Book of Abstracts

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Discrete comparison principle for the time-fractional diffusion equation

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We prove a discrete comparison principle (equivalent to a discrete maximum principle) for the L1 discretisation of the Caputo time derivative and the standard 3-point discretisation of the spatial derivative in the time-fractional initial-boundary value problem $D_t^{\alpha}u - p\Delta u + c(x,t)u = f$, where p > 0 but no assumption is made on the sign of c. (Previously, any discrete comparison principle relied on the assumption that $c \ge 0$.) The result reveals why one needs a certain condition on the temporal mesh that has been assumed by several authors when analysing numerical methods for this problem. Then this comparison principle is used to give a new error analysis for the case $c \ge 0$ by means of a barrier function. All the analysis can be extended to certain other discretisations of the fractional derivative.

KEY WORDS: Discrete comparison principle, L1 scheme, weak singularity, convergence analysis

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Backward difference formulae: The energy technique for (sub)diffusion equation

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In combination with the Grenander–Szegő theorem, we observe that a relaxed positivity condition on multipliers, milder than the basic requirement of the Nevanlinna–Odeh multipliers that the sum of the absolute values of their components is strictly less than 1, makes the energy technique applicable to the stability analysis of BDF methods for parabolic equations with selfadjoint elliptic part. This is particularly useful for the six-step BDF method for which we show that no Nevanlinna–Odeh multipliers exist. We introduce multipliers satisfying the positivity property for the six-step BDF method and establish stability of the method for parabolic equations [1] and subdiffusion equation [2, 3].

KEY WORDS: (Sub)diffusion equation, six-step BDF method, energy technique, multipliers, stability estimate

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- 3. Jiankang Shi and Minghua Chen, Correction of high-order BDF convolution quadrature for fractional Feynman-Kac equation with Lévy flight, J. Sci. Comput. 85:28 (2020)

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A spectrally accurate approximation to Subdiffusion equations using the log orthogonal functions

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We develop and analyze a spectral-Gelerkin method for solving subdiffusion equations, which contain Caputo fractional derivatives with order $\nu \in (0, 1)$. The basis functions of our spectral method are constructed by applying a log mapping to Laguerre functions, and have already been proved to be suitable to approximate functions with fractional power singularities in [1]. We provide rigorous regularity and error analysis which show that the scheme is spectrally accurate, i.e., the convergence rate depends only on regularity of problem data. The proof relies on the approximation properties of some reconstruction of the basis functions as well as the sharp regularity estimate in some weighted Sobolev spaces. Numerical experiments fully support the theoretical results and show the efficiency of the proposed spectral-Galerkin method. We also develop fully discrete scheme with the proposed spectral method in time and Galerkin finite element method in space, and apply the proposed techniques to subdiffusion equations with time dependent diffusion coefficients as well as to the nonlinear time-fractional Allen-Cahn equation.

KEY WORDS: Log orthogonal functions, subdiffusion equation, singularity, error analysis, spectral accuracy

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Numerical algorithm for the space-time fractional Fokker-Planck system with two internal states

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The fractional Fokker-Planck system with multiple internal states is derived in [Xu and Deng, Math. Model. Nat. Phenom., **13**, 10 (2018)], where the space derivative is Laplace operator. If the jump length distribution of the particles is power law instead of Gaussian, the space derivative should be replaced with fractional Laplacian. This paper focuses on solving the two-state Fokker-Planck system with fractional Laplacian. We first provide a priori estimate for this system under different regularity assumptions on the initial data. Then we use L_1 scheme to discretize the time fractional derivatives and finite element method to approximate the fractional Laplacian operators. Furthermore, we give the error estimates for the space semidiscrete and fully discrete schemes without any assumption on regularity of solutions. Finally, the effectiveness of the designed scheme is verified by one- and two-dimensional numerical experiments.

KEY WORDS: Fractional Fokker-Planck system, multiple internal states, Riemann-Liouville fractional derivative, fractional Laplacian, L_1 scheme, finite element method, error estimates

^{1.} DX Nie, J Sun, WH Deng, Numerical algorithm for the space-time fractional Fokker-Planck system with two internal states, Numerische Mathematik, 146(3), 481-511, 2020.

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Rational approximation schemes for computing operator functions $E_{\alpha,\beta}(-\mathcal{L}t^{\gamma})v$ and $\mathcal{L}^{-\alpha}f$

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In this talk we shall focus on two approximation problems arising from solving fractional differential equations numerically. Let $E_{\alpha,\beta}(t)$ denote the two-parameter Mittag-Leffler function and \mathcal{L} be the positive definite elliptic operator. We shall present two rational approximation schemes correspondingly for $E_{\alpha,\beta}(-\mathcal{L}t^{\gamma})$ and $\mathcal{L}^{-\alpha}$ such that $E_{\alpha,\beta}(-\mathcal{L}t^{\gamma})v$ and $\mathcal{L}^{-\alpha}f$ can be evaluated efficiently for $\forall v, f \in H^{-1}$. Rigorous error analysis will be carried out then sharp error bounds follow. We will also give some numerical examples to illustrate the efficiency and robustness of our schemes.

KEY WORDS: Mittag-Leffler functions, fractional power of elliptic operators, rational approximation

^{1.} Beiping Duan and Zhimin Zhang, A rational approximation scheme for computing Mittag-Leffler function with discrete elliptic operator as input, J. of Scientific Computing, DOI: 10.1007/s10915-021-01495-y.

Beiping Duan, Raytcho Lazarov, Joseph Pasciak. Numerical Approximation of Fractional Powers of Elliptic Operators. IMA J. of Numerical Analysis, 40(3), 1746–1771(2020).

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Optimal H^1 spatial convergence of a fully discrete finite element method for the time-fractional Allen-Cahn equation

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A time-fractional Allen-Cahn problem is considered, where the spatial domain Ω is a bounded subset of \mathbb{R}^d for some $d \in \{1, 2, 3\}$. New bounds on certain derivatives of the solution are derived. These are used in the analysis of the numerical method [1] (the L1 discretisation and Alikhanov's L2-1_{σ} discretisation of the Caputo derivative on suitably graded temporal meshes, with a standard finite element discretization of the spatial diffusion term, and Newton linearization of the nonlinear driving term), showing that the computed solution achieves the optimal rate of convergence in the Sobolev $H^1(\Omega)$ norm. (Previous papers considered only convergence in $L^2(\Omega)$.) Numerical results confirm our theoretical findings.

KEY WORDS: Time-fractional, Finite element method, Caputo derivative, Superconvergence

^{1.} Chaobao Huang and Martin Stynes, Optimal H^1 spatial convergence of a fully discrete finite element method for the time-fractional Allen-Cahn equation, Adv.Comput.Math., 2020, 46(4):63.

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Efficient algorithm and applications of the magnetohydrodynamic coupled fractional model

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In this paper, the problem of unsteady magnetohydrodynamic (MHD) flow and heat transfer of generalized second grade fluid through porous medium is investigated. The second grade fluid with a fractional derivative is used for the constitutive equation, and the fractional heat conduction equation is considered, which combined into a fractional coupled flow and heat transfer model. Then numerical scheme with the second-order fractional backward difference formula in the temporal direction and a spectral method in the spatial direction is proposed. The fully discrete scheme is obtained and proved to be stable and convergent with second order accuracy in time and spectral accuracy in space. Moreover, to decrease the memory requirement and computational cost of the time fractional fractional operator, a fast algorithm is presented and the convergence analysis of the numerical scheme with fast algorithm is also proved strictly. We also implement some numerical examples to further support the theoretical analysis. At last, an unsteady MHD flow of generalized second grade fluid through porous medium with fractional heat transfer is considered. The effects of the involved parameters on velocity profiles, temperature field, and concentration field are shown graphically and analyzed in detail.

KEY WORDS: Fractional coupled equations, Convergence analysis, Magnetohydrodynamics, Fast algorithm, Numerical simulation

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Discovering the subdiffusion model in an unknown medium

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The subdiffusion phenomenon is now widely recognized in many engineering and physical applications. The mathematical models for subdiffusion involve several parameters, e.g., diffusion coefficient, potential, initial and boundary conditions along with the order of derivation. Sometimes some of these parameters are not readily available, but one can measure additional information about the solution. Then one natural question is how much we can say about the mathematical model. In this talk, I will discuss several theoretical and computational results on determining the order of derivation and other parameters when the other problem data are not fully specified. The talk is based on joint works with Yavar Kian and Zhi Zhou.

KEY WORDS: numerical reconstruction, inverse problems, time-fractional diffusion

Pointwise-in-time a posteriori error control for time-fractional parabolic equations

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For time-fractional parabolic equations with a Caputo time derivative of order $\alpha \in (0, 1)$, we give pointwise-in-time a posteriori error bounds in the spatial L_2 and L_{∞} norms. Hence, an adaptive mesh construction algorithm is applied for the L1 method, which yields optimal convergence rates $2 - \alpha$ in the presence of solution singularities.

KEY WORDS: fractional-order parabolic equation, a posteriori error estimates, L1 scheme, pointwisein-time error bounds

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Exponential convolution quadrature for nonlinear subdiffusion equations with nonsmooth initial data

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An exponential type of convolution quadrature is proposed as a time-stepping method for the nonlinear subdiffusion equation with bounded measurable initial data. The method combines contour integral representation of the solution, quadrature approximation of contour integrals, multistep exponential integrators for ordinary differential equations, and locally refined stepsizes to resolve the initial singularity. The proposed k-step exponential convolution quadrature can have kth-order convergence for bounded measurable solutions of the nonlinear subdiffusion equation based on natural regularity of the solution with bounded measurable initial data.

KEY WORDS: subdiffusion equation, time-fractional, nonlinear, nonsmooth initial data, high order, convolution quadrature, exponential integrator, locally refined stepsizes

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Logarithmic asymptotics: analysis and computation

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This report includes a series of work with Drs. Zhiqiang Li and Zhen Wang [1, 2, 3, 4]. The so-called logarithmic asymptotics indicates that the solution to the evolution equation has algebraic asymptotics in the sense of logarithmic function. It is often used to characterize the ultra slow process, such as creep in igneous rocks. In this talk, we mainly introduce the logarithmic asymptotics and regularity of the solution to the Caputo-Hadamard fractional evolution equation. Based on these theoretical analysis, we construct the reliable numerical algorithms to numerically solve it.

KEY WORDS: Logarithmic asymptotics, Caputo-Hadamard derivative, finite difference method, local Discontinuous Galerkin finite method

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Some novel schemes to capture the initial dramatic evolutions of nonlinear subdiffusion equations

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The solution of the nonlinear subdiffusion equation has the initial layer and its initial energy may decay very fast. Therefore, it is important to investigate the evolution of the solution at the beginning. Based on smoothing transformation, we present some novel schemes to capture the initial dramatic evolutions in this talk. Meanwhile, the proposed time discretization is particularly effective for models with the small α and their interesting numerical phenomena are reported.

 KEY WORDS: Nonlinear subdiffusion equations, boundary layer, novel schemes, smooth transformation

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L1/LDG method for the generalized time-fractional Burgers equation

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This talk mainly introduces the L1/LDG method for the generalized time-fractional Burgers equation [1]. According to the regularity of the solution of the equation at the initial time, the L1 method on uniform or non-uniform meshes is used to discretize the fractional derivative in the sense of Caputo with derivative order in (0, 1), and the local discontinuous Galerkin (LDG) method is used in space. The fully discrete schemes for both situations are established and analyzed. It is shown that the derived schemes are numerically stable and convergent.

KEY WORDS: Caputo derivative, L1 scheme, Local discontinuous Galerkin method, Stability, Convergence

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Convergence analysis of collocation solutions in continuous piecewise polynomial spaces for Volterra integral equations

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Volterra integral equations are closely related to fractional differential equations. In this talk, we mainly focus on the convergence of collocation solutions in continuous piecewise polynomial spaces for second-kind Volterra integral equations (VIEs). First, it is shown that the collocation solutions for second-kind VIEs with smooth kernels are uniformly convergent (as the mesh diameter tends to zero) only for certain sets of collocation points. Then, we study the analogous convergence properties of the collocation solutions for second-kind VIEs with weakly singular kernels, both with respect to uniform and graded meshes.

KEY WORDS: Volterra integral equations, collocation methods, continuous piecewise polynomial spaces, convergence analysis

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Asymptotically compatible energy laws of L1-type schemes for time-fractional Allen-Cahn equation

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In this talk, we consider L1-type schemes with variable time-steps for time fractional Allen-Cahn equation. The proposed schemes are shown to be unconditionally stable (in a variational energy sense), and is maximum bound preserving. Interestingly, the discrete energy stability results can recover the classical energy dissipation law when the fractional order $\alpha \rightarrow 1$. That is, our schemes can asymptotically preserve the energy dissipation law in the $\alpha \rightarrow 1$ limit. As a by product, we build up a reversible transformation between the L1-type formula of the Riemann-Liouville derivative and the L1-type formula of the Caputo derivative, with the help of a class of discrete orthogonal convolution kernels. This is the first time such a *discrete* transformation is established between two discrete fractional derivatives.

KEY WORDS: Time-fractional Allen-Cahn equation, asymptotic preserving, energy stability, maximum principle, adaptive time-stepping

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Numerical analysis of time fractional diffusion problems with low regularity data

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We focus on numerical analysis for time fractional subdiffusion problems with order $\alpha \in (0, 1)$. Weak solution is introduced and regularity results are established in Sobolev space and Besov space, respectively. Then a time-stepping discontinuous Galerkin scheme is proposed and the optimal rate is derived with nonsmooth data. Besides, a time-spectral algorithm is considered and the "doubling" convergence rate $1 + 2\alpha$ is proved rigorously. Finally, several numerical experiments are provided to validate our theoretical results.

KEY WORDS: Fractional diffusion equation, weak solution, regularity, nonsmooth data, discontinuous Galerkin method, time-spectral algorithm, optimal error estimate

- 1. H. Luo and X. Xie. Optimal error estimation of a time-spectral method for fractional diffusion problems with low regularity data. arXiv:2106.03100, 2021.
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Barrier function local and global analysis of an L1 finite element method for a multiterm time-fractional initial-boundary value problem

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An initial-boundary value problem of the form $\sum_{i=1}^{l} q_i D_t^{\alpha_i} u(x,t) - \Delta u = f$ is considered, where each $D_t^{\alpha_i}$ is a Caputo fractional derivative of order $\alpha_i \in (0, 1)$ and the spatial domain Ω lies in \mathbb{R}^d for $d \in \{1, 2, 3\}$. To solve the problem numerically, we apply the L1 discretisation to each fractional derivative on a graded temporal mesh, together with a standard finite element method for the spatial derivatives on a quasiuniform spatial mesh. A new proof of the stability of this method, which is more complicated than the l = 1 case of a single fractional derivative, is given using barrier functions; this powerful new technique leads to sharp error estimates in $L^2(\Omega)$ and $H^1(\Omega)$ at each time level t_m that show precisely the improvement in accuracy of the method as one moves away from the initial time t = 0. (A result of this type has not previously been derived for this multiterm problem.) Consequently, while for global optimal accuracy one needs a mesh that is strongly graded when all the α_i are near zero, for local optimal accuracy away from t = 0 one needs a much less severe mesh grading. Numerical experiments show the sharpness of our theoretical results.

KEY WORDS: Multiterm time-fractional problem, L1 scheme, barrier function

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Numerical Methods for Several Fractional PDEs

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In this talk, several numerical methods for time/space fractional PDEs will be discussed. Firstly, we will talk about numerical methods for space fractional differential equations, including finite difference methods, finite element methods, and differential quadrature methods (meshless method). We emphasize that the finite element methods and differential quadrature methods are effective on complex domains. Secondly, we will focus on time fractional PDEs with nonlinear source term and discuss the convergence of L1 scheme and WSGD scheme combined with the finite element method, separately, and the optimal error estimations for those schemes will be given. At last, some conclusions are given on those methods.

KEY WORDS: finite element method, differential quadrature method, irregular domain, optimal error estimation

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Long time behavior of numerical solutions to time fractional differential equations

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Compared with the standard diffusion model, the time fractional subdiffusion equation has two typical characteristics: first, the solution has low regularity near the initial time; second, the solution has a polynomial decay rate over a long time. The first question has been well studied with many important results. We will focus on the second question. Based on the Volterra integral form of the equation, we introduce a class of CM-preserving numerical scheme. This kind of numerical scheme is proved to have many elegant properties, including good numerical stability and accurate preservation of the long decay rate of the linear subdiffusion equation.

KEY WORDS: fractional subdiffusion equation, CM-perserving schemes, polynomial decay rate

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Analysis of Fractional Models Arisen from Electromagnetic Wave Propagations in Dispersive Media

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Electromagnetic wave propagations in dispersive media– materials with a frequency-dependent electric permittivity are ubiquitous. The polarization response of the material leads to a temporal convolutional constitutive relation in the Maxwell's system. In this talk, we shall discuss the Maxwell's equations in a Havriliak-Negami (H-N) medium, which include the relatively known Cole-Cole (C-C) and Davidson-Cole (D-C) models as special cases. In general, for the H-N model, the convolutional polarization relation has a complicated singular kernel in terms of the Mittag-Leffler (ML) function. However, for the C-C and D-C models, it can be formulated as a time-fractional equation involving Caputo and tempered fractional derivatives respectively. Here, we focus on the numerical analysis of the H-N model in terms of energy dissipation and unconditionally stable discretization and also study an interesting differential-integral wave equation reduced from the Cole-Cole model.

This talk will be largely based on the recent joint works [1, 2, 3].

KEY WORDS: Time-fractional polarization, temporal convolution, dispersive media, energy law, stability

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X-Spectral Methods for Some Differential Equations

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In this talk I will present extended spectral methods for some classes of integro-differential equations, making use of fractional polynomials, also known as Muntz polynomials, for approximating solutions having low regularity. Basic approximation properties of the Muntz polynomials, including error estimates for the weighted projection and interpolation operators, are discussed. We will show how to construct and analyze efficient X-spectral methods based on the Muntz polynomial approximation. The potential application of the new methods covers a number of well-known problems, including classical elliptic equations having corner singularities, integro-differential equations with weakly singular kernels, fractional differential equations, and so on.

KEY WORDS: Spectral methods, fractional polynomials, integro-fractional differential equations

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Fast convolution quadrature for fractional operators

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We present a unified fast memory-saving method for the approximation of the fractional integral and derivative operators. Our method simplifies Lubich's fast method [SISC, 28 (2006) 421–438] in both theory and implementations. Numerical experiments support the theoretical results.

KEY WORDS: Fractional integral and derivatives, convolution quadrature, composite trapezoidal rule

Convergence analysis of the time-stepping numerical methods for time-fractional nonlinear subdiffusion equations

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In 1986, Dixon and McKee developed a discrete fractional Grönwall inequality [1] which can be seen as a generalization of the classical discrete Grönwall inequality. However, this generalized discrete Grönwall inequality and its variant [2] have not been widely applied in the numerical analysis of the time-stepping methods for the time-fractional evolution equations. The main purpose of this paper is to show how to apply the generalized discrete Grönwall inequality to prove the convergence of a class of time-stepping numerical methods for time-fractional nonlinear subdiffusion equations, including the popular fractional backward difference type methods of order one and two, and the fractional Crank-Nicolson type methods. We obtain the optimal L^2 error estimate in space discretization for multi-dimensional problems. The convergence of the fast time-stepping numerical methods is also proved in a simple manner. The present work unifies the convergence analysis of several existing time-stepping schemes. Numerical examples are provided to verify the effectiveness of the present method.

KEY WORDS: Time-fractional nonlinear subdiffusion equations, discrete fractional Grönwall inequality, fast time-stepping methods, convergence

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Analysis of the variable-step L1 scheme for the 2D time-fractional Swift-Hohenberg equation

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The variable-step L1 scheme for the time-fractional Swift-Hohenberg equation will be shown in this talk. We first consider the energy stability of the variable-step L1 scheme by constructing the modified discrete energy, and then extend our result to get the estimate of numerical solutions. By applying the discrete orthogonal convolution kernels, the L2 norm convergence of the proposed scheme is obtained. A key ingredient in the proof of the error estimates is the construction of the transformation for the approximation of the temporal derivative. With this transformation, we can then use positive semi-definiteness of the discrete orthogonal convolution kernels and the discrete Gronwall inequality to obtain the optimal error estimates. Numerical experiments are presented to confirm the theoretical results. On the simulation side, the comparison with the classical case shows the sub-diffusion property of the fractional models.

KEY WORDS: Swift-Hohenberg equation; L1 scheme; Energy stability; Convergence analysis

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Optimal control of variable-order time-fractional PDEs

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We study a distributed optimal control problem governed by a variable-order time-fractional diffusion equation in multiple space dimensions. The well-posedness of the proposed model and the smoothing properties of their solutions are proved, based on which the corresponding fully-discrete finite element methods are analyzed. Numerical experiments are carried out to substantiate the theoretical analysis.

KEY WORDS: Variable-order, time-fractional diffusion equation, optimal control, well-posedness and regularity, optimal-order error estimate

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Numerical analysis of backward subdiffsion problems: an application of error analysis in terms of data regularity

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We study the numerical scheme for approximately solving the backward problem of subdiusion equation involving a fractional derivative in time with order $\alpha \in (0, 1)$. After using quasiboundary value method to regularize the "mildly" ill-posed problem, we propose a fully discrete scheme by applying finite element method in space and convolution quadrature in time. The analysis of the proposed scheme relies heavily on smoothing properties of solution operators and some nonstandard error estimate for the direct problem in terms of problem data regularity. The theoretical results are useful to balance discretization parameters, regularization parameterand noise level.

KEY WORDS: fractional subdiffusion, backward problem, quasi-boundary value method, finite element method, convolution quadrature, error analysis

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