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FAST NUMERICAL SOLVERS FOR SUBDIFFUSION PROBLEMS WITH SPATIAL INTERFACES

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Abstract. This paper develops novel fast numerical solvers for subdiffusion problems with spatial interfaces. These problems are modeled by partial differential equations that contain both fractional order and conventional first order time derivatives. The former is non-local and approximated by L1 and L2 discretizations along with fast evaluation algorithms based on approximation by sums of exponentials. This results in an effective treatment of the "long-tail" kernel of subdiffusion. The latter is local and hence conventional implicit Euler or Crank-Nicolson discretizations can be used. Finite volumes are utilized for spatial discretization based on consideration of local mass conservation. Interface conditions for mass and fractional fluxes are incorporated into these fast solvers. Computational complexity and implementation procedures are briefly discussed. Numerical experiments demonstrate accuracy and efficiency of these new fast solvers.

Key words. Caputo and Riemann-Liouville derivatives, fast numerical solvers, fractional order fluxes, interface problems, subdiffusion, sum of exponentials (SOE).

1. Introduction

Anomalous diffusion happens in many physical, chemical, and biological processes [7, 8, 30, 33, 37, 44]. It is known that subdiffusion is a measure of cytoplasmic crowdedness in living cells [44] and anomalous diffusion in cardiac tissues is an index of myocardial microstructure [7].

Mathematically, subdiffusion is modeled by partial differential equations with fractional order time derivatives in Caputo, Riemann-Liouville, or other forms [8, 30].

The work in [11] offers a kind of guide to identify some common pitfalls in fractional-order differential problems. Approximation of fractional derivatives by polynomial interpolation is the common idea: L1, L2 schemes [30] and fractional linear multistep methods [25, 26, 27, 28]. [11] also discusses that the effect of the solution regularity on the accuracy of the numerical scheme for fractional-derivative problems briefly. Furthermore, because of the non-locality of the fractional-order operator, nested mesh techniques [14, 10], the fast fourier transform algorithm [15, 16] and kernel compression scheme [2, 3, 4] are mentioned for a fast, efficient and reliable treatment of fractional-derivative problems.

The conventional discretization methods applied to the frational partial differential equations [24, 23, 39, 40, 36, 48] also involve computation for the entire time period and/or across the whole domain and hence are very expensive. Therefore, fast PDE numerical solvers have been developed to overcome these disadvantages [12, 17, 36, 43, 46, 47, 48, 38]. Various techniques have been developed, e.g., approximation of kernels by sums of exponentials [17, 36, 46], and parallelization in time [45].

Subdiffusion may happen simultaneously in subdomains that are separated by spatial interfaces. Time-fractional anomalous diffusion models are used in [13]

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for simulations of transport processes in heterogeneous binary media for which interface conditions are established. Subdiffusive flow in a composite medium with a communicating interface has been investigated in [34]. In [42], 1-dim moving interface problems governed by subdiffusion is investigated. More work can be found in [9].

However, fast numerical solvers for subdiffusion problems with spatial interfaces are not yet available in the literature, to the best of our knowledge. There are well developed numerical methods in [13] for subdiffusion problems with spatial interfaces and nonlinear terms, but no discussion on fast solvers. Fast solvers are undoubtedly important for this type of problems. Our paper intends to fill this gap.

Our fast solvers rely on a special treatment of the convolutional kernel. Specifically, the integral for the Caputo derivative is split as a *recent past term* and a *history term* (the so-called "long-tail"). Based on approximation of the negative kernel by a sum of exponentials [5, 6], a recurrence formula is established for the history term and efficient time-marching schemes are developed (See Sections 3 and 5 for details). Moreover, interface conditions are naturally incorporated. It is interesting to notice that similar notion for handling kernels was applied in an early work on parabolic problems [41].

The rest of this paper is organized as follows. Section 2 describes the governing equations and interface conditions. Section 3 briefly reviews the L1, L2 temporal discretizations on graded meshes and then establishes fast evaluation algorithms based on approximation of negative power kernels by sums of exponentials. Section 4 focuses on spatial discretization using finite volumes. Section 5 develops fast numerical solvers for subdiffusion problems with spatial interfaces by combining the implicit Euler or Crank-Nicolson discretization for the conventional 1st order time derivative with the fast L1 or L2 evaluation algorithms for the fractional order derivatives. Stability analysis of the direct/fast L1 + back-Euler solvers for a simplified model is presented in Section 6. Section 7 discusses computational complexity and implementation of the fast solvers. Section 8 presents numerical experiments. The paper is concluded with remarks in Section 9.

2. Mathematical Models for Subdiffusion Problems with Spatial Interfaces

In essence, such problems involve subdiffusion with different diffusion indexes in subdomains that are separated by interfaces. For ease of representation, we consider two 1-dim or 2-dim subdomains Ω_1, Ω_2 that are separated by one interface Γ. Specifically, we consider the following governing equations

$$(1)\qquad \begin{cases} \partial_t u - {}_0^R\mathrm{D}_t^{1-\alpha_1}\, \nabla\cdot(A_1(\boldsymbol{x})\nabla u) = f_1(\boldsymbol{x},t) & \text{in } \Omega_1\times(0,T], \\ \partial_t u - {}_0^R\mathrm{D}_t^{1-\alpha_2}\, \nabla\cdot(A_2(\boldsymbol{x})\nabla u) = f_2(\boldsymbol{x},t) & \text{in } \Omega_2\times(0,T], \end{cases}$$

where $\Omega = \Omega_1 \cup \Omega_2$ is an open bounded connected domain in $\mathbb{R}^d (d = 1, 2)$,

(i) The time-fractional indices $\alpha_i \in (0, 1)$ for $i = 1, 2$;
(ii) $A_i(\boldsymbol{x}) = \left[a_{j,k}^{(i)}(\boldsymbol{x})\right]_{1\le j,k\le d}, i = 1, 2$ are the diffusion tensors that are symmetric, bounded, and uniformly positive-definite on Ω_i;
(iii) The source terms $f_i \in L^2(\Omega)$ for $i = 1, 2$.