Numer. Math. Theor. Meth. Appl. Vol. **14**, No. 4, pp. 893-919
doi: 10.4208/nmtma.OA-2020-0020 November 2021

A Note on Parallel Preconditioning for the All-at-Once Solution of Riesz Fractional Diffusion Equations

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Received 8 May 2020; Accepted (in revised version) 14 March 2021

Abstract. The p-step backward difference formula (BDF) for solving systems of ODEs can be formulated as all-at-once linear systems that are solved by parallel-in-time preconditioned Krylov subspace solvers (see McDonald *et al.* [36] and Lin and Ng [32]). However, when the BDFp ($2 \leq p \leq 6$) method is used to solve time-dependent PDEs, the generalization of these studies is not straightforward as p-step BDF is not selfstarting for $p \geq 2$. In this note, we focus on the 2-step BDF which is often superior to the trapezoidal rule for solving the Riesz fractional diffusion equations, and show that it results into an all-at-once discretized system that is a low-rank perturbation of a block triangular Toeplitz system. We first give an estimation of the condition number of the all-at-once systems and then, capitalizing on previous work, we propose two block circulant (BC) preconditioners. Both the invertibility of these two BC preconditioners and the eigenvalue distributions of preconditioned matrices are discussed in details. An efficient implementation of these BC preconditioners is also presented, including the fast computation of dense structured Jacobi matrices. Finally, numerical experiments involving both the one- and two-dimensional Riesz fractional diffusion equations are reported to support our theoretical findings.

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AMS subject classifications: 65F08, 15B05, 65M22, 35R11

Key words: Backwards difference formula, all-at-once discretization, parallel-in-time preconditioning, Krylov subspace solver, fractional diffusion equation.

1. Introduction

In this paper, we are particularly interested in the efficient numerical solution of evolutionary partial differential equations (PDEs) with both first order temporal derivative and space fractional-order derivative(s). These models arise in various scientific applications in different fields including physics [3], bioengineering [35], hydrology [37], and finance [44], etc., owing to the potential of fractional calculus to describe rather accurately natural processes which maintain long-memory and hereditary properties in complex systems [27, 35]. In particular, fractional diffusion equations can provide an adequate and accurate description of transport processes that exhibit anomalous diffusion, for example subdiffusive phenomena and Lévy fights [38], which cannot be modelled properly by second-order diffusion equations. As most fractional diffusion equations can not be solved analytically, approximate numerical solutions are sought by using efficient numerical methods such as, e.g., (compact) finite difference [9, 10, 25, 31, 37, 46], finite element [54] and spectral (Galerkin) methods [51,52,56].

Many numerical techniques proposed in the literature for solving this class of problems are the common time-stepping schemes. They solve the underlying evolutionary PDEs with space fractional derivative(s) by marching in time sequentially, one level after the other. As many time steps may be usually necessary to balance the numerical errors arising from the spatial discretization, these conventional time-stepping schemes can be very time-consuming. This concern motivates the recent development of parallel-in-time (PinT) numerical solutions for evolutionary PDEs (especially with space fractional derivative(s)) including, e.g., the inverse Laplace transform method [40], the MGRIT method [14, 18, 50, 54], the exponential integrator [15] and the parareal method [49]. A class of PinT methods, i.e., the space-time methods, solves the evolutionary PDEs at all the time levels simultaneously by performing an all-at-once discretization that results into a large-scale linear system that is typically solved by preconditioned Krylov subspace methods c.f., e.g., [2, 4, 7, 16, 20, 29, 34, 41, 42, 47] for more details. However, most of them only focus on the numerical solutions of one-dimensional space fractional diffusion equations [20, 29, 42, 57] due to the huge computational cost required for high-dimensional problems.

Recently, McDonald *et al.* proposed in [36] a block circulant (BC) preconditioner to accelerate the convergence of Krylov subspace methods for solving the all-at-once linear system arising from p-step BDF temporal discretization of evolutionary PDEs. Parallel experiments with the BC preconditioner in [36] are reported by Goddard and Wathen in [19]. In [32], a generalized version of the BC preconditioner has been proposed by Lin and Ng who introduced a parameter $\alpha \in (0, 1)$ into the top-right