamma = 1$ (standard diffusion):

$$y(x,t) = \cos(2\pi x)\mathrm{e}^{-4\pi^2 t}, \tag{75}$$

$$y(x,t) \approx \cos(2\pi x)(1 - 4\pi^2 t + \mathrm{O}(t^2)). \tag{76}$$

We have compared these solutions with the results from numerical simulations based on the implicit numerical scheme outlined in Section 2. In Fig. 2 we show the absolute error in the predicted value of $y(0,0.1)$ as a function of the time step Δt for the special cases $\gamma = 1/2$ and $\gamma = 1$. We see the absolute error increases linearly for $\gamma = 1$ (lower curve in this figure) and like $\Delta t^{1/2}$ for $\gamma = 1/2$ (upper curve).

Clearly the absolute error in the numerical solution of the fractional diffusion equation cannot be accounted for solely on the basis of the preceding local error analysis. The local error of the Euler approximation, $\mathrm{O}(\Delta t)$, is larger than the local error in the L1 approximation, $\mathrm{O}(\Delta t^{1+\gamma})$. However the global error in the solution has a γ dependence, $\mathrm{O}(\Delta t)$ for $\gamma = 1$ and $\mathrm{O}(\Delta t^{1/2})$ for $\gamma = 1/2$, suggesting that the accumulation of errors from the L1 approximation is greater than the accumulation of errors from the Euler approximation. The following comments are also relevant in this context. The derivative of the exact solution

$$\frac{\partial y(x,t)}{\partial t} = \cos(2\pi x)\sum_{k=1}^{\infty}\frac{(-4\pi^2)^k}{\Gamma(\gamma k)}t^{\gamma k-1} \tag{77}$$

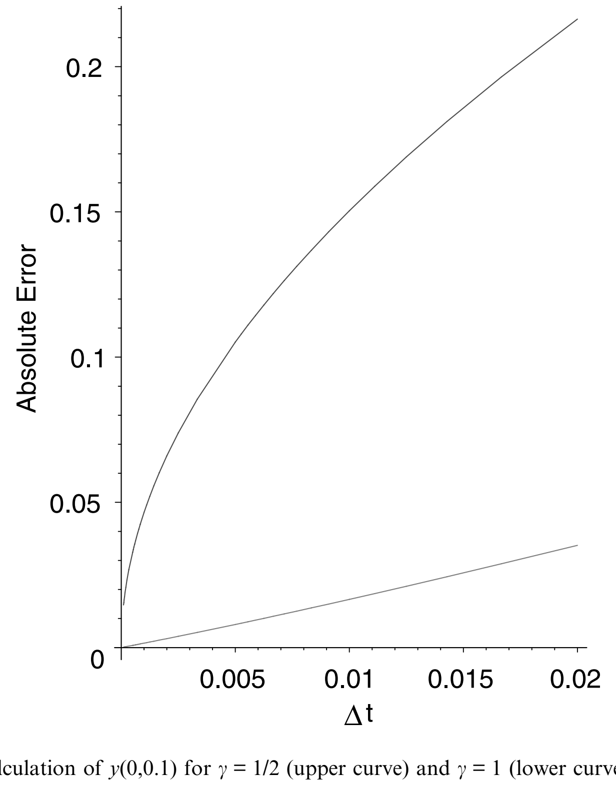

Fig. 2. Absolute error in the calculation of $y(0,0.1)$ for $\gamma = 1/2$ (upper curve) and $\gamma = 1$ (lower curve) for varying time step size, Δt.

is unbounded as $t \to 0+$ for $0 < \gamma < 1$. Hence the solution $y(x,t)$ cannot be expressed as a Taylor series about $t = 0$ as was assumed in the local error analysis. The singularity at $t = 0$ results in a large initial error in the Euler scheme which is further propagated (via the memory effect) in the L1 scheme.

4. Stability

In this section we have considered the stability of the implicit numerical method described in Section 2 for solving the fractional diffusion equation

$$\frac{\partial y}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \frac{\partial^2 y}{\partial x^2} \tag{78}$$

for $0 < \gamma \leqslant 1$. The numerical solution is governed by the difference equations

$$\begin{aligned} y_j^{k+1} - y_j^k = \frac{\mathrm{d}\Delta t^\gamma}{\Gamma(1+\gamma)\Delta x^2} \Bigg\{ & \frac{\gamma}{k^{1-\gamma}} \left(y_{j+1}^1 - 2y_j^1 + y_{j-1}^1 \right) \\ & + \sum_{l=1}^{k} \alpha_{k-l+1}(\gamma) \left(\left(y_{j+1}^{l+1} - 2y_j^{l+1} + y_{j-1}^{l+1} \right) - \left(y_{j+1}^l - 2y_j^l + y_{j-1}^l \right) \right) \Bigg\}, \end{aligned} \tag{79}$$

where $y_j^k \approx y((j-1)\Delta x, (k-1)\Delta t)$ and

$$\alpha_s(\gamma) = s^\gamma - (s-1)^\gamma. \tag{80}$$

To investigate the stability of this system we set $y_j^k = \delta_k \mathrm{e}^{\mathrm{i}qj\Delta x}$ where q is a real spatial wave number and let $\rho = \Delta t^\gamma / \Gamma(1+\gamma)\Delta x^2$ in Eq. (79), then

$$\begin{aligned} \delta_{k+1}\mathrm{e}^{\mathrm{i}qj\Delta x} - \delta_k \mathrm{e}^{\mathrm{i}qj\Delta x} = \rho \Bigg\{ & \frac{\gamma}{k^{1-\gamma}} \left(\delta_1 \mathrm{e}^{\mathrm{i}q(j+1)\Delta x} - 2\delta_1 \mathrm{e}^{\mathrm{i}qj\Delta x} + \delta_1 \mathrm{e}^{\mathrm{i}q(j-1)\Delta x} \right) \\ & \times \sum_{l=1}^{k} \alpha_{k-l+1}(\gamma) \left(\left(\delta_{l+1} \mathrm{e}^{\mathrm{i}q(j+1)\Delta x} - 2\delta_{l+1} \mathrm{e}^{\mathrm{i}qj\Delta x} + \delta_{l+1} \mathrm{e}^{\mathrm{i}q(j-1)\Delta x} \right) \right. \\ & \left. - \left(\delta_l \mathrm{e}^{\mathrm{i}q(j+1)\Delta x} - 2\delta_l \mathrm{e}^{\mathrm{i}qj\Delta x} + \delta_l \mathrm{e}^{\mathrm{i}q(j-1)\Delta x} \right) \right) \Bigg\}. \end{aligned} \tag{81}$$

The numerical method is unconditionally stable if $|\delta_{k+1}/\delta_k| \leqslant 1$ for all k, q, ρ, Δx and γ.

Dividing Eq. (81) by $\mathrm{e}^{\mathrm{i}qj\Delta x}$ and using the identity

$$\mathrm{e}^{\mathrm{i}q\Delta x} - 2 + \mathrm{e}^{-\mathrm{i}q\Delta x} = -4\sin^2\left(\frac{q\Delta x}{2}\right), \tag{82}$$

we arrive at the difference equation

$$\delta_{k+1} = \delta_k - 4\rho\sin^2\left(\frac{q\Delta x}{2}\right) \left\{ \frac{\gamma}{k^{1-\gamma}} \delta_1 + \sum_{l=1}^{k} \alpha_{k-l+1}(\gamma)(\delta_{l+1} - \delta_l) \right\}. \tag{83}$$

If $k \geqslant 2$ we can rearrange this expression for the ratio

$$\frac{\delta_{k+1}}{\delta_k} = 1 - V\alpha_2(\gamma) - V\left\{ \frac{\delta_1}{\delta_k}\mu_k(\gamma) + \sum_{l=2}^{k-1} \beta_{k-l+2}(\gamma) \frac{\delta_l}{\delta_k} \right\}, \tag{84}$$

where:

$$V = \frac{U}{1+U}, \tag{85}$$

$$U = 4\rho \sin^2\left(\frac{q\Delta x}{2}\right), \tag{86}$$

$$\beta_s(\gamma) = \alpha_s(\gamma) - \alpha_{s-1}(\gamma) = s^\gamma - 2(s-1)^\gamma + (s-2)^\gamma, \tag{87}$$

$$\mu_k(\gamma) = \frac{\gamma}{k^{1-\gamma}} - \alpha_k(\gamma) = \frac{\gamma}{k^{1-\gamma}} - (k^\gamma - (k-1)^\gamma). \tag{88}$$

The sum in Eq. (84) is only evaluated if $k \geqslant 3$ otherwise it is taken to be zero.

We first consider some special cases. If $k = 1$ then from Eq. (83) we have

$$\frac{\delta_2}{\delta_1} = 1 - \gamma V \leqslant 1. \tag{89}$$

If $\gamma = 1$ (standard diffusion) we find

$$\frac{\delta_2}{\delta_1} = 1 - V \tag{90}$$

for $k = 1$ and

$$\frac{\delta_{k+1}}{\delta_k} = 1 - V\alpha_2(1) - V\left\{\frac{\delta_1}{\delta_k}\mu_k(1) + \sum_{l=1}^{k-1}\beta_{k-l+2}(1)\frac{\delta_l}{\delta_k}\right\} = 1 - V \tag{91}$$

for $k \geqslant 2$; since $\mu_k(1) = \beta_{k+1}(1) = 0$ and $\alpha_2(1) = 1$. Thus

$$\frac{\delta_{k+1}}{\delta_k} = 1 - V \leqslant 1 \quad \forall k \tag{92}$$

and so in the case of standard diffusion we recover the well known result that the implicit method is unconditionally stable.

If $\gamma = 0$ then we find

$$\frac{\delta_{k+1}}{\delta_k} = 1 \tag{93}$$

for all $k \geqslant 1$; since $\mu_k(0) = \beta_{k+1}(0) = 0$ and $\alpha_2(0) = 0$.

It remains to consider $0 < \gamma < 1$. In Fig. 3 we have plotted the ratio δ_{k+1}/δ_k for $k = 1,2,3,4$ and $k = 10$ over a range of γ. Results are shown for two values of V. With these k values we observe the following pattern of behaviour: (i) δ_{k+1}/δ_k is a monotonic decreasing function of γ; (ii) $\delta_{k+1}/\delta_k \leqslant 1$ for all γ; (iii) $\delta_{k+1}/\delta_k \geqslant \delta_k/\delta_{k-1}$.

We now establish through series expansions that $\delta_{k+1}/\delta_k \leqslant 1$ for all γ in the range $0 < \gamma \ll 1$ and all k. Note that if $\gamma = 0$ then

$$\frac{\delta_j}{\delta_{j+1}} = 1 \quad \forall j \tag{94}$$

and thus

$$\frac{\delta_l}{\delta_k} = \prod_{j=l}^{k-1}\frac{\delta_j}{\delta_{j+1}} = 1 \quad \forall l < k. \tag{95}$$

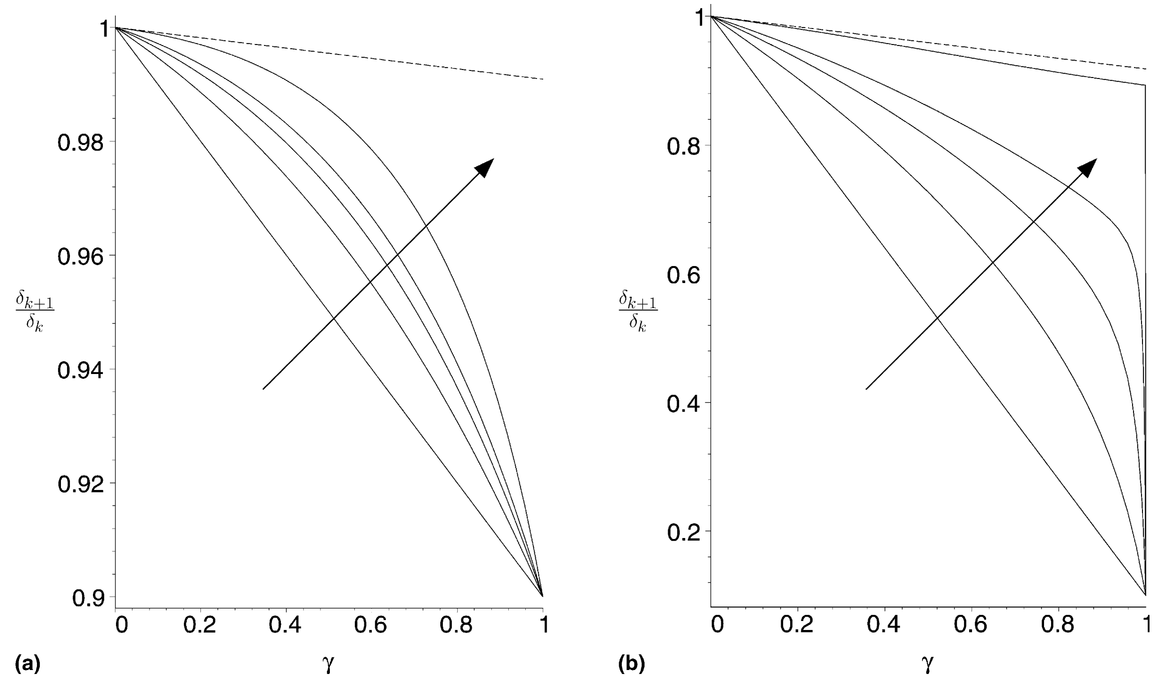

Fig. 3. Comparison of the ratios δ_{k+1}/δ_k for $k = 1,2,3,4$ and $k = 10$ with (a) $V = 0.1$, (b) $V = 0.9$. The straight dashed line is a plot of $1 - \gamma V/10$ versus γ. The arrow indicates the direction of increasing k. In each of these plots, $\delta_{k+1}/\delta_k > \delta_k/\delta_{k-1}$. Note the different vertical scales in (a) and (b).

Then without loss of generality we have

$$\frac{\delta_l}{\delta_k} = 1 + \mathrm{O}(\gamma). \tag{96}$$

We also have the expansions:

$$\alpha_k(\gamma) = \gamma \log k - \gamma \log(k-1) + \mathrm{O}(\gamma^2), \tag{97}$$

$$|\mu_k(\gamma)| = \gamma \log k - \gamma \log(k-1) - \frac{\gamma}{k} + \mathrm{O}(\gamma^2), \tag{98}$$

$$|\beta_s(\gamma)| = 2\gamma \log(s-1) - \gamma \log(s-2) - \gamma \log(s) + \mathrm{O}(\gamma^2). \tag{99}$$

We now substitute these expansions, Eqs. (96)–(99) into Eq. (84) and simplify to obtain the result

$$\frac{\delta_{k+1}}{\delta_k} = 1 - \frac{\gamma V}{k} + \mathrm{O}(\gamma^2). \tag{100}$$

Thus $\delta_{k+1}/\delta_k \leqslant 1$ for k finite and γ sufficiently small.

We have not been able to prove algebraically that the method is unconditionally stable for all γ in the range $0 < \gamma < 1$ but the pattern of results in Fig. 3 and the series expansions above are consistent with

$$1 - \gamma V \leqslant \frac{\delta_j}{\delta_{j-1}} \leqslant 1 - \gamma \frac{V}{j-1}, \quad j = 2, 3, \ldots k. \tag{101}$$

It is possible to use the above bounds inductively to find additional bounds on δ_{k+1}/δ_k. First we note the following results from Eq. (101):

$$\frac{\delta_j}{\delta_{j-1}} \leqslant 1, \tag{102}$$

$$\frac{\delta_1}{\delta_k} = \frac{\delta_l}{\delta_k}\prod_{j=1}^{l-1}\frac{\delta_j}{\delta_{j+1}} \geqslant \frac{\delta_l}{\delta_k}, \tag{103}$$

$$\frac{\delta_1}{\delta_k} = \prod_{j=1}^{k-1}\frac{\delta_j}{\delta_{j+1}} \leqslant \left(\frac{1}{1-\gamma V}\right)^{k-1}. \tag{104}$$

It now follows from Eqs. (101)–(103) and Eq. (84) together with $\mu_k \leqslant 0$ and $\beta_{k-l+2} \leqslant 0$ that

$$\frac{\delta_{k+1}}{\delta_k} \leqslant 1 - V\alpha_2(\gamma) + V\frac{\delta_1}{\delta_k}\left(|\mu_k(\gamma)| + \sum_{l=2}^{k-1}|\beta_{k-l+2}(\gamma)|\right). \tag{105}$$

To simplify this further we sum over l:

$$\sum_{l=2}^{k-1}\beta_{k-l+2}(\gamma) = \sum_{l=2}^{k-1}\alpha_{k-l+2}(\gamma) - \alpha_{k-l+1}(\gamma), \tag{106}$$

$$\sum_{l=2}^{k-1}\beta_{k-l+2}(\gamma) = \sum_{l=1}^{k-2}\alpha_{k-l+1}(\gamma) - \sum_{l=2}^{k-1}\alpha_{k-l+1}(\gamma), \tag{107}$$

$$\sum_{l=2}^{k-1}\beta_{k-l+2}(\gamma) = \alpha_k(\gamma) - \alpha_2(\gamma) \tag{108}$$

and use the definition for $\mu_k(\gamma)$ to obtain the identity

$$\alpha_2(\gamma) - |\mu_k(\gamma)| - \sum_{l=2}^{k-1}|\beta_{k-l+2}(\gamma)| = \frac{\gamma}{k^{1-\gamma}}. \tag{109}$$

We thus have the bound

$$\frac{\delta_{k+1}}{\delta_k} \leqslant 1 - V\alpha_2(\gamma) + V\frac{\delta_1}{\delta_k}\left(\alpha_2(\gamma) - \frac{\gamma}{k^{1-\gamma}}\right). \tag{110}$$

It is also possible to find more restrictive bounds including $\delta_{k+1}/\delta_k < 1$ for a restricted range of γ but more generally we have found it necessary to explore numerical results for the ratios. We have undertaken extensive numerical simulations of the difference equations, Eqs. (84) and (89) with $\delta_1 = 1, U = 10^6$, and for various values of γ. Results from these simulations are shown in Figs. 4 and 5.

In Fig. 4 we have made a Log–Log plot of the value δ_k versus k for $k = 1,2,\ldots,1000$ and we find that the long term behaviour is $O(k^{-\gamma})$. This long term behaviour is similar to the long-term behaviour of the Mittag–Leffler Function [33]

$$E_\gamma\left(-q^2 t^\gamma\right) \sim \frac{t^{-\gamma}}{\Gamma(1-\gamma)q^2}, \tag{111}$$

which describes the decay of the Fourier modes, q, of the fractional diffusion equation [33]. Since the stability of the implicit numerical scheme is in essence governed by the decay of the discrete Fourier modes

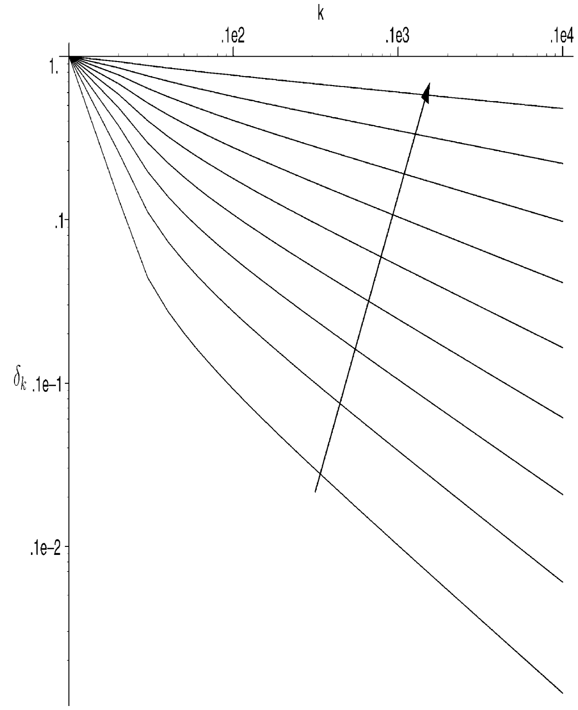

Fig. 4. Log–Log plot of the numerical estimates of δ_k for $k = 1,2,\ldots,1000$ and for $\gamma = 0.1(0.1)0.9$ decreasing in value in the direction of the arrow.

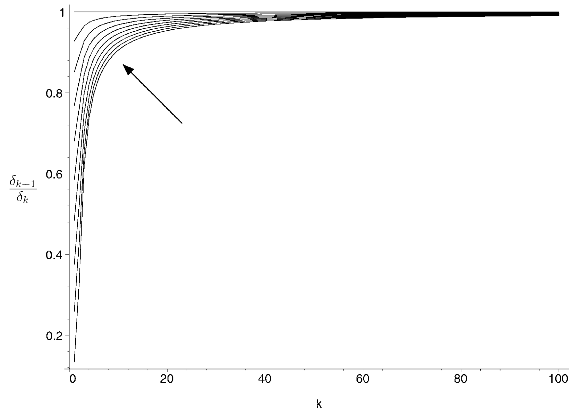

Fig. 5. Comparison of the ratios δ_{k+1}/δ_k for $k = 2,3,\ldots,100$ and for values of $\gamma = 0(0.1)0.9$ decreasing in the direction of the arrow.

in a discrete Fourier transform of the fractional diffusion equation the correspondence between the $O(k^{-\gamma})$ and $O(t^{-\gamma})$ decay rates is further evidence in support of the stability of the numerical method.

Finally, in Fig. 5 we have plotted the ratio δ_{k+1}/δ_k for $k = 1,2,\ldots,100$ for various values of γ and we find that in all cases this ratio is indeed less than one. Here, we have omitted in the plot values of $k > 100$ simply to distinguish the behaviour of different γ values for small k. For larger values of k the ratio remains bounded from above by one (not shown).

5. Summary

In this paper we have investigated the stability and accuracy of an implicit numerical method for solving the fractional diffusion equation

$$\frac{\partial y}{\partial t} = \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \frac{\partial^2 y}{\partial x^2}, \tag{112}$$

where $0 < \gamma \leqslant 1$. We have shown that the method has accuracy $O(\Delta x^2)$ in the spatial grid size and $O(\Delta t^{1+\gamma})$ in the fractional time step. We have also provided algebraic and numerical evidence that the method is unconditionally stable. These results complement other recent studies on the stability and accuracy of finite difference schemes for anomalous diffusion modelled with fractional partial differential equations [23,21]. The numerical methods that we have developed in this paper can also be applied to the fractional Fokker–Planck equation [3] and to fractional reaction–diffusion equations [4,5] where it has the same accuracy and stability.

A systematic study of the global accuracy of our implicit method remains an area for future research.

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