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Efficient solution of two-sided nonlinear space-fractional diffusion equations using fast Poisson preconditioners

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ABSTRACT

We develop a fast Poisson preconditioner for the efficient numerical solution of a class of two-sided nonlinear space-fractional diffusion equations in one and two dimensions using the method of lines. Using the shifted Grünwald finite difference formulas to approximate the two-sided (i.e. the left and right Riemann–Liouville) fractional derivatives, the resulting semi-discrete nonlinear systems have dense Jacobian matrices owing to the non-local property of fractional derivatives. We employ a modern initial value problem solver utilising backward differentiation formulas and Jacobian-free Newton–Krylov methods to solve these systems. For efficient performance of the Jacobian-free Newton–Krylov method it is essential to apply an effective preconditioner to accelerate the convergence of the linear iterative solver. The key contribution of our work is to generalise the fast Poisson preconditioner, widely used for integer-order diffusion equations, so that it applies to the two-sided space-fractional diffusion equation. A number of numerical experiments are presented to demonstrate the effectiveness of the preconditioner and the overall solution strategy.

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1. Introduction

The concept of fractional derivatives, and their applications to modelling anomalous diffusion are widely recognised by engineers and mathematicians. Fractional derivatives model diffusion-type processes where the underlying particle motion deviates from Brownian motion [1]. A typical example where non-Brownian motion gives rise to anomalous diffusion is particle transport in heterogeneous porous media. Zhang et al. [2] have given an excellent review of fractional models and field applications in this area. Perhaps the best-known experiments are the gradient tracer tests performed in a subsurface aquifer system at the Macrodispersion Experiment (MADE) test site. Benson et al. [3] and others have analysed the data from these experiments and concluded that they are consistent with a fractional-order model of dispersion, where the standard Fickian term is replaced with a fractional derivative.

Transport in porous media is by no means the only area in which fractional models of diffusion are found. Magin [4] gives an excellent account of numerous applications in the area of bioengineering, including fractional impedance, fractional dielectrics and fractional kinetics. Some even more recently proposed fractional models include those for magnetic resonance signal attenuation in human tissue [5], controlled drug delivery systems [6], and migration of water through cell walls in wood [7].

Fractional models present additional challenges for numerical solution methods, compared to integer-order models. A wide variety of techniques have been developed, including finite difference and related methods ([8–15]), finite element

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methods [16–18], finite volume methods [19,20], spectral methods [21,22], mesh-free methods [23,24], all of which are tailored to specific forms of fractional equations.

In this paper we consider the two-sided, nonlinear space-fractional diffusion equation

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = \kappa(u,\mathbf{x},t)\sum_{\ell=1}^{d}\left[p_\ell \frac{\partial^{\alpha_\ell} u(\mathbf{x},t)}{\partial (x_\ell)^{\alpha_\ell}} + (1-p_\ell)\frac{\partial^{\alpha_\ell} u(\mathbf{x},t)}{\partial (-x_\ell)^{\alpha_\ell}}\right] + S(u,\mathbf{x},t) \tag{1}$$

on the finite domain $0 < x_\ell < L_\ell$ with homogeneous Dirichlet boundary conditions and initial condition $u(\mathbf{x},0) = u_0(\mathbf{x})$. The fractional orders are assumed to satisfy $1 < \alpha_\ell \leqslant 2$.

The unknown function $u(\mathbf{x},t)$ can be interpreted as representing the concentration of a particle plume undergoing anomalous diffusion. The inclusion of both left and right Riemann–Liouville derivatives allows the modelling of flow regime impacts from either side of the domain. The diffusion coefficient $\kappa(u,\mathbf{x},t)$ is assumed positive, and the forcing function $S(u,\mathbf{x},t)$ models sources or sinks. Meerschaert and Tadjeran [9] give the interpretation of the skewnesses $p_\ell \in [0,1]$ in terms of forward and backward jump probabilities at the particle scale.

For compactness, we have presented Eq. (1) in its general form. In this paper, we will consider the one- and two-dimensional cases ($d = 1$ and $d = 2$ respectively). When considering the one-dimensional case we will generally drop the subscripts on α, p, L, and x. When considering the two-dimensional case, we will set $x_1 = x$ and $x_2 = y$.

The left and right Riemann–Liouville derivatives in Eq. (1) are defined by (with subscripts dropped for clarity) [25]:

$$\frac{\partial^\alpha u(x,y,t)}{\partial x^\alpha} = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_a^x \frac{u(\xi,y,t)}{(x-\xi)^{\alpha-1}}\,\mathrm{d}\xi \tag{2}$$

and

$$\frac{\partial^\alpha u(x,y,t)}{\partial (-x)^\alpha} = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_x^b \frac{u(\xi,y,t)}{(\xi-x)^{\alpha-1}}\,\mathrm{d}\xi. \tag{3}$$

The limits of integration a and b in these definitions are the subject of some discussion in the literature. We shall elaborate more on this in Section 4. For the finite interval $[0,L]$ presently being considered, the values of these limits are simply $a = 0$ and $b = L$.

To put the present work in context, we begin by discussing some of the key numerical methods that have been proposed to solve various special cases of Eq. (1). Meerschaert and Tadjeran considered finite difference methods for the one-dimensional, one-sided, linear case [8]. They showed that discretisation of the fractional derivatives using standard (non-shifted) Grünwald formulas led to unstable methods when the fractional order α satisfies $1 < \alpha \leqslant 2$. To overcome this, they proposed a method utilising shifted Grünwald formulas, which they showed to be stable, and first order accurate in space. Extensions of this method to address two-sided problems [9], two-dimensional problems [26] and solutions with second order spatial accuracy [27] followed soon after.

A defining characteristic of these methods is the density of the matrices they generate. For example, discretising the one-dimensional, two-sided space-fractional diffusion equation with Meerschaert and Tadjeran's [9] approach results in a fully dense matrix. This has serious implications on the efficiency of the numerical scheme, which must deal with $\mathcal{O}(N^2)$ storage and $\mathcal{O}(N^3)$ factorisation costs, where N is the number of nodes in the mesh. Furthermore, the expense of evaluating the discrete equations scales as $\mathcal{O}(N^2)$, again due to the non-local nature of the fractional derivatives and in contrast to the $\mathcal{O}(N)$ scaling for non-fractional discretisations.

In more recent times, a number of authors have addressed the issue of high computational expense associated with the solution of space-fractional equations. Several different approaches have been explored, with many papers employing a mixture of these approaches in various fascinating ways.

Krylov subspace methods have been a popular approach, owing to their ability to solve linear systems and compute matrix functions without the need to operate directly on dense matrices. Yang et al. [17,20,28] and Burrage et al. [18] used Krylov subspace methods for computing matrix functions to solve fractional Laplacian equations. Moroney and Yang [29] and Wang and Wang [30] used Krylov subspace methods to solve the two-sided space-fractional diffusion equation in one dimension, with the former authors considering nonlinear problems and the latter authors considering linear problems with an advection term.

Preconditioning has been a common theme in many of these papers, since it is well known that Krylov subspace methods generally require an effective preconditioner in order to perform satisfactorily. Yang et al. [17,20,28] developed preconditioners based on eigenvalue deflation. Burrage et al. [18] considered both algebraic multigrid and incomplete LU preconditioning. Moroney and Yang [29] developed a banded preconditioner.

The use of fast transform methods has also proved popular of late. Wang et al. [31] showed how to exploit the Toeplitz-like structure of the coefficient matrix for the one-dimensional, two-sided, linear space-fractional diffusion equation to derive an efficient $\mathcal{O}(N\log^2 N)$ method. Wang and Wang [30] also utilised fast Fourier transforms to efficiently compute the matrix–vector products in their Krylov subspace method. Pang and Sun [32] have proposed a multigrid method utilising fast Fourier transforms, also for the one-dimensional, two-sided, linear problem. Bueno-Orovio et al. [22] have considered

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