MAFELAP 2019 abstracts for the mini-symposium Numerical methods for nonlocal problems

Organisers: Bangti Jin and Buyang Li

THE RATIONAL SPDE APPROACH FOR GAUSSIAN RANDOM FIELDS WITH GENERAL SMOOTHNESS

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A popular approach for modeling and inference in spatial statistics is to represent Gaussian random fields as solutions to stochastic partial differential equations (SPDEs) of the form $L^\beta u = W$, where W is Gaussian white noise, L is a second-order differential operator, and $\beta > 0$ is a parameter that determines the smoothness of u. However, this approach has been limited to the case $2\beta \in \mathbb{N}$, which excludes several important covariance models and makes it necessary to keep β fixed during inference.

We introduce a new method, the rational SPDE approach, which is applicable for any $\beta > 0$ and therefore remedies the mentioned limitation. The presented scheme combines a finite element discretization in space with a rational approximation of the function $x^{-\beta}$ to approximate u. For the resulting approximation, an explicit rate of strong convergence to u is derived and we show that the method has the same computational benefits as in the restricted case $2\beta \in \mathbb{N}$ when used for statistical inference and prediction. Numerical experiments are performed to illustrate the accuracy of the method, and an application to climate reanalysis data is presented.

ON NUMERICAL APPROXIMATIONS OF THE SPECTRAL FRACTIONAL LAPLACIAN VIA THE METHOD OF SEMIGROUPS

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As it is well-known, there are several (non-equivalent) ways of defining fractional operators in bounded domains. In this talk we will focus on the so-called spectral fractional Laplacian. Following the heat semi-group formula we consider a family of operators which are boundary conditions dependent and discuss a suitable approach for their numerical discretizations. We will also discuss the numerical treatment of the associated homogeneous boundary value problems. In the end we will talk about possible extensions that can be treated with our approach such as non-homogeneous boundary conditions and discretizations of fractional operators in the whole space.

References

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[3] F. del Teso, J. Endal, E. R. Jakobsen. *Robust numerical methods for nonlocal (and local) equations of porous medium type. Part II: Schemes and experiments.* SIAM J. Numer. Anal., **56(6)**: 3611–3647, (2018).

NONLOCAL (AND LOCAL) NONLINEAR DIFFUSION EQUATIONS. BACKGROUND, ANALYSIS, AND NUMERICAL APPROXIMATION

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We will consider finite-difference schemes for nonlocal (and local) nonlinear diffusion equations posed in $\mathbb{R}^N \times (0, T)$. Properties needed to perform numerical analysis are going to be discussed. The numerical approximations will converge to the solutions of the equations studied under minimal assumptions including assumptions that lead to very irregular solutions. In other words, the schemes we introduce are robust in the sense that they converge under very unfavourable conditions. Numerical simulations will also be presented.

NUMERICAL ANALYSIS OF SUBDIFFUSION WITH A TIME-DEPENDENT COEFFICIENT

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In the past few years, the numerical analysis of the subdiffusion equation has witnessed impressive progress. However, most works are concerned with the case of a time-independent diffusion coefficient, and the analysis techniques are not directly applicable to the case of a time-dependent coefficient. In this talk, we present some recent works on the error analysis for the case of a time-dependent coefficient, and illustrate the theory with numerical experiments.

NUMERICAL APPROXIMATION OF SEMILINEAR SUBDIFFUSION EQUATIONS WITH NONSMOOTH INITIAL DATA

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We consider the numerical approximation of a semilinear fractional order evolution equation involving a Caputo derivative in time of order $\alpha \in (0,1)$. Assuming a Lipschitz continuous nonlinear source term and an initial data $u_0 \in \dot{H}^\nu(\Omega)$, $\nu \in [0,2]$, we discuss existence, stability, and provide regularity estimates for the solution of the problem. For a spatial discretization via piecewise linear finite elements, we establish optimal $L^2(\Omega)$-error estimates for cases with smooth and nonsmooth initial data, extending thereby known results derived for the classical semilinear parabolic problem. We further investigate fully implicit and linearized time-stepping schemes based on a convolution quadrature in time generated by the backward Euler method. Our main result provides pointwise-in-time optimal $L^2(\Omega)$-error estimates for both numerical schemes. Numerical examples in one- and two-dimensional domains are presented to illustrate the theoretical results.

BARRIER FUNCTIONS IN THE ERROR ANALYSIS FOR FRACTIONAL-DERIVATIVE PARABOLIC PROBLEMS ON QUASI-GRADED MESHES

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An 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 this problem, building on [N. Kopteva, Error analysis of the L1 method on graded and uniform meshes for a fractional-derivative problem in two and three dimensions, Math. Comp., 2019], we give a simple and general numerical-stability analysis using barrier functions, which yields sharp pointwise-in-time error bounds on quasi-graded temporal meshes with arbitrary degree of grading. L1-type and higher-order discretizations in time are considered in combination with finite element spatial discretiztions. In particular, those results imply that milder (compared to the optimal) grading yields optimal convergence rates in positive time. Our theoretical findings are illustrated by numerical experiments.

STABLE AND CONVERGENT FULLY DISCRETE INTERIOR–EXTERIOR COUPLING OF MAXWELL'S EQUATIONS

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Maxwell's equations are considered with transparent boundary conditions, for initial conditions and inhomogeneity having support in a bounded, not necessarily convex three-dimensional domain or in a collection of such domains. The numerical method only involves the interior domain and its boundary. The transparent boundary conditions are imposed via a time-dependent boundary integral operator that is shown to satisfy a coercivity property. The stability of the numerical method relies on this coercivity and on an anti-symmetric structure of the discretized equations that is inherited from a weak first-order formulation of the continuous equations. The method proposed here uses a discontinuous Galerkin method and the leapfrog scheme in the interior and is coupled to boundary elements and convolution quadrature on the boundary. The method is explicit in the interior and implicit on the boundary. Stability and convergence of the spatial semi-discretisation are proven, and with a computationally simple stabilization term, this is also shown for the full discretization.

OPTIMAL CONTROL IN A BOUNDED DOMAIN FOR WAVE PROPAGATING IN THE WHOLE SPACE: COUPLED THROUGH BOUNDARY INTEGRAL EQUATIONS

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This paper is concerned with an optimal control problem in a bounded-domain Ω_0 under the constraint of a wave equation in the whole space. The problem is regularized and then reformulated as an initial-boundary value problem of the wave equation in a bounded domain $\Omega \supset \overline{\Omega}_0$ coupled with a set of boundary integral equations on $\partial\Omega$ taking account of wave propagation through the boundary. The well-posedness and stability of the reformulated problem are proved. A fully discrete finite element method is proposed for solving the reformulated problem. In particular, the wave equation in the bounded domain is discretized by an averaged central difference method in time, and the boundary integral equations are discretized in time by using the convolution quadrature generated by the second-order backward difference formula. The finite and boundary element methods are used for spatial discretization of the wave equation and the boundary integral equations, respectively. The stability and convergence of the numerical method are also proved. Finally, the spatial and temporal convergence rates are validated numerically in 2D.

AFEM FOR THE FRACTIONAL LAPLACIAN

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For the discretization of the integral fractional Laplacian $(-\Delta)^s$, $0 < s < 1$, based on piecewise linear functions, we present and analyze a reliable weighted residual *a posteriori* error estimator. In order to compensate for a lack of L^2-regularity of the residual in the regime $3/4 < s < 1$, this weighted residual error estimator includes as an additional weight a power of the distance from the mesh skeleton. We prove optimal convergence rates for an h-adaptive algorithm driven by this error estimator in the framework of [Carstensen, Feischl, Page, Praetorius, axioms of adaptivity, CAMWA 2014]. Key to the analysis of the adaptive algorithm are novel local inverse estimates for the fractional Laplacian.

COMPUTATIONAL SOLUTIONS FOR FRACTIONAL DIFFUSION EQUATIONS

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VARIABLE ORDER, DIRECTIONAL $\mathcal{H}^2$-MATRICES FOR HELMHOLTZ PROBLEMS WITH COMPLEX FREQUENCY

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The sparse approximation of high-frequency Helmholtz-type integral operators has many important physical applications such as problems in wave propagation and wave scattering. The discrete system matrices are huge and densely populated; hence their sparse approximation is of outstanding importance. In our talk we will generalize the directional $\mathcal{H}^2$-matrix techniques from the "pure" Helmholtz operator $Lu = -\Delta u + z^2 u$ with $z = -ik, k$ real, to general complex frequencies z with $\mathrm{Re}(z) > 0$. In this case, the fundamental solution decreases exponentially for large arguments. We will develop a new admissibility condition which contain $\mathrm{Re}(z)$ and $\mathrm{Im}(z)$ in an explicit way and introduce the approximation of the integral kernel function on admissible blocks in terms of frequency-dependent directional expansion functions. We present an error analysis which is explicit with respect to the expansion order and with respect to the real and imaginary part of z. This allows us to choose the variable expansion order in a quasi-optimal way depending on $\mathrm{Re}(z)$ but independent of, possibly large, $\mathrm{Im}(z)$. The complexity analysis is explicit with respect to $\mathrm{Re}(z)$ and $\mathrm{Im}(z)$ and shows how higher values of $\mathrm{Re}(z)$ reduce the complexity. In certain cases, it even turns out that the discrete matrix can be replaced by its nearfield part.

Numerical experiments illustrate the sharpness of the derived estimates and the efficiency of our sparse approximation.

FAST AND PARALLEL RUNGE-KUTTA APPROXIMATION OF SUBDIFFUSION EQUATIONS

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A highly parallel algorithm for the numerical solution of inhomogeneous linear time-fractional differential equations of the type

$$D_t^\alpha u(t) = Au(t) + f(t) \text{ for } t \in (0, T) \text{ and } u(0) = 0$$

is presented. Here D_t^α is a (Caputo) fractional derivative, and $(A, D(A))$ a closed, densely defined, sectorial linear operator in some Banach space defined on $D(A)$.

The algorithm requires the solution of $\mathcal{O}(\log(1/h)\log(1/\varepsilon))$ linear systems in parallel, where h is the time step size required to resolve the inhomogeneity f and ε is the required accuracy. Additionally the solution of $\mathcal{O}(N\log(1/h)\log(1/\varepsilon))$ scalar linear inhomogeneous differential equations $\dot{y}(t) = \lambda y(t) + f(t)$ on certain time intervals is needed. The basic ingredients of the algorithm are the variation of constants formula, the Cauchy integral representation for the approximation of the operator exponential and the discretization of contour integrals using $\mathcal{O}(\log(1/h))$ contours with $\mathcal{O}(\log(1/\varepsilon))$ quadrature points each. Details of the basic algorithm can be found in [M. Fischer, Fast and Parallel Runge–Kutta Approximation of Fractional Evolution Equations. SIAM Journal on Scientific Computing 41:2, 2019, A927-A947].

In the numerical example the operator A will be the Laplacian with appropriate boundary conditions, discretized by the finite element method.

FINITE VOLUME METHODS FOR THE FRACTIONAL KLEIN-KRAMERS EQUATION

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The fractional Klein-Kramers equation describes the process of subdiffusion in the presence of an external force field in phase space. We present a family of finite volume schemes for the fractional Klein-Kramers equation, that includes first or second order schemes in phase space, and implicit or explicit schemes in time. We prove, for the open domain, that the schemes satisfy the positivity preserving property. For a bounded domain in space we consider two types of boundary conditions, absorbing boundary conditions and reflecting boundary conditions. The inclusion of boundary conditions leads to some technical complications that require changes in the finite volume schemes near the boundary. Numerical tests are presented in the end.

UNCONDITIONALLY CONVERGENT $L1$-GALERKIN FEMS FOR NONLINEAR TIME-FRACTIONAL SCHRÖDINGER EQUATIONS

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In this work, a linearized $L1$-Galerkin finite element method is proposed to solve the multi-dimensional nonlinear time-fractional Schrödinger equation. In terms of a temporal-spatial error splitting argument, we prove that the finite element approximations in L^2-norm and L^∞-norm are bounded without any time stepsize conditions. More importantly, by using a discrete fractional Gronwall type inequality, optimal error estimates of the numerical schemes are obtained unconditionally, while the classical analysis for multi-dimensional nonlinear fractional problems always required certain time-step restrictions dependent on the spatial mesh size. Numerical examples are given to illustrate our theoretical results.

LAPLACE TRANSFORM METHOD FOR SOLVING FRACTIONAL CABLE EQUATION WITH NONSMOOTH DATA

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We introduce two time discretization schemes for solving time fractional cable equation. The time derivative is approximated by using the backward Euler method and the second order backward difference formula, respectively. The Riemann-Liouville fractional derivatives are approximated by using the backward Euler convolution quadrature method and the second order backward difference convolution quadrature method, respectively. The nonsmooth data error estimates with the convergence orders $O(k)$ and $O(k^2)$ are proved in detail. Instead of using the discretized operational calculus approach to prove the nonsmooth data error estimates of the time discretization schemes for solving time fractional cable equation as used in literature, we directly bound the kernel function in the resolvent and obtain the nonsmooth data error estimates. To the best of our knowledge, this is the first work to consider the nonsmooth data error estimates for solving time fractional cable equation by directly bound the kernel function in the resolvent. This argument may be applied to consider the nonsmooth data error estimates for solving time fractional cable equation where the Riemann-Liouville fractional derivatives are approximated by using other schemes, for example, L1 scheme.

FORMULATION OF NONLOCAL BOUNDARY VALUE PROBLEM AND ITS ASYMPTOTIC ANALYSIS

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Nonlocal-type models are a class of emerging mathematical physics equations. A common feature of these equations is the involving of nonlocal integral operators. This feature presents some troubles to formulate boundary value problems of nonlocal type. Besides, conceptually, nonlocal models should be considered some kind of relaxation for the classical local differential models. In this talk, we propose the formulation of nonlocal boundary value problems of elliptic type, and study the asymptotic convergence rate between the nonlocal boundary value problems and their local counterparts.

CORRECTION OF HIGH-ORDER BDF CONVOLUTION QUADRATURE FOR FRACTIONAL EVOLUTION EQUATIONS

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We develop proper correction formulas at the starting $k-1$ steps to restore the desired k^{th}-order convergence rate of the k-step BDF convolution quadrature for discretizing evolution equations involving a fractional-order derivative in time. The desired k^{th}-order convergence rate can be achieved even if the source term is not compatible with the initial data, which is allowed to be nonsmooth. We provide complete error estimates for the subdiffusion case $\alpha \in (0,1)$, and sketch the proof for the diffusion-wave case $\alpha \in (1,2)$. Extensive numerical examples are provided to illustrate the effectiveness of the proposed scheme.