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Fast alternating-direction finite difference methods for three-dimensional space-fractional diffusion equations

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ABSTRACT

Fractional diffusion equations model phenomena exhibiting anomalous diffusion that cannot be modeled accurately by second-order diffusion equations. Because of the nonlocal property of fractional differential operators, numerical methods for space-fractional diffusion equations generate dense or even full coefficient matrices with complicated structures. Traditionally, these methods were solved via Gaussian elimination, which requires computational work of $O(N^3)$ per time step and $O(N^2)$ of memory to store where N is the number of spatial grid points in the discretization. The significant computational work and memory requirement of these methods makes a numerical simulation of three-dimensional space-fractional diffusion equations computationally prohibitively expensive. We present an alternating-direction implicit (ADI) finite difference formulation for space-fractional diffusion equations in three space dimensions and prove its unconditional stability and convergence rate provided that the fractional partial difference operators along x-, y-, z-directions commute. We base on the ADI formulation to develop a fast iterative ADI finite difference method, which has a computational work count of $O(N \log N)$ per iteration at each time step and a memory requirement of $O(N)$. We also develop a fast multistep ADI finite difference method, which has a computational work count of $O(N \log^2 N)$ per time step and a memory requirement of $O(N \log N)$. Numerical experiments of a three-dimensional space-fractional diffusion equation show that these both fast methods retain the same accuracy as the regular three-dimensional implicit finite difference method, but have significantly improved computational cost and memory requirement. These numerical experiments show the utility of the fast method.

1. Introduction

In the last few decades increasingly more diffusion processes were found not to obey the classical Fickian diffusion equation. Recent studies show that fractional diffusion equations provide an adequate and accurate description of these anomalous diffusion processes, which cannot be modeled properly by second-order diffusion equations [3,5,22]. However, because of the nonlocal nature of fractional differential operators, numerical methods for fractional diffusion equations raise numerical difficulties that were not encountered in the numerical methods for second-order diffusion equations. In the context of space-fractional diffusion equations, the corresponding numerical methods often generate dense or even full coefficient matrices [6,7,13,14,16,21]. Traditionally, these methods were solved via Gaussian elimination, which requires $O(N^3)$ of computational work per time step and $O(N^2)$ of memory to store where N is the number of spatial grid points in the discretization. Consequently, the numerical simulation of space-fractional diffusion equations can be very expensive, especially in three space dimensions. Therefore, development of fast and faithful numerical methods with efficient storage for space-fractional diffusion equations is of fundamental importance for the applications of fractional diffusion equations.

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Meerschaert and Tadjeran [17,18] utilized a shifted Grünwald–Letnikov difference approximation to develop an implicit Euler finite difference method for space-fractional diffusion equations in one space dimension. They went on to prove that the Meerschaert–Tadjeran method is unconditional stable and has a first-order convergence in space and time. In [16] Meerschaert, Scheffler, and Tadjeran used the idea of the classical alternating-direction method [15,24] to develop an alternating-direction implicit (ADI) Euler method to solve a one-sided space-fractional diffusion equations in two space dimensions and proved that the Meerschaert–Scheffler–Tadjeran ADI method is unconditionally stable and has first-order convergence rate in space and time. Moreover, the method has a significantly improved computational work of $O(N^{3/2})$ but still has a memory requirement of $O(N^2)$. However, the improved work count no longer holds true for a general two-sided problem in two space dimensions.

The bottleneck on the computational cost and memory requirement for the numerical methods for space-fractional diffusion equations was broken up recently by one of the authors in [30]. In [30] we proved that the stiffness matrix of the Meerschaert–Tadjeran method for the space-fractional diffusion equations in one space dimension can be decomposed as a sum of diagonal-multiply-Toeplitz matrices. We utilized these facts and applied an operator-splitting technique to the Meerschaert–Tadjeran method to develop a fast operator-splitting finite difference method for the space-fractional diffusion equations in one space dimension. The method has a computational work account of $O(N\log^2 N)$ per time step and has a memory requirement of $O(N\log N)$, while retaining the accuracy of the Meerschaert–Tadjeran method. In [31] we utilized the Toeplitz-like structure of the stiffness matrix to solve the Meerschaert–Tadjeran method directly by a conjugate gradient type fast solver. The resulting fast algorithm has a computational cost of $(N\log N)$ per iteration at each time step and a memory requirement of $O(N)$ for space-fractional diffusion equations in one space dimension.

Subsequently, we developed fast numerical methods for space-fractional diffusion equations in multiple space dimensions. In [29] we developed a fast alternating-direction implicit finite difference method for two-sided space-fractional diffusion equations in two space dimensions with decoupled x and y derivatives. In the paper we used the fast operator-splitting finite difference method developed in [30] to solve the resulting one-dimensional systems. The resulting method has a computational work count of $O(N\log^2 N)$ per time step and a memory requirement of $O(N\log N)$. In [25,27] we proved that the stiffness matrix of the Meerschaert–Tadjeran finite difference method for the space-fractional diffusion equations in two space dimensions can be decomposed as combinations of matrices of block-Toeplitz–Toeplitz-block structure and developed a fast conjugate gradient type iterative algorithm for the numerical method. This fast algorithm has a computational cost of $(N\log N)$ per iteration at each time step and a memory requirement of $O(N)$.

The objectives of this paper can be summarized as follows:

- We develop a fast multistep ADI finite difference method for space-fractional diffusion equations in three space dimensions. As for the fast solution of the resulting one-dimensional systems of space-fractional diffusion equations, we implement the following two options.
  - We employ the idea of the fast operator-splitting in [30] for the resulting one-dimensional systems to come up with a fast multistep ADI finite difference method. The would result in a computational work count of $O(N\log^2 N)$ per time step and a memory requirement of $O(N\log N)$ for the space-fractional diffusion equations in three space dimensions.
  - Alternatively, we use a fast conjugate gradient type iterative solver to solve the Meerschaert–Tadjeran finite difference method for the one-dimensional systems. The resulting method has a computational cost of $(N\log N)$ per iteration at each time step and a memory requirement of $O(N)$.
- The full Meerschaert–Tadjeran finite difference method for the space-fractional diffusion equations in three space dimensions can be solve by a fast conjugate gradient type of iterative solver [25,27]. The would result in a computational work count of $O(N\log N)$ per iteration per time step and a memory requirement of $O(N)$ for the space-fractional diffusion equations in three space dimensions. It is unclear from these work and memory counts which method is computationally more efficient and there has been no comparison of these fast methods reported in the literature either. We carry out preliminary numerical experiments to investigate the performance of and comparison among all the three fast solution methods in the context of space-fractional diffusion equations in three space dimensions.
- Another motivation for the development of ADI methods arises from the numerical simulation of nonlinear advection-diffusion transport equations with anomalous diffusion in multiple space dimensions [2,9]. Since there is no efficient solvers for Riemann problems of nonlinear hyperbolic conservation laws in multiple space dimensions, fast front tracking method based on the efficient solution of one-dimensional Riemann problem of hyperbolic conservation laws has been combined with dimensional splitting to efficiently solve hyperbolic conservation laws in multiple space dimensions [10,12]. Hence, the ADI methods for space-fractional diffusion equations and the fast front tracking methods based on dimensional splitting for hyperbolic conservation laws can naturally be combined in the efficient numerical solution of nonlinear advection-diffusion equations with anomalous diffusion in multiple space dimensions.

The rest of the paper is organized as follows. In Section 2 we outline the space-fractional diffusion equation we attempt to solve and present the corresponding finite difference method. In Section 3 we present an ADI finite difference formulation. In Section 4 we prove the unconditional stability and convergence rate of the ADI formulation. In Section 5 we develop a fast conjugate gradient squared iterative solver to solve the resulting one-dimensional systems from the ADI formulation. In Section 6 we develop a fast multistep ADI finite difference method. In Section 7 we conduct numerical experiments to examine the performance of the ADI methods developed in Sections 5 and 6 and to investigate the comparison of these