Recent Progress in Nonlocal Modeling, Analysis and Computation

June 14-18, 2020

Venue: Zoom ID 971 9237 0490

南方科技大学
SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY

杰曼诺夫数学中心
SUSTech International Center for Mathematics

国家天元数学东南中心
Tianyuan Mathematical Center in Southeast China

Program

(Beijing time GMT+8)

June 14		
Tutorial session, Chair: Jiang Yang		
09:00--11:00	Xiaochuan Tian	An Invitation to Nonlocal and Fractional Models, part one: Nonlocal Models
15:00--17:00	Zhi Zhou	An Invitation to Nonlocal and Fractional Models, part two: Fractional Models
Opening (20:30--20:40), Chair: Xiaoming Wang		
Evening session, Chair: Qiang Du		
20:40--21:15	Max Gunzburger	Approximate Euclidean Balls for the Efficient Assembly of Finite Element Stiffness Matrices for Nonlocal Models
21:15--21:50	Kuang Huang	Traffic Flow with Nonlocal Velocity Control: A global Stability Analysis

June 15

Morning session, Chair: Jie Shen		
08:30--09:05	Juncheng Wei	Nonlocal Mazzeo-Pacard Program
09:05--09:40	Raytcho Lazarov	Solution of Spectral Fractional Elliptic Problems: A Concise Overview
09:40--10:15	Tadele Mengesha	A Fractional Korn's Inequality with Applications to Regularity Estimates for Nonlocal Estimates
Afternoon session I, Chair: Zhi Zhou		
15:00--15:35	Bangti Jin	Incomplete Iterative Schemes for Subdiffusion
15:35--16:10	Zuoqiang Shi	PDE-based Methods for Interpolation on High Dimensional Point Cloud
Afternoon session II, Chair: Zuoqiang Shi		
16:30--17:05	Martin Stynes	A Frequent Weakness in Error Estimates for Numerical Methods for Time-fractional Initial-boundary Value Problems
17:05--17:40	Xinlong Feng	Numerical Simulation of Binary Fluid–surfactant Phase Field Model Coupled with Geometric Curvature on the Curved Surface
Evening session, Chair: Tao Tang		
20:30--21:05	Ricardo H. Nochetto	Local Error Estimates for Nonlocal Problems
21:05--21:40	William Rundell	The Role of the Subdiffusion Operator in Inverse Problems

June 16

Morning session, Chair: Masahiro Yamamoto		
08:30--09:05	Jin Cheng	A Linear Nonlocal Model for Outbreak of COVID-19 and Parameter Identification
09:05--09:40	Olena Burkovska	A Nonlocal Cahn-Hilliard Model with A Nonsmooth Potential Permitting Sharp Interfaces
09:40--10:15	Marta D'Elia	A Unified Theoretical and Computational Nonlocal Framework: Generalized Nonlocal Vector Calculus and Physics-informed Neural Networks
Afternoon session I, Chair: Espen R. Jakobsen		
15:00--15:35	Markus J. Melenk	Hp-FEM for the Spectral Fractional Laplacian in Polygons
15:35--16:10	Yanping Chen	Two-grid Methods for Maxwell's Equations in A Cole-Cole Dispersive Medium
Afternoon session II, Chair: Bangti Jin		
16:30--17:05	Masahiro Yamamoto	On An Initial Boundary Value Problem for Generalized Time-fractional Partial Differential Equation
17:05--17:40	Yubin Yan	An Analysis of the L1 Scheme for Stochastic Subdiffusion Problem Driven by Integrated Space-time White Noise
Evening session, Chair: Raytcho Lazarov		
20:30--21:05	Xavier Ros-Oton	The Neumann Problem for the Fractional Laplacian
21:05--21:40	Andrea Bonito	Numerical Simulations of Surface Quasi-Geostrophic Flows: Dunford-Taylor Method and Maximum Principle

June 17

Morning session, Chair: Xiaochuan Tian		
08:30--09:05	Robert Lipton	Nonlocal Fracture Modeling
09:05--09:40	Jinqiao Duan	Most Probable Transition Pathways in Stochastic Dynamics of a Gene Regulation System
09:40--10:15	Lili Ju	A Conservative Nonlocal Convection-diffusion Model and Asymptotically Compatible Finite Difference Discretization
Afternoon session I, Chair: Li-Lian Wang		
15:00--15:35	Weihua Deng	Functional Distribution of Multimodal Diffusion: Multiscale Modeling and Computation
15:35--16:10	Espen R. Jakobsen	Discretization of PDEs with Nonlocal Diffusion Terms, nonlinear and Possibly Degenerate Models
Afternoon session II, Chair: Jilu Wang		
16:30--17:05	Tao Zhou	Variable-step Time-stepping for Nonlocal Problems
17:05--17:40	Honglin Liao	Adaptive Time-stepping Schemes for Some Time Fractional Phase Field Models
Evening session, Chair: Lili Ju		
20:30--21:05	Yue Yu	An Asymptotically Compatible Meshfree Formulation for Neumann-type Boundary Condition on Nonlocal Problems
21:05--21:40	Hong Wang	Variable-order Fractional PDEs: Modeling, Analysis and Approximation

June 18

Morning session, Chair: Zhi Zhou		
08:30--09:05	Zhimin Zhang	Superconvergent Points for Fractional Differentiation of Polynomial Spectral Interpolation
09:05--09:40	Buyang Li	Subdiffusion with Time-Dependent Coefficients: Improved Regularity and Second-Order Time Stepping
09:40--10:15	Zhiping Mao	Fractional Phase Field Crystal Modelling: Analysis, Approximation and Pattern Formation
Afternoon session I, Chair: Weihua Deng		
15:00--15:35	Zhonghua Qiao	L-infinity Stable Numerical Methods for Nonlocal Allen-Cahn and Cahn-Hilliard Equations
15:35--16:10	Jiwei Zhang	Fast Algorithm and Numerical Analysis for Subdiffusion Equations
Afternoon session II, Chair: Zhonghua Qiao		
16:30--17:05	Li-Lian Wang	Towards Fast and Accurate Computation of Stiffness Matrix of Integral Fractional Laplacian in Multiple Dimensions: FEM and Spectral Methods
17:05--17:40	Jilu Wang	Well-posedness and Numerical Approximation of A Fractional Diffusion Equation with A Nonlinear Variable Order
Evening session, Chair: Chuanju Xu		
20:30--21:05	Changpin Li	L1/LDG Method for the Caputo-Hadamard Fractional Partial Differential Equation
21:05--21:40	Sheng Chen	Log Spectral Method and its Application to Fractional Problems

Title & Abstract

Numerical Simulations of Surface Quasi-Geostrophic Flows: Dunford-Taylor Method and Maximum Principle

Andrea Bonito (bonito@math.tamu.edu)

Texas A&M University

We consider the surface quasi-geostrophic (SQG) flow system modeling the dynamic of the buoyancy at the poles. In this advection dominated setting, fractional operators allow for a dimension reduction of the computational domain. Continuous linear finite elements for the space discretizations and three stages Runge-Kutta method for the time discretizations are analyzed. The positive and negative fractional powers of elliptic operators are represented using Dunford-Taylor integrals [1,2] and thus only require the solution to standard reaction-diffusion problems for their approximations. To cope with the hyperbolic nature of the system, we propose in the spirit of [3], a flux corrected transport limiting algorithm coupling a low order maximum principle preserving scheme with a higher order scheme. The resulting numerical method satisfies a maximum principle under a typical CFL condition. It is formally third order in time and second order in space. We illustrate the performances of our algorithm on different benchmarks. We also discuss a numerical study of freely decaying turbulence to exhibit the intricate nature of the SQG system.

[1] A. Bonito, W. Lei and J. Pasciak, Numerical approximation of the integral fractional Laplacian, Numer. Math., 142 (2019).

[2] A. Bonito and J. Pasciak, Numerical approximation of fractional powers of elliptic operators, Math. Comp., 84 (2015).

[3] J.-L. Guermond and B. Popov, Invariant domains and second-order continuous finite element approximation for scalar conservation equations, SIAM J. Numer. Anal., 55 (2017).

A Nonlocal Cahn-Hilliard Model with A Nonsmooth Potential Permitting Sharp Interfaces

Olena Burkovska (Orkburkovskao@ornl.gov)

Oak Ridge National Laboratory

We present a nonlocal Cahn-Hilliard model with a nonsmooth potential of double-well obstacle type that promotes sharp interfaces in the solution. To capture long-range interactions between particles, we set up a nonlocal Ginzburg-Landau energy functional which recovers the classical (local) model for vanishing nonlocal interactions. In contrast to the local Cahn-Hilliard problem that always leads to diffuse interfaces, the proposed nonlocal model can lead to a strict separation into pure phases of the substance. Here, the lack of smoothness of the potential is essential to guarantee the aforementioned sharp-interface property. Mathematically, this introduces additional inequality constraints that, in a weak form, lead to a coupled system of variational inequalities which at each time instance can be restated as a constrained optimization problem. We prove the well-posedness and regularity of the semi-discrete and continuous in time weak solutions and derive the conditions under which pure phases are admitted. Moreover, we discuss discretization of the problem based on finite elements and implicit-explicit time stepping methods that can be realized efficiently. We illustrate our theoretical findings through several numerical experiments.

Log Spectral Method and its Application to Fractional Problems

Sheng Chen

Beijing Computational Science Research Center

We present a new class of orthogonal functions, log orthogonal functions (LOFs), which are constructed by applying a log mapping to the Laguerre functions. We develop basic approximation theory for these new orthogonal functions and compare the new basis with the classical orthogonal polynomials. The error analysis and numerical results show that the method based on the new orthogonal functions is particularly suitable for functions which have weak singularities at one endpoint, and can lead to exponential convergent rates, as opposed to low algebraic rates if usual orthogonal polynomials are used. Further, we apply them to several typical fractional differential equations whose solutions exhibit weak singularities. Numerical experiments fully support the theoretical results and show the efficiency of the proposed spectral Galerkin method.

Two-grid Methods for Maxwell's Equations in A Cole-Cole Dispersive Medium

Yanping Chen (yanpingchen@scnu.edu.cn)

South China Normal University

In this talk, we propose a modified two-grid method(MTGM) built upon the mixed finite element scheme for solving the time-fractional Maxwell's equations in Cole-Cole dispersive media. Different from many other classical approaches, this modified algorithm makes sure that the first family of Nedelec edge finite elements perform the same adequate approximation properties in the L^2 norm comparing with the second family of Nedelec elements. Firstly, we get the global superconvergence results on the coarse mesh; then we take the postprocessing solutions on the coarse mesh into the second step as the correction values. Theoretical analysis shows the optimal accuracy, and the numerical experiments presented confirm the theoretical results.

A Linear Nonlocal Model for Outbreak of COVID-19 and Parameter Identification

Jin Cheng (jcheng@fudan.edu.cn)

Fudan University

The novel coronavirus pneumonia (COVID-19) is a major event in the world. Whether we can establish the mathematical models to describe the characteristics of epidemic spread and evaluate the effectiveness of the control measures we have taken is a question of concern. From January 26, 2020, our team began to conduct research on the modeling of new crown epidemic. A kind of linear nonlocal dynamical system model with time delay is proposed to describe the development of covid-19 epidemic. Based on the public data published by the government, the information of transmission rate, isolation rate and other information that can not be directly observed in the process of epidemic development is obtained through inversion method, and on the basis of that, a "reasonable" prediction of the development of the epidemic is made. To provide some reasonable data support for government decision-making and various needs of the public.

A Unified Theoretical and Computational Nonlocal Framework: Generalized Nonlocal Vector Calculus and Physics-informed Neural Networks

Marta D’Elia (mdelia@sandia.gov)

Sandia National Laboratories

Nonlocal models provide an improved predictive capability thanks to their ability to capture effects that classical partial differential equations fail to capture. Among these effects we have multiscale behavior and anomalous behavior such as super- and sub-diffusion. These models have become popular for a broad range of applications, including mechanics, subsurface flow, turbulence, plasma dynamics, heat conduction and image processing. However, their improved accuracy comes at a price of many modeling and numerical challenges. In this work we focus on the estimation of model parameters, often unknown, or subject to noise. In particular, we address the problem of model identification in presence of sparse measurements. Our approach to this inverse problem is based on the combination of 1. Machine Learning and Physical Principles and 2. a Unified Nonlocal Vector Calculus and Versatile Surrogates such as neural networks (NN). The outcome is a flexible tool that allows us to learn existing and new nonlocal operators. We refer to our technique as nPINNs (nonlocal Physics-Informed Neural Networks); here, we model the nonlocal solution with a NN and we solve an optimization problem where we minimize the residual of the nonlocal equation and the misfit with measured data. The result of the optimization are the weights and biases of the NN and the set of unknown model parameters. In this talk we briefly present the unified vector calculus, introduce nPINNs, describe its properties, and provide several numerical results that illustrate our findings, including an application to turbulence. This is a joint work with M. Gulian, G. Pang, M. Parks, and G. E. Karniadakis.

Functional Distribution of Multimodal Diffusion: Multiscale Modeling and Computation

Weihua Deng (dengwh@lzu.edu.cn)

Lanzhou University

It has been widely recognized that anomalous diffusion is a very general phenomenon in the natural world, which is characterized by the nonlinear evolution of mean-squared displacement with respect to time, i.e., $\langle x^2(t) \rangle \propto t^{\beta}$ with $\beta \neq 1$. The common examples are $\beta < 1$ for a subdiffusive continuous-time random walk with a divergent first moment of waiting time and $\beta > 1$ for a Lévy flight with a divergent second moment of jump length. The common feature of the two typical anomalous diffusive processes is their single mode of the motions. However, a particle moving in a complex or even seemingly simple structures might present simultaneous modes, such as the tracing particle under the effect of a flow acting in the phase space of chaotic Hamiltonian systems. Functional is a class of statistical observables, having wide applications in almost all disciplines. This talk will discuss the multiscale modeling and computation of functional distribution for diffusion with multiple modes.

Most Probable Transition Pathways in Stochastic Dynamics of a Gene Regulation System

Jinqiao Duan (duan@iit.edu)

Illinois Institute of Technology

Dynamical systems arising in biophysics are often subject to random fluctuations. The noisy fluctuations may be Gaussian or non-Gaussian, which are modeled by Brownian motion or α-stable Levy motion, respectively. Non-Gaussianity of the noise manifests as nonlocality at a "macroscopic" level. Stochastic dynamical systems with non-Gaussian noise (modeled by α-stable Levy motion) have attracted a lot of attention recently. The non-Gaussianity index α is a significant indicator for various dynamical behaviors. Transition phenomena are special events for evolution from one metastable state to another in stochastic dynamical systems, caused by the interaction between nonlinearity and uncertainty. Examples for such events are phase transition, pattern change, gene transcription, climate change, abrupt change, extreme transition, and other rare events. The most probable transition pathways are the maximal likely (in the sense of optimizing a probability or an action functional) trajectory between metastable states. The speaker will present recent work on analyzing and computing the most probable transition pathways for stochastic dynamical systems, in the context of the Onsager-Machlup action functionals.

Numerical Simulation of Binary Fluid–surfactant Phase Field Model Coupled with Geometric Curvature on the Curved Surface

Xinlong Feng (fxlmath@xju.edu.cn)

Xinjiang University

In this work, we consider the numerical simulation of the binary fluid–surfactant phase field model coupled with geometric curvature on the curved surface. By taking account of the effect of the curvature, we firstly modify the free energy of the fluid–surfactant system, which results a new phase field model on the curved surface. Then, based on the SAV method, we study the numerical schemes, which consist of a surface FEM for the spatial discretization, and first- and second-order implicit schemes for the temporal discretization. Finally, numerical examplesare shown to verify the theoretical prediction.

Approximate Euclidean Balls for the Efficient Assembly of Finite Element Stiffness Matrices for Nonlocal Models

Max Gunzburger (mgunzburger@fsu.edu)

Florida State University

In many nonlocal models, interactions are limited to bounded neighborhoods that are usually chosen to be Euclidean balls so that for grid-based discretizations, one has to deal with intersections of balls with grid cells. As a result, the assembly process of finite element stiffness matrices faces the challenge of constructing the partial elements (having curved boundaries) created by the intersections of the ball and elements. A further challenge is the construction of quadrature rules over those partial elements. Through the use of approximate balls (e.g., several polygonal approximations of Euclidean balls) we mitigate the challenges of dealing with ball-element intersections and of the selection of quadrature rules. We study, both theoretically and computationally, the relative accuracy and efficiency of the several approaches we develop. This is a joint work with Marta D'Elia and Christian Vollman.

Discretization of PDEs with Nonlocal Diffusion Terms, nonlinear and Possibly Degenerate Models

Espen R. Jakobsen (espen.jakobsen@ntnu.no)

Norwegian University of Science and Technology

An important source of nonlocal PDEs are different types of anomalous diffusion phenomena. From mainly linear equations in probability and finance, to nonlinear equations in mechanics and control theory. In this talk we focus on three types of quite different nonlinear and possibly degenerate models: HJB-equations from control theory, conservation laws, and porous medium equations. We will explain that they can be discretized in a unified and consistent way using similar finite difference quadrature type of schemes. In all cases we present stability and convergence results in simplified model examples, and we also present error estimates. We comment on the different mathematical techniques used for the proofs and sketch some arguments. The talk can be seen as a very compact synthesis of more than 15 years of research, and includes recently published results as well as some of the earliest numerical results for every model class discussed. Some of the results predates results for linear PDEs.

Incomplete Iterative Schemes for Subdiffusion

Bangti Jin (b.jin@ucl.ac.uk)

University College London

In this talk, we develop efficient incomplete iterative scheme for the numerical solution of the subdiffusion model involving a Caputo derivative of order in time. It is based on piecewise linear Galerkin finite element method in space and convolution quadrature in time and solves one linear algebraic system inexactly by an iterative algorithm at each time step. We present theoretical results for both smooth and nonsmooth solutions, using novel weighted estimates of the time-stepping scheme. The analysis indicates that with the number of iterations at each time level chosen properly, the error estimates are nearly identical with that for the exact linear solver, and the theoretical findings provide guidelines on the choice. Illustrative numerical results are presented to complement the theoretical analysis.

A Conservative Nonlocal Convection-diffusion Model and Asymptotically Compatible Finite Difference Discretization

Lili Ju (ju@math.sc.edu)

University of South Carolina

In this talk, we first present a nonlocal convection-diffusion model, in which the convection term is constructed in a special upwind manner so that mass conservation and maximum principle are maintained. The well-posedness of the proposed nonlocal model and its convergence to the classical local convection-diffusion model are established. A quadrature-based finite difference discretization is then developed to numerically solve the nonlocal problem and it is shown to be consistent and unconditionally stable. We further demonstrate that the numerical scheme is asymptotically compatible, that is, the approximate solutions of the nonlocal problem converge to the exact solution of the corresponding local problem when the mesh size and the horizon parameter decrease zero. Some numerical experiments are also performed to complement the theoretical analysis.

Traffic Flow with Nonlocal Velocity Control: A global Stability Analysis

Kuang Huang (kh2862@columbia.edu)

Columbia University

The emerging automated and connected vehicle technologies allow vehicles to perceive and process traffic information in a wide range. When those vehicles were put on highways, how would traffic flows be changed? How to design the vehicles so that passengers could benefit from the change? To answer the questions, nonlocal models are a good framework to describe nonlocal interactions between vehicles and analyze the impact of nonlocal interactions on traffic flows.

In this talk, I will discuss a particular nonlocal traffic flow model that assumes vehicles control their velocities in reaction to the nonlocal traffic density. By applying a global stability analysis to the model, we obtain that, under suitable assumptions on how the nonlocal information is utilized, the nonlocal traffic flow is stable around the uniform flow and all traffic jams dissipate in a short period.

Solution of Spectral Fractional Elliptic Problems: A Concise Overview

Raytcho Lazarov (raytcho.lazarov@gmail.com)

Texas A&M University

The purpose of the talk is to present some new results in numerics for the problem ${\mathcal A}^\alpha u =f$. Here ${\mathcal A}$ is a self-adjoint and coercive elliptic operator defined on a dense subset of $L^2(\Omega)$, with Ω a bounded Lipschitz domain and $0< \alpha < 1$. We discuss the discretizations ${\mathcal A}_h$ of ${\mathcal A}$ by finite difference or finite element methods on a mesh with mesh-size h and survey the existence, stability, error, and positivity of the solution of the system ${\mathcal A}_h^\alpha u_h =f_h$. The fractional power of the operators $ {\mathcal A}$ and $ {\mathcal A}_h$ are defined through their spectrum. For solving this system we show that the methods of Bonito and Pasciak (Numerical approximation of fractional powers of elliptic operators, Math.Comp., 2015), Vabishchevich (Numerically solving equations with fractional powers of elliptic operators, JCP, 282, 2015) and Nochetto, Ot\'arola, and Salgado (A PDE Approach to Fractional Diffusion, Foundations of Comput. Math., 2015) are all based on rational approximations $r(z)$ of z^α on $(0,1]$. Instead of $u_h = {\mathcal A}_h^{-\alpha} f_h$ these methods introduce $w_h= r({\mathcal A}_h^{-1})f_h$, with $r(z) \in %$ in the set of rational functions $ {\mathcal R}_k= \{ P_k(z)/Q_k(z)\}$, $P_k(z)$, $Q_k(z)$ polynomials of degree k, such that ${\mathcal A}_h^{-\alpha} \approx r({\mathcal A}_h^{-1})$. Consequently $w_h \approx u_h$. Second, we argue and computationally show that the best uniform rational approximation (BURA), $$ r(z)= r_{\alpha,k}(z) := {\arg \min}_{s(z)\in {\mathcal R}_k}\, \| s(z) - z^{\alpha} \|_{L^\infty[0,1]},$$ studied by S. Harizanov, R.Lazarov, P. Marinov, S. Margenov, and J. Pasciak (Analysis of numerical methods for spectral fractional elliptic equations based on BURA, JCP, 2020) gives a new method, which is as good as the above methods and in many cases significantly outperforms them in therms of efficiency, parallelization, and robustness.

Subdiffusion with Time-Dependent Coefficients: Improved Regularity and Second-Order Time Stepping

Buyang Li (buyang.li@polyu.edu.hk)

Hong Kong Polytechnic University

This article concerns second-order time discretization of subdiffusion equations with time-dependent diffusion coefficients. High-order differentiability and regularity estimates are established for subdiffusion equations with time-dependent coefficients. Using these regularity results and a perturbation argument of freezing the diffusion coefficient, we prove that the convolution quadrature generated by the second-order backward differentiation formula, with proper correction at the first time step, can achieve second- order convergence for both nonsmooth initial data and incompatible source term. Numerical experiments are consistent with the theoretical results.

L1/LDG Method for the Caputo-Hadamard Fractional Partial Differential Equation

Changpin LI (lcp@shu.edu.cn)

Shanghai University

In this talk, we introduce L1/LDG method for the time fractional partial differential equation, where the time fractional derivative is in the sense of Caputo-Hadamard. We first introduce the Hadamard fractional calculus and the associated integral transform. Then we study the regularity and decay estimate of the solution to the considered equation. Since the equation model has a time fractional derivative, its solution very likely behaves a certain weak regularity at the initial time. If its solution is suitable smooth, then we can use the L1 scheme on uniform meshes to approximate the time derivative, and use the local discontinuous Galerkin (LDG) method to approach the space derivative. If the solution has a certain weak regularity at the initial time, we use the L1 scheme on non-uniform meshes (i.e., grading meshes) and we still use the LDG method in space direction. The fully discrete schemes for both situations are established and analyzed. Numerical examples are displayed which support the theoretical analysis.

Adaptive Time-stepping Schemes for Some Time Fractional Phase Field Models

Honglin Liao (liaohl@csrc.ac.cn)

Nanjing University of Aeronautics and Astronautics

Adaptive second-order Crank-Nicolson time-stepping methods are developed for the time-fractional molecular beam epitaxial models. Based on the piecewise linear interpolation, the Caputo's fractional derivative is approximated by a novel second-order formula, which is naturally suitable for a general class of nonuniform meshes and essentially preserves the positive semi-definite property of integral kernel. The resulting time-stepping schemes are energy stable on nonuniform time meshes, and are computationally efficient in multiscale time simulations when combined with adaptive time steps, such as are appropriate for accurately resolving the intrinsically initial singularity of solution and for efficiently capturing the fast dynamics away initial time.

Nonlocal Fracture Modeling

Robert Lipton (lipton@lsu.edu)

Louisiana State University

We consider a non-local model for calculating dynamic fracture. The force interaction is derived from a double well strain energy density function, resulting in a non- monotonic material model. The fracture set emerges from the model and is part of the dynamics. The non-local model is seen to encode the well known kinetic relation between crack driving force and crack tip velocity seen in classic fracture theories. We conclude with a numerical analysis of the model and several computational examples. This is joint work with Prashant Jha.

Fractional Phase Field Crystal Modelling: Analysis, Approximation and Pattern Formation

Zhiping Mao (zhiping_mao@brown.edu)

Brown University

We consider a Fractional Phase Field Crystal Model in which the classical Swift-Hohenberg equation (SHE) is replaced by a fractional order Swift-Hohenberg equation (FSHE) equation which reduces to the classical case when the fractional order $\beta=1$. It is found that choosing the value of β appropriately leads to FSHE giving a markedly superior fit to experimental measurements of the structure factor than obtained using the SHE ($\beta=1$) for a number of crystalline materials. The improved fit to the data provided by the fractional partial differential equation prompts our investigation of a Fractional Phase Field Crystal (FPFC) model based on the fractional free energy functional. It is shown that the FSHE is well-posed and exhibits the same type of pattern formation behavior as the SHE, which is crucial for the success of the PFC model, independently of the fractional exponent β. This means that the FPFC model inherits the early successes of the FPC model such as physically realistic predictions of the phase diagram etc. and, therefore, provides a viable alternative to the classical PFC model.

Hp-FEM for the Spectral Fracdtional Laplacian in Polygons

Markus J. Melenk (melenk@tuwien.ac.at)

Technische Universitaet Wien

For the spectral fractional Laplacian in polygons we present two types of discretizations that converge at an exponential rate. The first one is based on the Caffarelli-Silvestre extension, which realizes the non-local fractional Laplacian as a Dirichlet-to-Neumann map of a (degenerate) elliptic boundary value problem (BVP). This BVP is amenable to a discretization by high order finite element method (hp-FEM). Exponential convergence of the hp-FEM can be achieved if the underlying meshes are suitably refined towards the edges of the polygon so as to resolve the boundary singularities and towards the vertices in order to capture the corner singularities. The second discretization is based on the so-called ``Balakrishnan" formula, an integral representation of the inverse of the spectral fractional Laplacian. The discretization of the integral leads to a collection of BVPs, which can be discretization by hp-FEM. Again, the use of meshes that are refined towards the vertices and the boundary leads to exponential convergence. The talk is based on joint work with C. Schwab (ETH Zurich) and L. Banjai (Heriot Watt University).

A Fractional Korn's Inequality with Applications to Regularity Estimates for Nonlocal Estimates

Tadele Mengesha (mengesha@utk.edu)

The University of Tennessee Knoxville

In this talk I will present a fractional version of the classical Korn's inequality. The inequality allows us to characterize fractional Sobolev spaces of vector fields via a norm that involves only the measure of the magnitude of projected difference quotients. The result is used to describe the energy space associated to a strongly coupled system of nonlocal equations related to a nonlocal continuum model via peridynamics. Moreover, the characterization permits us to apply classical space embeddings in proving that weak solutions to the nonlocal system enjoy both improved differentiability and improved integrability. This is based on ongoing and joint work with James M. Scott.

Local Error Estimates for Nonlocal Problems

Ricardo H. Nochetto (rhn@math.umd.edu)

University of Maryland

The integral fractional Laplacian of order $s \in (0,1)$ is a nonlocal operator. It is known that solutions to the Dirichlet problem involving such an operator exhibit an algebraic boundary singularity regardless of the domain regularity. This, in turn, deteriorates the global regularity of solutions and as a result the global convergence rate of the numerical solutions. For finite element discretizations, we derive {\em local} error estimates in the H^s-seminorm and show optimal convergence rates in the interior of the domain by only assuming meshes to be shape-regular. These estimates quantify the fact that the reduced approximation error is concentrated near the boundary of the domain. We illustrate our theoretical results with several numerical examples. This is joint work with J.P. Borthagaray and D. Leykekhman.

L-infinity Stable Numerical Methods for Nonlocal Allen-Cahn and Cahn-Hilliard Equations

Zhonghua Qiao (zhonghua.qiao@polyu.edu.hk)

The Hong Kong Polytechnic University

In this talk, we will first investigate the first and second order Runge-Kutta ETD schemes for the nonlocal Allen-Cahn equation. The discrete maximum bound principles will be established without any restrictions on the numerical solutions. Then we will present first and second order stabilized semi-implicit schemes for the nonlocal Cahn-Hilliard equation. With a combination of the higher-order consistency estimates and the convergence analysis, we justify the L-infinity bound of the numerical solution of the first order stabilized semi-implicit scheme for the nonlocal Cahn-Hilliard equation.

The Neumann Problem for the Fractional Laplacian

Xavier Ros-Oton (xavier.ros-oton@math.uzh.ch)

University of Zurich

We study a Neumann problem for the fractional Laplacian. We start with some basic properties, such as its variational formulation, probabilistic interpretation, existence of solutions, and then turn our attention to their regularity.

The Role of the Subdiffusion Operator in Inverse Problems

William Rundell (rundell@math.tamu.edu)

Texas A&M University

The recent decade has seen enormous number of papers of inverse problems for diffusion equations involving the sub diffusion operator. This talk will try and give an overview of the role this plays for uniqueness and ill-conditioning as opposed to the classical situation.

PDE-based Methods for Interpolation on High Dimensional Point Cloud

Zuoqiang Shi (zqshi@mail.tsinghua.edu.cn)

Tsinghua University

Interpolation on high dimensional point cloud provides a fundamental model in many data analysis and machine learning problems. In this talk, we will present some PDE based methods to do interpolation on point cloud. Applications in image processing and machine learning are shown to demonstrate the performance of our methods.

A Frequent Weakness in Error Estimates for Numerical Methods for Time-fractional Initial-boundary Value Problems

Martin Stynes (m.stynes@csrc.ac.cn)

Beijing Computational Science Research Center

Time-fractional initial-boundary value problems of the form $D_t^\alpha u-p \partial^2 u/\partial x^2 +cu=f$ are considered, where $D_t^\alpha u$ is a Caputo fractional derivative of order $\alpha\in (0,1)$. As $\alpha\to 1^-$, we prove that the solution u converges, uniformly on the space-time domain, to the solution of the classical parabolic initial-boundary value problem where $D_t^\alpha u$ is replaced by $\partial u/\partial t$. Nevertheless, most of the rigorous analyses of numerical methods for this time-fractional problem have error bounds that blow up as $\alpha\to 1^-$, as we demonstrate. We show that in some cases these analyses can be modified to obtain robust error bounds that do not blow up as $\alpha\to 1^-$.

An Invitation to Nonlocal and Fractional Models, part one: Nonlocal Models

Xiaochuan Tian (xtian@math.utexas.edu)

University of Texas at Austin

There has been a growing interest in the study of nonlocal models as more general and sometimes more realistic alternatives to the conventional PDE models. We will devote two tutorial talks on the introduction of nonlocal and fractional models. In this first talk, we will focus on the nonlocal models with a finite range of nonlocal interactions, which serve as bridges connecting the classical PDEs, nonlocal discrete models and the fractional differential equations (which will be introduced in the second talk). This talk will cover topics including nonlocal modeling, nonlocal calculus and numerical analysis for the nonlocal models.

Variable-order Fractional PDEs: Modeling, Analysis and Approximation

Hong Wang (hwang@math.sc.edu)

University of South Carolina

Fractional PDEs model challenge phenomena like anomalously diffusive transport and long-range interactions or memory effect characterized by non-Gaussian heavy tail behaviors more accurately than integer order diffusion PDEs do, because they were derived via a continuous time random walk (CTRW) assuming that the mean waiting time has power-law decaying tails. But classical FPDE was shown to yield nonphysical initial or boundary singularity, which makes it unrealistic to conduct error estimates of numerical approximations to FPDEs assuming their true solutions smooth. Moreover, in many applications the structure of porous materials may change, which leads to the change of the fractional order via the Hurst index. This leads to variable-order FPDEs. Moreover, variable-order FPDEs provide a physically relevant approach to fix the nonphysical singularity of classical constant-order FPDEs. In this talk we will go over the modeling, analysis and approximation of variable-order FPDEs.

Well-posedness and Numerical Approximation of A Fractional Diffusion Equation with A Nonlinear Variable Order

Jilu Wang (jiluwang@csrc.ac.cn)

Beijing Computational Science Research Center

In this work, we prove well-posedness and regularity of solutions to a fractional diffusion equation with a variable fractional order that may depend on the unknown solution. We present linearly implicit time discretization for the equation, and present rigorous analysis for the convergence of numerical solutions based on proved regularity results.

Towards Fast and Accurate Computation of Stiffness Matrix of Integral Fractional Laplacian in Multiple Dimensions: FEM and Spectral Methods

Li-Lian Wang (lilian@ntu.edu.sg)

Nanyang Technological University

PDEs involving integral fractional Laplacian in multiple dimensions pose significant numerical challenges due to the nonlocality and singularity of the operator. In this talk, we report our recent attempts towards fast and accurate computation of the underlying stiffness matrix. For the rectangular or L-shaped domain, each entry of stiffness matrix associated with the tensorial FEM can be expressed explicitly by some one-dimensional integral, which can be evaluated accurately. In particular, for the uniform grids, the matrix is Toepliz or block Toepliz. The key is to implement in the Fourier domain, where the Fourier transform of basis can be derived explicitly. We also develop fast Fourier-like spectral methods for integral fractional Laplacian in R^d based on the Dumford-Taylor formulation of the fractional Laplacian, which leads to diagonal stiffness matrix. This talk is based on several works jointed with Changtao Sheng (NTU), Huiyuan Li (CAS), Jie Shen (Purdue Univ.), Tao Tang (BNU-HKBU) and/or Huifang Yuan (SUSTech).

Nonlocal Mazzeo-Pacard Program

Juncheng Wei (jcwei@math.ubc.ca)

University of British Columbia

I will discuss recent progress on nonlocal Mazzeo-pacard program for nonlocal Yamabe problem. To execute this program, some basic techniques in ordinary differential equations are extended to nonlocal differential equations, such as variation of parameter formula, Wronskian, initial value problems, etc.

On An Initial Boundary Value Problem for Generalized Time-fractional Partial Differential Equation

Masahiro Yamamoto (myama@ms.u-tokyo.ac.jp)

University of Tokyo

We consider an initial boundary value problem for partial differential equation with Caputo-type time derivative admitting some kernel function. First we define such a generalized Caputo derivative in fractional Sobolev spaces and prove that it is an isomorphism. Then we prove the well-posedness of the weak solution for the initial boundary value problem and more regular solution. Finally we show a maximum principle.

An Analysis of the L1 Scheme for Stochastic Subdiffusion Problem Driven by Integrated Space-time White Noise

Yubin Yan (y.yan@chester.ac.uk)

University of Chester

We consider the strong convergence of the numerical methods for solving stochastic subdiffusion problem driven by an integrated space-time white noise. The time fractional derivative is approximated by using the L1 scheme and the time fractional integral is approximated with the Lubich's first order convolution quadrature formula. We use the Euler method to approximate the noise in time and use the truncated series to approximate the noise in space. The spatial variable is discretized by using the linear finite element method. Applying the idea in Gunzburger \et (Math. Comp. 88(2019), pp. 1715-1741), we express the approximate solutions of the fully discrete scheme by the convolution of the piecewise constant function and the inverse Laplace transform of the resolvent related function. Based on such convolution expressions of the approximate solutions, we obtain the optimal convergence orders of the fully discrete scheme in spatial multi-dimensional cases by using the Laplace transform method and the corresponding resolvent estimates.

An Asymptotically Compatible Meshfree Formulation for Neumann-type Boundary Condition on Nonlocal Problems

Yue Yu (yuy214@lehigh.edu)

Lehigh University

In this paper we consider nonlocal models with a finite nonlocal horizon parameter characterizing the range of nonlocal interactions, and consider the treatment of Neumann-like boundary conditions that have proven challenging for discretizations of nonlocal models. We
propose a new generalization of classical local Neumann conditions by converting the local flux (in diffusion problems) or traction load (in peridynamics) to correction terms in the nonlocal model, which provides an estimate for the nonlocal interactions of each point with points outside the domain. To obtain an asymptotically compatible scheme, we utilize a recently introduced optimization-based quadrature framework to numerically discretizethe nonlocal Neumann-type problem. In this meshfree framework, surface effects for problems involving bond-breaking are automatically captured without modifying the model, which is especially attractive in handling material fracture. We numerically verify the consistency of our approach with a series of static problems with analytic solution, demonstrate the first order convergence for problems involving curvilinear surfaces and corners. We also quantitatively validate the applicability of the approach to realistic problems by reproducing high-velocity impact results from the Kalthoff-Winkler experiments.

Fast Algorithm and Numerical Analysis for Subdiffusion Equations

Jiwei Zhang (jiweizhang@whu.edu.cn)

Wuhan University

We first develop a fast algorithm to significantly reduce the computational cost and storage to evaluate the Caputo derivative. After that, we introduce the numerical analysis for nonuniform time-stepping schemes.To the end, we develop a general framework for the stability and convergence analysis with three tools: a family of complementary discrete convolution kernels, a discrete fractional Gronwall inequality and a global (convolutional) consistency analysis, which is not limited to a special time mesh by building a convolution structure of local truncation error.

Superconvergent Points for Fractional Differentiation of Polynomial Spectral Interpolation

Zhimin Zhang (zzhang@math.wayne.edu)

CSRC and WSU

For polynomial interpolation, we identify those points where fractional derivatives converge faster than the best possible global rate. It is found that those points are different for different order of fractional derivatives. In addition, the superconvergent gain decreases as the fractional derivative order (<1) decreases.

Variable-step Time-stepping for Nonlocal Problems

Tao Zhou (tzhou@lsec.cc.ac.cn)

Chinese Academy of Sciences

We discuss some numerical analysis aspects of variable-step time stepping approximations for nonlocal problems, which include time-fractional PDEs, Volterra integral equations, ect.

An Invitation to Nonlocal and Fractional Models, part two: Fractional Models

Zhi Zhou (zhi.zhou@polyu.edu.hk)

Hong Kong Polytechnic University

In the second part of tutorial, we will focus on the fractional calculus and its application. During the past two decades, fractional models have attracted considerable attention. The main advantage of the fractional operators is that provides excellent instruments for the description of (long-range) memory and non-local properties of various materials and processes. The talk will cover some basic knowledge of fractional calculus, modeling of fractional models, and related numerical analysis.