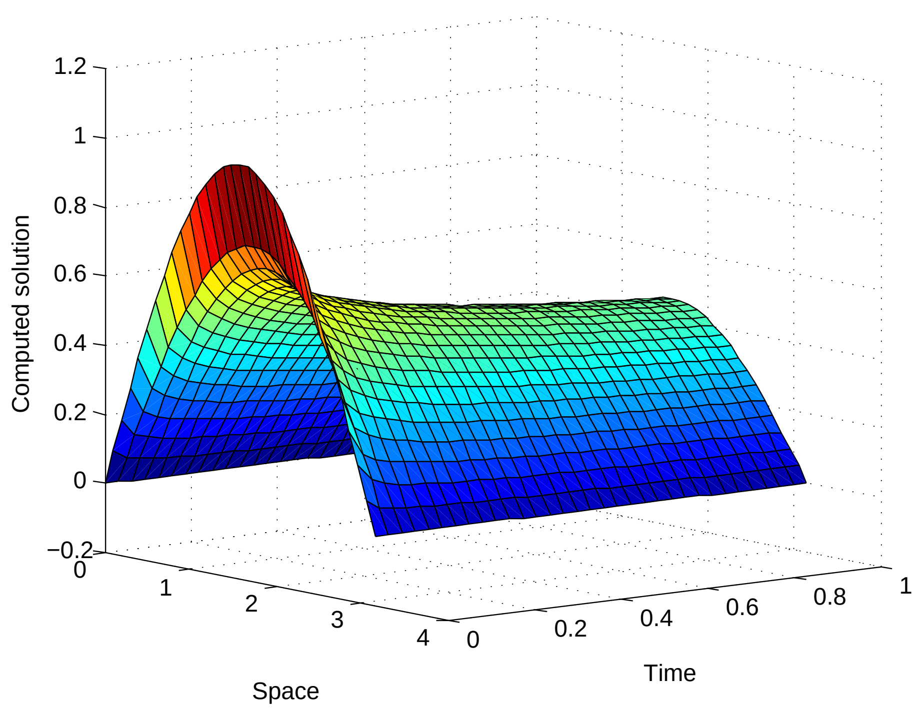
Book of Abstracts

6th Annual Conference

Numerical Methods for
Fractional-Derivative Problems

Beijing Computational Science Research Center

11–13 August 2022



Modified BDF2 schemes for subdiffusion models with a singular source term

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The aim of this paper is to study the time stepping scheme for approximately solving the subdiffusion equation with a weakly singular source term. In this case, many popular time stepping schemes, including the correction of high-order BDF methods, may lose their high-order accuracy. To fill in this gap, in this paper, we develop a novel time stepping scheme, where the source term is regularized by using a k-fold integral-derivative and the equation is discretized by using a modified BDF2 convolution quadrature. We prove that the proposed time stepping scheme is second-order, even if the source term is nonsmooth in time and incompatible with the initial data. Numerical results are presented to support the theoretical results.

KEY WORDS: Subdiffusion, modified BDF2 schemes, singular source term, error estimate

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Algorithm and analysis for the anomalous Feynman-Kac equation

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We derive the Feynman-Kac equation governing the functional distribution of anomalous diffusion. Then we discuss its well-posedness, regularity, and numerical schemes.

KEY WORDS: Numerical discretization, Feynman-Kac equation, Well-posedness, Regularity

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¶This work was supported in part by the National Natural Science Foundation of China under grant 12071195.

A quadrature scheme for steady-state diffusion equations involving fractional power of regularly accretive operator

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In this talk we present a quadrature scheme to numerically solve the nonlocal diffusion equation $(\mathcal{A}^\alpha + b\mathcal{I})u = f$ with $\mathcal{A}^\alpha$ the α-th power of the regularly accretive operator $\mathcal{A}$. Rigorous error analysis is carried out and sharp error bounds (up to some negligible constants) are obtained. The error estimates include a wide range of cases in which the regularity index and spectral angle of $\mathcal{A}$, the smoothness of f, the size of b and α are all involved. The quadrature scheme is exponentially convergent with respect to the step size and is root-exponentially convergent with respect to the number of solves. Some numerical tests will be presented to verify the sharpness of our estimates. Furthermore, both the scheme and the error bounds can be utilized directly to solve and analyze time-dependent problems.

KEY WORDS: fractional powers of regularly accretive operators, quadrature scheme, nonlocal diffusion equations

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A fast finite volume method for spatial fractional diffusion equations on nonuniform meshes

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In this work, a fast finite volume method is proposed for the initial and boundary value problems of spatial fractional diffusion equations on nonuniform meshes. The discretizations of the Riemann-Liouville fractional derivatives lead to unstructured dense coefficient matrices, differing from the Toeplitz-like structure under the uniform mesh. The fast algorithm is proposed by using the sum-of-exponentials (SOE) technique to the spatial kernel $x^{\alpha-1}$, $\alpha \in (0,1)$. Then, the matrix-vector multiplications of the resulting coefficient matrices could be implemented in $\mathcal{O}(m \log^2 m)$ operations, where m denotes the size of matrices. Iterative solvers are preferably applied to obtain the numerical solution. The proposed fast scheme is proved to be unconditionally stable for sufficiently accurate SOE approximation. Meanwhile, a banded preconditioner is exploited to accelerate the Krylov subspace method. Numerical experiments are provided to demonstrate the efficiency of the proposed fast algorithm.

KEY WORDS: Finite volume method, spatial fractional diffusion equations, sum-of-exponentials technique, fast algorithm

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¶This work was supported in part by the National Natural Science Foundation of China under grant 12101123.

High-order two-grid finite difference algorithm and its application in nonlinear time-fractional biharmonic problems

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In this work, we propose a basic implementation framework of the high-order two-grid finite difference algorithm, in which the cubic spline interpolation operator is introduced and its linearity and boundedness are discussed. As an application, the above two-grid algorithm is used to solve the nonlinear time fractional biharmonic equation. In this method, the well-known Alikhanov's approximation on graded meshes is presented to deal with the weak singularity at initial time $t = 0$, while compact difference method based on order reduction is employed to approximate the spatial second-order and fourth-order derivatives. And then, α-robust and optimal error estimates with the order of $\mathcal{O}\left(N^{-\min\{r\alpha,2\}} + h^4 + H^8\right)$ in the sense of L^2 and L^∞ norms are unconditionally proved, where N, H and h are the number of temporal unknowns, coarse grid mesh size, and fine grid mesh size, respectively. Numerical examples are provided to verify the effectiveness and efficiency of the proposed two-grid algorithm. To the best of our knowledge, this seems to be the first work about the construction and application of two-grid algorithm based on the high-order difference method.

KEY WORDS: Compact difference method, cubic spline interpolation, two-grid, nonlinear time fractional biharmonic equation, unconditional and optimal error estimate

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¶This work was supported in part by the National Natural Science Foundation of China under grants 11971482 and 12131014.

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

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A semilinear initial-boundary value problem with a Caputo time derivative of fractional order $\alpha \in (0, 1)$ is considered, solutions of which typically exhibit a singular behaviour at an initial time. For L1-type discretizations of this problem, we employ the method of upper and lower solutions to obtain sharp pointwise-in-time error bounds on quasi-graded temporal meshes with arbitrary degree of grading [1]. In particular, those results imply (similarly to the case of linear equations [2]) that milder (compared to the optimal) grading yields the optimal convergence rate $2 - \alpha$ in positive time, while quasi-uniform temporal meshes yield first-order convergence in positive time. Furthermore, under appropriate conditions on the nonlinearity, the method of upper and lower solutions immediately implies that, similarly to the exact solutions, the computed solutions lie within a certain range. Semi-discretizations in time and full discretizations using finite differences and finite elements in space are addressed. The theoretical findings are illustrated by numerical experiments. In the second part of the talk, we shall discuss the pointwise-in-time a posteriori error control, in the spirit of [3] but for the semilinear case, for which we shall employ [4].

KEY WORDS: fractional-order parabolic equation, semilinear, L1 scheme, graded temporal mesh, arbitrary degree of grading, pointwise-in-time error bounds, a posteriori error estimates

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An exponential spectral method using VP means for semilinear subdiffusion equations with rough data

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A new spectral method is constructed for the linear and semilinear subdiffusion equations with possibly discontinuous rough initial data. The new method effectively combines several computational techniques, including the contour integral representation of the solutions, the quadrature approximation of contour integrals, the exponential integrator using the de la Vallée Poussin means of the source function, and a decomposition of the time interval geometrically refined towards the singularity of the solution and the source function. Rigorous error analysis shows that the proposed method has spectral convergence for the linear and semilinear subdiffusion equations with bounded measurable initial data and possibly singular source functions under the natural regularity of the solutions.

KEY WORDS: Semilinear subdiffusion equation, singularity, spectral method, exponential integrator, VP means, geometric decomposition, contour integral, quadrature approximation

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1. Buyang Li, Yanping Lin, Shu Ma, Qiqi Rao: An exponential spectral method using VP means for semilinear subdiffusion equations with rough data.

Applications of Padé approximation in solving time-fractional differential equations

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The significant computational work and memory requirement of the numerical methods for fractional PDEs imposes a serious challenge for solving these models. Much efforts have been made to overcome the numerical difficulties. The rational approximation technique is one of the most important strategies. In this talk we consider the special case of the rational approximation. We first review the existing works of the rational approximation in solving time-fractional differential equations. We hence discuss a new approach based on the approximation of the Laplace spectrum of the convolution kernel by Padé approximation. To illustrate the performance of proposed approach, we design numerical schemes for some time-fractional differential equations using the approach, which include fractional ODEs, PDEs with tempered fractional boundaries. We discuss the error estimates of proposed numerical scheme by Padé approximation. We also present some numerical examples to verify our theoretical results.

KEY WORDS: Padé approximation, fractional derivatives, time fractional PDEs

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Approximation formulae for Caputo-Hadamard fractional derivatives and their applications in large time integration

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In this talk, three kinds of numerical formulas are proposed for approximating the Caputo-Hadamard fractional derivatives, which are called L1-2 formula, L2-1_σ formula, and H2N2 formula, respectively. Among them, the numerical formulas L1-2 and L2-1_σ are for order $\alpha \in (0,1)$ with (3-α)-th order convergence, and H2N2 formula is for order $\alpha \in (1,2)$ with (3-α)-th order convergence too, where the theoretical convergence order has been verified by the illustrative examples. Finally, these three new formulas are applied to large time integration of fractional differential systems.

KEY WORDS: Caputo-Hadamard derivative, L1-2 formula, L2-1_σ formula, H2N2 formula

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¶This work was partially supported by the National Natural Science Foundation of China under grant no. 11872234

Sharp pointwise-in-time error estimate of L1 scheme for nonlinear subdiffusion equations

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An essential feature of the subdiffusion equations with the ŠÁ-order time fractional derivative is the weak singularity at the initial time. The weak regularity of the solution is usually characterized by a regularity parameter $\sigma \in (0,1) \cup (1,2)$. Under this general regularity assumption, we here obtain the pointwise-in-time error estimate of the widely used L1 scheme for nonlinear subdiffusion equations. To the end, we present a refined discrete fractional-type Gr¡§onwall inequality and a rigorous analysis for the truncation errors. Numerical experiments are provided to demonstrate the effectiveness of our theoretical analysis.

KEY WORDS: Sharp pointwise-in-time error estimate, L1 scheme,nonlinear subdiffusion equations,non-smooth solutions

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¶This work was supported in part by the National Natural Science Foundation of China under grant 111171162.

An efficient numerical method on modified space-time sparse grid for time-fractional diffusion equation with nonsmooth data

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In this paper, we focus on developing a high efficient algorithm for solving time-fractional diffusion equation (TFDE). For TFDE, the initial function or source term is usually not smooth, which can lead to the low regularity of exact solution. And such low regularity have a marked impact on the convergence rate of numerical method. In order to improve the convergence rate of the algorithm, we introduce the space-time sparse grid (STSG) method to solve TFDE. In our study, we employ the sine basis for spatial discretization, and all the sine coefficients can be divided into several levels. The sine coefficients with different levels are discretized by temporal basis with different scales, which can lead to the STSG method. Under certain conditions, the function approximation on standard STSG can achieve the accuracy order $\mathcal{O}(2^{-Jd})$ with $\mathcal{O}(2^J J)$ degrees of freedom for $d = 1$ and $\mathcal{O}(2^{Jd})$ degrees of freedom for $d > 1$, where d is the spatial dimension, and J denotes the maximal level of sine coefficients. However, the standard STSG is not suitable to simulate the singularity of TFDE at the initial time. To overcome this, we integrate the full grid into the STSG, and obtain the modified STSG. Then, the modified STSG is used to construct the fully discrete scheme for solving TFDE. The great advantage of STSG method can be shown in the comparative numerical experiment.

KEY WORDS: Time-fractional diffusion equation, Space-time sparse grid, Sine pseudospectral method, L1 difference method, Hierarchical basis

¶This work is supported by NSF of China (Nos. 12071403, 11971412), Scientific Research Foundation of Hunan Provincial Education Department of China (Nos. 21A0108, 20B566).

Discrete gradient structure of the second-order integral averaged formula for nonlinear integro-differential models

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The discrete gradient structure and the positive definiteness of discrete fractional integrals or derivatives are fundamental to the numerical stability in long-time simulation of nonlinear integro-differential models. We bulid up a discrete gradient structure for a class of second-order variable-step approximations of fractional Riemann-Liouville integral and fractional Caputo derivative. Then certain variational energy dissipation laws at discrete levels of the corresponding variable-step Crank-Nicolson type methods are established for time-fractional Allen-Cahn and time-fractional Klein-Gordon type models. They are shown to be asymptotically compatible with the associated energy law of the classical Allen-Cahn and Klein-Gordon equations in the associated fractional order limits. Numerical examples together with an adaptive time-stepping procedure are provided to demonstrate the effectiveness of our second-order methods.

KEY WORDS: integral averaged approximation; discrete gradient structure; time-fractional Allen-Cahn model; time-fractional Klein-Gordon model; discrete variational energy law

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¶This work was supported in part by the National Natural Science Foundation of China under grants 12071216, 12101510 and 12071373, the NSF of Sichuan Province under grant 2022NSFSC1789, and the Guanghua Talent Project of SWUFE.

A global dynamics preserving method for a class of time-fractional epidemic model with reaction-diffusion

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We use an L1 finite difference method to discretize a time-fractional reaction-diffusion epidemic model with generalized incidence rate. The L1 finite difference method preserves the positivity and boundness properties of the continuous epidemic model. Furthermore, the dynamic properties of the proposed discrete system are studied. The global asymptotic stability of autonomous systems with L1 scheme is investigated by Lyapunov's direct method. By constructing a new discrete Lyapunov function, we prove the global asymptotic stability of disease-free equilibrium point and endemic equilibrium point.

KEY WORDS: time fractional, epidemic model, global stability, Lyapunov function

¶This work was supported in part by the National Natural Science Foundation of China under grants 12101039.

An efficient spectral method for the fractional Schrödinger equation on the real line

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The fractional Schrödinger equation (FSE) on the real line arises in a broad range of physical settings and their numerical simulation is challenging due to the nonlocal nature and the power law decay of the solution at infinity. In this paper, we propose a new spectral discretization scheme for the FSE in space based upon Malmquist-Takenaka functions. We show that this new discretization scheme achieves much better performance than existing discretization schemes in the case where the underlying FSE involves the square root of the Laplacian, while in other cases it also exhibits comparable or even better performance. Numerical experiments are provided to illustrate the effectiveness of the proposed method.

KEY WORDS: Fractional Laplacian, fractional Schrödinger equation, Malmquist-Takenaka functions, spectral Galerkin method

¶This work was supported by the National Natural Science Foundation of China under grant 11671160.

Efficient Monte Carlo Methods for fractional PDEs in High Dimensions

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In this talk, we introduce a Monte Carlo method for solving PDEs involving an integral fractional Laplacian (IFL) on any bounded domain in arbitrary dimensions. We first construct a new Feynman-Kac representation based on the Green function for the fractional Laplacian operator on the unit ball in arbitrary dimensions. Then an algorithm is proposed for solving fractional PDEs in the complex domain, inspired by the "walk-on-spheres" algorithm proposed in [Kyprianou, Osojnik, and Shardlow, IMA J. Numer. Anal.(2018)]. The proposed method finds it remarkably efficient in solving fractional PDEs: it only needs to evaluate the integrals of expectation form over a series of inside ball tangent boundaries with the known Green function. Moreover, we carry out the error estimates of the proposed method for the n-dimensional unit ball. Finally, ample numerical results are presented to demonstrate the robustness and effectiveness of this approach for fractional PDEs in unit disk and complex domains, and even in ten-dimensional cases.

KEY WORDS: Integral fractional Laplacian, Green function, Monte Carlo method, Spherical coordinate

¶This work was supported by Shanghai Pujiang Program 21PJ1403500, the Fundamental Research Funds for the Central Universities 2021110474 and Shanghai Post-doctoral Excellence Program 2021154.

Numerical stability of Grünwald-Letnikov method for time fractional delay differential equations

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This paper is concerned with the numerical stability of time fractional delay differential equations (F-DDEs) based on Grünwald-Letnikov (GL) approximation for the Caputo fractional derivative. In particular, we focus on the numerical stability region and the Mittag-Leffler stability. Using the boundary locus technique, we first derive the exact expression of the numerical stability region in the parameter plane, and show that the fractional backward Euler scheme is not $\tau(0)$-stable, which is different from the backward Euler scheme for integer DDE models. Secondly, we prove the numerical Mittag-Leffler stability for the numerical solutions provided that the parameters fall into the numerical stability region, by employing the singularity analysis of generating function. Our results show that the numerical solutions of F-DDEs are completely different from the classical integer order DDEs, both in terms of $\tau(0)$-stability and the long-time decay rate. Numerical examples are given to confirm the theoretical results.

KEY WORDS: Fractional DDEs, numerical stability, boundary locus technique, singularity analysis, generating function.

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Numerical Analysis of Some Singular Partial Differential Equations with Logarithmic Nonlinearity

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The presence of logarithmic nonlinear term of the form $f(u) = u\log(|u|)$ in parabolic PDEs or Schrödinger's equations brings about significant challenges in both numerical discretization and analysis. The nonlinear term is non-differentiable but Hölder continuous at $u = 0$, and the underlying energy does not have a definite sign. Such PDEs exhibit richer and unusual dynamics that may not possess for general PDEs with smooth nonlinear terms. In this talk, we shall present our recent attempts for such problems and introduce some new tools for the analysis. This presentation is based on joint works with Dr. Yan Jingye and Dr. Boya Zhou.

KEY WORDS: Logarithmic Schrödinger's equations, Hölder continuity, linearized scheme, Positive solutions, ground states

¶This work was supported in part by the National Natural Science Foundation of China under grant 91430216.

Error estimation of a discontinuous Galerkin method for time fractional subdiffusion problems with nonsmooth data

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A numerical analysis is provided for a piecewise constant discontinuous Galerkin method for time fractional subdiffusion problems. The regularity of weak solution is firstly established by using variational approach and Mittag-Leffler function. Then several optimal error estimates are derived with low regularity data. Finally, numerical experiments are conducted to verify the theoretical results.

KEY WORDS: time fractional subdiffusion, weak solution, low regularity, discontinuous Galerkin method, optimal error estimate, Laplace transform.

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¶This work was supported in part by the National Natural Science Foundation of China under grant 11771312.

Sinc methods based on the single and double exponential transformations for high-order fractional differential equations

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This report mainly applies the Sinc method to solve higher-order fractional differential equations, which is divided into the following two parts: Firstly, we apply the Sinc-Galerkin method to solve the fourth-order fractional evolution equation with a weak singular kernel. From which, the time derivative and Riemann-Liouville fractional integral term are approximated by the Crank-Nicolson method and the trapezoidal convolution quadrature rule, respectively. Then a fully discrete scheme is formulated by employing the Sinc-Galerkin approximation. The exponential convergence rate in space of proposed method are derived. In addition, some properties of the Toeplitz matrix generated by the composite Sinc function at the Sinc node are extended to the cases of arbitrary order in the preliminary knowledge. Secondly, we apply the Sinc-collocation method to solve the eighth-order nonlinear boundary value problem with variable coefficients. From which, we derive the exponential convergence of the Sinc-collocation method based on the double exponential transformation applied to eighth-order boundary value problems. Then using Kantorovich's theorem, we obtain the exponential convergence of the non-linear eighth-order ordinary differential equation. Besides, we extend the analytical results to the arbitrary even-order case. Numerical experiments verify the accuracy and effectiveness of the above two schemes.

KEY WORDS: Fractional evolution equation, Kantorovich's theorem, Sinc-Galerkin and collocation, exponential convergence

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¶This work was supported in part by the National Natural Science Foundation of China under grant 12071127.

A unified fast method for the fractional operators

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Time-dependent fractional partial differential equations typically require huge amounts of memory and computational time, especially for long-time integration, which taxes computational resources heavily for high-dimensional problems. Here, we first analyze existing numerical methods of sum-of-exponentials for approximating the kernel function in constant-order fractional operators, and identify the current pitfalls of such methods. In order to overcome the pitfalls, an improved sum-of-exponentials is developed and verified. We also present several sum-of-exponentials for the approximation of the kernel function in variable-order fractional operators. Subsequently, based on the sum-of-exponentials, we propose a unified framework for fast time-stepping methods for fractional integral and derivative operators of constant and variable orders. We test the fast method based on several benchmark problems, including fractional initial value problems, the time-fractional AllenšCCahn equation in two and three spatial dimensions, and the Schrodinger equation with nonreflecting boundary conditions, demonstrating the efficiency and robustness of the proposed method. The convergence analysis of the fast method is also displayed. The results show that the present fast method significantly reduces the storage and computational cost especially for longtime integration problems

KEY WORDS: Sum-of-exponentials, contour quadrature, fractional integral and derivative operators, fast time-stepping methods, time-fractional AllenšCCahn equation, nonreflecting boundary conditions

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Numerical study for the nonlinear fractional complex Ginzburg-Landau equation in finite difference setting

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Five types of numerical methods are conducted to solve two-dimensional nonlinear fractional complex Ginzburg-Landau equation finite difference setting. They include BDF2-ADI methods [1], compact BDF2-ADI methods [1], Crank-Nicolson method [2], Compact Crank-Nicolson method [4] and Exponential Runge-Kutta method [5]. Detailed error analysis are proved. We give the preconditioned GMRES method with a block circulant preconditioner to speed up the convergence rate of the iteration. Meanwhile, fast Fourier transformation is utilized to reduce the complexity for calculating the discretized systems. Numerical experiments are illustrated to compare the efficiency of a part of numerical methods.

KEY WORDS: fractional complex Ginzburg-Landau equation, compact, exponential Runge-Kutta method, preconditioner

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¶This work was supported in part by high-level talents project of Zhejiang Sci-tech University.

Solution landscape of space-fractional problems and model comparison

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High-index saddle dynamics provides an effective means to compute the any-index saddle points and construct the solution landscape. We prove error estimates for Euler discretization of high-index saddle dynamics by resolving the difficulties such as the strong nonlinearity and the orthonormalization procedure in the numerical scheme [1]. Then we propose a fast algorithm for the variable-order spectral fractional Laplacian, which reduces the computational cost from $O(M^2 \ln M)$ to $O(M \ln^2 M)$ where M refers to the size of the problem. Based on this fast algorithm, we apply the high-index saddle dynamics to construct the solution landscape of space-fractional phase field problems and then compare the impacts of variable fractional order and variable coefficient from the point of view of the solution landscape [2].

KEY WORDS: Fractional Laplacian, variable-order, solution landscape, saddle dynamics

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¶This work was supported in part by the National Natural Science Foundation of China No. 12050002 and 21790340, the National Key Research and Development Program of China No. 2021YFF1200500, the International Postdoctoral Exchange Fellowship Program (Talent-Introduction Program) No. YJ20210019, and the China Postdoctoral Science Foundation No. 2021TQ0017 and 2021M700244.

Fast predictor-corrector methods for solving nonlinear time-fractional differential equations

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A second-order predictor-corrector method of [Nguyen and Jang, Fract. Calc. Appl. Anal. 2017] is generalised to graded meshes to solve nonlinear fractional initial-value problems whose typical solutions have a weak singularity at the initial time. In comparison with existing predictor-corrector methods in the literature, this new method significantly improves the numerical accuracy while reducing the computational cost. Moreover, to increase its computational efficiency still further, a corresponding fast algorithm based on the sum-of-exponentials approximation to the kernel of the scheme is described. An error analysis is given for problems whose right-hand sides satisfy a Lipschitz condition. The method (and its fast variant) are then extended to solve the nonlinear time-fractional Benjamin-Bona-Mahony-Burgers (BBMB) initial-boundary value problem, combined with a standard discretisation of the spatial derivatives on a uniform mesh. Estimates are derived for the discrete H^1-norm errors in the computed solution for the BBMB problem; to enable this analysis, a new Gronwall inequality is proved. A fast high-order predictor-corrector method is also derived by applying the quadratic interpolation polynomial approximation for the integral function. Finally, several numerical experiments show the sharpness of our theoretical error bounds for both problems.

KEY WORDS: Predictor-corrector method, Time-fractional Benjamin-Bona-Mahony-Burgers equation, Sum-of-exponentials approximation, Gronwall inequality

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¶This work was supported in part by the National Natural Science Foundation of China (12101037, 12001163, 12171025 and NSAF-U1930402), the China Postdoctoral Science Foundation (2021M690322).

Inverse potential problem for subdiffusion from terminal observation

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In this talk, we consider the inverse problem of recovering a potential coefficient in the fractional subdiffusion model from the terminal observational data. We shall present conditional stability estimates in Sobolev spaces which further inspires proper numerical algorithm and relevant error analysis. The argument relies on refined properties of solution operators involving two-parameter Mittag–Leffler functions. The efficiency and accuracy of the proposed algorithm are illustrated with several numerical examples.

KEY WORDS: inverse potential problem, iterative algorithm, conditional stability, fully discrete scheme, error analysis

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¶This work was supported in part by the Hong Kong RGC grant 15304420.