INTERNATIONAL JOURNAL OF COMPUTERS AND COMMUNICATIONS
DOI: 10.46300/91013.2022.16.2 Volume 16, 2022

ADI methods for three-dimensional fractional diffusions

Moreno Concezzi, Renato Spigler
Department of Mathematics and Physics,
University "Roma Tre", Rome, Italy,

***Abstract*—ADI methods can be generalized to solve numerically multidimensional fractional diffusion equations, which describe fluid flows through porous media better than classical diffusion equations. A new, unconditionally stable, second-order and well balanced in space, third-order in time ADI scheme has been constructed and its convergence accelerated by an extrapolation technique coupled with the *PageRank* algorithm.**

***Index Terms*—anomalous (fractional) diffusion in three dimensions; Alternating Direction Implicit (ADI) methods; extrapolation; PageRank.**

I. Introduction

Diffusive flow problems occur in a number of applications, and hence have been extensively studied. Important examples are provided by seepage flows, groundwater hydraulics, and fluid dynamics in porous media; see [10], [2], e.g.. In 1856, H. Darcy [5] derived his celebrated equation, the "Darcy's law", that is $\mathbf{q} = -\mathbf{K}\,\nabla p$, where p is the pressure, $\mathbf{q} = (q_1, q_2, q_3)$ the fluid velocity, the indices referring to the three directions, x, y, and z, and $\mathbf{K} = (K_1, K_2, K_3)$ the percolation tensor. Below, we assume $\mathbf{K}$ diagonal. Darcy obtained such a rule through experiments on saturated flows of water through a column of soil, In heterogeneous media, when the flow is continuous and the Darcy's law holds, choosing the main directions of the percolation as the coordinate directions and neglecting gravity effects, the partial differential equation (PDE) describing a single-phase isothermal seepage flow can be written as

$$\nu^{-1} p_t = \nabla\cdot(\mathbf{K}\,\nabla p) + f(x_1, x_2, x_3, t),\ (x_1, x_2, x_3) \in \Omega, \quad (1)$$

[16], [7], [11], where p_t denotes time partial derivative and Ω is a given open bounded domain of $\mathbf{R}^3$ where the percolation occurs. The associated boundary conditions are given by $p(x_1, x_2, x_3, t)|_{\partial\Omega} = \Phi(x_1, x_2, x_3, t)$, and the initial condition by $p(x_1, x_2, x_3, 0) = \varphi(x_1, x_2, x_3)$, for suitable functions Φ, φ; ν^{-1} is the specific storage coefficient (taken constant), and $f(x_1, x_2, x_3, t)$ is some source or sink term.

Equation (1) was derived assuming the seepage flow to be continuous, and the Darcy's law does *not* hold in general for real seepage flows. Hence, in 1998 J. He [7] proposed a modified form of the Darcy's law, formulating it in terms of *fractional* Riemann-Liouville derivatives [14], that is as

$$\mathbf{q} = -\mathbf{K}\,\nabla^{\alpha} p, \qquad \nabla^{\alpha} := \left(\frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}}, \frac{\partial^{\alpha_2}}{\partial x_2^{\alpha_2}}, \frac{\partial^{\alpha_3}}{\partial x_3^{\alpha_3}}\right),$$

where the operator ∇^{α}, with $\alpha := (\alpha_1, \alpha_2, \alpha_3)$, was introduced. The more general equation for seepage flow with fractional derivatives was thus obtained,

$$\nu^{-1} p_t = \partial_i^{\beta_i}\left(K_i \partial_i^{\alpha_i} p\right) + f(x_1, x_2, x_3, t), \quad (2)$$

where $\partial_i \beta_i \equiv \partial^{\beta_i}/\partial x_i$, and we used the summation convention. Here, $0 < \beta_i < 1$, $0 < \alpha_i \leq 1$, and $1 < \beta_i + \alpha_i \leq 2$, for $i = 1, 2, 3$.

Given the importance but, at the same time, the unavailability of analytic solutions to *fractional* partial differential equations (fPDEs), many authors have proposed, over the years, numerical methods to solve them, see [9], [17], [15], [21], [18], [19], [20], e.g. Yet, numerical methods for handling efficiently high-dimensional fPDEs seem to be rather few.

In this paper, we consider the 3D fPDE in (2) on the bounded domain, $\Omega := \prod_{i=1}^{3}(0, L_i)$, and the time interval $(0, T]$. We assume that such a fractional equation has a unique and sufficiently smooth solution, when subject to Dirichlet boundary conditions, and some initial condition. The fractional operators involved Riemann-Liouville derivatives of order α_i, β_i, with respect to x_i. Other useful definitions of fractional derivatives exist, and among these, the Grünwald-Letnikov fractional derivative is for us most relevant, see [14], while the so-called *shifted* Grünwald-Letnikov derivative will be used in the numerical schemes. Fractional Riermann-Liouville derivatives of sufficiently regular functions coincide with those intended in the sense of Grünwald-Letnikov as well as in the sense of Caputo [14].

We construct a new, well "balanced", fractional version of the Alternating Direction Implicit (ADI) method, to solve numerically 3D diffusion fPDEs. Our algorithm is *unconditionally stable* for every fractional order of space derivatives, *second-order* accurate *in space*, and *third-order* accurate *in time*. Its convergence can be sped up adopting an extrapolation technique, along with an optimization realized through Google's *PageRank* algorithm.

Composing the two Grünwald-Letnikov fractional derivatives [14], the fPDE above becomes

$$\nu^{-1} p_t = K_i \partial_i^{\gamma_i} p + f(x, y, z, t) \quad \text{in}\, \Omega \times (0, T], \quad (3)$$

where we set $\gamma_i := \beta_i + \alpha_i$, for $i = 1, 2, 3$, and the K_i's are positive constants. Below, we construct a "fractional Alternating Direction Implicit" (fADI) scheme to solve numerically such a problem.

II. fADI schemes

We discretize space and time, as usual, setting $x_i^m := m_i h_i$ for $m_i = 0, 1, 2, \ldots, M_i$, $h_i := \frac{L_i}{M_i}$, and similarly for the time variable. The numerical approximation to $p(x_1^{m_1}, x_2^{m_2}, x_3^{m_3}, t^n)$, provided by the scheme at such points will be denoted by $p^n_{m_1,m_2,m_3}$, and similarly for the source term, f, and the boundary and initial values. The first-order derivative $\partial_t p$ in (3) is approximated by finite differences, and assume that p is sufficiently regular, so that the operators $\partial_i^{\gamma_i}$ can be discretized using the shifted fractional Grünwald-Letnikov derivative. Thus, we obtain the implicit scheme

$$\begin{aligned}
&\frac{p^{n+1}_{m_1,m_2,m_3} - p^n_{m_1,m_2,m_3}}{\tau} \\
&= \frac{K_i}{h_i^{\gamma_i}} \sum_{s=0}^{m_i+1} g_{\gamma_i,s}\, p^{n+1}_{m_i+1-s,m_2,m_3} \\
&+ \frac{K_2}{h_2^{\gamma_2}} \sum_{s=0}^{m_2+1} g_{\gamma_2,s}\, p^{n+1}_{m_1,m_2+1-s,m_3} \\
&+ \frac{K_3}{h_3^{\gamma_3}} \sum_{s=0}^{m_3+1} g_{\gamma_3,s} p^{n+1}_{m_1,m_2,m_3+1-s} + f^{n+1}_{m_1,m_2,m_3},
\end{aligned} \tag{4}$$

where the coefficients g's are defined in [14]. The fractional discrete operator

$$\delta_1^{\gamma_1} p^{n+1}_{m_1,m_2,m_3} := \frac{1}{h_1^{\gamma_1}} \sum_{s=0}^{m_1+1} g_{\gamma_1,s} p^{n+1}_{m_1+1,m_2,m_3}, \tag{5}$$

is known to provide an $\mathcal{O}(h_1)$ approximation of the Grünwald-Letnikov shifted fractional derivative of order γ_1, see [13], etc. The scheme in (4) can be rewritten in a more compact form as

$$\begin{aligned}
&(1 - K_1\tau\delta_1^{\gamma_1} - K_2\tau\delta_2^{\gamma_2} - K_3\tau\delta_3^{\gamma_3})\, p^{n+1}_{m_1,m_2,m_3} \\
&= p^n_{m_1,m_2,m_3} + \tau f^n_{m_1,m_2,m_3}.
\end{aligned} \tag{6}$$

In can be shown that the scheme in (4) has a *local truncation* error of order $\mathcal{O}(\tau) + \sum_{i=1}^3 \mathcal{O}(h_i)$, and is *unconditionally* stable.

Equation (6) (or (4)) yields a *linear* system of equations for $p^{n+1}_{m_1,m_2,m_3}$. Others than in the classical ADI method, such a system is not sparse, but a *large dense* linear system of equations. This calls for suitable efficient numerical methods, hopefully also unconditionally stable.

As in the classical ADI methods, we split the computations into three steps, corresponding to the three directions, x_1, x_2, and x_3, each step requiring a reduced computational load. An extra, higher-order, term is added to the left-hand side of equation (6), so to factor the operator into three parts, without affecting the overall convergence rate,

$$\begin{aligned}
&(K_1K_2\tau^2\delta_1^{\gamma_1}\delta_2^{\gamma_2} + K_1K_3\tau^2\delta_1^{\gamma_1}\delta_3^{\gamma_3} \\
&+ K_2K_3\tau^2\delta_2^{\gamma_2}\delta_3^{\gamma_3} - K_1K_2K_3\tau^3\delta_1^{\gamma_1}\delta_2^{\gamma_2}\delta_3^{\gamma_3})\, p^{n+1}_{m_1,m_2,m_3}.
\end{aligned} \tag{7}$$

Thus, we obtain the scheme

$$\begin{aligned}
&(1 - K_1\tau\delta_1^{\gamma_1})(1 - K_2\tau\delta_2^{\gamma_2})(1 - K_3\tau\delta_3^{\gamma_3})\, p^{n+1}_{m_1,m_2,m_3} \\
&= p^n_{m_1,m_2,m_3} + \tau f^n_{m_1,m_2,m_3}.
\end{aligned} \tag{8}$$

Splitting (8) in the three dimensions, we obtain the *unbalanced* scheme, which provides the solution at time t^{n+1},

$$(1 - K_1\tau\delta_1^{\gamma_1})\, p^{n+1/3}_{m_1,m_2,m_3} = p^n_{m_1,m_2,m_3} + \tau f^n_{m_1,m_2,m_3}, \tag{9}$$

$$(1 - K_2\tau\delta_2^{\gamma_2})\, p^{n+2/3}_{m_1,m_2,m_3} = p^{n+1/3}_{m_1,m_2,m_3}, \tag{10}$$

and

$$(1 - K_3\tau\delta^{\gamma_3})\, p^{n+1}_{m_1,m_2,m_3} = p^{n+2/3}_{m_1,m_2,m_3}, \tag{11}$$

which turns out to be of the first order in space [10].

We propose now a new *balanced* splitting of the ADI scheme in (8), which provides the solution at time t^{n+1} through three more balanced steps, obtained replacing the previous right-hand sides with $p^n_{m_1,m_2,m_3} + \frac{\tau}{3} f^n_{m_1,m_2,m_3}$, $p^{n+1/3}_{m_1,m_2,m_3} + \frac{\tau}{3} f^n_{m_1,m_2,m_3}$, and $p^{n+2/3}_{m_1,m_2,m_3} + \frac{\tau}{3} f^n_{m_1,m_2,m_3}$, respectively.

It can be shown that such second choice provides an algorithm second-order accurate in space and third-order in time [4].

Since the "load" represented by the source term enters this second scheme in a more balanced way, it is expected that such an algorithm performs better when there is little anisotropy, i.e., when the fractional orders γ_i, $i = 1, 2, 3$, do not differ appreciably.

Taking into account the boundary values $p^{n+1/3}_{0,m_2,m_3}$ and $p^{n+2/3}_{M_1,m_2,ma-3}$, we can construct the coefficients of the matrix, say A, of the linear system concerning the first step, see [4]. Then, using the boundary values $p^{n+2/3}_{m_1,0,m_3}$ and $p^{n+2/3}_{m_1,M_2,m_3}$, we obtain the matrix, say B, of the linear system concerning te second step. For each fixed (m_1, m_3), such a matrix presents some similarity with A. Finally, using the boundary values $p^{n+1}_{m_1,m_2,0}$ and $p^{n+1}_{m_1,m_2,M_3}$, we obtain the matrix C of the linear system concerning the third step, which, again, for each fixed (m_1, m_2), is analogous to A.

Examining the three matrices A, B, C, above, it can be seen that, at each time step, it is only required to solve, for each fixed pair (m_2, m_3) (at each x_1-level) a linear upper *triangular* system of size $M_1 - 1$, and similarly for the other systems. We refer to [4] for more details.

III. Numerical implementation

Here we apply our numerical method to solve 3D fractional diffusion problems. An example is given to illustrate its performance.

Our algorithm can be *optimized*, achieving an appreciable *acceleration*, exploiting Google's *PageRank* algorithm [8]. This method will be associated to an *extrapolation* technique, which determines the coefficients which make it optimal. A considerable amount of CPU time can be saved just resorting to the *extrapolation* technique [1]. This procedure also increases the accuracy of our algorithm up to the *third order* in time, see [3], [12]. The *extrapolated solution*, $q^n(\tau)$, is evaluated as

$$q^n(\tau) = \psi_1\, p^n(\tau) + \psi_2\, p^n\left(\frac{3}{4}\tau\right) + \psi_3\, p^n\left(\frac{\tau}{2}\right) + \psi_4\, p^n\left(\frac{\tau}{4}\right), \tag{12}$$

where the coefficients ψ's are suitably determined, see [4]. Here we have displayed the dependence of p^n on τ.

IV. A NUMERICAL EXAMPLE

Let the linear three dimensional fPDE

$$\begin{aligned} &\nu^{-1}\partial_t p = K_{11}\ {}_0D_1^{\alpha}p + K_{21}\ {}_1D_2^{\alpha}p + K_{12}\ {}_0D_2^{\beta}p \\ &+K_{22}\ {}_2D_2^{\beta}p + K_{13}\ {}_0D_3^{\gamma}p + K_{23}\ {}_3D_2^{\gamma}p \\ &+d_1\,\partial_1 p + d_2\,\partial_2 p + d_3\,\partial_3 p + f(x_1,x_2,x_3,t), \end{aligned} \tag{13}$$

where ${}_aD_b^{\alpha}p$ denotes the fractional Riemann-Liouville derivative of p of order α, in the interval $[a,b]$, be considered on the domain $(x_1,x_2,x_3)\in[0,2]^3$, $0<t\le T$, with

$$\begin{aligned} K_{11} &= \Gamma(3-\alpha)\,x_1^{\alpha}, & K_{21} &= \Gamma(3-\alpha)(2-x_1)^{\alpha} \\ K_{12} &= \Gamma(3-\beta)\,x_2^{\beta}, & K_{22} &= \Gamma(3-\beta)(2-x_2)^{\beta} \\ K_{13} &= \Gamma(3-\gamma)\,x_1^{\gamma}, & K_{23} &= \Gamma(3-\gamma)(2-x_3)^{\gamma}, \end{aligned}$$

$$d_i = \frac{1}{4}x_i, \quad i=1,2,3,$$

and the forcing term

$$\begin{aligned} &f(x_1,x_2,x_3,t) \\ &:= -4\,e^{-t}x_1^2x_2^2x_3^2(x_1-2)(x_2-2) \\ &(x_3-2)(3x_1x_2x_3-5x_1-5x_2-5x_3+8) \\ &-[l_{\alpha}(x_1,x_3,t)+l_{\gamma}(x-3,x_1,t)+l_{\alpha}(x_2,x_1,t) \\ &+l_{\beta}(x_1,x_2,t)+l_{\beta}(x_3,x_2,t)+l_{\gamma}(x_2,x_3,t)]. \end{aligned} \tag{14}$$

Here $l_{\delta}(u,v,t) := g(u,t)\,h_{\delta}(v)$, being $g(u,t) := 32\,e^{-t}u^2(2-u)^2$, and

$$h_{\delta}(u) := u^2+(2-u)^2-\frac{3(u^3+(2-u)^3)}{3-\delta}+\frac{3(u^4+(2-u)^4)}{(3-\delta)(4-\delta)},$$

where δ can be α, β or γ.

Dirichlet homogeneous boundary conditions are imposed, as well as the initial condition

$$p(x_1,x_2,x_3,0) = 4x_1^2(2-x_1)^2x_2^2(2-x_2)^2x_3^2(2-x_3)^2.$$

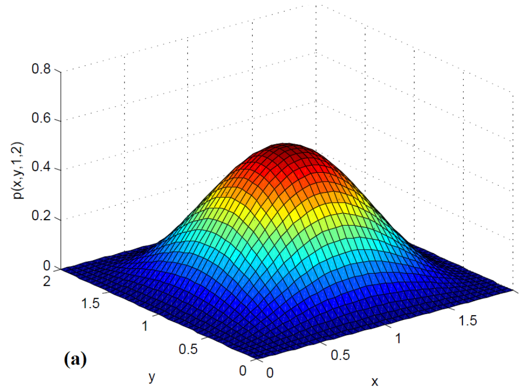
The analytical solution to such a problem is given by

$$p(x_1,x_2,x_3,t) = 4x_1^2e^{-t}(2-x_1)^2x_2^2(2-x_2)^2x_3^2(2-x_3)^2,$$

see [6], and it is used to *validate* our 3D algorithm and test its performance.

TABLE I
L^{∞} AND L^2 NORM DISCREPANCIES FOR THE EXAMPLE, WHEN THE *balanced* SCHEME IS USED, AT TIME $T=1$, FOR SEVERAL VALUES OF N, AND $\tau=h=2/N$.

(α,β,γ)	N	$\Vert q^n_{fADI}-q^n_{ADI}\Vert_\infty$	$\Vert q^n_{fADI}-q^n_{ADI}\Vert_2$
$(1.2,1.2,1.2)$	256	6.1758 E-7	3.8458 E-6
	512	2.2548 E-7	7.8442 E-7
$(1.4,1.5,1.6)$	256	2.8287 E-7	1.1205 E-6
	512	3.7852 E-8	3.7854 E-7
$(1.9,1.9,0.9)$	256	1.1582 E-7	5.7852 E-7
	512	1.7855 E-8	5.0023 E-7
$(2.0,2.0,2.0)$	256	8.1158 E-8	8.7852 E-7
	512	1.7852 E-8	6.7852 E-8



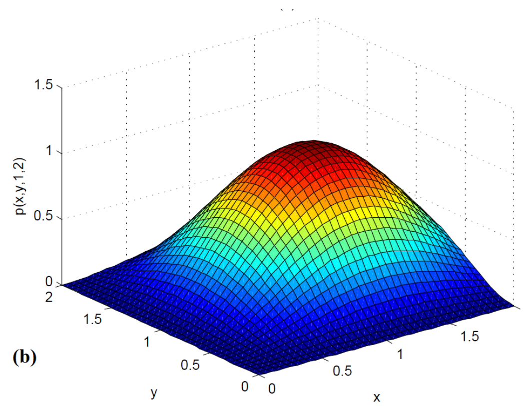


Fig. 1. (a) Classical solution (obtained by a fine grid numerical ADI method with $\tau=h/16$ and $h=1/64$), and (b) exact (analytical) fractional diffusion solution with $(\alpha,\beta,\gamma)=(1.4,1.5,1.6)$, for $x_3=1$ and $T=2$. The same forcing function was used in both cases.

Fig. 1 shows clearly the effect of replacing ordinary derivatives, (α,β,γ) = $(2,2,2)$, with fractional derivatives. Here, (α,β,γ) = $(1.4,1.5,1.6)$, which implies *anomalous* diffusion.

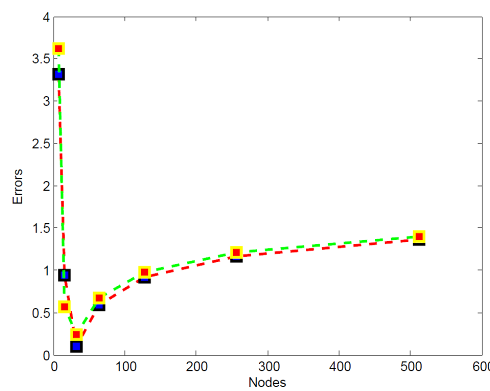


Fig. 2. Absolute numerical error between the exact and the numerical solution of the fPDE of the Example, at $T=2$, with $(\alpha,\beta,\gamma)=(1.4,1.5,1.6)$.

Fig. 2 shows the numerical errors $\Vert q^n - P^n\Vert$, in the L^2 and L^{∞} norms, on a log-scale, being $P^n \equiv p(x_{m_1},x_{m_2},x_{m_3},t^n)$ the exact solution to the fPDE, and $q^n \equiv q,\tau$ is its approximation given obtained through equation (12).

V. Conclusion

An ADI method has been constructed to solve numerically multidimensional fractional diffusion equations. The algorithm is unconditionally stable, second-order in space, third-order in time, and its convergence can be made faster by some extrapolation strategy and the *PageRank* algorithm. The scheme is better balanced with repect to previously existing schemes, assigning an equal weight to the three steps, in each space direction. More details can be found in [4].

Acknowledgment

This work was supported, in part, by the Italian GNFM-INdAM.

References

[1] Chen, S.,Liu, F., *ADI-Euler and extrapolation methods for the two dimensional fractional advection-dispersion equation*, J. Appl. Math. Comp., **26**, 295-311, 2008.

[2] Chou, H., Lee, B., and Chen, C, *The transient infiltration process for seepage flow from cracks*, Western Pacific Meeting, Advances in Subsurface Flow and Transport: Eastern and Western Approaches III, Eos Trans. AGU, 2006.

[3] Concezzi, M., Spigler, R., *Numerical solution of two-dimensional fractional diffusion equations by a high-order ADI method*, Commun. Appl. Ind. Math., 2013, printed online; **3**, No. 2 (2012), in print. [http://dx.doi.org/10.1685/journal.caim.421]

[4] Concezzi, M., Spigler, R., *An ADI method for the numerical solution of 3D fractional reaction-diffusion equations in porous media*, 2014, submitted.

[5] Darcy, H., *Les fontaines publique de la Ville de Dijon*, Western Paris, France: Dalmont, 1856.

[6] Deng, W., Chen, M., *Efficient numerical algorithms for three-dimensional fractional partial differential equations*, arXiv:1303.4628v1, 2013.

[7] He, J., *Approximate analytical solution for seepage flow with fractional derivatives in porous media*, Comput. Methods Appl. Mech. Eng. **167**, 57-68, 1998.

[8] Kamvar, S., Haveliwala, T., Manning, C., and Golub, G., *Extrapolation Methods for Accelerating PageRank Computations*, Welfth International World Wide Web Conference, 2003.

[9] Liu, F., Anh, V., Turner, I., Zhunag, P.*Numerical simulation for solute transport in fractal porous media*, ANZIAM J. **45**, 461-473., 2004.

[10] Liu, Q., Liu, F., Turner, I., and Anh, V., *Numerical simulation for the $3D$ seepage flow with fractional derivatives in porous media*, IMA J. Appl. Math. **74** , 178-200, 2009.

[11] Luo, Z.-J., Zhang, Y.-Y., and Wu, Y.-X., *Finite element numerical simulation of three-dimensional seepage control for deep foundation pit dewatering*, Hydrodyn. **20**, 596-602, 2008.

[12] Marchuk, G.I., and Shaidurov, V.V., *Difference Methods and Their Extrapolations*, Springer-Verlag, New York, 1983.

[13] Meerschaert, M. M. and Tadjeran, C., *Finite difference approximations for fractional advection-dispersion flow equations*, J. Comput. Appl. Math. **172**, 65-77. 2004.

[14] Podlubny, I., *Fractional Differential Equations*, New York: Academic Press, 1999.

[15] Roop, J. P., *Computational aspects of FEM approximation of fractional advection dispersion equations on bounded domains in R^2*, J. Comput. Appl. Math. **193**, 243-268, 2006.

[16] Rushton, K. R. and Redshaw, S. C, *Seepage and Groundwater Flow*, Brisbane, Australia: Wiley-Interscience Publication, 1979.

[17] Shen, S. and Liu, F., *Error analysis of an explicit finite difference approximation for the space fractional diffusion with insulated ends*, ANZIAM J. **46**, 871-887, 2005.

[18] Smith, D.D., *Numerical Solution of Partial Differential Equations: Finite Difference Methods*, Oxford Applied Mathematics and Computing Sciences Series, Oxford University Press, 1990.

[19] Yu, Q., Liu, F., Anh, V., and Turner, I., *Solving linear and nonlinear space-time fractional reaction-diffusion equations by Adomian decomposition method*, Int. J. Numer. Methods Eng. **74**, 138-158., 2008.

[20] Zhang, H., Liu, F., and Anh, V., *Numerical approximation of Lévy-Feller diffusion equation and its probability interpretation*, J. Comput. Appl. Math. **206**, 1098-1115, 2007.

[21] Zhuang, P., and Liu, F., *Implicit difference approximation for the time fractional diffusion equation*, J. Appl. Math. Comput. **22**, 87-99, 2006.