Journal of Computational Mathematics
Vol.44, No.3, 2026, 670–699.
http://www.global-sci.org/jcm
doi:10.4208/jcm.2504-m2024-0235

ROTHE METHOD AND NUMERICAL ANALYSIS FOR A SUB-DIFFUSION EQUATION WITH CLARKE SUBDIFFERENTIAL*

Yujie Li and Chuanju Xu[1)]
School of Mathematical Sciences and Fujian Provincial Key Laboratory of Mathematical Modeling and High Performance Scientific Computing, Xiamen University, Xiamen 361005, China
Email: cjxu@xmu.edu.cn

Abstract

This paper is devoted to the study of a sub-diffusion equation involving a Clarke subdifferential boundary condition. It describes transport of particles governed by the anomalous diffusion in media with boundary semipermeability. The weak formulation of the model problem results in a time fractional parabolic hemivariational inequality. We first construct an abstract hemivariational evolutionary inclusion and prove its unique solvability using a time-discretization approximation, known as the Rothe method. In addition, a numerical approach based on a finite difference scheme in time and finite dimensional approximation in space is proposed and analyzed for the abstract problem. These results are then applied to establish the convergence of the numerical solution of the model problem. Under appropriate regularity assumptions, an optimal order error estimate for the linear finite element method is derived. Some numerical examples are provided to support the theoretical results.

Mathematics subject classification: 35S10, 47J20, 49J27, 65M06, 65M12.
Key words: Numerical analysis, Fractional hemivariational inequality, Sub-diffusion equation, Rothe method, Clarke subdifferential.

1. Introduction

Anomalous diffusion has been an active area of research in the physics community since the introduction of continuous time random walks by Montroll and Weiss [45]. One of the main characteristics of anomalous diffusion is the nonlinear behaviour of the mean square displacement, i.e. $\langle x^2(t)\rangle \propto t^\alpha$ ($\alpha < 1$ and $\alpha > 1$ correspond to subdiffusion and superdiffusion, respectively), which is, in general, related to a stochastic process with non-Markovian characteristics. This kind of diffusion process is found in various complex systems, which usually no longer follow Gaussian statistics, and thus Fick's second law fails to describe the related transport behaviour. Examples can be found in various fields ranging from biophysics (e.g. transport of large molecules in living cells [15, 53]), to geophysics and ecology (e.g. tracer diffusion in subsurface hydrology [7]).

Fractional partial differential equations (FPDEs) have been widely regarded as a complementary tool in the description of anomalous transport processes [42]. For the classical theory of fractional derivatives and FPDEs, the reader is referred to [10,48]. In particular, time fractional

* Received October 18, 2024 / Revised version received February 17, 2025 / Accepted April 3, 2025 / Published online June 18, 2025 /
1) Corresponding author

diffusion equations (TFDEs), which is obtained from the standard diffusion equations by replacing the first-order time derivative with a fractional derivative of order α $(0 < \alpha < 1)$, appear to be useful for the mathematical description of anomalous subdiffusion, related to long waiting times between particle jumps [41]. A number of scholars are devoted to the investigation of the analytical solutions to the TFDEs or the multi-term TFDEs [1,11,24–26]. Luchko and Yamamoto [38] obtained some uniqueness and existence results for a general TFDE. Liu *et al.* [36] extended the time fractional diffusion wave equation to a generalized form in the sense of the regularized version of the k-Hilfer-Prabhakar fractional operator involving the k-Mittag function and found a novel and general solution.

From the numerical aspect, there exist a lot of work related to construction of time stepping methods for time-fractional differential equations; see, e.g. [2,13,14,35,39,40,52,54,57]. In the existing work, the finite difference approximation of the fractional derivative is the most studied one. This type of time stepping methods makes use of piecewise linear/quadratic interpolation approximation at each subinterval, results in the widely-used L1 scheme [35,52], L2-1_σ scheme [2], and L2 scheme [40]. Some other work involves the storage reduction and singularity treatment at the starting point. Much efforts have been made in developing fast numerical methods to recover the desired convergence order for solutions of low regularity; see, e.g. [4,5,8,17,27,28,31,32,34,37,51].

In this paper, we focus on a time fractional diffusion equation involving a Clarke subdifferential boundary condition. Let Ω be a bounded Lipschitz domain in $\mathbb{R}^d$ with $d = 2, 3$ and the boundary $\partial\Omega$ is Lipschitz continuous. Assume $\partial\Omega$ is divided into two disjoint measurable parts Γ_1 and Γ_2 and the measure of Γ_1 is positive. The outward unit normal vector at $\partial\Omega$ is denoted by $\boldsymbol{\nu}$. We are concerned with the evolutionary process on the time interval $[0, T]$ with a given $T > 0$. The pointwise formulation of our model problem is

Problem 1.1. Find $u : \Omega \times (0, T) \to \mathbb{R}$ such that for all $t \in (0, T)$,

$$\begin{aligned}
&{}_0D_t^\alpha u(x,t) - \Delta u(x,t) = f(x,t) && \text{in } \Omega \times (0,T), \\
&u(x,t) = 0 && \text{on } \Gamma_1 \times (0,T), \\
&-\frac{\partial u(x,t)}{\partial \nu} \in \partial j\big(u(x,t)\big) && \text{on } \Gamma_2 \times (0,T), \\
&u(x,0) = u_0(x) && \text{in } \Omega.
\end{aligned}$$

Here the unknown function u represents the density of particles and ${}_0D_t^\alpha u(x,t)$ denotes the time Caputo fractional derivative of u introduced in the next section. In addition, ∂j denotes the Clarke subdifferential of a locally Lipschitz continuous function j. It is worth mentioning that the traditional diffusion equation with a Clarke subdifferential boundary condition has been considered in [47]. Han and Wang [23] studied the numerical solution of that model and derived an optimal error estimate of a finite element method.

Clarke subdifferential is a multivalued operator, widely used in fields such as contact mechanics and fluid dynamics to represent nonsmooth relations between variables that include jumps. Roughly speaking, the Clarke subdifferential introduced in Problem 1.1 as the boundary condition of the anomalous diffusion equation is targeted at simulating the process of pollutants in groundwater entering the aquifer through soil. As a porous medium, the complex structure and adsorption characteristics of soil will significantly affect the transport of pollutants. In addition, the difference in physical properties between aquifer and soil will also lead to a nonsmooth relationship between diffusion flux and solute concentration at the boundary. Therefore, compared