

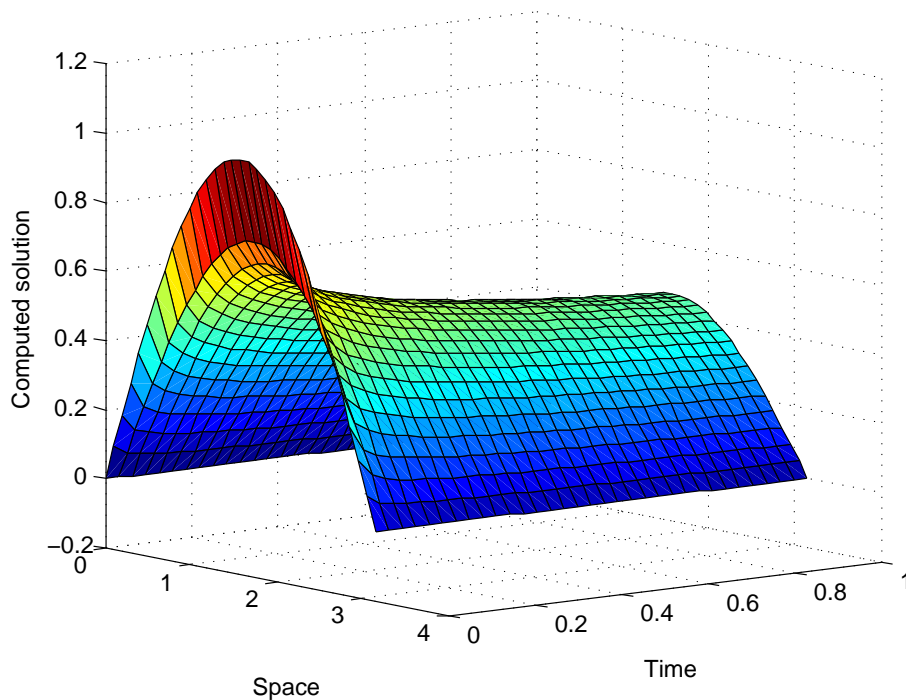
Book of Abstracts

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Numerical Methods for
Fractional-Derivative Problems

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On spectral Petrov-Galerkin method for solving optimal control problem governed by fractional diffusion equations with fractional Noise

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In this paper, a spectral Petrov-Galerkin method is developed to solve an optimal control problem governed by a two-sided space-fractional diffusion-reaction equation with additive fractional noise. In order to compensate weak singularities of the solution near boundaries, regularities of both the fractional noise and the optimal control problem are analyzed in weighted Sobolev space. The spectral Petrov-Galerkin method is presented by employing truncated spectral expansion of the fractional Brownian motion (fBm) type noise, and error estimates are given based on the obtained regularity of the optimal control problem. Numerical experiments are carried out to verify the theoretical findings.

KEY WORDS: optimal control problem, diffusion-reaction problems, fractional Brownian motion, weighted Sobolev space, error estimate

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Pointwise-in-time error estimates of some numerical methods for multi-term subdiffusion equations

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In this talk, we consider the time-fractional initial-boundary problems of parabolic type. Previously, global error bounds for computed numerical solutions to such problems have been provided by Liao et al. (SIAM J. Numer. Anal. 2018, 2019) and Stynes et al. (SIAM J. Numer. Anal. 2017). In this talk we show how the concept of complete monotonicity can be combined with these older analyses to derive local error bounds (i.e., error bounds that are sharper than global bounds when one is not close to the initial time $t = 0$). Our new approach is used to bound the global and local errors in the numerical solution of a multi-term time-fractional diffusion equation, using the L1 scheme or GL scheme for the temporal discretisations of each fractional derivative. These error bounds are α -robust. Numerical results show they are sharp.

KEY WORDS: Complete Monotonicity, Multi-Term Time-Fractional, Local Error Estimates, L1 Scheme, Grünwald–Letnikov Scheme

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High-order BDF convolution quadrature for subdiffusion models with a singular source term

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Anomalous diffusion is often modelled in terms of the subdiffusion equation, which can involve a weakly singular source term. For this case, many predominant time stepping methods, including the correction of high-order BDF schemes [JIN, LI, AND ZHOU, SIAM J. Sci. Comput., 39 (2017), A3129–A3152], may suffer from a severe order reduction. To fill in this gap, we propose a smoothing method for time stepping schemes, where the singular term is regularized by using a m -fold integral-differential calculus and the equation is discretized by the k -step BDF convolution quadrature, called ID m -BDF k method. We prove that the desired k th-order convergence can be recovered even if the source term is a weakly singular and the initial data is not compatible. Numerical experiments illustrate the theoretical results.

KEY WORDS: subdiffusion equation, smoothing method, ID m -BDF k method, singular source term, error estimate

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Efficient Numerical Methods for the Integral Fractional Laplacian

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Due to its extraordinary modeling capabilities, the nonlocal fractional-order Laplacian has recently attracted increasing scientific and engineering attention in the past decade. However, the nonlocal operators bring up new challenges in discretization, computation and analysis for the associated PDEs. To cope with these difficulties, we present two efficient numerical methods, the radial basis functions and neural-network methods. For both methods, we discuss their convergence analysis. Some numerical examples are provided to demonstrate their efficiency and accuracy.

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Unconditional energy dissipation law and optimal error estimate of fast L1 schemes for a time-fractional Cahn-Hilliard problem

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In this talk, we will investigate a fully discrete semi-implicit stabilized scheme for the time-fractional Cahn-Hilliard equation, which adopts the nonuniform fast L1 scheme in time and the mixed finite element method in space. By using the temporal-spatial splitting technique, the boundedness of L^∞ -norm of the computed solution U_h^n is obtained. Combining this boundedness, the unconditional optimal error estimate is given without certain temporal restrictions dependent on the spatial mesh size. Moreover, with the help of the boundedness of $\|U_h^n\|_\infty$ and the positive definiteness of L1 kernels, it's shown that the proposed scheme preserves the modified discrete energy dissipation property. Finally, numerical experiments are provided to further verify our theoretical convergent results.

KEY WORDS: Time-fractional Cahn-Hilliard equations, Energy dissipation laws, Weak singularity, Mixed finite element methods

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Fractional collocation method for third-kind Volterra integral equations with nonsmooth solutions

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In this talk, we develop a collocation method for solving third-kind Volterra integral equations. In order to achieve high order convergence for problems with nonsmooth solutions, we construct a collocation scheme on a modified graded mesh using a basis of fractional polynomials, depending on a certain parameter λ . For the proposed method, we derive an error estimate in the L^∞ -norm, which shows that the optimal order of global convergence can be obtained by choosing the appropriate parameter λ and modified mesh, even when the exact solution has low regularity. Numerical experiments confirm the theoretical results and illustrate the performance of the method.

KEY WORDS: Third-kind Volterra integral equation, nonsmooth solution, fractional polynomial, collocation method, error estimate

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Recent results on pointwise-in-time a posteriori error control for time-fractional parabolic equations

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I will start with a review of [1], which was presented at the 2021 edition of this workshop. 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 time stepping algorithm is applied for the L1 method, which yields optimal convergence rates $2 - \alpha$ in the presence of solution singularities. Interestingly, the proposed time stepping algorithm yields the grids similar to a-priori-constructed optimal grids in [2, 3].

In the main part of the talk, we shall discuss recent extensions of the proposed methodology to variable-coefficient multiterm time-fractional subdiffusion equations [4], and to the case of higher-order discretizations [5]. The stable implementation of the proposed algorithm will also be addressed [5].

KEY WORDS: fractional-order parabolic equation, a posteriori error estimates, L1 scheme, pointwise-in-time error bounds, time stepping algorithm, multiterm time-fractional subdiffusion, higher-order schemes

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High-order splitting finite element methods for the subdiffusion equation with limited smoothing property*

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In contrast with the diffusion equation which smoothens the initial data to C^∞ for $t > 0$ (away from the corners/edges of the domain), the subdiffusion equation only exhibits limited spatial regularity. As a result, one generally cannot expect high-order accuracy in space in solving the subdiffusion equation with nonsmooth initial data. In this paper, a new splitting of the solution is constructed for high-order finite element approximations to the subdiffusion equation with nonsmooth initial data. The method is constructed by splitting the solution into two parts, i.e., a time-dependent smooth part and a time-independent nonsmooth part, and then approximating the two parts via different strategies. The time-dependent smooth part is approximated by using high-order finite element method in space and convolution quadrature in time, while the steady nonsmooth part could be approximated by using smaller mesh size or other methods that could yield high-order accuracy. Several examples are presented to show how to accurately approximate the steady nonsmooth part, including piecewise smooth initial data, Dirac–Delta point initial data, and Dirac measure concentrated on an interface. The argument could be directly extended to subdiffusion equations with nonsmooth source data. Extensive numerical experiments are presented to support the theoretical analysis and to illustrate the performance of the proposed high-order splitting finite element methods.

KEY WORDS: subdiffusion, limited smoothing property, nonsmooth data, finite element method, high-order, convolution quadrature, error estimate

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Numerical approximations to ψ fractional derivativeEnyu Fan*, Changpin Li* Martin Stynes†

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A generalised fractional derivative (the ψ -Caputo derivative) is studied. Generalizations of standard discretizations are constructed for this derivative: L1, L1-2, L2-1 $_{\sigma}$ for derivatives of order $\alpha \in (0, 1)$, and L2, H2N2, L2 $_1$ for derivatives of order $\alpha \in (1, 2)$. These new discretizations extend known results for the standard Caputo derivative, the Caputo-Hadamard derivative, etc. Numerical examples are given to demonstrate their performance.

KEY WORDS: ψ -Caputo derivative, L1 discretisation, L1-2 discretisation, L2-1 $_{\sigma}$ discretisation, L2 discretisation, H2N2 discretisation, L2 $_1$ discretisation, truncation error

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Combined L1-spectral methods for time fractional Cahn-Hilliard equations

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The solution of the time fractional Cahn-Hilliard equation has the initial layer and the equation's energy may decay fast at certain time. To capture the evolutions effectively, the time discretization is done by combining the transformed L1 scheme and the standard L1-scheme on the nonuniform meshes. The spatial discretization is archived by the Fourier-pseudo spectral method. The fully-discrete scheme is proved to be energy-stable. And the convergence results of the schemes is obtained. Numerical experiments are given to confirm the theoretical results.

KEY WORDS: time fractional Cahn-Hilliard equations, initial layer, L1-schemes, energy-stable schemes

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On discontinuous and continuous approximations to second-kind Volterra integral equations

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Collocation and Galerkin methods in the discontinuous and globally continuous piecewise polynomial spaces, in short, denoted as DC, CC, DG and CG methods respectively, are employed to solve second-kind Volterra integral equations (VIEs) with smooth or weakly singular kernels. It is proved that the quadrature DG and CG (QDG and QCG) methods obtained from the DG and CG methods by approximating the inner products by suitable numerical quadrature formulas, are equivalent to the DC and CC methods, respectively. In addition, the fully discretised DG and CG (FDG and FCG) methods are equivalent to the corresponding fully discretised DC and CC (FDC and FCC) methods. The convergence theories are established for DC, CC, DG and CG methods. In particular, it is proved that the CC (CG) method for second-kind VIEs possesses a similar convergence to the DC (DG) method for first-kind VIEs. Numerical examples illustrate the theoretical results.

KEY WORDS: Volterra integral equations, collocation methods, Galerkin methods, convergence

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Efficient and Accurate Numerical Methods Using the Accelerated Spectral Deferred Correction for Solving Fractional Differential Equations

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We develop an efficient and accurate spectral deferred correction (SDC) method for fractional differential equations (FDEs) by extending the algorithm in [1] for classical ordinary differential equations (ODEs). Specifically, we discretize the resulted Picard integral equation by the SDC method and accelerate the convergence of the SDC iteration by using the generalized minimal residual algorithm (GMRES). We first derive the correction matrix of the SDC method for FDEs and analyze the convergence region of the SDC method. We then present several numerical examples for stiff and non-stiff FDEs including fractional linear and nonlinear ODEs as well as fractional phase field models, demonstrating that the accelerated SDC method is much more efficient than the original SDC method, especially for stiff problems. Furthermore, we resolve the issue of low accuracy arising from the singularity of the solutions by using a geometric mesh, leading to highly accurate solutions compared to uniform mesh solutions at almost the same computational cost. Moreover, for long-time integration of FDEs, using the geometric mesh leads to great computational savings as the total number of degrees of freedom required is relatively small.

KEY WORDS: Stiff problem, Generalized minimal residual, Geometric mesh refinement, Long time evolution, Fractional phase field models

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Local analysis of an L1/finite element method for a time-fractional singularly perturbed reaction-diffusion problem

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An initial-boundary value problem of the form $D_t^\alpha - \varepsilon^2 D_x^2 u + bu = f$ is considered on the space-time domain $\Omega \times (0, T]$, with Dirichlet initial and boundary conditions, where D_t^α is a Caputo fractional derivative of order $\alpha \in (0, 1)$ and $\varepsilon \ll 1$ is a positive constant. Bounds on the solution u and its derivatives are proved via a solution decomposition and a maximum principle; these bounds show that the solution has a weak singularity at the initial time $t = 0$ and also has layers (caused by the small parameter ε) at the boundaries of the spatial domain Ω . We apply the L1 discretisation to fractional derivative on a graded temporal mesh, together with a standard finite element method for the spatial derivatives on a Shishkin spatial mesh. Using our bounds on the derivative of the solution, local in time error estimates, which are uniform in the singular perturbation parameter ε , are derived.

KEY WORDS: Time-fractional, singularly perturbed, L1 scheme, finite element method, Shishkin mesh

A grid-overlay finite difference method for the fractional Laplacian on arbitrary bounded domains

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We present a grid-overlay finite difference method for the numerical approximation of the fractional Laplacian on arbitrary bounded domains. The method uses an unstructured simplicial mesh and an overlay uniform grid for the underlying domain and constructs the approximation based on a uniform-grid finite difference approximation and a data transfer from the unstructured mesh to the uniform grid. The method takes full advantage of both uniform-grid finite difference approximation in efficient matrix-vector multiplication via the fast Fourier transform and unstructured meshes for complex geometries. We show that its stiffness matrix is similar to a symmetric and positive definite matrix and thus invertible if the data transfer has full column rank and positive column sums. Piecewise linear interpolation is studied as a special example for the data transfer. We prove that the full column rank and positive column sums of linear interpolation is guaranteed if the spacing of the uniform grid is smaller than or equal to a positive bound proportional to the minimum element height of the unstructured mesh. Moreover, we propose a sparse preconditioner for the iterative solution of the resulting linear system for the homogeneous Dirichlet problem of the fractional Laplacian. Numerical examples demonstrate that the new method has similar convergence behavior as existing finite difference and finite element methods and that the sparse preconditioning is effective. Furthermore, the new method can readily be incorporated with existing mesh adaptation strategies. Numerical results obtained by combining with the so-called MMPDE moving mesh method are also presented.

KEY WORDS: Fractional Laplacian, finite difference, arbitrary domain, mesh adaptation, overlay grid, nonlocal

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A fractional PDE model for describing dynamic responses of viscoelastic beams

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Vibrations are prevalent in mechanical or biological systems, which may be unwanted or even destructive in many circumstances. Their precise characterization and modeling is crucial in the design and determination of the dynamic durability of the systems and can provide insights into disease evolution, and is the key to develop effective ways to mitigate the impact of unwanted vibrations to optimize the performance, to extend the durability of the systems in engineering applications, and to develop replacements that restore the structures and functionality of damaged organs in medical industry.

Many modern structures are subjected to challenging conditions, such as high temperatures and high tensile stresses. In these circumstances conventional metals may creep significantly, which is one of the main causes of system failure. This has led to the development of creep-resistant superalloys and ceramic matrix composite materials, which exhibit viscoelastic behaviors. Viscoelastic materials, such as natural and synthetic biomaterials, smart materials, polymers, and elastomers, exhibit both elastic characteristic of solid and viscous behavior of fluid. They have been widely used in many applications.

In this talk we go over a fractional PDE model for describing dynamic responses of viscoelastic beams. If time permits, we will discuss some extensions to more general beams as well as their mathematical and numerical analysis.

KEY WORDS: viscoelastic beams, dynamic responses, fractional partial differential equation

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High-order schemes based on extrapolation for semilinear fractional differential equation

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By rewriting the Riemann-Liouville fractional derivative as Hadamard finite-part integral and with the help of piecewise quadratic interpolation polynomial approximations, we obtain a numerical scheme for approximating the Riemann-Liouville fractional derivative of order $\alpha \in (1, 2)$. The error has the asymptotic expansion $(d_3\tau^{3-\alpha} + d_4\tau^{4-\alpha} + d_5\tau^{5-\alpha} + \dots) + (d_2^*\tau^4 + d_3^*\tau^6 + d_4^*\tau^8 + \dots)$ at any fixed time $t_N = T, N \in \mathbb{Z}^+$, where $d_i, i = 3, 4, \dots$ and $d_i^*, i = 2, 3, \dots$ denote some suitable constants and $\tau = T/N$ denotes the step size. Based on this discretization, a new scheme for approximating the linear fractional differential equation of order $\alpha \in (1, 2)$ is derived and its error is shown to have a similar asymptotic expansion. As a consequence, a high-order scheme for approximating the linear fractional differential equation is obtained by extrapolation. Further we introduce a high-order scheme for approximating a semilinear fractional differential equation. Several numerical experiments are conducted to show that the numerical results are consistent with our theoretical results.

KEY WORDS: Hadamard finite-part integral, extrapolation, semilinear problem, high-order method

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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 Allen–Cahn 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, fast time-stepping method, fractional integral and derivative operators, convergence

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On τ matrix-based approximate inverse preconditioning technique for solving spatial fractional diffusion equations

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In this talk, we will explore the special structure of the discretized linear systems from the spatial fractional diffusion equations. The coefficient matrices of the resulting discretized systems have a diagonal-plus-Toeplitz structure. Standard circulant preconditioners may not work for such Toeplitz-like linear systems. However, because the resulting Toeplitz matrix is symmetric positive definite, then we can employ the τ matrix to approximate it. By making use of the piecewise interpolation polynomials, we propose a new approximate inverse preconditioner to handle the diagonal-plus-Toeplitz coefficient matrices. The τ matrix-based approximate inverse preconditioning technique can be implemented very efficiently by using discrete sine transforms. Theoretically, we have proved that the spectrum of the resulting preconditioned matrices are clustered around one. Thus, Krylov subspace methods with the proposed preconditioners converge very fast. To demonstrate the efficiency of the new preconditioners, numerical experiments are implemented. The numerical results show that with the proper interpolation node numbers, the performance of the τ -matrix based splitting preconditioning technique is better than the other tested preconditioners.

KEY WORDS: Spatial fractional diffusion equation, preconditioning, Krylov subspace method, τ matrix, approximate inverse

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Accelerated schemes of compact difference methods for space-fractional sine-Gordon equations with distributed delay

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In this talk, for quickly solving one- and two-dimensional space-fractional sine-Gordon equations with distributed delay, we suggest several accelerated schemes of direct compact difference (DCD) methods. For one-dimensional (1D) problems, with a function transformation, we construct an indirect compact difference (ICD) method, which requires less calculation cost than the corresponding DCD method, and prove under the appropriate conditions that ICD method has second-order (resp. forth-order) calculation accuracy in time (resp. space). By extending the argument for 1D case, we further obtain an ICD method for solving two-dimensional (2D) problems and derive the similar convergence result. For ICD and DCD methods of 2D problems, we also give their alternative direction implicit (ADI) schemes. Moreover, for the fast implementations of ICD method of 1D problems and indirect ADI method of 2D problems, we further present their acceleration strategies. Finally, with a series of numerical experiments, the findings in this paper are further confirmed.

KEY WORDS: Space-fractional sine-Gordon equations with distributed delay, direct/indirect compact difference methods, alternative direction implicit scheme, error analysis, fast implementation

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Do we need decay-preserving error estimate for solving parabolic equations with the initial singularity?

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The solutions with weakly initial singularity arises in a wide variety of equations, for example, diffusion and subdiffusion equations. When the well-known L1 scheme is used to solve the subdiffusion equations with weak singularity, numerical simulations show that this scheme can produce various convergence rates for different choices of model parameters (i.e., domain size, final time T , and reaction coefficient κ). In fact, this elusive phenomenon can be found in other numerical methods for reaction-diffusion equations such as the backward Euler (IE) scheme, Crank-Nicolson (C-N) scheme, and BDF2 scheme. The current theory in the literatures cannot explain why there exists two different convergence regimes, which has been puzzling us for a long while, and motivating us to study this inconsistency between the standard convergence theory and numerical experiences. In this talk, we provide a general methodology to systematically obtain error estimates that incorporate the exponential decaying feature of the solution. We call this novel error estimate decay-preserving error estimate and apply it to aforementioned IE, C-N, and BDF2 schemes. Our estimates reveal that the various convergence rates are caused by the trade-off between the two components in different model parameter regimes. In this way, we are able to capture different states of the convergence rate, for which the traditional error estimates fail, since we take the model parameters into account and thus retain more properties of the continuous solution. In addition, the alpha-robust estimates for L1 and Alikhanov's schemes on general nonuniform meshes are also reported. The works are jointed with Zhimin Zhang and Chengchao Zhao.

KEY WORDS: subdiffusion equations, nonuniform time mesh, discrete Grönwall inequality, α -robust error estimate

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Analysis and numerical approximation of space-fractional boundary value problems in one and two space dimensions

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Space-fractional boundary value problems provide adequate descriptions for challenging phenomena such as the anomalous diffusion. We introduce some recent progresses on the mathematical analysis and numerical methods to space-fractional boundary value problems in one space dimension, and then provide an extension to a two-dimensional problem via the spectral-type method of solid harmonic polynomials, as well as proving a decomposition of the fractional Laplacian in two space dimensions.

KEY WORDS: space-fractional, diffusion, variable coefficient, fractional Laplacian

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A unified design of energy stable schemes with variable steps for fractional gradient flows and nonlinear integro-differential equations

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A unified discrete gradient structure of the second order nonuniform integral averaged approximations for the Caputo fractional derivative and the Riemann-Liouville fractional integral is established in this paper. The required constraint of the step-size ratio is weaker than that found in literatures. With the proposed discrete gradient structure, the energy stability of the variable step Crank-Nicolson type numerical schemes is derived immediately, which is essential to the long-time simulations of the time fractional gradient flows and the nonlinear integro-differential models. The discrete energy dissipation laws fit seamlessly into their classical counterparts as the fractional indexes tend to one. In particular, it provides a framework for the stability analysis of variable step numerical schemes based on the scalar auxiliary variable type approaches. The time fractional Swift-Hohenberg model and the time fractional sine-Gordon model are taken as two examples to elucidate the theoretical results at great length. Extensive numerical experiments using the adaptive time-stepping strategy are provided to verify the theoretical results in the time multi-scale simulations.

KEY WORDS: time fractional gradient flow, nonlinear integro-differential equation, nonuniform time steps, discrete gradient structure, scalar auxiliary variable, energy stability

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A bilateral preconditioning for an L2-type all-at-once system arising from time-space fractional PDEs

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Time-space fractional Bloch-Torrey equations (TSFBTEs) are developed by some researchers to investigate the relationship between diffusion and fractional-order dynamics. In this talk, we concentrate on design a bilateral preconditioning for all-at-once system from multidimensional TSFBTEs. Firstly, we propose an implicit difference scheme for this equation by employing an L2-type formula. Then, we prove the stability and the convergence of the proposed scheme. Based on such a numerical scheme, an L2-type all-at-once system is derived and solved in a parallel-in-space pattern. Based on the special structure of its coefficient matrix, we propose a bilateral preconditioning strategy to accelerate the convergence of Krylov subspace solvers. We theoretically show that the condition number of the preconditioned matrix is uniformly bounded by a constant. Several numerical examples are provided to test the proposed scheme and preconditioning technique.

KEY WORDS: Preconditioning, All-at-once system, Toeplitz matrix, Parallel-in-space, L2-type difference scheme

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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 many parameters, e.g., diffusion coefficient, potential, initial and boundary conditions, source 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 several parameters from one measurement when the other problem data are not fully specified.

KEY WORDS: inverse problem, subdiffusion, lateral boundary measurement, unknown medium, uniqueness, numerical algorithm

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