REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggesstions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA, 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any oenalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.
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1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
08-09-2022	Final Report	23-Sep-2015 - 31-May-2022

4. TITLE AND SUBTITLE
Final Report: Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics and Applications

5a. CONTRACT NUMBER
W911NF-15-1-0562

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611103

6. AUTHORS

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
67451-NC-MUR.98

12. DISTRIBUTION AVAILIBILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			George Karniadakis
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RPPR Final Report
as of 08-Sep-2022

Agency Code: 21XD

Proposal Number: 67451NCMUR **Agreement Number: W911NF-15-1-0562**
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Report Date: 31-Aug-2022 Date Received: 08-Sep-2022
Final Report for Period Beginning 23-Sep-2015 and Ending 31-May-2022
Title: Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics and Applications
Begin Performance Period: 23-Sep-2015 **End Performance Period:** 31-May-2022
Report Term: 0-Other

Submitted By: George Karniadakis Email: george@anailytica.com
Phone: (401) 369-5743

Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: **STEM Participants:**

Major Goals: This MURI project is the vision of a team of researchers from Brown University, Michigan State University, Columbia University, University of South Carolina, and Rice University with overlapped interests and complementary expertise on theory, numerical methods, and applications of fractional PDEs (FPDEs). Our overarching goal is the development of a seamless integration of theory and algorithms for data-driven FPDEs, while targeting the common themes of conservation, monotonicity, adaptive refinement, and high-order accuracy in the context of simulations of multiphase flows, turbulence, fluid-structure interactions, hydrology, and solid mechanics. We envision a combined mathematical and computational framework, where the fractional operators can be constructed based on available data, hence providing model validation for the specific phenomenon but also a tailor-based simulation capability that can be scaled to real-life applications. The proposed research plan emphasizes a dynamic integration of six main research areas that form the pillars of our integrated approach:

• Research Area 1: Theory of non-local operators and stochastic interpretation of fractional operators.
• Research Area 2: Numerical solution of fractional PDEs with emphasis on variable fractional order.
• Research Area 3: Fast solvers for dense linear systems with linear/quasi-linear computational complexity.
• Research Area 4: Stochastic FPDEs and determination of the fractional order directly by available data.
• Research Area 5: Applications to fluid and solid mechanics, fluid-structure interactions, two-phase flows, turbulence and reactive system with front propagation.
• Research Area 6: High performance computing & developing opensource software for fractional problems.

Accomplishments: There has been great progress in the five years on all research six areas, in recruiting excellent postdocs and PhD students, in participating in conferences with invited and contributed talks as well as on organizing mini-symposia and workshops on FPDEs. The add-on helped us to start three new areas on machine learning, fractional photonics, stochastic FPDEs, and opensource software for fractional problems. In the following, we provide a summary of progress by each co-PI. First, we provide some highlights on all our activities and then we present the report of each PI.

MURI Highlights
- More than 197 papers have been published or submitted on all six research areas of MURI.
- More than 70 invited and plenary talks by MURI personnel.
- Volume on numerical methods in Handbook of FPDEs.
- Several minisymposia and two workshops organized by MURI PIs.
- New research focusing on 2D & 3D fractional Laplacians in bounded domains with emphasis on boundary conditions and their stochastic interpretation. 11-author revised paper.

- New research focusing on machine learning, fractional photonics, stochastic fractional PDEs and opensource software enabled by the add-on funding.
- Fractional models of turbulent polymer drag reduction at high Reynolds number.
- Combine FPDE and molecular dynamics to efficiently simulate anomalous diffusive transport in heterogeneous porous materials with nanoscale pores.
- Non-local modeling of ion diffusion in battery systems & experiments.
- We discovered new fractional phase-field/non-local equations for interface problems.
- New opensource software at Brown (fractional NEKTAR), Uath (Nektar++) and MSU (FracFit).

Training Opportunities: Nothing to Report

Results Dissemination: Nothing to Report

Honors and Awards: Awards:

George Karniadakis received the SIAM/ACM Prize in Computational Science and Engineering (2021) for advancing spectral elements, reduced-order modeling, uncertainty quantification, dissipative particle dynamics, fractional PDEs, and scientific machine learning, while pushing applications to extreme computational scales and mentoring many leaders.

The PI Qiang Du also received recognition as he was awarded the TJR Hughes Medal by the USACM (US Association of Computational Mechanics) at the USNCCM 2021 for his “numerous innovative contributions to computational physics and computational fluid mechanics, and unwavering service to the scientific computing community."

Honors and Awards (Karniadakis)
1. SIAM/ACM Computational Science and Engineering Award, 2021
2. Elected to the National Academy of Engineering, 2022
3. Vannevar Bush Faculty Fellowship, 2022

Protocol Activity Status:

Technology Transfer: Nothing to Report

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Project Contribution:
National Academy Member: N

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Project Contribution:
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Project Contribution:
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Project Contribution:
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Project Contribution:
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Project Contribution:
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RPPR Final Report
as of 08-Sep-2022

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Project Contribution:
National Academy Member: N

ARTICLES:

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2016.01.015
Volume: 310 Issue: First Page #: 63
Date Submitted: 7/14/16 12:00AM Date Published: 4/1/16 8:00AM
Publication Location:
Article Title: A fast finite volume method for conservative space-fractional diffusion equations in convex domains
Authors: Jinhong Jia, Hong Wang
Keywords: Anomalous diffusion; Circulant matrix; Conjugate gradient squared method; Fast Fourier transform; Space-fractional diffusion equation; Toeplitz matrix; Volume penalization
Abstract: We develop a fast finite volume method for variable-coefficient, conservative space-fractional diffusion equations in convex domains via a volume-penalization approach. The method has an optimal storage and an almost linear computational complexity. The method retains second-order accuracy without requiring a Richardson extrapolation. Numerical results are presented to show the utility of the method.
Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Applied Mathematics and Computation
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.amc.2016.01.031
Volume: 280 Issue: First Page #: 86
Date Submitted: 7/14/16 12:00AM Date Published: 4/1/16 4:00AM
Publication Location:
Article Title: Uniform estimates for characteristics-mixed finite method for transient advection-dominated diffusion problems in two-dimensional space
Authors: Huanzhen Chen, Lei Gao, Hong Wang
Keywords: Transient advection-dominated diffusion equations; Characteristics-mixed finite element method; Uniform error estimates; Numerical experiments
Abstract: We prove uniform error estimates for the characteristics-mixed finite element method for two-dimensional transient convection-dominated diffusion equations, in the sense that the generic constants in the error estimates depend linearly on certain Sobolev norms of the true solution but not on the scaling diffusion parameter ?. Numerical experiments are presented to confirm our theoretical findings.
Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1007/s10915-016-0196-7
Volume: Issue: First Page #:
Date Submitted: 7/14/16 12:00AM Date Published: 3/1/16 5:00AM
Publication Location:
Article Title: Accuracy of Finite Element Methods for Boundary-Value Problems of Steady-State Fractional Diffusion Equations
Authors: Hong Wang, Danping Yang, Shengfeng Zhu
Keywords: Fractional diffusion equation Fractional Galerkin method High-order error estimate Indirect finite element method Regularity of solution
Abstract: Optimal-order error estimates in the energy norm and the L2 norm were previously proved in the literature for finite element methods of Dirichlet boundary-value problems of steady-state fractional diffusion equations under the assumption that the true solutions have desired regularity and that the solution to the dual problem has full regularity for each right-hand side. We show that the solution to the homogeneous Dirichlet boundary-value problem of a one-dimensional steady-state fractional diffusion equation of constant coefficient and source term is not necessarily in the Sobolev space H1.
Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: J Sci Computing
Publication Identifier Type: DOI Publication Identifier: 10.1007/s10915-017-0433-8
Volume: Issue: First Page #:
Date Submitted: 8/27/21 12:00AM Date Published: 4/13/17 3:04PM
Publication Location:
Article Title: POD Reduced-Order Modeling of Time-Fractional Partial Differential Equations with Applications in Parameter Identification
Authors: Hongfei Fu, Hong Wang, Zhu Wang
Keywords: Time-fractional partial differential equations · Proper orthogonal decomposition · Reduced-order model · Parameter identification · L-M regularization
Abstract: In this paper, a reduced-order model (ROM) based on the proper orthogonal decomposition and the discrete empirical interpolation method is proposed for efficiently simulating time-fractional partial differential equations (TFPDEs). Both linear and nonlinear equations are considered.We demonstrate the effectiveness of the ROMby several numerical examples, in which the ROMachieves the same accuracy of the full-ordermodel (FOM) over a long-term simulation while greatly reducing the computational cost. The proposed ROM is then regarded as a surrogate of FOM and is applied to an inverse problem for identifying the order of the time-fractional derivative of the TFPDE model. Based on the Levenberg– Marquardt regularization iterative method with the Armijo rule, we develop a ROM-based algorithm for solving the inverse problem. For cases in which the observation data is either uncontaminated or contaminated by random noise, the proposed approach is able to achieve accurate parameter estimation.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computer Methods in Applied Mechanics and Engineering
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cma.2016.03.018
Volume: 305 Issue: First Page #: 376
Date Submitted: 7/14/16 12:00AM Date Published: 6/1/16 4:00AM
Publication Location:
Article Title: A fractional phase-field model for two-phase flows with tunable sharpness: Algorithms and simulations
Authors: Fangying Song, Chuanju Xu, George Em Karniadakis
Keywords: Fractional Allen–Cahn equation; Sharp interface; Eulerian method; ADI; Spectral method; Variable fractional order
Abstract: We develop a fractional extension of a mass-conserving Allen–Cahn phase field model that describes the mixture of two incompressible fluids. The fractional order controls the sharpness of the interface, which is typically diffusive in integer-order phase-field models. The model is derived based on an energy variational formulation. An additional constraint is employed to make the Allen–Cahn formulation mass-conserving and comparable to the Cahn–Hilliard formulation but at reduced cost. The spatial discretization is based on a Petrov–Galerkin spectral method whereas the temporal discretization is based on a stabilized ADI scheme both for the phase-field equation and for the Navier–Stokes equation. We demonstrate the spectral accuracy of the method with fabricated smooth solutions and also the ability to control the interface thickness between two fluids with different viscosity and density in simulations of two-phase flow in a pipe and of a rising bubble.
Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1137/141001299
Volume: 37 Issue: 6 First Page #:
Date Submitted: 8/26/21 12:00AM Date Published: 1/1/15 3:00PM
Publication Location:
Article Title: A Generalized Spectral Collocation Method with Tunable Accuracy for Variable-Order Fractional Differential Equations
Authors: Fanhai Zeng, Zhongqiang Zhang, George Em Karniadakis
Keywords: singular basis, Jacobi polynomials, differentiation matrices, fractional boundary value problems, space-fractional Burger's equation, variable fractional order
Abstract: We develop spectral collocation methods for fractional differential equations with variable order with two end-point singularities. Specifically, we derive three-term recurrence relations for both integrals and derivatives of the weighted Jacobi polynomials of the form $(1+x)^{\mu_1}(1-x)^{\mu_2}P_{j}^{a,b}(x) \,({a,b, \mu_1,\mu_2>-1})$, which leads to the desired differentiation matrices. We apply the new differentiation matrices to construct collocation methods to solve fractional boundary value problems and fractional partial differential equations with two end-point singularities. We demonstrate that the singular basis enhances greatly the accuracy of the numerical solutions by properly tuning the parameters μ_1 and μ_2, even for cases for which we do not know explicitly the form of singularities in the solution at the boundaries. Comparison with other existing methods shows the superior accuracy of the proposed spectral collocation method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1137/17M1113060
Volume: 39 Issue: 3 First Page #:
Date Submitted: 8/26/21 12:00AM Date Published: 1/1/17 10:00AM
Publication Location:
Article Title: A Petrov--Galerkin Spectral Method of Linear Complexity for Fractional Multiterm ODEs on the Half Line
Authors: Anna Lischke, Mohsen Zayernouri, George Em Karniadakis
Keywords: C0-continuous element; Modal basis/test functions; Non-local assembling/scattering; Boundary/interior singularities; History fading analysis; Spectral convergence
Abstract: We develop a new C 0-continuous Petrov–Galerkin spectral element method for one-dimensional fractional elliptic problems of the form 0D? x u(x) ? ?u(x) = f (x), ? ? (1, 2], subject to homogeneous boundary conditions. We formulate a new procedure for assembling the global linear system from elemental (local) mass and stiffness matrices. We also investigate two distinct choices of basis/test functions: (i) local basis/test functions, and (ii) local basis with global test functions. We show that the former choice leads to a better-conditioned system and accuracy, while the latter results in ill-conditioned linear systems, and therefore, that is not an efficient and a proper choice of test function. Finally, we perform a systematic numerical study of non-local effects via full and partial history fading in order to further enhance the efficiency of the scheme.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2017.07.052
Volume: 348 Issue: First Page #: 694
Date Submitted: 8/26/21 12:00AM Date Published: 11/1/17 8:00AM
Publication Location:
Article Title: Discovering variable fractional orders of advection–dispersion equations from field data using multi-fidelity Bayesian optimization
Authors: Guofei Pang, Paris Perdikaris, Wei Cai, George Em Karniadakis
Keywords: spectral accuracy, linear complexity, singular solutions, tunable accuracy, distributed order
Abstract: We present a new tunably accurate Laguerre Petrov-Galerkin spectral method for solving linear multiterm fractional initial value problems with derivative orders at most one and constant coefficients on the half line. Our method results in a matrix equation of special structure which can be solved in O(N logN) operations. We also take advantage of recurrence relations for the generalized associated Laguerre functions (GALFs) in order to derive explicit expressions for the entries of the stiffness and mass matrices, which can be factored into the product of a diagonal matrix and a lower-triangular Toeplitz matrix. The resulting spectral method is efficient for solving multiterm fractional differential equations with arbitrarily many terms, which we demonstrate by solving a ♀ fty-term example.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Probabilistic Engineering Mechanics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.probengmech.2017.06.002
Volume: 54 Issue: First Page #: 2
Date Submitted: 8/26/21 12:00AM Date Published: 10/1/18 4:00AM
Publication Location:
Article Title: Nonlinear random vibrations of plates endowed with fractional derivative elements
Authors: Giovanni Malara, Pol D. Spanos
Keywords: Nonlinear plate, Statistical linearization, Boundary element method, Fractional calculus
Abstract: This paper deals with the problem of determining the nonlinear response of a plate endowed with fractional derivative elements and exposed to random loads. It shows that an approximate solution of the nonlinear fractional partial differential equation governing the plate vibrations can be obtained via a statistical linearization based approach. The approach is implemented by considering a time-dependent representation of the response involving the eigen-functions of the linear problem. This representation allows deriving a nonlinear fractional ordinary differential equation governing the variation of the time-dependent part of the response, which is linearized in a mean square sense. Then, an iterative procedure provides the response statistics and power spectral density functions.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Procedia Engineering
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.proeng.2017.09.144
Volume: 199 Issue: First Page #: 18
Date Submitted: 8/26/21 12:00AM Date Published:
Publication Location:
Article Title: Random Vibrations of Nonlinear Continua Endowed with Fractional Derivative Elements
Authors: Pol D. Spanos, Giovanni Malara
Keywords: continuum mechanics, fractional derivative, boundary element method, statistical linearization
Abstract: In this paper, two techniques are proposed for determining the large displacement statistics of random exciting continua endowed with fractional derivative elements: Boundary Element Method (BEM) based Monte Carlo simulation; and Statistical Linearization (SL). The techniques are applied to the problem of nonlinear beam and plate random response determination in the case of colored random external load. The BEM is implemented in conjunction with a Newmark scheme for estimating the system response in the time domain in conjunction with repeated simulations, while SL is used for estimating efficiently and directly, albeit iteratively, the response statistics.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1137/16M1078197
Volume: 39 Issue: 4 First Page #:
Date Submitted: 8/26/21 12:00AM Date Published: 1/1/17 5:00AM
Publication Location:
Article Title: Computing Fractional Laplacians on Complex-Geometry Domains: Algorithms and Simulations
Authors: Fangying Song, Chuanju Xu, George Em Karniadakis
Keywords: eigenvalue problem, spectral element method, fractional Laplacian, fractional diffusion, fractional phase-field equations
Abstract: We consider a fractional Laplacian defined in bounded domains by the eigendecomposition of the integer-order Laplacian, and demonstrate how to compute very accurately (using the spectral element method) the eigenspectrum and corresponding eigenfunctions in twodimensional prototype complex-geometry domains. We then employ these eigenfunctions as trial and test bases to first solve the fractional diffusion equation, and subsequently to simulate two-phase flow based on the Navier–Stokes equations combined with a fractional Allen–Cahn mass-preserving model. A key point to the effectiveness of an exponential convergence of this approach is the use of a weighted Gram–Schmidt orthonormalization of the eigenfunctions that guarantees accurate projection and recovery of spectral accuracy for smooth solutions. We demonstrate that even when only part of the eigenspectrum is computed accurately we can still obtain exponential convergence if we employ the complete set of the eigenvectors of the disc
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1137/16M1076083
Volume: 39 Issue: 1 First Page #:
Date Submitted: 8/26/21 12:00AM Date Published: 2/1/17 5:00AM
Publication Location:
Article Title: A Generalized Spectral Collocation Method with Tunable Accuracy for Fractional Differential Equations with End-Point Singularities
Authors: Fanhai Zeng, Zhiping Mao, George Em Karniadakis
Keywords: singular basis, Jacobi polyfractonomials, Jacobi polynomials, differentiation matrices, space-fractional Burgers equation
Abstract: We generalize existing Jacobi–Gauss–Lobatto collocation methods for variable-order fractional differential equations using a singular approximation basis in terms of weighted Jacobi polynomials of the form (1 ± x)?Pa,b j (x), where ? > ?1. In order to derive the differentiation matrices of the variable-order fractional derivatives, we develop a three-term recurrence relation for both integrals and derivatives of these weighted Jacobi polynomials, hence extending the three-term recurrence relationship of Jacobi polynomials. The new spectral collocation method is applied to solve fractional ordinary and partial differential equations with endpoint singularities. We demonstrate that the singular basis enhances greatly the accuracy of the numerical solution by properly tuning the parameter ?, even for cases where we do not know explicitly the form of singularity in the solution at the boundaries.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computers & Mathematics with Applications
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.camwa.2016.11.018
Volume: 73 Issue: 6 First Page #: 1286
Date Submitted: 8/26/21 12:00AM Date Published: 3/1/17 5:00AM
Publication Location:
Article Title: Efficient two-dimensional simulations of the fractional Szabo equation with different time-stepping schemes
Authors: Fangying Song, Fanhai Zeng, Wei Cai, Wen Chen, George Em Karniadakis
Keywords: Direction splitting Fractional diffusion-wave equation Wave propagation Viscoelastic media Second-order convergence
Abstract: The modified Szabo wave equation is one of the various models that have been developed to model the power law frequency-dependent attenuation phenomena in lossy media.The purpose of this study is to develop two different efficient numerical methods for the two-dimensional Szabo equation and to compare the relative merits of each method. In both methods we employ the ADI scheme to split directions, however, we use different time discretization. Specifically, in the first ADI method (ADI-I) we include a third-order correction term to achieve second-order convergence for smooth solutions, hence extending the work of Sun and Wu (2006). In the second ADI method (ADI-II), we employ the scheme in Zeng et al. (submitted for publication) to two-dimensional fractional wave equation using multiple correction terms to enhance accuracy for non-smooth solutions.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2017.01.048
Volume: 336 Issue: First Page #: 143
Date Submitted: 8/26/21 12:00AM Date Published: 5/1/17 4:00AM
Publication Location:
Article Title: Fractional Burgers equation with nonlinear non-locality: Spectral vanishing viscosity and local discontinuous Galerkin methods
Authors: Zhiping Mao, George Em Karniadakis
Keywords: Fractional conservation laws Spectral element method SVV Fractional LDG High-order methods
Abstract: We consider the viscous Burgers equation with a fractional nonlinear term as a model involving non-local nonlinearities in conservation laws, which, surprisingly, has an analytical solution obtained by a fractional extension of the Hopf–Cole transformation. We use this model and its inviscid limit to develop stable spectral and discontinuous Galerkin spectral element methods by employing the concept of spectral vanishing viscosity (SVV). For the global spectral method, SVV is very effective and the computational cost is O(N2), which is essentially the same as for the standard Burgers equation. We also develop a local discontinuous Galerkin (LDG) spectral element method to improve the accuracy around discontinuities, and we again stabilize the LDG method with the SVV operator. Finally, we solve numerically the inviscid fractional Burgers equation both with the spectral and the spectral element LDG methods. We study systematically the stability and convergence of both methods and determ
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computer Methods in Applied Mechanics and Engineering
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cma.2017.01.020
Volume: 318 Issue: First Page #: 193
Date Submitted: 8/26/21 12:00AM Date Published: 5/1/17 4:00AM
Publication Location:
Article Title: A tunable finite difference method for fractional differential equations with non-smooth solutions
Authors: Xuejuan Chen, Fanhai Zeng, George Em Karniadakis
Keywords: Weighted shifted Gr¨unwald–Letnikov formula; Correction terms; Fractional boundary value problems; Space-fractional Allen–Cahn equation; Singularities
Abstract: In this work, a finite difference method of tunable accuracy for fractional differential equations (FDEs) with end-point singularities is developed. Modified weighted shifted Grunwald–Letnikov (WSGL) formulas are proposed to approximate the left and right Riemann–Liouville fractional operators, which show better accuracy than the original WSGL formulas, due to the use of the correction terms. Finite difference schemes are constructed to solve two fractional boundary value problems and a space-fractional Allen–Cahn equation. Even if the singularity of the considered FDEs is unknown, satisfactory numerical solutions can still be obtained by suitably tuning the correction terms. Various numerical examples are presented to verify the effectiveness of the present method, and comparisons with other known methods are also made that demonstrate higher accuracy of the current method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1137/16M1070323
Volume: 38 Issue: 5 First Page #:
Date Submitted: 8/26/21 12:00AM Date Published: 1/1/16 5:00AM
Publication Location:
Article Title: Implicit-Explicit Difference Schemes for Nonlinear Fractional Differential Equations with Nonsmooth Solutions
Authors: Wanrong Cao, Fanhai Zeng, Zhongqiang Zhang, George Em Karniadakis
Keywords: time-fractional derivatives, IMEX schemes, low regularity, multirate systems, multiterm fractional derivatives
Abstract: We propose second-order implicit-explicit (IMEX) time-stepping schemes for nonlinear fractional differential equations with fractional order 0 < ? < 1. From the known structure of the nonsmooth solution and by introducing corresponding correction terms, we can obtain uniformly second-order accuracy from these schemes. We prove the convergence and linear stability of the proposed schemes. Numerical examples illustrate the flexibility and efficiency of the IMEX schemes and show that they are effective for nonlinear and multirate fractional differential systems as well as multiterm fractional differential systems with nonsmooth solutions.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computer Methods in Applied Mechanics and Engineering
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cma.2016.05.030
Volume: 308 Issue: First Page #: 443
Date Submitted: 8/26/21 12:00AM Date Published: 8/1/16 4:00AM
Publication Location:
Article Title: Fractional-order uniaxial visco-elasto-plastic models for structural analysis
Authors: J.L. Suzuki, M. Zayernouri, M.L. Bittencourt, G.E. Karniadakis
Keywords: Fractional-order constitutive laws; History-dependent visco-elasto-plasticity; Large strains; Time-fractional integration
Abstract: We propose two fractional-order models for uniaxial large strains and visco-elasto-plastic behavior of materials in structural analysis. Fractional modeling seamlessly interpolates between the standard elasto-plastic and visco-elasto-plastic models, takinginto account the history (memory) effects of the accumulated plastic strain to specify the state of stress. To this end, we develop two models, namely M1 and M2, corresponding to visco-elasto-plasticity considering a rate-dependent yield function and viscoplastic regularization, respectively. Finally, we develop the so called fractional return-mapping algorithm for solving the nonlinear system of the equilibrium equations developed for each model.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2015.11.058
Volume: 307 Issue: First Page #: 15
Date Submitted: 8/26/21 12:00AM Date Published: 2/1/16 5:00AM
Publication Location:
Article Title: Fast difference schemes for solving high-dimensional time-fractional subdiffusion equations
Authors: Fanhai Zeng, Zhongqiang Zhang, George Em Karniadakis
Keywords: Subdiffusion Fractional linear multistep method ADI Fast Poisson solver Compact finite difference Unconditional stability Convergence
Abstract: In this paper, we focus on fast solvers with linearithmic complexity in space for high-dimensional time-fractional subdiffusion equations. Firstly, we present two alternating direction implicit (ADI) finite difference schemes for the two-dimensional time-fractional subdiffusion equation that are convergent of order (1 +?)in time, where ?(0 <?<1) is the fractional order. Secondly, we develop two finite difference schemes which admit fast solvers without applying ADI techniques for two-dimensional time-fractional subdiffusion. Lastly, we extend these fast solvers to three-dimensional time-fractional subdiffusion. All the non-ADI difference methods are unconditionally stable and convergent with order two in time and order twoor four in space. We also present several numerical experiments to verify the theoretical results.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1137/16M1073121
Volume: 39 Issue: 3 First Page #:
Date Submitted: 8/26/21 12:00AM Date Published: 1/1/17 5:00AM
Publication Location:
Article Title: Petrov--Galerkin and Spectral Collocation Methods for Distributed Order Differential Equations
Authors: Ehsan Kharazmi, Mohsen Zayernouri, George Em Karniadakis
Keywords: distributed Sobolev space, distributed bilinear forms, modal basis, nodal basis, fractional Lagrange interpolants, spectral convergence, stability analysis, error analysis, uncertainty quanti♀cation
Abstract: Distributed order fractional operators offer a rigorous tool for mathematical modeling of multiphysics phenomena, where the differential orders are distributed over a range of values rather than being just a fi♀xed integer/fraction as in standard/fractional ODEs/PDEs. We develop two spectrally accurate schemes, namely, a Petrov-Galerkin spectral method and a spectral collocation method for distributed order fractional differential equations. We defi♀ne the underlying distributed Sobolev space and the associated norms, where we carry out the corresponding discrete stability and error analyses of the proposed scheme. In the collocation scheme, we employ fractional (nonpolynomial) Lagrange interpolants satisfying the Kronecker delta property at the collocation points. Subsequently, we obtain the corresponding distributed differentiation matrices to be employed in the discretization of the strong problem.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computer Methods in Applied Mechanics and Engineering
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cma.2017.08.029
Volume: 327 Issue: First Page #: 478
Date Submitted: 8/26/21 12:00AM Date Published: 12/1/17 5:00AM
Publication Location:
Article Title: Second-order numerical methods for multi-term fractional differential equations: Smooth and non-smooth solutions
Authors: Fanhai Zeng, Zhongqiang Zhang, George Em Karniadakis
Keywords: FODEs; Time-fractional diffusion-wave equation; Shifted Grünwald–Letnikov formula; Low regularity
Abstract: Starting with the asymptotic expansion of the error equation of the shifted Grünwald–Letnikov formula, we derive a new modified weighted shifted Grünwald–Letnikov (WSGL) formula by introducing appropriate correction terms. We then apply one special case of the modified WSGL formula to solve multi-term fractional ordinary and partial differential equations, and we prove the linear stability and second-order convergence for both smooth and non-smooth solutions when the regularity of the solutions is known. We show theoretically and numerically that numerical solutions with good accuracy can be obtained with only a few correction terms. Moreover, the correction terms can be tuned according to the fractional derivative orders without explicitly knowing the analytical solutions. Numerical simulations verify the theoretical results and demonstrate that the new WSGL formula leads to better performance compared to other known numerical approximations with similar resolution.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1137/140985536
Volume: 37 Issue: 4 First Page #:
Date Submitted: 8/26/21 12:00AM Date Published: 1/1/15 5:00AM
Publication Location:
Article Title: Tempered Fractional Sturm--Liouville EigenProblems
Authors: Mohsen Zayernouri, Mark Ainsworth, George Em Karniadakis
Keywords: regular/singular tempered fractional Sturm–Liouville operators, well-posedness, tempered Jacobi poly-fractonomial, spectral approximation, Petrov–Galerkin method
Abstract: Continuum-time random walk is a general model for particle kinetics, which allows for incorporating waiting times and/or non-Gaussian jump distributions with divergent second moments to account for Levy flights. Exponentially tempering the probability distribution of the waiting times and the anomalously large displacements results in tempered-stable Levy processes with finite moments, where the fluid (continuous) limit leads to the tempered fractional diffusion equation. The development of fast and accurate numerical schemes for such nonlocal problems requires a new spectral theory and suitable choice of basis functions. In this study we introduce two classes of regular and singular tempered fractional Sturm-Liouville problems of two kinds (TFSLP-I and TFSLP-II). We further develop a Petrov–Galerkin spectral method for solving tempered fractional ODEs, followed by the corresponding stability and convergence analysis which validates the achieved spectral convergence in our simulations.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Numerical Analysis
Publication Identifier Type: DOI Publication Identifier: 10.1137/16M1103622
Volume: 56 Issue: 1 First Page #: 24
Date Submitted: 8/26/21 12:00AM Date Published: 1/1/18 5:00AM
Publication Location:
Article Title: A Spectral Method (of Exponential Convergence) for Singular Solutions of the Diffusion Equation with General Two-Sided Fractional Derivative
Authors: Zhiping Mao, George Em Karniadakis
Keywords: two-sided fractional di♂erential equation, two-sided Jacobi polyfractonomial, Petrov{Galerkin method, error estimate, spectral convergence
Abstract: An open problem in the numerical solution of fractional partial differential equations(FPDEs) is how to obtain high-order accuracy for singular solutions; even for smooth right-handsides solutions of FPDEs are singular. Here, we consider the one-dimensional diffusion equation with general two-sided fractional derivative characterized by a parameter p 2 [0; 1]; for p = 1=2 we recover the Riesz fractional derivative, while for p = 1, 0 we obtain the one-sided fractional derivative. We employ a Petrov{Galerkin projection in a properly weighted Sobolev space with (two-sided) Jacobi polyfracnomials as basis and test functions. In particular, we derive these two-sided Jacobi polyfractonomials as eigenfunctions of a Sturm-Liouville problem with weights uniquely determined by the parameter p.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Numerical Analysis
Publication Identifier Type: DOI Publication Identifier: 10.1137/17M1151791
Volume: 56 Issue: 5 First Page #: 3010
Date Submitted: 8/26/21 12:00AM Date Published: 1/1/18 5:00AM
Publication Location:
Article Title: A Riesz Basis Galerkin Method for the Tempered Fractional Laplacian
Authors: Zhijiang Zhang, Weihua Deng, George Em Karniadakis
Keywords: tempered fractional Laplacian, Galerkin schemes, B-spline and Riesz basis, preconditioning
Abstract: The fractional Laplacian ??/2 is the generator of the ?-stable Levy process, which is the scaling limit of the L´evy flight. Due to the divergence of the second moment of the jump length of the Levy flight, it may not be a suitable physical model in many practical applications. However, using a parameter ? to exponentially temper the isotropic power law measure of the jump length leads to the tempered L´evy flight, which has finite second moment. For a short time the tempered Levy flight exhibits the dynamics of L´evy flight, while after a sufficiently long time it turns to normal diffusion. In the current work, we present new computational methods for the tempered fractional Laplacian equation, including the cases with the homogeneous and nonhomogeneous generalized Dirichlet type boundary conditions. We prove the well-posedness of the Galerkin weak formulation and provide convergence analysis of the single scaling B-spline and multiscale Riesz bases finite element methods.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computers & Mathematics with Applications
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.camwa.2016.11.023
Volume: 73 Issue: 6 First Page #: 1233
Date Submitted: 8/26/21 12:00AM Date Published: 3/1/17 5:00AM
Publication Location:
Article Title: A divide-and-conquer fast finite difference method for space–time fractional partial differential equation
Authors: Hongfei Fu, Michael K. Ng, Hong Wang
Keywords: Anomalous diffusion Divide-and-conquer method Finite difference method Krylov subspace iterative solver Space–time fractional partial differential equation
Abstract: We develop a fast finite difference method (FDM) for space–time FPDE: (i) We utilize the Toeplitz-like structure of the coefficient matrix to develop a matrix-free preconditioned fast Krylov subspace iterative solver to invert the coefficient matrix at each time step. (ii) We utilize a divide-and-conquer strategy, a recursive direct solver, to handle the temporal coupling of the numerical scheme. The fast method has an optimal memory requirement of O(MN) and an approximately linear computational complexity of O(NM(log N + log2 M)), without resorting to any lossy compression. Numerical experiments show the utility of the method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Fractional Calculus and Applied Analysis
Publication Identifier Type: DOI Publication Identifier: 10.1515/fca-2017-0005
Volume: 20 Issue: 1 First Page #:
Date Submitted: 8/26/21 12:00AM Date Published: 1/1/17 5:00AM
Publication Location:
Article Title: A preconditioned fast finite difference method for space-time fractional partial differential equations
Authors: Hongfei fu, Hong Wang
Keywords: anomalous di♂usion, ♀nite di♂erence method, space-time discretization, space-time fractional diffusion equation, Krylov subspace method
Abstract: We develop a fast space-time ♀nite difference method for space-time fractional diffusion equations by fully utilizing the mathematical structure of the scheme. A circulant block preconditioner is proposed to further reduce the computational costs. The method has optimal-order memory requirement and approximately linear computational complexity. The method is not lossy, as no compression of the underlying numerical scheme has been employed. Consequently, the method retains the stability, accuracy, and, in particular, the conservation property of the underlying numerical scheme. Numerical experiments are presented to show the efficiency and capacity of long time modeling of the new method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Discrete & Continuous Dynamical Systems - B
Publication Identifier Type: DOI Publication Identifier: 10.3934/dcdsb.2017178
Volume: 22 Issue: 9 First Page #: 3529
Date Submitted: 8/26/21 12:00AM Date Published:
Publication Location:
Article Title: A preconditioned fast Hermite finite element method for space-fractional diffusion equations
Authors: Meng Zhao, Aijie Cheng, Hong Wang
Keywords: Anomalous di♂usion, space-fractional di♂usion equation, hermite ♀nite element, block Toeplitz matrix, fast Fourier transform, preconditioned conjugate gradient squared method.
Abstract: We develop a fast Hermite ♀nite element method for a one-dimensional space-fractional diffusion equation, by proving that the stiffness matrix of the method can be expressed as a Toeplitz block matrix. Then a block circulant preconditioner is presented. Numerical results are presented to show the utility of the fast method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1007/s10915-016-0316-4
Volume: 71 Issue: 2 First Page #: 660
Date Submitted: 8/26/21 12:00AM Date Published: 11/1/16 4:00AM
Publication Location:
Article Title: Mixed-Type Galerkin Variational Principle and Numerical Simulation for a Generalized Nonlocal Elastic Model
Authors: Lueling Jia, Huanzhen Chen, Hong Wang
Keywords: Generalized nonlocal elastic model · Fractional derivative equation · Mixed-type variational principle · Mixed-type finite element procedure · Fast algorithm
Abstract: A mixed-type Galerkin variational principle is proposed for a generalized nonlocal elastic model. The solvability and regularity of its solution is naturally derived through the Lax–Milgram lemma, from which a solvability criterion is inferred for a Fredholm integral equation of the first kind. A mixed-type finite element procedure is therefore developed and the existence and uniqueness of the discrete solution is proved. Numerical error bounds for the unknown and the intermediate variable are proved. By carefully exploring the structure of the coefficient matrices of the numerical method, we develop a fast conjugate gradient algorithm , which reduces the computations to O(NlogN) per iteration and the memory to O(N). The use of the precondition significantly reduces the number of iterations. Numerical results show the utility of the method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computer Methods in Applied Mechanics and Engineering
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cma.2016.08.020
Volume: 311 Issue: First Page #: 280
Date Submitted: 8/26/21 12:00AM Date Published: 11/1/16 4:00AM
Publication Location:
Article Title: A fast collocation method for a static bond-based linear peridynamic model
Authors: Xuhao Zhang, Hong Wang
Keywords: Fast collocation method; Nonlocal diffusion model; Peridynamic model
Abstract: We develop a fast collocation method for a steady-state bond-based linear peridynamic model in two space dimensions. The method reduces the computational work from O(N2) per Krylov subspace iteration in a traditional collocation method toO(N log N) and the memory requirement from O(N2) in a collocation method to O (N), where N is the number of unknowns in the discrete system. Furthermore, the method reduces the computational work of evaluating and assembling the stiffness matrix, which often constitutes a major portion of the overall computational work, from O(N2) in a collocation method to O(N). The significant reduction of the CPU times and storage in the fast collocation method is achieved by carefully exploring the structure of the stiffness matrix of the collocation method without any lossy compression involved. In other words, the fast method is evaluated in an equivalent but more efficient manner.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2016.11.003
Volume: 330 Issue: First Page #: 114
Date Submitted: 8/26/21 12:00AM Date Published: 2/1/17 5:00AM
Publication Location:
Article Title: A fast collocation method for a variable-coefficient nonlocal diffusion model
Authors: Che Wang, Hong Wang
Keywords: Fast collocation method Fractional diffusion equation Nonlocal diffusion model Nonlocal model
Abstract: We develop a fast collocation scheme for a variable-coefficient nonlocal diffusion model, for which a numerical discretization would yield a dense stiffness matrix. The development of the fast method is achieved by carefully handling the variable coefficients appearing inside the singular integral operator and exploiting the structure of the dense stiffness matrix. The resulting fast method reduces the computational work from O(N3) required by a commonly used direct solver to O(NlogN)per iteration and the memory requirement from O(N2)to O (N). Furthermore, the fast method reduces the computational work of assembling the stiffness matrix from O(N2)to O(N). Numerical results are presented to show the utility of the fast method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computers & Mathematics with Applications
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.camwa.2017.02.008
Volume: 73 Issue: 7 First Page #: 1546
Date Submitted: 8/26/21 12:00AM Date Published: 4/1/17 4:00AM
Publication Location:
Article Title: An hp-Galerkin method with fast solution for linear peridynamic models in one dimension
Authors: Zhengguang Liu, Aijie Cheng, Hong Wang
Keywords: Galerkin methods Peridynamic model Toeplitz matrix Fast Fourier transform hp-Galerkin method
Abstract: In this paper, fast Galerkin and hp-Galerkin finite element methods are introduced and analyzed to solve a steady-state peridynamic model. We present a fast solution technique to accelerate non-square Toeplitz matrix–vector multiplications arising from piecewise-linear, piecewise-quadratic and piecewise-cubic Galerkin methods. This fast solution technique is based on a fast Fourier transform and depends on the special structure of coefficient matrices, and it helps to reduce the computational work from O(N3) required by traditional methods to O(Nlog2N) and the memory requirement from O(N2) to O(N) without using any lossy compression, where N is the number of unknowns. The peridynamic model admits solutions having jump discontinuities. For problems with discontinuous solutions, we therefore introduce a piecewise-constant Galerkin method and give an h- and p-refinement algorithm.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1007/s10915-017-0478-8
Volume: 74 Issue: 2 First Page #: 1009
Date Submitted: 8/26/21 12:00AM Date Published: 6/1/17 4:00AM
Publication Location:
Article Title: A Fast Finite Difference Method for Three-Dimensional Time-Dependent Space-Fractional Diffusion Equations with Fractional Derivative Boundary Conditions
Authors: Meng Zhao, Hong Wang, Aijie Cheng
Keywords: Anomalous diffusion · Finite difference method · Fractional derivative boundary condition · Space-fractional diffusion equation · Stability and convergence analysis · Maximum-minimum principle · Toeplitz matrix
Abstract: We develop a fast finite difference method for time-dependent variable-coefficient space-fractional diffusion equations with fractional derivative boundary-value conditions in three-dimensional spaces. Fractional differential operators appear in both the equation and the boundary conditions. Because of the nonlocal nature of the fractional Neumann boundary operator, the internal and boundary nodes are strongly coupled together in the coupled linear system. The stability and convergence of the finite difference method are discussed. For the implementation, the development of the fast method is based upon a careful analysis and delicate decomposition of the structure of the coefficient matrix. The fast method has approximately linear computational complexity perKrylov subspace iteration and an optimal order memory requirement. Numerical results are presented to show the utility of the method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Mathematical Methods in the Applied Sciences
Publication Identifier Type: DOI Publication Identifier: 10.1002/mma.4367
Volume: 40 Issue: 14 First Page #: 5018
Date Submitted: 8/27/21 12:00AM Date Published: 2/1/17 5:00AM
Publication Location:
Article Title: A mixed-type Galerkin variational formulation and fast algorithms for variable-coefficient fractional diffusion equations
Authors: Yongshan Li, Huanzhen Chen, Hong Wang
Keywords: mixed-type Galerkin variational formulation; fractional diffusion equation; finite element; solvability; error bounds; fast algorithm
Abstract: We consider the variable-coefficient fractional diffusion equations with two-sided fractional derivative. By introducing an intermediate variable, we propose a mixed-type Galerkin variational formulation and prove the existence and uniqueness of the variational solution. On the basis of the formulation, we develop a mixed-type finite element procedure on commonly used finite element spaces and derive the solvability of the finite element solution and the error bounds for the unknown and the intermediate variable. For the Toeplitz-like linear system generated by discretization, we design a fast conjugate gradient normal residual method to reduce storage and computing cost. Numerical experiments are included to verify our theoretical findings.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Chaos, Solitons & Fractals
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.chaos.2017.04.042
Volume: 102 Issue: First Page #: 473
Date Submitted: 8/27/21 12:00AM Date Published: 9/1/17 4:00AM
Publication Location:
Article Title: A variable-order fractional differential equation model of shape memory polymers
Authors: Zheng Li, Hong Wang, Rui Xiao, Su Yang
Keywords: Variable-order fractional differential equation Shape-memory polymer Parameter identification
Abstract: A shape-memory polymer (SMP) is capable of memorizing its original shape, and can acquire a temporary shape upon deformation and returns to its permanent shape in response to an external stimulus such as a temperature change. SMPs have been widely used industrial and medical applications. Previously, differential equation models were developed to describe SMPs and their applications. However, these models are often of very complicated form, which require accurate numerical simulations. In this paper we argue that a variable-order fractional differential equation model of the shape-memory behavior is more suitable than constant-order fractional differential equation models in terms of modeling the memory behavior of SMPs. We develop a numerical method to simulate the variable-order model and, in particular, to identify the unknown variable order of the model. Numerical experiments are presented to show the utility of the method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1007/s10915-017-0433-8
Volume: 74 Issue: 1 First Page #: 220
Date Submitted: 8/27/21 12:00AM Date Published: 4/1/17 4:00AM
Publication Location:
Article Title: POD/DEIM Reduced-Order Modeling of Time-Fractional Partial Differential Equations with Applications in Parameter Identification
Authors: Hongfei Fu, Hong Wang, Zhu Wang
Keywords: Time-fractional partial differential equations · Proper orthogonal decomposition · Discrete empirical interpolation method · Reduced-order model · Parameter identification
Abstract: In this paper, a reduced-order model (ROM) based on the proper orthogonal decomposition and the discrete empirical interpolation method is proposed for efficiently simulating time-fractional partial differential equations (TFPDEs). Both linear and nonlinear equations are considered.We demonstrate the effectiveness of the ROMby several numerical examples, in which the ROMachieves the same accuracy of the full-ordermodel (FOM) over a long-term simulation while greatly reducing the computational cost. The proposed ROM is then regarded as a surrogate of FOM and is applied to an inverse problem for identifying the order of the time-fractional derivative of the TFPDE model. Based on the Levenberg– Marquardt regularization iterative method with the Armijo rule, we develop a ROM-based algorithm for solving the inverse problem. For cases in which the observation data is either uncontaminated or contaminated by random noise, the proposed approach is able to achieve accurate parameter estimation.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2017.06.036
Volume: 347 Issue: First Page #: 20
Date Submitted: 8/27/21 12:00AM Date Published: 10/1/17 4:00AM
Publication Location:
Article Title: A space–time fractional phase-field model with tunable sharpness and decay behavior and its efficient numerical simulation
Authors: Zheng Li, Hong Wang, Danping Yang
Keywords: Fast solution method Fractional partial differential equation Fractional phase-field model Tunable decay behavior Tunable sharpness
Abstract: We present a space–time fractional Allen–Cahn phase-field model that describes the transport of the fluid mixture of two immiscible fluid phases. The space and time fractional order parameters control the sharpness and the decay behavior of the interface via a seamless transition of the parameters. Although they are shown to provide more accurate description of anomalous diffusion processes and sharper interfaces than traditional integer-order phase-field models do, fractional models yield numerical methods with dense stiffness matrices. Consequently, the resulting numerical schemes have significantly increased computational work and memory requirement. We develop a lossless fast numerical method for the accurate and efficient numerical simulation of the space–time fractional phase-field model. Numerical experiments shows the utility of the fractional phase-field model and the corresponding fast numerical method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computers & Mathematics with Applications
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.camwa.2017.09.003
Volume: 75 Issue: 6 First Page #: 2031
Date Submitted: 8/27/21 12:00AM Date Published: 3/1/18 5:00AM
Publication Location:
Article Title: A fast finite difference method for distributed-order space-fractional partial differential equations on convex domains
Authors: Jinhong Jia, Hong Wang
Keywords: Finite difference method for fractional differential equation on convex domain Multi-term fractional differential equation Distributed-order fractional differential equation
Abstract: Fast numerical methods were previously developed for space-fractional PDEs on multidimensional rectangular domains, without resorting to lossy compression, but rather, via the exploration of the tensor-product form of the Toeplitz-like decompositions of the stiffness matrices. In this paper, we develop a fast finite difference method for distributed order space-fractional PDEs on a general convex domain in multiple space dimensions. The fast method has an optimal order storage requirement and almost linear computational complexity, without any lossy compression. Numerical experiments show the utility of the method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2018.01.002
Volume: 373 Issue: First Page #: 1000
Date Submitted: 8/27/21 12:00AM Date Published: 11/1/18 4:00AM
Publication Location:
Article Title: An integrated fractional partial differential equation and molecular dynamics model of anomalously diffusive transport in heterogeneous nano-pore structures
Authors: Meng Zhao, Shuai He, Hong Wang, Guan Qin
Keywords: Anomalous diffusive transport Fractional partial differential equation Molecular dynamics simulation Multiscale model Nano-scale porous material Upscaling
Abstract: Fluid flows confined in nano-pore structures exhibit physical behaviors that are not observed in large-scale structures. Molecular dynamics simulation has been used for modeling nano-scale fluid flows at nanoscale, but is deemed to be computationally very expensive and is often limited to problems with simple geometry. We develop an integrated fractional partial differential equation and molecular dynamics upscaling modeling of anomalously diffusive transport in heterogeneous nano-pore structures, which has a significantly improved computational efficiency and memory requirement over the molecular dynamics simulation. Representative applications demonstrate the usage of the new model, which takes the model a few hours on a laptop that would otherwise require a molecular dynamics simulation in the matter of at least 100 years of CPU time on a parallel computer.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Numerical Analysis
Publication Identifier Type: DOI Publication Identifier: 10.1137/17M1118245
Volume: 56 Issue: 6 First Page #: 3249
Date Submitted: 8/27/21 12:00AM Date Published: 1/1/18 5:00AM
Publication Location:
Article Title: Time Discretization of a Tempered Fractional Feynman--Kac Equation with Measure Data
Authors: Weihua Deng, Buyang Li, Zhi Qian, Hong Wang
Keywords: tempered fractional operators, Feynmann-Kac equation, integral representation, convolution quadrature, convergence
Abstract: A feasible approach to study tempered anomalous dynamics is to analyze its functional distribution, which is governed by the tempered fractional Feynman-Kac equation. The main challenges of numerically solving the equation come from the time-space coupled nonlocal operators and the complex parameters involved. In this work, we introduce an efficient time-stepping method to discretize the tempered fractional Feynman{Kac equation by using the Laplace transform representation of convolution quadrature. Rigorous error estimate for the discrete solutions is carried out in the measure norm. Numerical experiments are provided to support the theoretical results.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Discrete & Continuous Dynamical Systems - B
Publication Identifier Type: DOI Publication Identifier: 10.3934/dcdsb.2017016
Volume: 22 Issue: 2 First Page #: 339
Date Submitted: 8/27/21 12:00AM Date Published:
Publication Location:
Article Title: Analysis of a nonlocal-in-time parabolic equation
Authors: Qiang Du, Jiang Yang, Zhi Zhou
Keywords: Nonlocal-in-time parabolic equation, nonlocal initial value problem, well-posedness, smoothing property, localization, Galerkin ♀nite element method, error estimates.
Abstract: In this paper, we consider an initial boundary value problem for nonlocal-in-time parabolic equations involving a nonlocal in time derivative. We fi♀rst show the uniqueness and existence of the weak solution of the nonlocal-in-time parabolic equation, and also the spatial smoothing properties. More- over, we develop a new framework to study the local limit of the nonlocal model as the horizon parameter approaches 0. Exploiting the spatial smoothing properties, we develop a semi-discrete scheme using standard Galerkin ♀nite element method for the spatial discretization, and derive error estimates dependent on data smoothness. Finally, extensive numerical results are presented to illustrate our theoretical fi♀ndings.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Discrete & Continuous Dynamical Systems - B
Publication Identifier Type: DOI Publication Identifier: 10.3934/dcdsb.2018110
Volume: 24 Issue: 1 First Page #: 231
Date Submitted: 8/27/21 12:00AM Date Published:
Publication Location:
Article Title: A comparative study on nonlocal diffusion operators related to the fractional Laplacian
Authors: Siwei Duo, Hong Wang, Yanzhi Zhang
Keywords: Fractional Laplacian; spectral fractional Laplacian; regional fractional Laplacian; peridynamic operator; extended homogeneous Dirichlet boundary condition; fractional Poisson equation.
Abstract: In this paper, we study four nonlocal diffusion operators, including the fractional Laplacian, spectral fractional Laplacian, regional fractional Laplacian, and peridynamic operator. These operators represent the infinitesimal generators of different stochastic processes, and especially their differences on a bounded domain are significant. We provide extensive numerical experiments to understand and compare their differences. We find that these four operators collapse to the classical Laplace operator. The eigenvalues and eigenfunctions of these four operators are different, and the k-th (for k 2 N) eigenvalue of the spectral fractional Laplacian is always larger than those of the fractional Laplacian and regional fractional Laplacian. The peridynamic operator can provide a good approximation to the fractional Laplacian, if the horizon size is sufficiently large. We find that the solution of the peridynamic model converges to that of the fractional Laplacian model.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Fractional Calculus and Applied Analysis
Publication Identifier Type: DOI Publication Identifier: 10.1515/fca-2017-0072
Volume: 20 Issue: 6 First Page #: 1356
Date Submitted: 8/27/21 12:00AM Date Published: 12/1/17 5:00AM
Publication Location:
Article Title: Wellposedness of Neumann boundary-value problems of space-fractional differential equations
Authors: Hong Wang, Danping Yang
Keywords: fractional differential equation, Neumann boundary value problem, wellposedness
Abstract: We conduct preliminary mathematical analysis of the wellposedness of different Neumann boundary-value problems of the FDEs. We prove that five out of the nine combinations of three different forms of FDEs that are closed by three types of Neumann boundary conditions are well posed and the remaining four do not admit a solution. In particular, for each form of the FDE there is at least one type of Neumann boundary condition such that the corresponding boundary-value problem is well posed, but there is also at least one type of Neumann boundary condition such that the corresponding boundary-value problem is ill posed. This fully demonstrates the subtlety of the study of FDE.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Chaos, Solitons & Fractals
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.chaos.2017.03.061
Volume: 102 Issue: First Page #: 361
Date Submitted: 8/27/21 12:00AM Date Published: 9/1/17 4:00AM
Publication Location:
Article Title: Asymptotically compatible schemes for space-time nonlocal diffusion equations
Authors: An Chen, Qiang Du, Changpin Li, Zhi Zhou
Keywords: Space-time nonlocal equation Well-posedness Local limit Fourier spectral method Quadrature-based finite difference Asymptotically compatibility
Abstract: In this paper, we study a space-time nonlocal diffusion model that reduces to the classical diffusion equation in the local limit. Firstly, we show the uniqueness and existence of the weak solution of the nonlocal model, and study the local limit of the nonlocal model as horizon parameters approach zero. Particularly, it is shown that the convergence is uniform at a rate of O (?+ ?2) , under certain regularity assumptions on initial and source data. Next we propose a fully discrete scheme, by exploiting the quadrature-based finite difference method in time and the Fourier spectral method in space, and show its stability. The nu- merical scheme is proved to be asymptotically compatible so that it preserves the local limiting behavior at the discrete level. Numerical experiments are provided to illustrate the theoretical results.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Communications in Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.4208/cicp.OA-2016-0033
Volume: 21 Issue: 1 First Page #: 16
Date Submitted: 8/27/21 12:00AM Date Published: 12/1/16 5:00AM
Publication Location:
Article Title: Artificial Boundary Conditions for Nonlocal Heat Equations on Unbounded Domain
Authors: Wei Zhang, Jiang Yang, Jiwei Zhang, Qiang Du
Keywords: Artificial boundary conditions, nonlocal models, Pad´e approximation, nonlocal heat equations, artificial boundary method.
Abstract: This paper is concerned with numerical approximations of a nonlocal heat equation define on an infinite domain. Two classes of artificial boundary conditions (ABCs) are designed, namely, nonlocal analog Dirichlet-to-Neumann-type ABCs (global in time) and high-order Pad´e approximate ABCs (local in time). These ABCs reformulate the original problem into an initial-boundary-value (IBV) problem on a bounded domain. For the global ABCs, we adopt a fast evolution to enhance computational efficiency and reduce memory storage. High order fully discrete schemes, both second-order in time and space, are given to discretize two reduced problems. Extensive numerical experiments are carried out to show the accuracy and efficiency of the proposed methods.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2016.11.028
Volume: 332 Issue: First Page #: 118
Date Submitted: 8/27/21 12:00AM Date Published: 3/1/17 5:00AM
Publication Location:
Article Title: Fast and accurate implementation of Fourier spectral approximations of nonlocal diffusion operators and its applications
Authors: Qiang Du, Jiang Yang
Keywords: Nonlocal diffusion operator Peridynamic operator Fourier spectral method Nonlocal Allen–Cahn equation Nonlocal Cahn–Hilliard equation Nonlocal phase-field crystal model
Abstract: This work is concerned with the Fourier spectral approximation of various integral differential equations associated with some linear nonlocal diffusion and peridynamic operators under periodic boundary conditions. For radially symmetric kernels, the nonlocal operators under consideration are diagonalizable in the Fourier space so that the main computational challenge is on the accurate and fast evaluation of their eigenvalues or Fourier symbols consisting of possibly singular and highly oscillatory integrals. For a large class of fractional power-like kernels, we propose a new approach based on reformulating the Fourier symbols both as coefficients of a series expansion and solutions of some simple ODE models. We then propose a hybrid algorithm that utilizes both truncated series expansions and high order Runge–Kutta ODE solvers to provide fast evaluation of Fourier symbols in both one and higher dimensional spaces.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Numerical Analysis
Publication Identifier Type: DOI Publication Identifier: 10.1137/15M1039857
Volume: 54 Issue: 3 First Page #: 1899
Date Submitted: 8/27/21 12:00AM Date Published: 1/1/16 5:00AM
Publication Location:
Article Title: Asymptotically Compatible Fourier Spectral Approximations of Nonlocal Allen--Cahn Equations
Authors: Qiang Du, Jiang Yang
Keywords: asymptotically compatible schemes, nonlocal models, Fourier spectral methods, nonlocal Allen–Cahn equations, error estimates
Abstract: We study Fourier spectral approximations of a nonlocal Allen–Cahn (NAC) equation that reduces to the conventional Allen–Cahn equation in the local limit. We show that the Fourier spectral methods are asymptotically compatible in the sense that they provide convergent approximations to both nonlocal and local models. Furthermore, we provide various error estimates. In particular, it is shown that the numerical solutions of nonlocal models converge to those of the corresponding local models uniformly at a rate of O(?2). This is achieved by first establishing a similar result for linear nonlocal diffusion equations. A careful investigation, both analytically and computationally, is made of the steady state solutions of NAC equations, demonstrating how discontinuities may appear in solutions and how they are related to model parameters.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Communications on Applied Mathematics and Computation
Publication Identifier Type: DOI Publication Identifier: 10.1007/s42967-019-0008-9
Volume: 1 Issue: 1 First Page #: 5
Date Submitted: 8/27/21 12:00AM Date Published: 3/1/19 5:00AM
Publication Location:
Article Title: Analysis and Approximation of Gradient Flows Associated with a Fractional Order Gross–Pitaevskii Free Energy
Authors: Mark Ainsworth, Zhiping Mao
Keywords: Fractional differential equation · Non-local energy · Well-posedness · Fourier spectral method
Abstract: We establish the well-posedness of the fractional PDE which arises by considering the gradient flow associated with a fractional Gross–Pitaevskii free energy functional and some basic properties of the solution. The equation reduces to the Allen–Cahn or Cahn–Hilliard equations in the case where the mass tends to zero and an integer order derivative is used in the energy. We study how the presence of a non-zero mass affects the nature of the solutions compared with the Cahn–Hilliard case. In particular, we show that, analogous to the Cahn–Hilliard case, the solutions consist of regions in which the solution is a piecewise constant (whose value depends on the mass and the fractional order) separated by an interface whose width is independent of the mass and the fractional derivative. However, if the average value of the initial data exceeds some threshold (which we determine explicitly), then the solution will tend to a single constant steady state.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computer Methods in Applied Mechanics and Engineering
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cma.2017.08.019
Volume: 327 Issue: First Page #: 4
Date Submitted: 8/27/21 12:00AM Date Published: 12/1/17 5:00AM
Publication Location:
Article Title: Aspects of an adaptive finite element method for the fractional Laplacian: A priori and a posteriori error estimates, efficient implementation and multigrid solver
Authors: Mark Ainsworth, Christian Glusa
Keywords: Non-local equations; Fractional Laplacian; Adaptive refinement
Abstract: We develop all of the components needed to construct an adaptive finite element code that can be used to approximate fractional partial differential equations, on non-trivial domains in d ? 1 dimensions. Our main approach consists of taking tools that have been shown to be effective for adaptive boundary element methods and, where necessary, modifying them so that they can be applied to the fractional PDE case. Improved a priori error estimates are derived for the case of quasi-uniform meshes which are seen to deliver sub-optimal rates of convergence owing to the presence of singularities. Attention is then turned to the development of an a posteriori error estimate and error indicators which are suitable for driving an adaptive refinement procedure. We assume that the resulting refined meshes are locally quasi-uniform and develop efficient methods for the assembly of the resulting linear algebraic systems and their solution using iterative methods, including the multigrid method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: International Journal of Numerical Analysis and Modeling
Publication Identifier Type: Publication Identifier:
Volume: 15 Issue: First Page #: 213
Date Submitted: 9/7/22 12:00AM Date Published: 3/13/17 7:58PM
Publication Location:
Article Title: UNIFORM Lp-BOUND OF THE ALLEN–CAHN EQUATION AND ITS NUMERICAL DISCRETIZATION
Authors: JIANG YANG, QIANG DU, AND WEI ZHANG
Keywords: Allen–Cahn Equations, maximum principle, operator splitting, uniform Lp-bound, Fourier spectral methods.
Abstract: Extensive experimental evidence highlight that scalar turbulence exhibits anomalous diffusion and stronger intermittency levels at small scales compared to that in fluid turbulence. This renders the corresponding subgrid-scale dynamics modeling for scalar turbulence a greater challenge to date. We develop a new large eddy simulation (LES) paradigm for efficiently and dynamically nonlocal LES modeling of the scalar turbulence. To this end, we formulate the underlying nonlocal model starting from the filtered Boltzmann kinetic transport equation, where the divergence of subgrid-scale scalar fluxes emerges as a fractional-order Laplacian term in the filtered advection-diffusion model, coding the corresponding supper-diffusive nature of scalar turbulence. Subsequently, we develop a robust data-driven algorithm for estimation of the fractional (non-integer) Laplacian exponent, where we on-the-fly calculate the corresponding model coefficient employing a new dynamic procedure. Our a priori t
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1137/17M1144696
Volume: 40 Issue: 4 First Page #:
Date Submitted: 8/27/21 12:00AM Date Published: 1/1/18 5:00AM
Publication Location:
Article Title: Hybrid Finite Element--Spectral Method for the Fractional Laplacian: Approximation Theory and Efficient Solver
Authors: Mark Ainsworth, Christian Glusa
Keywords: fractional laplacian, ♀nite element-spectral method, numerical approximation
Abstract: A numerical scheme is presented for approximating fractional order Poisson problems in two and three dimensions. We derive an a priori error estimate which takes account of the error arising from using an approximation in place of the true eigenvalues. We further present a strategy for choosing approximations of the eigenvalues based on Weyl's law and ♀nite element discretizations of the eigenvalue problem. The system of linear algebraic equations arising from the hybrid FEM-spectral scheme is decomposed into blocks which can be solved effectively using standard iterative solvers such as multigrid and conjugate gradient. Numerical examples in two and three dimensions suggest that the approach is quasi-optimal in terms of complexity.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: SIAM Journal on Numerical Analysis
Publication Identifier Type: DOI Publication Identifier: 10.1137/16M1075302
Volume: 55 Issue: 4 First Page #: 1689
Date Submitted: 8/27/21 12:00AM Date Published: 1/1/17 5:00AM
Publication Location:
Article Title: Analysis and Approximation of a Fractional Cahn--Hilliard Equation
Authors: Mark Ainsworth, Zhiping Mao
Keywords: fractional Cahn-Hilliard equation, mass conservation, stability, L1 boundedness, Fourier spectral method, error estimates
Abstract: We derive a fractional Cahn-Hilliard equation (FCHE) by considering a gradient flow in the negative order Sobolev space. The existence of a unique solution is established and it is shown that the equation preserves mass for all positive values of fractional order and that it indeed reduces the free energy. We are able to show that the Fourier{Galerkin method delivers a spectral rate of convergence for the FCHE in the case of a semidiscrete approximation scheme. Finally, we present results obtained using computational simulation of the FCHE for a variety of choices of fractional order. An examination of the coarsening rates of the FCHE reveals that the asymptotic rate is rather insensitive to the value and, as a consequence, is close to the well-established rate observed for the classical Cahn{Hilliard equation.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Chaos, Solitons & Fractals
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.chaos.2017.05.022
Volume: 102 Issue: First Page #: 264
Date Submitted: 8/27/21 12:00AM Date Published: 9/1/17 4:00AM
Publication Location:
Article Title: Well-posedness of the Cahn–Hilliard equation with fractional free energy and its Fourier Galerkin approximation
Authors: Mark Ainsworth, Zhiping Mao
Keywords: Fractional Cahn–Hilliard equation Non-local energy Well-posedness Fourier spectral method Error estimates
Abstract: We study the well-posedness of the Cahn–Hilliard equation in which the gradient term in the free energy is replaced by a fractional derivative. We begin by establishing the existence and uniqueness of a Fourier-Galerkin approximation and then derive a number of priori estimates for the Fourier-Galerkin scheme. Compactness arguments are then used to deduce the existence and uniqueness of the solution to the fractional Cahn–Hilliard equation. An estimate for the rate of convergence of the Fourier-Galerkin approximation is then obtained. Finally, we present some numerical illustrations of typical solutions to the fractional Cahn–Hilliard equation and how they vary with the fractional order ?and the parameter ?. In particular, we show how the width ? of the diffuse interface depends on ?and ?, and derive the scaling law ?= O (? 1 /?) which is verified numerically.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Scientific Computing
Publication Identifier Type: DOI Publication Identifier: 10.1007/s10915-018-0800-0
Volume: 78 Issue: 2 First Page #: 1087
Date Submitted: 8/27/21 12:00AM Date Published: 8/1/18 4:00AM
Publication Location:
Article Title: Error Estimates of Spectral Galerkin Methods for a Linear Fractional Reaction–Diffusion Equation
Authors: Zhongqiang Zhang
Keywords: Regularity · Weighted spaces · Optimal error estimate · Spectral methods · Fractional Laplacian
Abstract: We consider a fractional diffusion equation with a reaction term in one dimensional space. We first establish the regularity in weighted Sobolev spaces. Thenwe present an optimal error estimate for a spectral Galerkin method for the equation and a sub-optimal error estimate for a spectral Petrov–Galerkin method. Numerical results suggest that the convergence order in a weighted L2-norm is 2? + 1 for smooth inputs where ? is the order of the fractional Laplacian.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computers & Mathematics with Applications
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.camwa.2016.07.026
Volume: 73 Issue: 6 First Page #: 892
Date Submitted: 8/27/21 12:00AM Date Published: 3/1/17 5:00AM
Publication Location:
Article Title: Applications of inverse tempered stable subordinators
Authors: Mahmoud S. Alrawashdeh, James F. Kelly, Mark M. Meerschaert, Hans-Peter Scheffler
Keywords: Inverse subordinator Poisson process Tempered stable Cauchy problem Fractional calculus
Abstract: The inverse tempered stable subordinator is a stochastic process that models power law waiting times between particle movements, with an exponential tempering that allows all moments to exist. This paper shows that the probability density function of an inverse tempered stable subordinator solves a tempered time-fractional diffusion equation, and its ‘‘folded’’ density solves a tempered time-fractional telegraph equation. Two explicit formulae for the density function are developed, and applied to compute explicit solutions to tempered fractional Cauchy problems, where a tempered fractional derivative replaces the first derivative in time. Several examples are given, including tempered fractional diffusion equations on bounded or unbounded domains, and the probability distribution of a tempered fractional Poisson process. It is shown that solutions to the tempered fractional diffusion equation have a cusp at the origin.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Mathematical Analysis and Applications
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jmaa.2016.11.055
Volume: 448 Issue: 2 First Page #: 1450
Date Submitted: 8/27/21 12:00AM Date Published: 4/1/17 4:00AM
Publication Location:
Article Title: Exponents of operator self-similar random fields
Authors: Gustavo Didier, Mark M. Meerschaert, Vladas Pipiras
Keywords: Operator self-similar random fields Gaussian random fields Operator scaling Operator self-similarity Anisotropy
Abstract: If X(cEt) and cHX(t) have the same finite-dimensional distributions for some pair of linear operators E and H, we say that the random vector field X(t) is operator self-similar. The exponents E and H are not unique in general, due to symmetry. This paper characterizes the possible set of range exponents H for a given domain exponent, and conversely, the set of domain exponents E for a given range exponent.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Water Resources Research
Publication Identifier Type: DOI Publication Identifier: 10.1002/2015WR018515
Volume: 52 Issue: 4 First Page #: 2462
Date Submitted: 8/27/21 12:00AM Date Published: 4/1/16 4:00AM
Publication Location:
Article Title: Backward fractional advection dispersion model for contaminant source prediction
Authors: Yong Zhang, Mark M. Meerschaert, Roseanna M. Neupauer
Keywords: Stable process · Fractional calculus · Long-range dependence · Local times · Sample paths · Local nondeterminism
Abstract: Tempered fractional stable motion adds an exponential tempering to the power-law kernel in a linear fractional stable motion, or a shift to the power-law filter in a harmonizable fractional stable motion. Increments from a stationary time series that can exhibit semi-long-range dependence. This paper develops the basic theory of tempered fractional stable processes, including dependence structure, sample path behavior, local times, and local nondeterminism.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Vibration and Control
Publication Identifier Type: DOI Publication Identifier: 10.1177/1077546314568696
Volume: 22 Issue: 9 First Page #: 2211
Date Submitted: 8/27/21 12:00AM Date Published: 2/1/15 5:00AM
Publication Location:
Article Title: Anisotropic fractional diffusion tensor imaging
Authors: Mark M Meerschaert, Richard L Magin, Allen Q Ye
Keywords: Diffusion tensor imaging, anomalous diffusion, fractional calculus, anisotropy, magnetic resonance imaging
Abstract: Traditional diffusion tensor imaging (DTI) maps brain structure by fitting a diffusion model to the magnitude of the electrical signal acquired in magnetic resonance imaging (MRI). Fractional DTI employs anomalous diffusion models to obtain a better fit to real MRI data, which can exhibit anomalous diffusion in both time and space. In this paper, we describe the challenge of developing and employing anisotropic fractional diffusion models for DTI. Since anisotropy is clearly present in the three-dimensional MRI signal response, such models hold great promise for improving brain imaging. We then propose some candidate models, based on stochastic theory.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Theoretical Probability
Publication Identifier Type: DOI Publication Identifier: 10.1007/s10959-016-0720-6
Volume: 31 Issue: 1 First Page #: 598
Date Submitted: 8/27/21 12:00AM Date Published: 11/1/16 4:00AM
Publication Location:
Article Title: Asymptotic Behavior of Semistable Lévy Exponents and Applications to Fractal Path Properties
Authors: Peter Kern, Mark M. Meerschaert, Yimin Xiao
Keywords: Lévy exponent · Operator semistable process · Semi-selfsimilarity · Hausdorff dimension · Packing dimension · Range · Graph · Multiple points · Recurrence · Transience Mathematics Subject Classification
Abstract: This paper proves sharp bounds on the tails of the Lévy exponent of an operator semistable law on Rd . These bounds are then applied to explicitly compute the Hausdorff and packing dimensions of the range, graph, and other random sets describing the sample paths of the corresponding operator semi-selfsimilar Lévy processes. The proofs are elementary, using only the properties of the Lévy exponent, and certain index formulae.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Water Resources Research
Publication Identifier Type: DOI Publication Identifier: 10.1002/2016WR019748
Volume: 53 Issue: 3 First Page #: 2559
Date Submitted: 8/27/21 12:00AM Date Published: 3/1/17 5:00AM
Publication Location:
Article Title: FracFit: A robust parameter estimation tool for fractional calculus models
Authors: James F. Kelly, Diogo Bolster, Mark M. Meerschaert, Jennifer D. Drummond, Aaron I. Packman
Keywords: FracFit is a parameter estimation tool based on four space-fractional and time-fractional models used by the hydrology community ┐ Parameter estimates are extracted from measured breakthrough curves using a weighted nonlinear least squares algorithm ┐ Future models may be implemented within the framework, allowing intercomparison of models
Abstract: Anomalous transport cannot be adequately described with classical Fickian advection-dispersion equations (ADE) with constant coefficients. Rather, fractional calculus models may be used, which capture salient features of anomalous transport (e.g., skewness and power law tails). FracFit is a parameter estimation tool based on space-fractional and time-fractional models used by the hydrology community. Currently, four fractional models are supported: 1) space-fractional advection-dispersion equation (sFADE), 2) time-fractional dispersion equation with drift (TFDE), 3) fractional mobile-immobile (FMIM) equation, and 4) temporally tempered Levy motion (TTLM). Model solutions using pulse initial conditions and continuous injections are evaluated using stable distributions or subordination integrals. Parameter estimates are extracted from measured breakthrough curves (BTCs) using a weighted nonlinear least squares (WNLS) algorithm.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Water Resources Research
Publication Identifier Type: DOI Publication Identifier: 10.1002/2016WR019668
Volume: 53 Issue: 4 First Page #: 3464
Date Submitted: 8/27/21 12:00AM Date Published: 4/1/17 4:00AM
Publication Location:
Article Title: Space?time duality for the fractional advection?dispersion equation
Authors: James F. Kelly, Mark M. Meerschaert
Keywords: The space-fractional advectiondispersion equation models anomalous transport in rivers with a space fractional derivative. Space-fractional models are mathematically equivalent to a corresponding time-fractional model . This equivalence resolves a controversy in the hydrological literature
Abstract: The fractional advection-dispersion equation replaces the second spatial derivative in the usual advection-dispersion equation with a fractional derivative in the spatial variable. It was first applied to tracer tests in underground aquifers, and later to tracer tests in rivers. An alternative model replaces the first time derivative with a fractional derivative in time. Previous work has shown that both models provide a reasonable fit to breakthrough curves in rivers, which has led to a controversy regarding the physically appropriate fractional model. This paper shows that the relevant space-fractional model is mathematically equivalent to the corresponding time-fractional model, thus resolving the controversy.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Stochastic Processes and their Applications
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.spa.2018.08.004
Volume: 129 Issue: 8 First Page #: 2850
Date Submitted: 8/27/21 12:00AM Date Published: 8/1/19 4:00AM
Publication Location:
Article Title: Relaxation patterns and semi-Markov dynamics
Authors: Mark M. Meerschaert, Bruno Toaldo
Keywords: Relaxation; Fractional calculus; Bernstein function; Semi-Markov process; Continuous time random walk; Semigroup
Abstract: Exponential relaxation to equilibrium is a typical property of physical systems, but inhomogeneities are known to distort the exponential relaxation curve, leading to a wide variety of relaxation patterns. Power law relaxation is related to fractional derivatives in the time variable. More general relaxation patterns are considered here, and the corresponding semi-Markov processes are studied. Our method, based on Bernstein functions, unifies three different approaches in the literature.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Mathematische Nachrichten
Publication Identifier Type: DOI Publication Identifier: 10.1002/mana.201700111
Volume: 291 Issue: First Page #: 2516
Date Submitted: 8/27/21 12:00AM Date Published: 8/1/18 4:00AM
Publication Location:
Article Title: Space-time fractional Dirichlet problems
Authors: Boris Baeumer, Tomasz Luks, Mark M. Meerschaert
Keywords: bounded domain, fractional Cauchy problem, infinitesimal generator, killed Feller process
Abstract: This paper establishes explicit solutions for fractional diffusion problems on bounded domains. It also gives stochastic solutions, in terms of Markov processes time-changed by an inverse stable subordinator whose index equals the order of the fractional time derivative. Some applications are given, to demonstrate how to specify a well-posed Dirichlet problem for space-time fractional diffusions in one or several variables. This solves an open problem in numerical analysis.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Stochastic Processes and their Applications
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.spa.2017.04.003
Volume: 128 Issue: 1 First Page #: 39
Date Submitted: 8/27/21 12:00AM Date Published: 1/1/18 5:00AM
Publication Location:
Article Title: Domain and range symmetries of operator fractional Brownian fields
Authors: Gustavo Didier, Mark M. Meerschaert, Vladas Pipiras
Keywords: Operator fractional Brownian field; Symmetry group; Anisotropy; Operator scaling; Operator self-similarity; Long range dependence
Abstract: An operator fractional Brownian field (OFBF) is a Gaussian, stationary increment Rn-valued random field on Rm that satisfies the operator self-similarity property {X(cE t)}t?Rm L={cH X(t)}t?Rm , c > 0, for two matrix exponents (E, H). In this paper, we characterize the domain and range symmetries of OFBF, respectively, as maximal groups with respect to equivalence classes generated by orbits and, based on a new anisotropic polar-harmonizable representation of OFBF, as intersections of centralizers. We also describe the sets of possible pairs of domain and range symmetry groups in dimensions (m, 1) and (2, 2).
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2018.02.014
Volume: 385 Issue: First Page #: 225
Date Submitted: 8/27/21 12:00AM Date Published: 5/1/19 4:00AM
Publication Location:
Article Title: A unified spectral method for FPDEs with two-sided derivatives; part I: A fast solver
Authors: Mehdi Samiee, Mohsen Zayernouri, Mark M. Meerschaert
Keywords: Anomalous transport High-dimensional FPDEs Diffusion-to-wave dynamics Jacobi poly-fractonomial Unified fast solver Spectral convergence
Abstract: We develop a unified Petrov–Galerkin spectral method for a class of fractional partial differential equations with two-sided derivatives and constant coefficients subject to homogeneous Dirichlet initial/boundary conditions. We employ the eigenfunctions of the fractional Sturm–Liouville eigen-problems of the first kind, called Jacobi poly-fractonomials, as temporal bases, and the eigen-functions of the boundary-value problem of the second kind as temporal test functions. Next, we construct our spatial basis/test functions using Legendre polynomials, yielding mass matrices being independent of the spatial fractional orders (?i, ?j, i, j =1, 2, ⋯, d). Furthermore, we formulate a novel unified fast linear solver for the resulting high-dimensional linear system based on the solution of generalized eigen-problem of spatial mass matrices with respect to the corresponding stiffness matrices, hence, making the complexity of the problem optimal.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2018.07.041
Volume: 385 Issue: First Page #: 244
Date Submitted: 8/27/21 12:00AM Date Published: 5/1/19 4:00AM
Publication Location:
Article Title: A unified spectral method for FPDEs with two-sided derivatives; Part II: Stability, and error analysis
Authors: Mehdi Samiee, Mohsen Zayernouri, Mark M. Meerschaert
Keywords: Well-posedness Discrete inf–supcondition Spectral convergence Jacobi poly-fractonomials Legendre polynomials
Abstract: We present the stability and error analysis of the unified Petrov–Galerkin spectral method, developed in [1], for linear fractional partial differential equations with two-sided derivatives and constant coefficients in any (1 +d)-dimensional space-time hypercube, d =1, 2, 3, ⋯, subject to homogeneous Dirichlet initial/boundary conditions. Specifically, we prove the existence and uniqueness of the weak form and perform the corresponding stability and error analysis of the proposed method. Finally, we perform several numerical simulations to compare the theoretical and computational rates of convergence.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Statistical Planning and Inference
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jspi.2018.09.010
Volume: 200 Issue: First Page #: 129
Date Submitted: 8/27/21 12:00AM Date Published: 5/1/19 4:00AM
Publication Location:
Article Title: Parameter estimation for ARTFIMA time series
Authors: Farzad Sabzikar, A. Ian McLeod, Mark M. Meerschaert
Keywords: time series, parameter estimation, tempered fractional difference
Abstract: The ARTFIMA model applies a tempered fractional difference to the standard ARMA time series. This paper develops parameter estimation methods for the ARTFIMA model, and demonstrates a new R package. Several examples illustrate the utility of the method.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational and Applied Mathematics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cam.2017.11.012
Volume: 339 Issue: First Page #: 161
Date Submitted: 8/27/21 12:00AM Date Published: 9/1/18 4:00AM
Publication Location:
Article Title: Anomalous diffusion with ballistic scaling: A new fractional derivative
Authors: James F. Kelly, Cheng-Gang Li, Mark M. Meerschaert
Keywords: Fractional calculus Anomalous diffusion Riesz derivative Stable distributions Lévy motion
Abstract: The goal of this paper is to find a governing equation for anomalous diffusion with ballistic scaling and arbitrary skewness. To address this problem, we propose a new operator called the Zolotarev derivative, which is valid for all orders 0 < ? ? 2. The Fourier symbol of this operator is related to the characteristic function of a stable random variable in the ZolotarevM parameterization. In the symmetric case, the Zolotarev derivative reduces to the well-known Riesz derivative. For ? ?= 1, the Zolotarev derivative is a linear combination of Riemann–Liouville fractional derivatives and a first derivative. For ? = 1, the Zolotarev derivative is a non-local operator that models ballistic anomalous diffusion. We prove that this operator is continuous with respect to ?. We derive generator, Caputo, and Riemann–Liouville forms of this operator and provide two examples.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational and Applied Mathematics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cam.2017.12.053
Volume: 336 Issue: First Page #: 408
Date Submitted: 8/27/21 12:00AM Date Published: 7/1/18 4:00AM
Publication Location:
Article Title: Boundary conditions for fractional diffusion
Authors: Boris Baeumer, Mihály Kovács, Mark M. Meerschaert, Harish Sankaranarayanan
Keywords: Fractional calculus Boundary value problem Numerical solution Well-posed
Abstract: This paper derives physically meaningful boundary conditions for fractional diffusion equations, using a mass balance approach. Numerical solutions are presented, and theoretical properties are reviewed, including well-posedness and steady state solutions. Absorbing and reflecting boundary conditions are considered, and illustrated through several examples. Reflecting boundary conditions involve fractional derivatives. The Caputo fractional derivative is shown to be unsuitable for modeling fractional diffusion, since the resulting boundary value problem is not positivity preserving.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: arXiv e-prints
Publication Identifier Type: Publication Identifier:
Volume: Issue: First Page #:
Date Submitted: 9/7/22 12:00AM Date Published:
Publication Location:
Article Title: Dynamic Nonlocal Passive Scalar Subgrid-Scale Turbulence Modeling
Authors: Hadi Seyedi, S., A. Akhavan-Safaei, and M. Zayernouri
Keywords: Fulids
Abstract: Extensive experimental evidence highlight that scalar turbulence exhibits anomalous diffusion and stronger intermittency levels at small scales compared to that in fluid turbulence. This renders the corresponding subgrid-scale dynamics modeling for scalar turbulence a greater challenge to date. We develop a new large eddy simulation (LES) paradigm for efficiently and dynamically nonlocal LES modeling of the scalar turbulence. To this end, we formulate the underlying nonlocal model starting from the filtered Boltzmann kinetic transport equation, where the divergence of subgrid-scale scalar fluxes emerges as a fractional-order Laplacian term in the filtered advection-diffusion model, coding the corresponding supper-diffusive nature of scalar turbulence. Subsequently, we develop a robust data-driven algorithm for estimation of the fractional (non-integer) Laplacian exponent, where we on-the-fly calculate the corresponding model coefficient employing a new dynamic procedure. Our a priori t
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Physics of Fluids
Publication Identifier Type: DOI Publication Identifier: 10.1063/5.0079461
Volume: 34 Issue: 3 First Page #: 035104
Date Submitted: 9/8/22 12:00AM Date Published: 3/1/22 10:00AM
Publication Location:
Article Title: A data-driven dynamic nonlocal subgrid-scale model for turbulent flows
Authors: S. Hadi Seyedi, Mohsen Zayernouri
Keywords: Physics
Abstract: Extensive experimental evidence highlight that scalar turbulence exhibits anomalous diffusion and stronger intermittency levels at small scales compared to that in fluid turbulence. This renders the corresponding subgrid-scale dynamics modeling for scalar turbulence a greater challenge to date. We develop a new large eddy simulation (LES) paradigm for efficiently and dynamically nonlocal LES modeling of the scalar turbulence. To this end, we formulate the underlying nonlocal model starting from the filtered Boltzmann kinetic transport equation, where the divergence of subgrid-scale scalar fluxes emerges as a fractional-order Laplacian term in the filtered advection-diffusion model, coding the corresponding supper-diffusive nature of scalar turbulence. Subsequently, we develop a robust data-driven algorithm for estimation of the fractional (non-integer) Laplacian exponent, where we on-the-fly calculate the corresponding model coefficient employing a new dynamic procedure. Our a priori t
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: arXiv preprint
Publication Identifier Type: Publication Identifier:
Volume: Issue: First Page #:
Date Submitted: 9/7/22 12:00AM Date Published: 11/12/21 9:56PM
Publication Location:
Article Title: A nonlocal spectral transfer model and new scaling law for scalar turbulence
Authors: Akhavan-Safaei, A., and M. Zayernouri
Keywords: Tubulance
Abstract: In this study, we revisit the spectral transfer model for the turbulent intensity in the passive scalar transport (under large-scale anisotropic forcing), and a subsequent modification to the scaling of scalar variance cascade is presented. From the modified spectral transfer model, we obtain a revised scalar transport model using fractionalorder Laplacian operator that facilitates the robust inclusion of the nonlocal effects originated from large-scale anisotropy transferred across the multitude of scales in the turbulent cascade. We provide an a priori estimate for the nonlocal model based on the scaling analysis of scalar spectrum, and later examine our developed model through direct numerical simulation. We present a detailed analysis on the evolution of the scalar variance, high-order statistics of scalar gradient, and important two-point statistical metrics of the turbulent transport to make a comprehensive comparison between the nonlocal model and its standard version. Finally,
Distribution Statement: 1-Approved for public release; distribution is unlimited.
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2021.110571
Volume: 446 Issue: First Page #: 110571
Date Submitted: 9/8/22 12:00AM Date Published: 12/1/21 5:00AM
Publication Location:
Article Title: Data-driven fractional subgrid-scale modeling for scalar turbulence: A nonlocal LES approach
Authors: Ali Akhavan-Safaei, Mehdi Samiee, Mohsen Zayernouri
Keywords: fractional viscoelasticity; quasi-linear-viscoelasticity; urinary bladder rheology; data-driven model selection; power-law relaxation
Abstract: We introduce a data-driven fractional modeling framework for complex materials, and particularly bio-tissues. From multi-step relaxation experiments of distinct anatomical locations of porcine urinary bladder, we identify an anomalous relaxation character, with two power-law-like behaviors for short/long long times, and nonlinearity for strains greater than 25%. The first component of our framework is an existence study, to determine admissible fractional viscoelastic models that qualitatively describe linear relaxation. After the linear viscoelastic model is selected, the second stage adds large-strain effects to the framework through a fractional quasi-linear viscoelastic approach for the nonlinear elastic response of the bio-tissue of interest. From single-step relaxation data of the urinary bladder, a fractional Maxwell model captures both short/long-term behaviors with two fractional orders, being the most suitable model for small strains at the first stage. For the second stage,
Distribution Statement: 1-Approved for public release; distribution is unlimited.
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Fluid Mechanics
Publication Identifier Type: DOI Publication Identifier: 10.1017/jfm.2021.955
Volume: 932 Issue: First Page #:
Date Submitted: 9/8/22 12:00AM Date Published: 12/1/21 5:00AM
Publication Location:
Article Title: Tempered fractional LES modeling
Authors: Mehdi Samiee, Ali Akhavan-Safaei, Mohsen Zayernouri
Keywords: turbulence modelling, computational methods, fractals
Abstract: The presence of non-local interactions and intermittent signals in the homogeneous isotropic turbulence grant multi-point statistical functions a key role in formulating a new generation of large-eddy simulation (LES) models of higher fidelity. We establish a tempered fractional-order modelling framework for developing non-local LES subgrid-scale models, starting from the kinetic transport. We employ a tempered Lévy-stable distribution to represent the source of turbulent effects at the kinetic level, and we rigorously show that the corresponding turbulence closure term emerges as the tempered fractional Laplacian, (?+?)?(?), for ??(0,1), ?? 1/2 and ?>0 in the filtered Navier–Stokes equations. Moreover, we prove the frame invariant properties of the proposed model, complying with the subgrid-scale stresses.
Distribution Statement: 1-Approved for public release; distribution is unlimited.
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: arXiv preprint
Publication Identifier Type: Publication Identifier:
Volume: Issue: First Page #:
Date Submitted: 9/8/22 12:00AM Date Published:
Publication Location:
Article Title: Fractional Modeling in Action: A Survey of Nonlocal Models for Subsurface Transport, Turbulent Flows, and Anomalous Materials
Authors: D'Elia, M., M. Gulian, J. Suzuki, and M. Zayernouri
Keywords: Fractional models · Nonlocal models · Anomalous diffusion · Stochastic processes · Subsurface transport · Turbulence · Anomalous materials
Abstract: Modeling of phenomena such as anomalous transport via fractional-order differential equations has been established as an effective alternative to partial differential equations, due to the inherent ability to describe large-scale behavior with greater efficiency than fully-resolved classical models. In this review article, we first provide a broad overview of fractional-order derivatives with a clear emphasis on the stochastic processes that underlie their use. We then survey three exemplary application areas – subsurface transport, turbulence, and anomalous materials – in which fractional-order differential equations provide accurate and predictive models. For each area, we report on the evidence of anomalous behavior that justifies the use of fractional-order models, and survey both foundational models as well as more expressive state-of-the-art models.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Fractal and Fractional
Publication Identifier Type: DOI Publication Identifier: 10.3390/fractalfract5040223
Volume: 5 Issue: 4 First Page #: 223
Date Submitted: 9/8/22 12:00AM Date Published: 11/1/21 4:00AM
Publication Location:
Article Title: A Data-Driven Memory-Dependent Modeling Framework for Anomalous Rheology: Application to Urinary Bladder Tissue
Authors: Jorge L. Suzuki, Tyler G. Tuttle, Sara Roccabianca, Mohsen Zayernouri
Keywords: fractional viscoelasticity; quasi-linear-viscoelasticity; urinary bladder rheology; datadriven model selection; power-law relaxation
Abstract: We introduce a data-driven fractional modeling framework for complex materials, and particularly bio-tissues. From multi-step relaxation experiments of distinct anatomical locations of porcine urinary bladder, we identify an anomalous relaxation character, with two power-lawlike behaviors for short/long long times, and nonlinearity for strains greater than 25%. The first component of our framework is an existence study, to determine admissible fractional viscoelastic models that qualitatively describe linear relaxation. After the linear viscoelastic model is selected, the second stage adds large-strain effects to the framework through a fractional quasi-linear viscoelastic approach for the nonlinear elastic response of the bio-tissue of interest. From single-step relaxation data of the urinary bladder, a fractional Maxwell model captures both short/long-term behaviors with two fractional orders, being the most suitable model for small strains at the first stage.
Distribution Statement: 1-Approved for public release; distribution is unlimited.
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Fractional Calculus and Applied Analysis
Publication Identifier Type: DOI Publication Identifier: 10.1515/fca-2021-0045
Volume: 24 Issue: 4 First Page #: 1035
Date Submitted: 9/8/22 12:00AM Date Published: 8/1/21 8:00AM
Publication Location:
Article Title: Censored Stable Subordinators and Fractional Derivatives
Authors: Qiang Du, Lorenzo Toniazzi, Zirui Xu
Keywords: fractional initial calue problem, censored stable subordinator, fractional relaxation equation, Mittag-Leffler function
Abstract: Based on the popular Caputo fractional derivative of order♀ in (0; 1), we de♀fine the censored fractional derivative on the positive half-line R+. This derivative proves to be the Feller generator of the censored (or resurrected) decreasing ♀-stable process in R+. We provide a series representation for the inverse of this censored fractional derivative. We are then able to prove that this censored process hits the boundary in a♀n finite time 1, whose expectation is proportional to that of the ♀rest passage time of the stable subordinator. We also show that the censored relaxation equation is solved by the Laplace transform of 1. This relaxation solution proves to be a completely monotone series, with algebraic decay one order faster than its Caputo counter part, leading, surprisingly, to a new regime of fractional relaxation models. Lastly, we discuss how this work identifies a new sub-diffusion model.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: arXiv e-prints
Publication Identifier Type: Publication Identifier:
Volume: Issue: First Page #:
Date Submitted: 9/8/22 12:00AM Date Published:
Publication Location:
Article Title: SECOND ORDER ACCURATE DIRICHLET BOUNDARY CONDITIONS FOR LINEAR NONLOCAL DIFFUSION PROBLEMS
Authors: HWI LEE AND QIANG DU
Keywords: Nonlocal models, nonlocal diffusion, peridynamics, smoothed particle hydrodynamics, nonlocal gradient, nonlocal boundary condition, extrapolation, nonlocal interactions kernel
Abstract: We present an approach to handle Dirichlet type nonlocal boundary conditions for nonlocal diffusion models with a finite range of nonlocal interactions. Our approach utilizes a linear extrapolation of prescribed boundary data. A novelty is, instead of using local gradients of the boundary data that are not available a priori, we incorporate nonlocal gradient operators into the formulation to generalize the finite differences-based methods which are pervasive in literature; our particular choice of the nonlocal gradient operators is based on the interplay between a constant kernel function and the geometry of nonlocal interaction neighborhoods. Such an approach can be potentially useful to address similar issues in peridynamics, smoothed particle hydrodynamics and other nonlocal models. We first show the well-posedness of the newly formulated nonlocal problems and then analyze their asymptotic convergence to the local limit as the nonlocality parameter shrinks to zero.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: arXiv preprint
Publication Identifier Type: Publication Identifier:
Volume: Issue: First Page #:
Date Submitted: 9/8/22 12:00AM Date Published:
Publication Location:
Article Title: Nonlocal diffusion models with consistent local and fractional limits
Authors: QIANG DU, XIAOCHUAN TIAN, AND ZHI ZHOU
Keywords: nonlocal models, nonlocal diffusion, peridynamics, fractional PDEs, well-posedness, inhomogeneous data
Abstract: For some spatially nonlocal diffusion models with a ♀finite range of nonlocal interactions measured by a positive parameter, we review their formulation de♀fined on a bounded domain subject to various conditions that correspond to some inhomogeneous data. We consider their consistency to similar inhomogeneous boundary value problems of classical partial differential equation (PDE) models as the nonlocal interaction kernel gets localized in the local limit, and at the same time, for rescaled fractional type kernels, to corresponding inhomogeneous nonlocal boundary value problems of fractional equations in the global limit. Such discussions help to delineate issues related to nonlocal problems de♀fined on a bounded domain with inhomogeneous data.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: arXiv preprint
Publication Identifier Type: Publication Identifier:
Volume: Issue: First Page #:
Date Submitted: 9/8/22 12:00AM Date Published:
Publication Location:
Article Title: Nonlocal Trace Spaces and Extension Results for Nonlocal Calculus
Authors: Qiang Du, Xiaochuan Tian, Cory Wright, Yue Yu
Keywords: Trace Theorem; Nonlocal Function Space; Inverse Trace Theorem; Trace Space; Finite Nonlocal Interactions; Extension Operator
Abstract: For a given Lipschitz domain, it is a classical result that the trace space of W1,p() is W1?1/p,p(?), namely any W1,p() function has a well-defined W1?1/p, p(?) trace on its codimension-1 boundary ? and any W1?1/p,p(?) function on ? can be extended to a W1,p() function. Recently, [26] characterizes the trace space for nonlocal Dirichlet problems involving integrodifferential operators with infinite interaction ranges, where the boundary datum is provided on the whole complement of the given domain Rd\ . In this work, we study function spaces for nonlocal Dirichlet problems with a finite range of nonlocal interactions, which naturally serves a bridging role between the classical local PDE problem and the nonlocal problem with infinite interaction ranges. For these nonlocal Dirichlet problems, the boundary conditions are normally imposed on a region with finite thickness volume which lies outside of the domain.
Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Fluid Mechanics
Publication Identifier Type: DOI Publication Identifier: 10.1017/jfm.2022.377
Volume: 942 Issue: First Page #:
Date Submitted: 9/8/22 12:00AM Date Published: 5/1/22 8:00AM
Publication Location:
Article Title: Theory and simulation of electrokinetic fluctuations in electrolyte solutions at the mesoscale
Authors: Mingge Deng, Faisal Tushar, Luis Bravo, Anindya Ghoshal, George Karniadakis, Zhen Li
Keywords: microscale transport, suspensions, general fluid mechanics
Abstract: Electrolyte solutions play an important role in energy storage devices, whose performance relies heavily on the electrokinetic processes at sub-micron scales. Although fluctuations and stochastic features become more critical at small scales, the long-range Coulomb interactions pose a particular challenge for both theoretical analysis and simulation of fluid systems with fluctuating hydrodynamic and electrostatic interactions. Here, we present a theoretical framework based on the Landau–Lifshitz theory to derive closed-form expressions for fluctuation correlations in electrolyte solutions, indicating significantly different decorrelation processes of ionic concentration fluctuations from hydrodynamic fluctuations, which provides insights for understanding transport phenomena of coupled fluctuating hydrodynamics and electrokinetics.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: arXiv preprint
Publication Identifier Type: Publication Identifier:
Volume: Issue: First Page #:
Date Submitted: 9/8/22 12:00AM Date Published:
Publication Location:
Article Title: Bayesian Physics-Informed Neural Networks for real-world nonlinear dynamical systems
Authors: Kevin Linka, Amelie Schäfer, Xuhui Meng, Zongren Zou, George Em Karniadakis, Ellen Kuh
Keywords: dynamical systems; machine learning; Neural Networks; Physics-Informed Neural Networks; Bayesian Inference; Bayesian Neural Networks
Abstract: Understanding real-world dynamical phenomena remains a challenging task. Across various scientific disciplines, machine learning has advanced as the go-to technology to analyze nonlinear dynamical systems, identify patterns in big data, and make decision around them. Neural networks are now consistently used as universal function approximators for data with underlying mechanisms that are incompletely understood or exceedingly complex. However, neural networks alone ignore the fundamental laws of physics and often fail to make plausible predictions. Here we integrate data, physics, and uncertainties by combining neural networks, physics-informed modeling, and Bayesian inference to improve the predictive potential of traditional neural network models. We embed the physical model of a damped harmonic oscillator into a fully-connected feedforward neural network to explore a simple and illustrative model system, the outbreak dynamics of COVID-19.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: IEEE Transactions on Neural Networks and Learning Systems
Publication Identifier Type: DOI Publication Identifier: 10.1109/TNNLS.2022.3178706
Volume: Issue: First Page #: 1
Date Submitted: 9/8/22 12:00AM Date Published:
Publication Location:
Article Title: DynG2G: An Efficient Stochastic Graph Embedding Method for Temporal Graphs
Authors: Mengjia Xu, Apoorva Vikram Singh, George Em Karniadakis
Keywords: Dynamic graph, multivariate Gaussian distribution, graph embedding, uncertainty quantification
Abstract: Dynamic graph embedding has gained great attention recently due to its capability of learning low-dimensional and meaningful graph representations for complex temporal graphs with high accuracy. However, recent advances mostly focus on learning node embeddings as deterministic “vectors” for static graphs, hence disregarding the key graph temporal dynamics and the evolving certainties associated with node embedding in the latent space. In this work, we propose an efficient stochastic dynamic graph embedding method (DynG2G) that applies an inductive feed-forward encoder trained with node triplet energy-based ranking loss. Every node per timestamp is encoded as a time-dependent probabilistic multivariate Gaussian distribution in the latent space, hence we are able to quantify the node embedding uncertainty on-the-fly.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: arXiv preprint
Publication Identifier Type: Publication Identifier:
Volume: Issue: First Page #:
Date Submitted: 9/8/22 12:00AM Date Published:
Publication Location:
Article Title: Convergence analysis of the time-stepping numerical methods for time-fractional nonlinear subdiffusion equations
Authors: Hui Zhang, Fanhai Zeng, Xiaoyun Jiang, George Em Karniadakis
Keywords: Time-fractional nonlinear subdiffusion equations; discrete fractional Gr¨onwall inequality; fast time-stepping methods; convergence.
Abstract: In 1986, Dixon and McKee developed a discrete fractional Gr¨onwall inequality [Z. Angew.Math. Mech., 66 (1986), pp. 535–544], which can be seen as a generalization of the classical discrete Gr¨onwall inequality. However, this generalized discrete Gr¨onwall inequality and its variant [SIAM J. Numer. Anal., 57 (2019), pp. 1524–1544] have not been widely applied in the numerical analysis of the time-stepping methods for the time-fractional evolution equations. The main purpose of this paper is to show how to apply the generalized discrete Gr¨onwall inequality to prove the convergence of a class of time-stepping numerical methods for time-fractional nonlinear subdiffusion equations, including the popular fractional backward difference type methods of order one and two, and the fractional Crank-Nicolson type methods. We obtain the optimal L2 error estimate in space discretization for multi-dimensional problems.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: International Journal of Multiphase Flow
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.ijmultiphaseflow.2021.103667
Volume: 141 Issue: First Page #: 103667
Date Submitted: 9/8/22 12:00AM Date Published: 8/1/21 8:00AM
Publication Location:
Article Title: Fluid-structure interactions in a flexible pipe conveying two-phase flow
Authors: X. Zheng, Z. Wang, M.S. Triantafyllou, G.E. Karniadakis
Keywords: Two-phase flowPhase-fieldPipe conveying fluidFluid-structure interactionSlug/churn flowDirect numerical simulation
Abstract: We present three-dimensional direct numerical simulation (DNS) results of a horizontal flexible pipe conveying two-phase incompressible flow at moderate Reynolds numbers (400 ?700). We find that the Reynolds number (Re) and the void fraction (?) essentially determine the onset of self-sustained oscillations in the two-fluid/pipe system. We employ a phase-field formulation to solve the Navier-Stokes coupled with the Cahn-Hilliard equation and the structure equation in an arbitrary Lagrangian Eulerian (ALE) framework. A spectral/hp element method is adopted for the fluid solver and a Galerkin method for the structure solver. We construct stability diagrams showing the transitions between different states of the two-fluid/pipe system. Specifically, we focus on the transition from a stable state to a planar oscillatory state and also to an out-of-plane oscillatory state as a function of four non-dimensional parameters, the Reynolds number Re, the void fraction ?.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computer Physics Communications
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cpc.2020.107695
Volume: 261 Issue: First Page #: 107695
Date Submitted: 9/8/22 12:00AM Date Published: 4/1/21 8:00AM
Publication Location:
Article Title: An open-source parallel code for computing the spectral fractional Laplacian on 3D complex geometry domains
Authors: Max Carlson, Xiaoning Zheng, Hari Sundar, George Em Karniadakis, Robert M. Kirby
Keywords: Fractional Laplacian Anomalous diffusion Eigen-decomposition, Surface quasi-geostrophic equation, open-source code
Abstract: We present a spectral element algorithm and open-source code for computing the fractional Laplacian defined by the eigenfunction expansion on finite 2D/3D complex domains with both homogeneous and nonhomogeneous boundaries. We demonstrate the scalability of the spectral element algorithm on large clusters by constructing the fractional Laplacian based on computed eigenvalues and eigenfunctions using up to thousands of CPUs. To demonstrate the accuracy of this eigen-based approach for computing the factional Laplacian, we approximate the solutions of the fractional diffusion equation using the computed eigenvalues and eigenfunctions on a 2D quadrilateral, and on a 3D cubic and cylindrical domain, and compare the results with the contrived solutions to demonstrate fast convergence.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational and Applied Mathematics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cam.2022.114298
Volume: 412 Issue: First Page #: 114298
Date Submitted: 9/8/22 12:00AM Date Published: 10/1/22 8:00AM
Publication Location:
Article Title: Block triangular preconditioning for stochastic Galerkin method
Authors: Dongwu Wang, Bin Zheng, Long Chen, Guang Lin, Jinchao Xu
Keywords: Stochastic Galerkin method, Polynomial chaos, Block triangular preconditioner, Multigrid
Abstract: In this paper, we develop a new block triangular preconditioner for solving partial differential equations with random coefficients. We prove spectral bounds for the preconditioned system. Several numerical examples are provided to demonstrate the efficiency of this preconditioner, especially for stochastic problems with large variance.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational and Applied Mathematics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cam.2022.114116
Volume: 408 Issue: First Page #: 114116
Date Submitted: 9/8/22 12:00AM Date Published: 7/1/22 8:00AM
Publication Location:
Article Title: A consistent and conservative Phase-Field method for multiphase incompressible flows
Authors: Ziyang Huang, Guang Lin, Arezoo M. Ardekani
Keywords: Multiphase incompressible flows, Phase-Field model, Consistent scheme, Mass conservation, Momentum conservation Large-density ratio
Abstract: In the present study, a consistent and conservative Phase-Field method, including both the model and scheme, is developed for multiphase flows with an arbitrary number of immiscible and incompressible fluid phases. The consistency of mass conservation and the consistency of mass and momentum transport are implemented to address the issue of physically coupling the Phase-Field equation, which locates different phases, to the hydrodynamics. These two consistency conditions, as illustrated, provide the ‘‘optimal’’ coupling because (i) the new momentum equation resulting from them is Galilean invariant and implies the kinetic energy conservation, regardless of the details of the Phase-Field equation, and (ii) failures of satisfying the second law of thermodynamics or the consistency of reduction of the multiphase flow model only result from the same failures of the Phase-Field equation but are not due to the new momentum equation.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Multiscale Modeling & Simulation
Publication Identifier Type: DOI Publication Identifier: 10.1137/21M1405289
Volume: 20 Issue: 2 First Page #: 618
Date Submitted: 9/8/22 12:00AM Date Published: 6/1/22 8:00AM
Publication Location:
Article Title: AMS-Net: Adaptive Multiscale Sparse Neural Network with Interpretable Basis Expansion for Multiphase Flow Problems
Authors: Yating Wang, Wing Tat Leung, Guang Lin
Keywords: multiscale flow dynamics, model reduction, adaptive method, sparse learning, deep neural network, interpretable machine learning
Abstract: In this work, we propose an adaptive sparse learning algorithm that can be applied to learn the physical processes and obtain a sparse representation of the solution given a large snapshot space. Assume that there is a rich class of precomputed basis functions that can be used to approximate the quantity of interest. For instance, in the simulation of a multiscale flow system, one can adopt mixed multiscale methods to compute velocity bases from local problems and apply the proper orthogonal decomposition method to construct bases for the saturation equation. We then design a neural network architecture to learn the coefficients of solutions in the spaces which are spanned by these basis functions. The information of the basis functions is incorporated in the loss function, which minimizes the differences between the downscaled reduced order solutions and reference solutions at multiple time steps.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Mathematical Geosciences
Publication Identifier Type: DOI Publication Identifier: 10.1007/s11004-022-09998-6
Volume: 54 Issue: 3 First Page #: 459
Date Submitted: 9/8/22 12:00AM Date Published: 3/1/22 10:00AM
Publication Location:
Article Title: Special Issue: Geostatistics and Machine Learning
Authors: Sandra De Iaco, Dionissios T. Hristopulos, Guang Lin
Keywords: s Geostatistics · Statistical learning · Machine learning · Spatial process · Gaussian process regression
Abstract: Recent years have seen a steady growth in the number of papers that apply machine learning methods to problems in the earth sciences. Although they have different origins, machine learning and geostatistics share concepts and methods. For example, the kriging formalism can be cast in the machine learning framework of Gaussian process regression. Machine learning, with its focus on algorithms and ability to seek, identify, and exploit hidden structures in big data sets, is providing new tools for exploration and prediction in the earth sciences. Geostatistics, on the other hand, offers interpretable models of spatial (and spatiotemporal) dependence. This special issue on Geostatistics and Machine Learning aims to investigate applications of machine learning methods as well as hybrid approaches combining machine learning and geostatistics which advance our understanding and predictive ability of spatial processes.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational Physics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.jcp.2021.110795
Volume: 449 Issue: First Page #: 110795
Date Submitted: 9/8/22 12:00AM Date Published: 1/1/22 10:00AM
Publication Location:
Article Title: A consistent and conservative Phase-Field model for thermo-gas-liquid-solid flows including liquid-solid phase change
Authors: Ziyang Huang, Guang Lin, Arezoo M. Ardekani
Keywords: Consistent model, Phase change, Solidification/melting, Multiphase flow, Fluid-structure interaction, Phase-Field
Abstract: In the present study, a consistent and conservative Phase-Field model is developed to study thermo-gas-liquid-solid flows with liquid-solid phase change. The proposed model is derived with the help of the consistency conditions and exactly reduces to the consistent and conservative Phase-Field method for incompressible two-phase flows, the fictitious domain Brinkman penalization (FD/BP) method for fluid-structure interactions, and the Phase-Field model of solidification of pure material. It honors the mass conservation, defines the volume fractions of individual phases unambiguously, and therefore captures the volume change due to phase change. The momentum is conserved when the solid phase is absent, but it changes when the solid phase appears due to the no-slip condition at the solid boundary. The proposed model also conserves the energy, preserves the temperature equilibrium, and is Galilean invariant.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

RPPR Final Report
as of 08-Sep-2022

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Journal of Computational and Applied Mathematics
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cam.2021.113674
Volume: 398 Issue: First Page #: 113674
Date Submitted: 9/8/22 12:00AM Date Published: 12/1/21 10:00AM
Publication Location:
Article Title: Flow-driven spectral chaos (FSC) method for long-time integration of second-order stochastic dynamical systems
Authors: Hugo Esquivel, Arun Prakash, Guang Lin
Keywords: Uncertainty quantification, Long-time integration, Stochastic flow map, Stochastic dynamics of structures, Flow-driven spectral chaos (FSC), TD-gPC
Abstract: For decades, uncertainty quantification techniques based on the spectral approach have been demonstrated to be computationally more efficient than the Monte Carlo method for a wide variety of problems, particularly when the dimensionality of the probability space is relatively low. The time-dependent generalized polynomial chaos (TD-gPC) is one such technique that uses an evolving orthogonal basis to better represent the stochastic part of the solution space in time. In this paper, we present a new numerical method that uses the concept of enriched stochastic flow maps to track the evolution of the stochastic part of the solution space in time. The computational cost of this proposed flow-driven stochastic chaos (FSC) method is an order of magnitude lower than TD-gPC for comparable solution accuracy.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: International Journal of Multiphase Flow
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.ijmultiphaseflow.2021.103727
Volume: 142 Issue: First Page #: 103727
Date Submitted: 9/8/22 12:00AM Date Published: 9/1/21 8:00AM
Publication Location:
Article Title: A consistent and conservative volume distribution algorithm and its applications to multiphase flows using Phase-Field models
Authors: Ziyang Huang, Guang Lin, Arezoo M. Ardekani
Keywords: multiphase volume
Abstract: In the present study, a consistent and conservative Phase-Field model is developed to study thermo-gas-liquid-solid flows with liquid-solid phase change. The proposed model is derived with the help of the consistency conditions and exactly reduces to the consistent and conservative Phase-Field method for incompressible two-phase flows, the fictitious domain Brinkman penalization (FD/BP) method for fluid-structure interactions, and the Phase-Field model of solidification of pure material. It honors the mass conservation, defines the volume fractions of individual phases unambiguously, and therefore captures the volume change due to phase change. The momentum is conserved when the solid phase is absent, but it changes when the solid phase appears due to the no-slip condition at the solid boundary. The proposed model also conserves the energy, preserves the temperature equilibrium, and is Galilean invariant.
Distribution Statement: 2-Distribution Limited to U.S. Government agencies only; report contains proprietary info
Acknowledged Federal Support: **Y**

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Partners

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I certify that the information in the report is complete and accurate:
Signature: George Karniadakis
Signature Date: 9/8/22 4:35PM

ARO MURI # 8 Project (2015): August 2018--Jan 2020
Progress Report
Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications

- **George Karniadakis & Mark Ainsworth, Brown University**
- **Qiang Du, Columbia University**
- **Mark Meerschaert & Mohsen Zayernouri, Michigan State University**
- **Pol Spanos, Rice University**
- **Hong Wang, University of South Carolina**
- **Add-On: Zhongqiang Zhang (WPI) and Robert M. Kirby (Uath)**

Background: This MURI project is the vision of a team of researchers from Brown University, Michigan State University, Columbia University, University of South Carolina and Rice University with overlapped interests and complementary expertise on theory, numerical methods and applications of fractional PDEs (FPDEs). Our overarching goal is the development of a seamless integration of theory and algorithms for data-driven FPDEs, while targeting the common themes of conservation, monotonicity, adaptive refinement and high-order accuracy in the context of simulations of multiphase flows, turbulence, fluid-structure interactions, hydrology and solid mechanics. We envision a combined mathematical and computational framework, where the fractional operators can be constructed based on available data, hence providing model validation for the specific phenomenon but also a tailor-based simulation capability that can be scaled to real-life applications. The proposed research plan emphasizes a dynamic integration of six main research areas that form the pillars of our integrated approach:

• *Research Area 1*: Theory of non-local operators and stochastic interpretation of fractional operators.
• *Research Area 2:* Numerical solution of fractional PDEs with emphasis on variable fractional order.
• *Research Area 3:* Fast solvers for dense linear systems with linear/quasi-linear computational complexity.
• *Research Area 4:* Stochastic FPDEs and determination of the fractional order directly by available data.
• *Research Area 5:* Applications to fluid and solid mechanics, fluid-structure interactions, two-phase flows, turbulence and reactive system with front propagation.
• *Research Area 6:* High performance computing & developing opensource software for fractional problems.

MURI Objectives

- To address the common physical themes of anomalous transport, exponentially accelerated fronts, non-Markovian behavior and long-range interactions, self-similarity and scaling, singular behavior, interfaces and finite-domain decorrelation effects.

- To develop rigorous mathematical theory, algorithms and software for data-driven fractional PDEs that will provide significant breakthroughs towards modeling, analyzing and subsequently controlling complex multiscale systems characterized by the aforementioned phenomena —in a computationally scalable way.
- To demonstrate the physical relevance and effectiveness of our framework in diverse applications of interest to DoD, characterized by the common themes of conservation, monotonicity, adaptive refinement and high-order accuracy.

Status of the Project

There has been great progress in the five years on all research six areas, in recruiting excellent postdocs and PhD students, in participating in conferences with invited and contributed talks as well as on organizing mini-symposia and workshops on FPDEs. The add-on helped us to start three new areas on machine learning, fractional photonics, stochastic FPDEs, and opensource software for fractional problems. In the following, we provide a summary of progress by each co-PI. First, we provide some highlights on all our activities and then we present the report of each PI.

MURI Highlights

- More than 197 papers have been published or submitted on all six research areas of MURI.
- More than 70 invited and plenary talks by MURI personnel.
- Volume on numerical methods in Handbook of FPDEs.
- Several minisymposia and two workshops organized by MURI PIs.
- New research focusing on 2D & 3D fractional Laplacians in bounded domains with emphasis on boundary conditions and their stochastic interpretation. 11-author revised paper.
- New research focusing on machine learning, fractional photonics, stochastic fractional PDEs and opensource software enabled by the add-on funding.
- Fractional models of turbulent polymer drag reduction at high Reynolds number.
- Combine FPDE and molecular dynamics to efficiently simulate anomalous diffusive transport in heterogeneous porous materials with nanoscale pores.
- Non-local modeling of ion diffusion in battery systems & experiments.
- We discovered new fractional phase-field/non-local equations for interface problems.
- New opensource software at Brown (fractional NEKTAR), Uath (Nektar++) and MSU (FracFit).

Michigan State University Report (co-PI: Mark Meerschaert)

(Research Areas 1, 2 & 5)

Personnel supported on the MURI grant: Postdoc James Kelly; PhD student Mehdi Samiee; PhD student Eduardo Demoraes. MSU Assistant Professor Mohsen Zayernouri, and Mark M Meerschaert (PI).

Summary: The MSU team has made substantial progress on numerical methods for fractional diffusion, theoretical foundations, and related problems in statistics and probability.

Highlights:

During the past year, the MSU MURI team has published results on:

- Theory and computer codes for fractional diffusion with Dirichlet /Neumann boundary conditions
- A new kind of fractional derivative that facilitates parameter estimation
- Theoretical results on heavy tailed processes and random fields

During the past year, the MSU MURI team had papers accepted on:

- Spectral methods for space-time fractional diffusion
- The general theory of space-nonlocal diffusion with Dirichlet boundary conditions
- The general theory of time-nonlocal diffusion
- Four chapters for the forthcoming *Handbook of Fractional Calculus*

During the past year, the MSU MURI team has submitted papers on:

- Numerical methods for the fractional Laplacian on bounded domains
- Two-sided fractional diffusion with Dirichlet /Neumann boundary conditions
- Spectral methods for distributed order space-time fractional diffusion
- Duality theory for space-fractional and time-fractional diffusion and hyperdiffusion
- Semi-fractional diffusion for problems with discrete scale invariance
- Parameter estimation for tempered fractional time series, to model turbulence

Publication list:

1. J.F. Kelly, C.G. Li and M.M. Meerschaert, Anomalous Diffusion with Ballistic Scaling: A New Fractional Derivative, *Journal of Computational and Applied Mathematics*, Vol. 339 (2018), pp. 161–178. Special Issue on Modern fractional dynamic systems and applications.
2. P. Kern, M.M. Meerschaert, and Y. Xiao, Asymptotic behavior of semistable Lévy exponents and applications to fractal path properties, *Journal of Theoretical Probability*, Vol. 31 (2018), No. 1, pp. 598–617.
3. B. Baeumer, M. Kovács, M.M. Meerschaert, and H. Sankaranarayanan, Boundary Conditions for Fractional Diffusion, *Journal of Computational and Applied Mathematics*, Vol. 336 (2018), pp. 408–424. Click here to download the R codes for this paper.
4. G. Didier, M.M. Meerschaert, and V. Pipiras, Domain and range symmetries of operator fractional Brownian fields, *Stochastic Processes and their Applications*, Vol. 128 (2018), No. 1, pp. 39–78.
5. A unified spectral method for FPDEs with two-sided derivatives; part I: A fast solver, *Journal of Computational Physics*, to appear (with Mohsen Zayernouri and Mehdi Samiee, Department of Computational Mathematics, Science and Engineering, Michigan State University).
6. The fractional advection-dispersion equation for contaminant transport, *Handbook of Fractional Calculus with Applications*, to appear (with James F. Kelly, Department of Statistics and Probability, Michigan State University).
7. Inverse subordinators and time fractional equations, *Handbook of Fractional Calculus with Applications*, to appear (with Erkan Nane, Department of Mathematics and

Statistics, Auburn University: and P. Vellaisamy, Department of Mathematics, Indian Institute of Technology Bombay).

8. Continuous time random walks and space-time fractional differential equations, *Handbook of Fractional Calculus with Applications*, to appear (with Hans-Peter Scheffler, Fachbereich Mathematik, University of Siegen, Germany).
9. Space-time fractional Dirichlet problems, *Mathematische Nachrichten*, to appear (with Boris Baeumer, Department of Mathematics and Statistics, University of Otago, Dunedin, New Zealand; and Tomasz Luks, Institut für Mathematik, Universität Paderborn, Germany).
10. A Unified Spectral Method for FPDEs with Two-sided Derivatives; Part II: Stability and Error Analysis, *Journal of Computational Physics*, to appear (with Mohsen Zayernouri and Mehdi Samiee, Department of Computational Mathematics, Science and Engineering, Michigan State University).
11. Relaxation patterns and semi-Markov dynamics, *Stochastic Processes and their Applications*, to appear (with Bruno Toaldo, Department of Statistical Sciences, Sapienza - University of Rome).
12. Lagrangian approximation of vector fractional differential equations, *Handbook of Fractional Calculus with Applications*, to appear (with Yong Zhang, Department of Geological Sciences, University of Alabama).
13. What Is the Fractional Laplacian? (with Anna Lischke, Guofei Pang, Mamikon Gulian, Fangying Song, Xiaoning Zheng, Zhiping Mao, Mark Ainsworth, and George Em Karniadakis, Division of Applied Mathematics, Brown University; Christian Glusa, Center for Computing Research, Sandia National Laboratory; and Wei Cai, Department of Mathematics, Southern Methodist University, Dallas, TX).
14. Parameter estimation for ARTFIMA time series, (with A. Ian McLeod, Department of Statistical and Actuarial Sciences, University of Western Ontario; and Farzad Sabzikar, Department of Statistics, Iowa State University).
15. Boundary conditions for two-sided fractional diffusion (with James F. Kelly, Department of Statistics and Probability, Michigan State University; and Harish Sankaranarayanan, Department of Statistics and Probability, Michigan State University).
16. Petrov-Galerkin Method for Fully Distributed-Order Fractional Partial Differential Equations (with Mohsen Zayernouri, Mehdi Samiee, and Ehsan Kharazmi, Department of Computational Mathematics, Science and Engineering, Michigan State University).
17. Semi-fractional diffusion equations (with Svenja Lage and Peter Kern, Mathematical Institute, Heinrich-Heine-University Düsseldorf, Germany).
18. Space-Time Duality and Fractional Hyperdiffusion (with James F. Kelly, Department of Statistics and Probability, Michigan State University).

Michigan State University: (co-PI: Mohsen Zayernouri)

(Research Areas 1, 2 & 5)

Personnel supported on the MURI grant: Postdoc Vikran Dharodi; PhD student Mehdi Samiee; PhD student Eduardo Demoraes, PhD student Ali Akhavan-Safaei, PhD student Seyedhadi Seyedi. MSU Assistant Professor Mohsen Zayernouri (PI).

Summary: The MSU team has made substantial progress on fractional subgrid-scale models for turbulence, operator-based uncertainty quantification, numerical methods for distributed-order

fractional PDEs in high-dimensions with fast solvers, stochastic phase-field models for material failure, fast and stable time-integration schemes for time-fractional problems, and fractional vibration and structure health monitoring of mechanical structures.

Highlights:

During the past year, the MSU MURI team has published results on:

- Theory and practice of Fractional Sensitivity Equation Method (FSEM) for constructing the fractional operators.
- Theory and computer codes for unified distributed-order FPDEs with Dirichlet boundary conditions.
- Spectral and spectral-element methods for advection-diffusion problems.
- Noise suppression using fractional shock absorbers/dampers.
- One chapter for the *Handbook of Fractional Calculus.*

During the past year, the MSU MURI team had papers accepted on:

- Operator-based uncertainty quantification for FPDEs.
- Fractional subgrid-scale LES models for incompressible isotropic turbulence.
- Fast and stable fractional IMEX time-integrators.

During the past year, the MSU MURI team has submitted papers on:

- Stochastic phase-field modeling of material failure.
- Phase-field based machine learning algorithm for predicting material failure.
- Automatic and self-singularity capturing schemes for fractional time-integrations.

Published (& in Press) Journal Papers:

1) M. Samiee, A. A Safaei, M. Zayernouri, (2020) ***A Fractional Subgrid-scale Model for Turbulent Flows: Theoretical Formulation and a Priori Study***, Physics of Fluid, in Press.

2) E. Kharazmi and M. Zayernouri, (2020) **Operator-Based Uncertainty Quantification of Stochastic Fractional PDEs**, *ASME Journal on Verification, Validation, and Uncertainty Quantification*, in Press.

3) M. Samiee E. Kharazmi, M. Meerschaert, M. Zayernouri, (2020) ***A*** **Unified Petrov-Galerkin Spectral Method and Fast Solver for Distributed-Order Partial Differential Equations***, Communications on Applied Mathematics and Computation*, in Press.

4) Y. Zhou, J. Suzuki, C. Zhang, and M. Zayernouri, (2020) **Fast Implicit-Explicit Time-Integration of Nonlinear Fractional Differential Equations***, Journal of Applied Numerical Mathematics.*

5) P. Varghaei, E. Kharazmi, J. Suzuki, and M. Zayernouri, (2020) **Nonlinear Vibration of Fractional Viscoelastic Cantilever Beam: Application to Structural Health Monitoring**, ASME Journal of Vibration and *Acoustics*, in Press.

6) M. Ari, R. Teymoori-Faal, M. Zayernouri, (2019) **Vibrations Suppression of Fractionally Damped Plates using Multiple Optimal Dynamic Vibration Absorbers,** *International Journal of Computer Mathematics, 1-24.*

7) M. Samiee, M. Zayernouri, and M. M. Meerschaert, (2019) **A Unified Spectral Method for FPDEs with Two-sided Derivatives; Part I: A Fast Solver**, *Journal of Computational Physics, 385, 225-243.*

8) M. Samiee, M. Zayernouri, and M. M. Meerschaert, (2019) **A Unified Spectral Method for FPDEs with Two-sided Derivatives; Part II: Stability and Error Analysis**, *Journal of Computational Physics, 385, 244-261*

9) A. Lischke, M. Zayernouri, Z. Zhang, (2019) **Spectral and Spectral Element Methods for Fractional Advection–Diffusion–Reaction Equations**, *Handbook of Fractional Calculus with Applications, Volume 3: Numerical Methods.*

Submitted Journal Manuscripts:

10) E. de Moraes, H. Salehi, and M. Zayernouri, (2020) **Data-Driven Failure Prediction in Brittle Materials: A Phase-Field based Machine Learning Framework**, submitted to *Engineering Applications of Artificial Intelligence*.

11) E. Kharazmi, Z. Mao, G. Pang, M. Zayernouri, and G. E. Karniadakis, (2020) **Fractional Calculus and Numerical Methods for Fractional PDEs**, *Paper Review (De Gruyter)*.

12) E. de Moraes, M. Zayernouri, M. Meerschaert, (2020), **An Integrated Sensitivity-Uncertainty Quantification Framework for Stochastic Phase-Field Modeling of Material Damage,** submitted to *Int. J. Numerical Methods in Engineering.*

13) J. Suzuki and M. Zayernouri, (2020) **A Data-Infused Self-Singularity-Capturing Scheme for Fractional Differential Equations***,* submitted to *Int. Journal of Computer Mathematics*.

Columbia University Report (co-PI: Qiang Du)

(Research Areas 1 & 5)

Progress report: July 2018-Dec 2019

The research team at Columbia, under the direction of Qiang Du, has actively participated in research supported by the MURI project and has sought after collaborations with other MURI team members.

Research team at Columbia:

Personnel supported on the grant at Columbia: PI Qiang Du was supported for one summer month by the grant; post-doc scholar Lorenzo Toniazzi (11/18-08/19) and graduate students Yunzhe Tao, Hwi Lee and Zirui Xu were partially supported for the year.
Unsupported research personnel: a couple of graduate students have been collaborating on the project, but they do not receive any support from this grant.

Research progress: as outlined in the proposal, the proposed work for the Columbia team focuses on the analysis and discretization of Fractional PDEs and nonlocal integral equations.

Highlight.
1. We published in 2019 a research monograph "Nonlocal Modeling, Analysis and Computation" [6] based on our NSF-CBMS conference lectures. 2. Our work has attracted much attention and recognition. In [21], our original framework for AC schemes for nonlocal models was further extended and it is published as a SIAM Review Digest Award paper (first issue, 2020).

Origin of Nonlocality.
While we focused on algorithmic development and analysis, we were also aware of important modeling issues and we studied the origin of nonlocality in a multiscale modeling context and its relations to model reduction and homogenization. Our findings were reported in [1]. A more special case study was given in [10].

Interpretation of nonlocal/fractional models.
We investigated the stochastic interpretations of nonlocal-in-time diffusion models [5]. This motivated us to study more general fractional differential equations via the analysis of censored fractional derivative and establish the well-posedness of the resulting equation and its solution behavior.

Nonlocal/fractional modeling.
We have studied nonlocal smoothing of well-known models of mechanics with the goal to understand how they affect numerical methods like the SPH discretization in CFD as well as the discretization of nonlocal elasticity models. We examined in particular the nonlocal analog of the linear Stokes equations and the Navier model of linear elasticity, and linear models of linear convection, with all of them depending on the suitable definitions of the nonlocal gradient operator. The latter is a key building block for the nonlocal smoothing of traditional PDEs, as well as for nonlocal models themselves. Our finding showed that there may be intrinsic instabilities associated with some of the popular forms of the nonlocal gradient on the continuum level, thus leading to discretizations that are also prone to instabilities and lack of robustness. We proposed alternatives that can help eliminating these instabilities for some model problems. Publications related to this line of works can be found in [12, 15, 16]. We also examined the nonlocal analog of classical two-point value problem and showed that one can expect second order accuracy with respect to the horizon parameter [14]. In light of possible discontinuous solutions for nonlocal diffusion models with integrable kernels, we developed hybrid continuous and discontinuous Galerkin approximations [13].

Algorithms for nonlocal/fractional models.
We continued the development of asymptotically compatible discontinuous Galerkin finite element approximations and quadrature-based finite difference schemes, as well as fast spectral methods for nonlocal models [2-4, 9, 18]. We studied applications of various stable time-stepping schemes to others considered nonlinear nonlocal phase field models [7, 8]. We have also done some initial investigations on the proper coupling of nonlocal models with local models on the continuum level using either seamless coupling approaches [11,19]. Other related topics include our study of the diffusion in battery systems [17], and the application of nonlocal diffusion layers for more robust and effective deep neural network design [20].

Reference and publications:

[1] Q. Du, B. Engquist, and X.C. Tian. Multiscale modeling, homogenization and nonlocal effects: mathematical and computational issues. Contemporary Mathematics, Celebrating 75th Anniversary of Mathematics of Computation, 2020.

[2] Q Du, L Ju, and J Lu. Analysis of fully discrete approximations for dissipative systems and application to time-dependent nonlocal diffusion problems. Journal of Scientific Computing, 78:1438–1466, 2019.
[3] Q. Du, L. Ju, and J. Lu. A discontinuous Galerkin method for one-dimensional time-dependent nonlocal diffusion problems. Mathematics of Computation, 88:123-147, 2019.
[4] Q. Du, Y. Tao, X. Tian, and J. Yang. Asymptotically compatible discretization of multidimensional nonlocal diffusion models and approximations of nonlocal Green's functions. IMA J. Numerical Analysis, 39:607-625, 2019.
[5] Q. Du, L. Toniazzi, and Z. Zhou. Stochastic representation of solution to nonlocal-in-time diffusion. Stochastic Processes and their Applications, 2020.
[6] Qiang Du. Nonlocal Modeling, Analysis, and Computation, volume CBMS-NSF conference series in applied mathematics 94. SIAM, 2019.
[7] Qiang Du, Lili Ju, Xiao Li, and Zhonghua Qiao. Stabilized linear semi-implicit schemes for the nonlocal Cahn-Hilliard equation. Journal of Computational Physics, 363:39–54, 2018.
[8] Qiang Du, Lili Ju, Xiao Li, and Zhonghua Qiao. Maximum principle preserving exponential time differencing schemes for the nonlocal Allen–Cahn equation. SIAM Journal on Numerical Analysis, 57(2):875–898, 2019.
[9] Qiang Du, Lili Ju, Jianfang Lu, and Xiaochuan Tian. A discontinuous Galerkin method with penalty for one-dimensional nonlocal diffusion problems. Communications on Applied Mathematics and Computation, 2(1):31–55, 2020.
[10] Qiang Du, Xiantao Li, and Liming Yuan. Analysis of coarse-grained lattice models and connections to nonlocal interactions. preprint, 2020.
[11] Qiang Du and Xiaochuan Tian. Heterogeneously localized nonlocal operators, boundary traces and variational problems. In Proceedings of the international congress of Chinese mathematicians, volume 43 of the ALM series, pages 217–236. International Press, 2018.
[12] Qiang Du and Xiaochuan Tian. Mathematics of smoothed particle hydrodynamics via a nonlocal stokes equation. Foundations of Computational Mathematics, pages 1–26, 2019.
[13] Qiang Du and Xiaobo Yin. A conforming dg method for linear nonlocal models with integrable kernels. J. Scientific Computing, 80:1913–1935, 2019.
[14] Qiang Du, Jiwei Zhang, and Chunxiong Zheng. On uniform second order nonlocal approximations to linear two-point boundary value problems. Communications in Mathematical Sciences, 17(6):1737-1755, 2019.
[15] H. Lee and Q Du. Asymptotically compatible SPH-like particle discretizations of one-dimensional linear advection models. SIAM Journal on Numerical Analysis, 57:127–147, 2019.
[16] H. Lee and Q Du. Nonlocal gradient operators with a nonspherical interaction neighborhood and their applications. ESAIM: Mathematical Modelling and Numerical Analysis, 2020.
[17] Yali Qiao, Zhi Zhou, Zhixing Chen, Sicen Du, Qian Cheng, Haowei Zhai, Nathan Joseph Fritz, Qiang Du, and Yuan Yang. Visualizing ion diffusion in battery systems by fluorescence microscopy: a case study on the dissolution of limn2o4. Nano Energy,45:68–74, 2018.

Recognition:

Qiang Du: AMS fellow, 2020.
SIAM Review Digest Paper Award, 2020.
ICM invited speaker, 2018.
All products acknowledge support from ARO grant W911NF-15-1-05

University of South Carolina Report (co-PI: Hong Wang)

(Research Area 1, 2 & 3)

Progress report: July 2018—Jan 2020

The research group at University of South Carolina, under the direction of Hong Wang, has actively participated in research supported by the MURI project.
During this time period, USC research group has focused on the study of variable-order FPDEs, which were listed on many research areas of the original research tasks.

1. *Variable-order FPDEs: well-posedness, smoothness and boundary conditions (Original proposal: Research Area 1) as well as numerical approximations (Research Area 2).*
   It is known that constant-order FPDEs can better model complex phenomena of anomalously diffusive transport and long-range spatial and temporal interactions more accurately then integer-order PDEs do. However, because they were derived via continuous time random walk (CTRW) as the number of jumps tends to infinity, the derived FPDEs hold away from the initial time and boundary. This explains why FPDEs exhibit solutions with nonphysical singularity near the initial time and the boundary. This causes numerical issues in their numerical approximations and makes many error estimates in the literature that were proved assuming the smoothness of solutions inappropriate.

   Besides, the order of FPDEs is related to the fractal dimension of the pore structure of the porous material. As the material structure changes (e.g., due to the growth of biomaterial), the order of FPDEs should change and yield variable-order FPDEs. Moreover, FPDEs with a properly chosen variable-order naturally eliminate the nonphysical singularity of their solutions.

   In papers (16)-(18) and (26) we proved well-posedness and regularity of variable-order time-fractional PDEs with a time-dependent variable order alpha(t). In paper (37) we extended the analysis to variable-order space-time FPDEs. In (41) we developed a finite element approximation to a variable-order time-fractional PDE and carried out the numerical analysis without artificially assuming the smoothness of the true solution.

   In (39) we proved well-posedness and regularity of a variable-order time-fractional PDE with a nonlinear variable order alpha(x,t,u) and derived a numerical approximation with a proved error estimate. In (32) we proved well-posedness and regularity of the boundary-value problem of a variable-order space-fractional diffusion equation with a space-dependent variable order alpha(x) and derived a numerical scheme with a proved error estimate.

2. *Development of fast numerical solvers for variable-order FPDEs (Research Area 3).*
   Because of the impact of the space or time-dependent variable order, the coefficient matrices of the numerical discretization do not have Toeplitz-like structure, so the fast numerical methods do not apply to variable-order FPDEs. In (36) we developed a fast numerical method for a variable-order space-fractional diffusion equation with a space-dependent variable order alpha(x). In (39) we developed a fast numerical method for a variable-order time-fractional PDE.

3. *Determination of variable order in variable-order FPDEs (Research Area 4).*

As the order of FPDEs is closely related to the fractal dimension of the porous material via the Hurst index, the variable orders of FPDEs provides a feasible mean to characterize the material change of the porous media. In (23) and (40) we proved the unique identifiability of the time-dependent variable order in a variable-order time-fractional PDE and the space-dependent variable order in a variable-order space-fractional diffusion equation, respectively. Numerical experiments showed the utility of the method.

Research publications (All acknowledged MURI support) since July 2018 (last report):

(1) W. Deng, B. Li, Z. Qian and H. Wang, Time discretization of a tempered fractional Feynman-Kac equation with measure data, SIAM J Numer Anal 56 (2018), 3249-3257.

(2) X. Guo, Y. Li and H. Wang, A high order finite difference method for tempered fractional diffusion equations with applications to the CGMY model, SIAM J Sci Comput} 40 (2018), A3322-3343.

(3) X. Guo, Y. Li and H. Wang, Tempered fractional diffusion equations for pricing multi-asset options under CGMY process, Computers & Math Appl 76 (2018), 1500-1514.

(4) L. Chen, J. Zhang, J. Zhao, W. Cao, H. Wang, J. Zhang, An accurate and efficient algorithm for the time-fractional molecular beam epitaxy model with slope selection, Computer Physics Communications, 245 (2019), 106842.

(5) N. Du, H. Sun, H. Wang, A preconditioned fast finite difference scheme for space-fractional diffusion equations in convex domains, Comput Appl Math, (2019) 38: 14.

(6) S. Duo and H. Wang, A fractional phase-field model using an infinitesimal generator of α stable Lévy process. J Comput Phys 384 (2019), 253-269.

(7) H. Fu, H. Liu, H. Wang, A finite volume method for two-dimensional Riemann-Liouville space-fractional diffusion equation and its efficient implementation, J Comput Phys 388 (2019), 316-334.

(8) H. Fu, Y. Sun, H. Wang and X. Zheng, Stability and convergence of a Crank–Nicolson finite volume method for space fractional diffusion equations. Appl Numer Math 139 (2019), 38-51.

(9) H. Fu and H. Wang, A preconditioned fast parareal finite difference method for space-time fractional partial differential equation. J Sci Comput 78 (2019), 1724-1743.

(10) J. Gao, M. Zhao, N. Du, X. Guo, H. Wang and J. Zhang, A finite element method for space-time directional fractional diffusion partial differential equations in the plane and its error analysis, J Comput Appl Math, 362 (2019), 354-365.

(11) J. Jia, H. Wang, A fast finite volume method for conservative space-time fractional diffusion equations discretized on space-time locally refined meshes, Comput Math Appl 78 (2019), 1345-1356.

(12) J. Jia, H. Wang, A fast finite volume method on locally refined meshes for fractional diffusion equations, East Asian J Appl Math, 9 (2019), 755--779.

(13) J. Liu, H. Fu, H. Wang, and X. Chai, A preconditioned fast quadratic spline collocation method for two-sided space-fractional partial differential equations, J Comput Appl Math 360 (2019), 138-156.

(14) F. Wang, H. Chen, H. Wang, Finite element simulation and efficient algorithm for fractional Cahn–Hilliard equation, J Comput Appl Math 356 (2019), 248-266.

(15) F. Wang, H. Chen, H. Wang, Least squared mixed Galerkin formulation for variable-coefficient fractional differential equations with D-N boundary condition, Math Meth Appl Sci 42 (2019), 4331-4342.

(16) H. Wang and X. Zheng, Analysis and numerical solution of a nonlinear variable-order fractional differential equation. Adv Comput Math 45 (2019), 2647–2675.

(17) H. Wang, and X. Zheng, Wellposedness and regularity of the variable-order time-fractional diffusion equations, J Math Anal Appl 475 (2019), 1778-1802.

(18) H. Wang, X. Zheng, A modified time-fractional diffusion equation and its finite difference method: Regularity and error analysis. Fract Cal Appl Anal 22 (2019), 1014-1038.

(19) T. Wang, F. Song, H. Wang, and G. E. Karniadakis, Fractional Gray–Scott model: Well-posedness, discretization, and simulations, Computer Methods Appl Mech Engrg 347 (2019), 1030-1049.

(20) S. Yang, H. Chen, H. Wang, Least-squared mixed variational formulation based on space decomposition for a kind of variable-coefficient fractional diffusion problems, J Sci Comput, 78 (2019), 687-709.

(21) J. Zhao, L. Chen, H. Wang, On power law scaling dynamics for time-fractional phase field models during coarsening. Commun Nonlinear Sci Numer Simul 70 (2019), 257-270.

(22) M. Zhao, H. Wang, Fast finite difference methods for space-time fractional partial differential equations in three space dimensions with nonlocal boundary conditions, Appl Numer Math 145 (2019), 411-428.

(23) X. Zheng, J. Cheng, H. Wang, Uniqueness of determining the variable fractional order in variable-order time-fractional diffusion equations, Inverse Problems, 35 (2019), 125002.

(24) X. Zheng, V. J. Ervin, and H. Wang, Spectral approximation of a variable coefficient fractional diffusion equation in one space dimension, Appl Math Comp 361 (2019), 98-111.

(25) X. Zheng, H. Liu, H. Wang, H. Fu, An efficient finite volume method for nonlinear distributed-order space-fractional diffusion equations in three space dimensions, J Sci Comput 80 (2019), 1395--1418.

(26) X. Zheng, H. Wang, Wellposedness and regularity of a nonlinear variable-order fractional wave equation, Appl Math Lett, 95 (2019), 29--35.

(27) P. Dai, Q. Wu, X. Zheng, H. Wang, An efficient matrix splitting preconditioning technique for two-dimensional unsteady space-fractional diffusion equations, J Comput Appl Math 371 (2020), 112673, DOI: 10.1016/j.cam.2019.112673.

(28) N. Du, X. Guo, H. Wang, A fast state-based peridynamic numerical model, Commun Comput Phys 27 (2020), 274--291.

(29) N. Du, X. Guo, H. Wang, Fast upwind and Eulerian-Lagrangian control volume schemes for time-dependent directional space-fractional advection-dispersion equations, J Comput Phys 405 (2020), 109127.

(30) T. Wang, X. Li, H. Wang, An error estimate of a Eulerian-Lagrangian localized adjoint method for a space-fractional advection diffusion equation, Int'l J Num Anal Modeling 17 (2020), 151--171.

(31) X. Zheng, V.J. Ervin, H. Wang, An indirect finite element method for variable-coefficient space-fractional diffusion equations and its optimal order error estimates, Commun Appl Math Comp 2 (2020), 147--162.

(32) X. Zheng, H. Wang, An optimal-order numerical approximation to variable-order space-fractional diffusion equations on uniform or graded meshes, SIAM Numer Anal 58 (2020), 330--352.

(33) C. Chen, H. Liu, X. Zheng, H. Wang, A two-grid MMOC finite element method for nonlinear variable-order time-fractional mobile/immobile advection–diffusion equations, Comput Math Appl, https://doi.org/10.1016/j.camwa.2019.12.008

(34) X. Zheng, H. Wang, Wellposedness and smoothing properties of history-state based variable-order time-fractional diffusion equations, J Appl Math Phys (ZAMP), 71 (2020), 34. https://doi.org/10.1007/s00033-020-1253-5

(35) H. Wang, Fast numerical methods for space-fractional partial differential equations. Handbook of Fractional Calculus with Applications. Vol. 3, Numerical Methods, Karniadakis (Ed.), 307–328, De Gruyter, Berlin, 2019.

(36) J. Jia, X. Zheng, H. Fu, P. Dai, H. Wang, A fast method for variable-order space-fractional diffusion equations, Numer Algorithm, https://doi.org/10.1007/s11075-020-00875-z

(37) X. Zheng, H. Wang, Wellposedness and regularity of a variable-order space-time fractional diffusion equation, Analysis and Applications.

(38) Z. Fang, H. Sun, H. Wang, A fast method for a variable-order time-fractional PDE, submitted.

(39) B. Li, H. Wang, J. Wang, Well-posedness and numerical approximation of a fractional diffusion equation with a nonlinear variable order, submitted.

(40) X. Zheng, J. Cheng and H. Wang, Uniqueness of determining the variable fractional order in the boundary-value problem of variable-order linear space-fractional diffusion equations with variable diffusivity coefficients.

(41) X. Zheng and H. Wang, Finite element approximations to variable-order time-fractional diffusion equations and their analysis without regularity assumptions of the solutions, submitted.

Invited talks by the USC team:

Conference presentations:

(1) H. Wang, "Fractional partial differential equations and fractional phase-field models", Workshop on phase-field modeling and simulation, Xiaman University, China, 11/14-11/15, 2018.

(2) H. Wang, "A new time-fractional partial differential equation model", Modeling with fractional PDEs: Statistical and Numerical Analysis, SIAM Conference on Computational Science and Engineering, Spokane, Washington, 2/25-3/1, 2019.

(3) X. Zheng, "On mathematical and numerical analysis for the variable-order fractional differential equations", Modeling with fractional PDEs: Statistical and Numerical Analysis, SIAM Conference on Computational Science and Engineering, Spokane, Washington, 2/25-3/1, 2019.

(4) H. Wang, "On mathematical modeling and analysis of fractional partial differential equations", The Third Workshop on Numerical Methods for Fractional-derivative

Problems, Beijing Computational Science Research Center, Beijing, China, 4/26-4/27, 2019.

(5) X. Zheng, "Wellposedness and regularity of variable-order time-fractional diffusion equations", The Third Workshop on Numerical Methods for Fractional-derivative Problems, Beijing Computational Science Research Center, Beijing, China, 4/26-4/27, 2019.

(6) H. Wang, "Modeling anomalously diffusive transport of solutes in highly heterogeneous subsurface porous media", Workshop on Environmental Chemistry and Numerical Simulation, Hohai University, Nanjing China, 5/15, 2019.

(7) H. Wang, "Fractional partial differential equations: modeling, analysis and numeric", Workshop on Analysis, Scientific Computing and Applications of PDEs, School of Mathematics and Statistics, Qilu University of Technology, Jinan, China, 5/18, 2019.

(8) H. Wang, "On fractional and integer-order partial differential equations", Workshop on Mathematical Analysis and Numerical Approximations of Partial Differential Equations, School of Mathematical Sciences, East China Normal University, Shanghai, China, 5/18-5/20, 2019.

(9) H. Wang, "Mathematical analysis and numerical approximations of an improved time-fractional partial differential equation model", International Conference on Mathematical Modeling and Numerical Methods, Ocean University of China, Qingdao, China, 5/30-6/2, 2019.

(10) H. Wang, "Uniqueness of determining the parameters of time-fractional diffusion equations", Workshop on Parameter Identifications of Mathematical Modeling, Beijing Computational Science Research Center, Beijing, China, 6/3-6/6, 2019.

(11) H. Wang, "Mathematical modeling and numerical approximations of space-time fractional advection-diffusion equations", Forum on Interface Problems, Beijing Computational Science Research Center, Beijing, China, 6/7, 2019.

(12) H. Wang, "Mathematical modeling, analysis and numerical approximations of fractional partial differential equations", Advanced Numerical Methods for Scientific Computation, Southern University of Science and Technology, Shenzhen, China, 6/15-6/17, 2019.

(13) H. Wang, "A variable-order time-fractional diffusion equation model", Sino-German Bilateral Symposium on Anomalous & Non-Ergodic Diffusion: Modeling,

Theory, Application & Simulation, School of Mathematics and Statistics, Lanzhou University, Lanzhou, China, 6/23-6/28, 2009.

(14) H. Wang, “Mathematical modeling and analysis of variable-order time-fractional diffusion equations”, 2019 International Workshop on Scientific Computing, School of Mathematical Sciences, Tianjin Normal University, Tianjin, China, 7/4-7/7, 2019.

(15) X. Zheng, “On the mathematical analysis of the variable-order time-fractional diffusion equations and applications to the numerical approximations and inverse problems”, Annual Conference on Computational Mathematics, Harbin, China, 7/31-8/4, 2019.

(16) X. Zheng, “Analysis and numerical simulations of variable-order time-fractional diffusion equations”, SIAM_SEAS, Knoxville, Tennessee, 9/20-9/22, 2019.

(17) H. Wang, “Inverting the variable-order in a variable-order time-fractional diffusion equation: analysis and computation”, Workshop on Optimal Control and Optimization on Nonlocal Models Special Semester on Optimization, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, 10/28-10/30, 2019.

(18) H. Wang, “A variable-order time-fractional PDE: modeling, analysis and numerical approximation", AMS Special Session on Analysis of Nonlocal Models, Joint Mathematics Meetings, Colorado Convention Center, Denver, 1/15-1/18, 2020.

Colloquium and seminar talks:

(1) H. Wang, “On numerical methods for advection-diffusion equations modeling subsurface flow and transport”, Ocean University of China, 9/12, 2018.

(2) H. Wang, “On mathematical modeling of flow and transport in subsurface”, Tianjin Normal University, 10/11, 2018.

(3) H. Wang, “Fractional partial differential equation: model and fast computation”, Tianjin Normal University, 10/11, 2018.

(4) X. Zheng, “A spectral method for the boundary value problem of fractional diffusion equation”, Graduate Colloquium, Department of Mathematics, University of South Carolina, 10/23, 2018.

(5) X. Zheng, “Mathematical and numerical analysis for the space-fractional diffusion equation”, College of Science, China University of Petroleum, 12/20, 2018.

(6) X. Zheng, “Fractional Calculus and its applications in nonlocal modeling”, School of Petroleum Engineering, China University of Petroleum, 12/22, 2018.

(7) H. Wang, “A new mathematical model of time-fractional diffusion equation”, School of Mathematics, Ocean University of China, Qingdao, China, 3/22, 2019.

(8) H. Wang, “A new time-fractional diffusion equation model with improved regularity estimate”, School of Mathematics, Fudan University, Shanghai, China, 5/6, 2019.

(9) X. Zheng, “Wellposedness and regularity of variable-order time-fractional diffusion equations”, School of Mathematical Sciences, Fudan University, 5/6, 2019.

(10) X. Zheng, “Wellposedness and regularity of variable-order time-fractional diffusion equations”, School of Mathematical Sciences, East China Normal University, 5/10, 2019.

(11) H. Wang, “On fractional partial differential equations: modeling and analysis”, Department of Mathematics, Shanghai University, Shanghai, China, 5/13, 2019.

(12) X. Zheng, “Wellposedness and regularity of variable-order time-fractional diffusion equations”, College of Science, Shanghai University, 5/14, 2019.

(13) H. Wang, “Variable-order time-fractional diffusion equations and the identification of their parameters”, School of Mathematical Sciences, Southeast University, Nanjing, China, 5/16, 2019.

(14) H. Wang, “Mathematical analysis and numerical approximations of variable-order time-fractional diffusion equations”, School of Mathematical Sciences, Southeast University, Nanjing, China, 5/17, 2019.

(15) X. Zheng, “Wellposedness and regularity of variable-order time-fractional diffusion equations”, College of Science, Southeast University, 5/17, 2019.

(16) X. Zheng, “An efficient finite volume method for nonlinear distributed-order space-fractional diffusion equations”, School of Mathematics and Information Sciences, Yantai University, 5/24, 2019.

(17) H. Wang, “Fractional partial differential equations”, IMS PDE Seminar, The Institute of Mathematical Sciences, The Chinese University of Hong Kong, 6/14, 2019.

(18) H. Wang, “Mathematical modeling and fast numerical methods of fractional partial differential equations”, Department of Mathematics, University of Macau, Macau, 6/19, 2019.

(19) H. Wang, “Mathematical modeling of subsurface porous medium flow and transport”, Geotechnical & Structuring Engineering Research Center, Shandong University, Jinan, China, 7/7, 2019.

(20) H. Wang, "Modeling and derivation of fractional partial differential equations", Mechanical Engineering Seminar, Department of Mechanical Engineering, Michigan State University, 9/10, 2019.

(21) H. Wang, "Variable-order time-fractional partial differential equations", FMATH Group Meeting, Department of Mechanical Engineering, Michigan State University, 9/13, 2019.

(22) X. Zheng, "Finite element approximations to variable-order fractional differential equations without regularity assumptions of the true solutions", Huicui College, China University of Petroleum, 12/25, 2019.

(23) X. Zheng, "Numerical approximation to a space-fractional diffusion equation with non-smooth data", School of Mathematics and Statistics, Shandong Normal University, 12/27, 2019.

(24) H. Wang, "A continuous time random walk modeling of fractional diffusion partial differential equations", Ocean University of China, Qingdao, China, 1/3, 2020.

(25) H. Wang, "Fractional partial differential equations: their continuous time random walk derivation and numerical simulation", Department of Mathematics, University of Macau, Macau, 1/7, 2020.

Other activities:

(1) Hong Wang and Zhongqiang Zhang organized a mini-symposium on Modeling with fractional PDEs: Statistical and Numerical Analysis, SIAM Conference on Computational Science and Engineering, Spokane, Washington, 2/25-3/1, 2019.

(2) Hong Wang and Zhongqiang Zhang organized a mini-symposium on Modelling with Fractional PDEs: Numerical Analysis and Applications, SIAM Annual Meeting, Toronto, 7/6-7/10,2020.

All products acknowledge support from ARO grant W911NF-15-1-0562.

Rice University Report (co-PI: Pol Spans)

(Research Areas 4 & 5)

Research Work on Dynamic Systems with Fractional Laplacian Operators under Deterministic and Stochastic Excitation

I. Introduction

Dynamic systems with fractional Laplacian operators have been examined. Both deterministic and stochastic excitation have been considered. The fractional Laplacian is an integro-differential

operator that is currently widely used in nonlocal models, such as the anomalous diffusion, which arises when a particle moves randomly in the space involving a random process that allows long jumps. In a bounded domain, there are different definitions of the fractional Laplacian, of which the Riesz-Marchaud and the Caputo-type representation have been examined in this research effort.

II. Boundary Element Approach

First, a BEM-based approximation scheme has been developed for a system endowed with the fractional Laplacian based on the Riesz-Marchaud definition. For a fractional diffusion equation, the algorithm is constructed by utilizing the integral representation of the fractional Poisson equation solution, as the analog equation, in which the unknown constants are determined by the BEM.

Second, properties of the Caputo-type fractional Laplacian have been examined. A BEM–based approach to determine the response of a dynamic system endowed with the fractional Laplacian term has been developed. The analog equation used in the BEM formulation is the classical Poisson equation. Then, based on the Caputo-type representation, the integral equation of the solution has been derived. The value of the fractional Laplacian of the response is updated progressively by matrix transformation of the unknown load. Related numerical results have validated the developed procedures.

The work has been presented at the 8th Computational Stochastic Mechanics Conference (CMS8) held in Paros, Greece 2018, June 10-14, 2018.
The paper is entitled “Boundary Element Method Based Approach for Estimating the Response of a System Governed by a Stochastic Nonlinear Fractional Diffusion Equation” with authors Yiyu Jiao, Giovanni Malara and Pol D. Spanos.

III. Statistical Linearization Approach

Determining the response of a stochastic system involving the fractional Laplacian operator is a daunting task. In this work, a novel expansion of the factional Laplacian has been attempted. Statistical linearization has been developed for an efficient determination, albeit approximate, of stochastic dynamic systems with fractional Laplacian terms.

First, a novel treatment of the fractional Laplacian has been introduced. The utilized eigenfunctions are calculated by a special integral transformation of the linear modes of the classical diffusion equation solution. The series expansion representation is equivalent to the Caputo-type definition.

Second, a statistical linearization approach has been developed for frequency domain analysis of the nonlinear fractional diffusion equations. The proposed expansion allows deriving a multi-degree-of-freedom nonlinear fractional ordinary differential equation. Such a system can be recast in a nonlinear matrix differential equation, which is linearized in a stochastic mean-square sense. Input-output relation and iterative scheme can then be applied to obtain the response statistics. Further, when the order of the fractional Laplacian is close to 2, the non-diagonal entries in the matrix can be ignored so that a simplified statistical linearization approximation can be developed.

The work on the novel expansion and complete statistical linearization has been presented by the

8th Computational Stochastic Mechanics Conference (CMS8) held in Paros, Greece 2018.

The paper is entitled "Statistical Linearization Approach for Calculating the Response Statistics of a System Governed by a Nonlinear Fractional Diffusion Equation" with authors Giovanni Malara, Yiyu Jiao and Pol D. Spanos.

IV. Large nonlinear vibrations of a beam excited by combined harmonic and random loads

A fundamental requirement in civil and mechanical engineering applications is the capacity to determine the response of a structural element subject to a prescribed load. For this purpose, a variety of techniques is available in the open literature for estimating the system response when the excitation is either harmonic or random. However, limited investigations have been undertaken in case of combined harmonic and random loads. This problem is important is several applications where, for instance, there are two distinct agents exciting simultaneously the system.

This work pursues an approximate approach for estimating the response of beam endowed by fractional derivative terms excited by the combined action of harmonic and random load. The beam equation is based on the assumption of large deformation. Further, it considers the contribution of fractional derivative elements representing, for instance, an external load on the structure. The load is of a separable type and the space-wise distribution of the harmonic and random loads is assumed identical.

The approach combines the harmonic balance and statistical linearization techniques for estimating the response statistics and the response spectrum. Indeed, the beam displacement is expanded by the linear modes of beam vibration. Then, by projecting the beam equation on the space of the linear modes, a system of nonlinear fractional ordinary differential equations (NFODE) governing the time varying amplitudes of the linear modes is obtained. Such a system of equations can be possibly solved by representing the solution as a superposition of a harmonic and of a random part. The harmonic part of the response is determined by utilizing the harmonic balance technique on the NFODE after considering ensamble averaging, while the random part of the response is determined from the NFODE by the statistical linearization technique. The response statistics can be determined by an iterative procedure involving the minimization of the mean square error of the system response. Relevant Monte Carlo data pertaining to a simply supported beam uniformly excited by a harmonic load combined with a random white noise will be used to ascertain the reliability of the proposed approach.

V. Personnel:

Y. Jiao, Graduate Student
G. Malara, Post-Graduate Fellow
P. Spanos, Faculty

Brown University Report (PI: George Karniadakis & co-PI: Mark Ainsworth)

(Research Areas 1-6)

Personnel: PI Karniadakis was supported for 3.05 months, and co-PI Ainsworth for 1.7 months. Moreover, Dr. He Li (4.9 months), Dr. Zhen Li (1 month), Dr. Zhiping Mao (12 months), Dr. Maziar Raissi (0.5 month), Dr. Guofei Pang (5 months), Dr. Alireza Yazdani (0.5 month), Dr. Mengjia Xu (1 month), and Dr. Xiaoning Zheng (3 months) participated as postdocs. The following PhD students were also supported by the MURI: Ansel Blumers (10 months), Anna Lischke (1 month), Lu Lu (2 months), Liu Yang (11 months), and Minglang Yin (10 months). In

addition, the following visiting scholars were supported by the MURI: Ladan Avazpour (6 months) and Kaixuan Zhang (5.5 month).

Research at Brown U: Mark Ainsworth

Hybrid finite element-spectral method for the fractional Laplacian: Approximation theory and efficient solver (M. Ainsworth and C. Glusa) [2]: A numerical scheme is presented for approximating fractional order Poisson problems in two and three dimensions. The scheme is based on reformulating the original problem posed over Ω on the extruded domain $C = \Omega \times [0, \infty)$ following [L. Caffarelli and L. Silvestre, Comm. Partial Differential Equations, 32 (2007), pp. 1245-1260]. The resulting degenerate elliptic integer order PDE is then approximated using a hybrid FEM-spectral scheme. Finite elements are used in the direction parallel to the problem domain Ω, and an appropriate spectral method is used in the extruded direction. The spectral part of the scheme requires that we approximate the true eigenvalues of the integer order Laplacian over Ω. We derive an a priori error estimate which takes account of the error arising from using an approximation in place of the true eigenvalues. We further present a strategy for choosing approximations of the eigenvalues based on Weyl's law and finite element discretizations of the eigenvalue problem. The system of linear algebraic equations arising from the hybrid FEM- spectral scheme is decomposed into blocks which can be solved effectively using standard iterative solvers such as multigrid and conjugate gradient. Numerical examples in two and three dimensions suggest that the approach is quasi-optimal in terms of complexity.

Aspects of an adaptive finite element method for the fractional Laplacian: a priori and a posteriori error estimates, efficient implementation and multigrid solver. (M. Ainsworth and C. Glusa) [1]: We develop all of the components needed to construct an adaptive finite element code that can be used to approximate fractional partial differential equations, on non-trivial domains in dimensions. Our main approach consists of taking tools that have been shown to be effective for adaptive boundary element methods and, where necessary, modifying them so that they can be applied to the fractional PDE case. Improved a priori error estimates are derived for the case of quasi-uniform meshes which are seen to deliver sub-optimal rates of convergence owing to the presence of singularities. Attention is then turned to the development of an a posteriori error estimate and error indicators which are suitable for driving an adaptive refinement procedure. We assume that the resulting refined meshes are locally quasi-uniform and develop efficient methods for the assembly of the resulting linear algebraic systems and their solution using iterative methods, including the multigrid method. The storage of the dense matrices along with efficient techniques for computing the dense matrix-vector products needed for the iterative solution is also considered. The performance and efficiency of the resulting algorithm is illustrated for a variety of examples.

Well-posedness of the Cahn-Hilliard equation with fractional free energy and its Fourier Galerkin approximation (M. Ainsworth and Z. Mao) [5]: We study the well-posedness of the Cahn-Hilliard equation in which the gradient term in the free energy is replaced by a fractional derivative. We begin by establishing the existence and uniqueness of a Fourier-Galerkin approximation and then derive a number of priori estimates for the Fourier-Galerkin scheme. Compactness arguments are then used to deduce the existence and uniqueness of the solution to the fractional Cahn-Hilliard equation. An estimate for the rate of convergence of the Fourier-

Galerkin approximation is then obtained. Finally, we present some numerical illustrations of typical solutions to the fractional Cahn-Hilliard equation and how they vary with the fractional order β and the parameter ϵ. In particular, we show how the width τ of the diffuse interface depends on ϵ and β, and derive the scaling law $\tau = O(\epsilon^{1/\beta})$ which is verified numerically.

Analysis and approximation of a fractional Cahn-Hilliard equation (M. Ainsworth and Z. Mao) [4]: We derive a fractional Cahn-Hilliard equation (FCHE) by considering a gradient flow in the negative order Sobolev space $H^{-\alpha}$, $\alpha \in [0,1]$, where the choice $\alpha = 1$ corresponds to the classical Cahn-Hilliard equation while the choice $\alpha = 0$ recovers the Allen-Cahn equation. The existence of a unique solution is established, and it is shown that the equation preserves mass for all positive values of fractional order α and that it indeed reduces the free energy. We then turn to the delicate question of the L^∞ boundedness of the solution and establish an L^∞ bound for the FCHE in the case where the nonlinearity is a quartic polynomial. As a consequence of the estimates, we are able to show that the Fourier-Galerkin method delivers a spectral rate of convergence for the FCHE in the case of a semi-discrete approximation scheme. Finally, we present results obtained using computational simulation of the FCHE for a variety of choices of fractional order α. It is observed that the nature of the solution of the FCHE with a general $\alpha > 0$ is qualitatively (and quantitatively) closer to the behavior of the classical Cahn--Hilliard equation than to the Allen-Cahn equation, regardless of how close to zero the value of α is. An examination of the coarsening rates of the FCHE reveals that the asymptotic rate is rather insensitive to the value of α and, as a consequence, is close to the well-established rate observed for the classical Cahn-Hilliard equation.

Towards an Efficient Finite Element Method for the Integral Fractional Laplacian on Polygonal Domains (M. Ainsworth and C. Glusa) [3]: We explore the connection between fractional order partial differential equations in two or more spatial dimensions with boundary integral operators to develop techniques that enable one to efficiently tackle the integral fractional Laplacian. In particular, we develop techniques for the treatment of the dense stiffness matrix including the computation of the entries, the efficient assembly and storage of a sparse approximation and the efficient solution of the resulting equations. The main idea consists of generalizing proven techniques for the treatment of boundary integral equations to general fractional orders. Importantly, the approximation does not make any strong assumptions on the shape of the underlying domain and does not rely on any special structure of the matrix that could be exploited by fast transforms. We demonstrate the flexibility and performance of this approach in a couple of two-dimensional numerical examples.

Well-posedness of the Cahn-Hilliard equation with fractional free energy and its Fourier-Galerkin approximation (M. Ainsworth and Z. Mao) [6]: We establish the well-posedness of the fractional PDE which arises by considering the gradient flow associated with a fractional Gross–Pitaevskii free energy functional and some basic properties of the solution. The equation reduces to the Allen–Cahn or Cahn–Hilliard equations in the case where the mass tends to zero and an integer order derivative is used in the energy. We study how the presence of a non-zero mass affects the nature of the solutions compared with the Cahn–Hilliard case. In particular, we show that, analogous to the Cahn–Hilliard case, the solutions consist of regions in which the solution is a piecewise constant (whose value depends on the mass and the fractional order) separated by an interface whose width is independent of the mass and the fractional derivative.

However, if the average value of the initial data exceeds some threshold (which we determine explicitly), then the solution will tend to a single constant steady state.

Fractional Phase Field Crystal Modelling: Analysis, Approximation and Pattern formation (M. Ainsworth and Z. Mao) [7]: 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.

Whilst the salient features of PFC and FPFC are identical, we expect more subtle features to differ. The prediction of grain boundary energy arising from a mismatch in orientation across a material interface is another notable success of the PFC model. The grain boundary energy can be evaluated numerically from the PFC model and compared with experimental measurements. The grain boundary energy is a derived quantity and is more sensitive to the nuances of the model. We compare the predictions obtained using the PFC and FPFC models with experimental observations of the grain boundary energy for several materials. It is observed that the FPFC model gives superior agreement with the experimental observation than those obtained using the classical PFC model, especially when the mismatch in orientation becomes larger.

References

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Research at Brown U: George Karniadakis

What Is the Fractional Laplacian? [1]: The fractional Laplacian in R^d, which we write as $(-\Delta)^{\alpha/2}$ with $\alpha \in (0,2)$, has multiple equivalent characterizations. Moreover, in bounded domains, boundary conditions must be incorporated in these characterizations in mathematically distinct ways, and there is currently no consensus in the literature as to which definition of the fractional Laplacian in bounded domains is most appropriate for a given application. The Riesz (or integral) definition, for example, admits a nonlocal boundary condition, where the value of a function u(x) must be prescribed on the entire exterior of the domain in order to compute its fractional Laplacian. In contrast, the spectral definition requires only the standard local boundary condition. These differences, among others, lead us to ask the question: "What is the fractional Laplacian?" We compare several commonly used definitions of the fractional Laplacian, and we use a quantitative approach to identify their practical differences. Indeed, the purpose of the present study is to identify features and differences in the solutions arising from the different commonly used definitions of the fractional Laplacian. This work provides useful information for researchers using the fractional Laplacian in developing new mathematical models, so that they may select the most appropriate definition for their application. We aim to compare different definitions on bounded domains using a collection of benchmark problems, in which we consider the fractional Poisson equation with both zero and nonzero boundary conditions, where the fractional Laplacian is defined according to the Riesz definition, the spectral definition, the directional definition, and the horizon-based nonlocal definition. We verify the accuracy of the numerical methods used in the approximations for each operator, and we focus on identifying differences in the features of the numerical solutions. In this work, we provide a quantitative assessment of new numerical methods as well as available state-of-the-art methods for discretizing the fractional Laplacian, and we present new results on the differences in features, regularity, and boundary behaviors of solutions to equations posed with these different definitions. We present stochastic interpretations and demonstrate the equivalence between some recent formulations. Through our efforts, we aim to further engage the research community in open problems and assist practitioners in identifying the most appropriate definition and computational approach to use for their mathematical models in addressing anomalous transport in diverse applications.

Petrov-Galerkin spectral method for FPDEs with end-point singularities [2]: We consider the 1-D diffusion equation with general two-sided fractional derivative characterized by a parameter $p \in [0, 1]$; for $p = 1/2$ we recover the Riesz fractional derivative while for $p = 1$, 0 we obtain the one-sided fractional derivative. We employ a Petrov-Galerkin projection in a properly weighted Sobolev space with (two-sided) Jacobi poly-fractonomials as basis and test functions. In particular, we derive these two-sided Jacobi poly-fractonomials as eigenfunctions of a Sturm-Liouville problem with weights uniquely determined by the parameter p. We provide a rigorous

analysis and obtain optimal error estimates that depend on the regularity of the forcing term, i.e., for smooth data (corresponding to singular solutions) we obtain exponential convergence while for smooth solutions we obtain algebraic convergence. We demonstrate the sharpness of our error estimates with numerical examples, and we present comparisons with a competitive spectral collocation method of tunable accuracy. We also investigate numerically deviations from the theory for inhomogeneous Dirichlet boundary conditions as well as for a fractional diffusion-reaction equation.

Spectral/spectral element methods using penalty for two-sided fractional differential equations with general boundary conditions [3, 13]: We first consider spectral approximations to the conservative form of the two-sided Riemann-Liouville (R-L) and Caputo fractional differential equations (FDEs) with nonhomogeneous Dirichlet (fractional and classical, respectively) and Neumann (fractional) boundary conditions. In particular, we develop a spectral penalty method (SPM) by using the Jacobi poly-fractonomial approximation for the conservative R-L FDEs while using the polynomial approximation for the conservative Caputo FDEs. We establish the well-posedness of the corresponding weak problems and analyze sufficient conditions for the coercivity of the SPM for different types of fractional boundary value problems. This analysis allows us to estimate the proper values of the penalty parameters at boundary points. We present several numerical examples to verify the theory and demonstrate the high accuracy of SPM, both for stationary and time dependent FDEs. Moreover, we compare the results against a Petrov-Galerkin spectral tau method (PGS-τ, an extension of [2]) and demonstrate the superior accuracy of SPM for all cases considered.

Secondly, we developed a multi-domain spectral collocation method for FPDEs in the Riemann–Liouville sense with Dirichlet boundary conditions by employing Jacobi Lagrangian interpolants to represent the solution in each element. We provide variable-order differentiation formulas, which can be computed efficiently for the multi-domain discretization taking into account the nonlocal interactions. We enforce the interface continuity conditions by matching the solution values at the element boundaries via the Lagrangian interpolants, and in addition we minimize the jump in (integer) fluxes using a penalty method. We analyze numerically the effect of the penalty parameter on the condition number of the global differentiation matrix and on the stability and convergence of the penalty collocation scheme. We demonstrate the effectiveness of the new method for the fractional Helmholtz equation of constant and variable-order using h−p refinement for different values of the penalty parameter. We also solve the fractional Burgers equation with constant and variable-order and compare with solutions obtained with a single domain spectral collocation method.

Fast solvers for adaptive finite element method and spectral element method applied to fractional differential equations using hierarchical matrix approximation [4, 5]: Firstly, we develop a robust and fast solver for the fractional differential equation (FDEs) involving the Riesz fractional derivative using an adaptive finite element method. It is based on the utilization of hierarchical matrices (H-Matrices) for the representation of the stiffness matrix resulting from the finite element discretization of the FDEs. We employ a geometric multigrid method for the solution of the algebraic system of equations. We combine it with an adaptive algorithm based on a posteriori error estimation. We use a posteriori error estimation based adaptive algorithm to deal with general-type singularities arising in the solution of the FDEs. Through various test

examples we demonstrate the efficiency of the method and the high accuracy of the numerical solution even in the presence of singularities. The proposed technique has been verified effectively through fundamental examples including Riesz, Left/Right Riemann–Liouville fractional derivative and, furthermore, it can be readily extended to more general fractional differential equations with different boundary conditions and low-order terms.

Secondly, we develop a fast solver for the spectral element method (SEM) applied to the two-sided fractional diffusion equation on uniform, geometric and graded meshes. By approximating the singular kernel with a degenerate kernel, we construct a H-matrix to represent the stiffness matrix of the SEM and provide error estimates verified numerically. We can solve efficiently the H-matrix approximation problem using a hierarchical LU decomposition method, which reduces the computational cost to $O(R^2N_d \log^2 N) + O(R^3N_d \log N)$, where R it is the rank of submatrices of the H-matrix approximation, Nd is the total number of degrees of freedom and N is the number of elements. However, we lose the high accuracy of the SEM. Thus, we solve the corresponding preconditioned system by using the H-matrix approximation problem as a preconditioner, recovering the high order accuracy of the SEM. The condition number of the preconditioned system is independent of the polynomial degree P and grows with the number of elements, but at modest values of the rank R is below order 10 in our experiments, which represents a reduction of more than 11 orders of magnitude from the un-preconditioned system; this reduction is higher in the two-sided fractional derivative compared to one-sided fractional derivative. The corresponding cost is $O(R^2N_d \log^2 N) + O(R^3N_d \log N) + (O(N_d^2)$. Moreover, by using a structured mesh (uniform or geometric mesh), we can further reduce the computational cost to $O(R^2N_d \log^2 N)+O(R^3N_d \log N)+O(P^2N \log N)$ for the preconditioned system. We present several numerical tests to illustrate the proposed algorithm using h and p refinements.

Fractional Gray-Scott model: well-posedness, discretization, and simulations [6]: The Gray-Scott (GS) model represents the dynamics and steady state pattern formation in reaction-diffusion systems and has been extensively studied in the past. In this paper, we consider the effects of anomalous diffusion on pattern formation by introducing the fractional Laplacian into the GS model. First, we prove that the continuous solutions of the fractional GS model are unique. We then introduce the Crank-Nicolson (C-N) scheme for time discretization and weighted shifted Grünwald difference operator for spatial discretization. We perform stability analysis for the time semi-discrete numerical scheme, and furthermore, we analyze numerically the errors with benchmark solutions that show second-order convergence both in time and space. We also employ the spectral collocation method in space and C-N scheme in time to solve the GS model in order to verify the accuracy of our numerical solutions. We observe the formation of different patterns at different values of the fractional order, which are quite different than the patterns of the corresponding integer-order GS model, and quantify them by using the radial distribution function (RDF). Finally, we discover the scaling law for steady patterns of the RDFs in terms of the fractional order $1 < \alpha \leq 2$.

Machine learning of space-fractional differential equations [7]: Data-driven discovery of "hidden physics" – i.e., machine learning of differential equation models underlying observed data – has recently been approached by embedding the discovery problem into a Gaussian Process regression of spatial data, treating and discovering unknown equation parameters as hyperparameters of a "physics informed" Gaussian Process kernel. This kernel includes the

parametrized differential operators applied to a prior covariance kernel. We extend this framework to the data-driven discovery of linear space-fractional differential equations. The methodology is compatible with a wide variety of space-fractional operators in Rd and stationary covariance kernels, including the Matérn class, and allows for optimizing the Matérn parameter during training. The main challenges to be addressed are a user-friendly way to perform fractional-order derivatives of covariance kernels, together with numerical methods that render such implementations feasible. Making use of the simple Fourier-space representation of *space-fractional* derivatives in Rd, we provide a unified set of integral formulas for the resulting Gaussian Process kernels. The shift property of the Fourier transform results in formulas involving d-dimensional integrals that can be efficiently treated using generalized Gauss-Laguerre quadrature. The implementation of fractional derivatives has several benefits. First, the method allows for discovering models involving fractional-order PDEs for systems characterized by heavy tails or anomalous diffusion, while bypassing the analytical difficulty of fractional calculus. Data sets exhibiting such features are of increasing prevalence in physical and financial domains. Second, a single fractional-order archetype allows for a derivative term of arbitrary order to be learned, with the order itself being a parameter in the regression. As a result, even when used for discovering integer-order equations, the proposed method has several benefits compared to previous works on data-driven discovery of differential equations; the user is not required to assume a "dictionary" of derivatives of various orders, and directly controls the parsimony of the models being discovered. We illustrate our method on several examples, including fractional-order interpolation of advection-diffusion and modeling relative stock performance in the S&P 500 with α-stable motion via a fractional diffusion equation.

Second-order numerical methods for multi-term fractional differential equations: Smooth and non-smooth solutions [8]: Starting with the asymptotic expansion of the error equation of the shifted Grunwald–Letnikov formula, we derive a new modified weighted shifted Grunwald–Letnikov (WSGL) formula by introducing appropriate correction terms. We then apply one special case of the modified WSGL formula to solve multi-term fractional ordinary and partial differential equations, and we prove the linear stability and second-order convergence for both smooth and non-smooth solutions when the regularity of the solutions is known. We show theoretically and numerically that numerical solutions with good accuracy can be obtained with only a few correction terms. Moreover, the correction terms can be tuned according to the fractional derivative orders without explicitly knowing the analytical solutions. Numerical simulations verify the theoretical results and demonstrate that the new WSGL formula leads to better performance compared to other known numerical approximations with similar resolution.

A new class of semi-implicit methods with linear complexity for nonlinear fractional differential equations [9]: We propose a new class of semi-implicit methods for solving nonlinear fractional differential equations and study their stability. Several versions of our new schemes are proved to be unconditionally stable by choosing suitable parameters. Subsequently, we develop an efficient strategy to calculate the discrete convolution for the approximation of the fractional operator in the semi-implicit method and we derive an error bound of the fast convolution. The memory requirement and computational cost of the present semi-implicit methods with a fast convolution are about $O(N \log n_T)$ and $O(Nn_T \log n_T)$, respectively, where N is a suitable positive integer and n_T is the final number of time steps. Numerical simulations, including the solution of a system of two nonlinear fractional diffusion equations with different

fractional orders in two-dimensions, are presented to verify the effectiveness of the semi-implicit methods.

Efficient Multistep methods for tempered fractional calculus: algorithms and simulations: [10] In this work, we extend the fractional linear multistep methods in [C. Lubich, SIAM J. Math. Anal., 17 (1986), pp.704–719] to the tempered fractional integral and derivative operators in the sense that the tempered fractional derivative operator is interpreted in terms of the Hadamard finite-part integral. We develop two fast methods, Fast Method I and Fast Method II, with linear complexity to calculate the discrete convolution for the approximation of the (tempered) fractional operator. Fast Method I is based on a local approximation for the contour integral that represents the convolution weight. Fast Method II is based on a globally uniform approximation of the trapezoidal rule for the integral on the real line. Both methods are efficient, but numerical experimentation reveals that Fast Method II outperforms Fast Method I in terms of accuracy, efficiency, and coding simplicity. The memory requirement and computational cost of Fast Method II are $O(Q)$ and $O(Q_{n_T})$, respectively, where n_T is the number of the final time steps and Q is the number of quadrature points used in the trapezoidal rule. The effectiveness of the fast methods is verified through a series of numerical examples for long-time integration, including a numerical study of a fractional reaction-diffusion model.

fPINNs: Fractional Physics-Informed Neural Networks: [11] Physics-informed neural networks (PINNs) are effective in solving integer-order partial differential equations (PDEs) based on scattered and noisy data. PINNs employ standard feedforward neural networks (NNs) with the PDEs explicitly encoded into the NN using automatic differentiation, while the sum of the mean-squared PDE-residuals and the mean-squared error in initial/boundary conditions is minimized with respect to the NN parameters. We extend PINNs to fractional PINNs (fPINNs) to solve space-time fractional advection-diffusion equations (fractional ADEs), and we demonstrate their accuracy and effectiveness in solving multi-dimensional forward and inverse problems with forcing terms whose values are only known at randomly scattered spatio-temporal coordinates (black-box forcing terms). A novel element of the fPINNs is the hybrid approach that we introduce for constructing the residual in the loss function using both automatic differentiation for the integer-order operators and numerical discretization for the fractional operators. We consider 1D time-dependent fractional ADEs and compare white-box (WB) and black-box (BB) forcing. We observe that for the BB forcing fPINNs outperform FDM. Subsequently, we consider multi-dimensional time-, space-, and space-time-fractional ADEs using the directional fractional Laplacian and we observe relative errors of 10^{-4}. Finally, we solve several inverse problems in 1D, 2D, and 3D to identify the fractional orders, diffusion coefficients, and transport velocities and obtain accurate results even in the presence of significant noise.

Stochastic Solution of Elliptic and Parabolic Boundary Value Problems for the Spectral Fractional Laplacian: [12] We prove and implement stochastic solution (or Feynman-Kac) formulas for boundary value problems involving the spectral fractional Laplacian with nonzero Dirichlet boundary condition. The main tools used in the proofs are the abstract Cauchy problem for Feller semigroups together with Balakrishnan's theory of fractional powers. We show the spectral fractional Laplacian with nonzero Dirichlet boundary conditions is the generator of an appropriate Feller semigroup for subordinate stopped Brownian motion, and obtain a stochastic

solution formula for the fractional heat equation in a bounded domain. We then obtain precise regularity and steady-state convergence properties of the parabolic problem using the eigenfunction expansion of the classical solution, which leads to estimates for the survival probability of subordinate stopped Brownian motion. These results allow us to take the long-time limit in the parabolic formula to establish a stochastic solution formula for the Dirichlet boundary value problem. These stochastic solution formulas for the spectral fractional Laplacian with nonzero boundary conditions are novel, and allow for efficient, embarrassingly parallel Monte Carlo solution of the boundary value problems. We discuss the discretization of these formulas, and verify them in dimensions two, three and sixteen with benchmark examples. We study the effect of the number of path samples and the time step size for path discretization on the accuracy of the solution.

A stabilized semi-implicit Fourier spectral method for nonlinear space-fractional reaction-diffusion equations: [14] The reaction-diffusion model can generate a wide variety of spatial patterns, which has been widely applied in chemistry, biology, and physics, even used to explain self-regulated pattern formation in the developing animal embryo. In this work, a second-order stabilized semi-implicit time-stepping Fourier spectral method for the reaction-diffusion systems of equations with space described by the fractional Laplacian is developed. We adopt the temporal-spatial error splitting argument to illustrate that the proposed method is stable without imposing the CFL condition, and an optimal L^2-error estimate in space is proved. We also analyze the linear stability of the stabilized semi-implicit method and obtain a practical criterion to choose the time step size to guarantee the stability of the semi-implicit method. Our approach is illustrated by solving several problems of practical interest, including the fractional Allen-Cahn, Gray-Scott and FitzHugh-Nagumo models, together with an analysis of the properties of these systems in terms of the fractional power of the underlying Laplacian operator, which are quite different from the patterns of the corresponding integer-order model.

A Universal Fractional Model of Wall-Turbulence: [15] Modeling of wall-bounded turbulent flows is still an open problem in classical physics, with only modest progress made in the last few decades beyond the so- called 'log law', which describes only the intermediate region in wall-bounded turbulence, i.e., $30 - 50y+$ to $0.1 - 0.2R+$ (in wall units) in a pipe of radius R. Here we propose a fundamentally new approach based on fractional calculus to model the entire mean velocity profile from the wall to the centerline of the pipe. Specifically, we represent the Reynolds stresses with a non-local fractional derivative of variable order that decays with the distance from the wall. Surprisingly, we find that this variable fractional order has a universal form for all Reynolds numbers and for three different flow types, i.e., channel flow, Couette flow, and pipe flow. We first use existing data bases from direct numerical simulations (DNS) to learn the variable fractional order function, and subsequently we test it against other DNS data and experimental measurements, including the Princeton superpipe experiments. Taken together, our findings reveal the continuous and decaying change of rate of turbulent diffusion from the wall as well as the strong non-locality of turbulent interactions that intensify away from the wall.

Discovering a universal variable-order fractional model for turbulent Couette flow using a physics-informed neural network: [16] The first fractional model for Reynolds stresses in wall-bounded turbulent flows was proposed by W. Chen. Here, we extend this formulation by

allowing the fractional order $\alpha(y)$ of the model to vary with the distance from the wall (y) for turbulent Couette flow. Using available direct numerical simulation (DNS) data, we formulate an inverse problem for $\alpha(y)$ and design a physics-informed neural network (PINN) to obtain the fractional order. Surprisingly, we found a universal scaling law for $\alpha(y+)$, where $y+$ is the non-dimensional distance from the wall in wall units. Therefore, we obtain a variable-order fractional model that can be used at any Reynolds number to predict the mean velocity profile and Reynolds stresses with accuracy better than 1%.

Nonlocal flocking dynamics: Learning the fractional order of PDEs from particle simulations: [17] Flocking refers to collective behavior of a large number of interacting entities, where the interactions between discrete individuals produce collective motion on the large scale. We employ an agent-based model to describe the microscopic dynamics of each individual in a flock and use a fractional partial differential equation (fPDE) to model the evolution of macroscopic quantities of interest. The macroscopic models with phenomenological interaction functions are derived by applying the continuum hypothesis to the microscopic model. Instead of specifying the fPDEs with an *ad hoc* fractional order for nonlocal flocking dynamics, we learn the effective nonlocal influence function in fPDEs directly from particle trajectories generated by the agent-based simulations. We demonstrate how the learning framework is used to connect the discrete agent-based model to the continuum fPDEs in one- and two-dimensional nonlocal flocking dynamics. In particular, a Cucker-Smale particle model is employed to describe the microscale dynamics of each individual, while Euler equations with non-local interaction terms are used to compute the evolution of macroscale quantities. The trajectories generated by the particle simulations mimic the field data of tracking logs that can be obtained experimentally. They can be used to learn the fractional order of the influence function using a Gaussian process regression model implemented with the Bayesian optimization. We show in one- and two-dimensional benchmarks that the numerical solution of the learned Euler equations solved by the finite volume scheme can yield correct density distributions consistent with the collective behavior of the agent-based system solved by the particle method. The proposed method offers new insights on how to scale the discrete agent-based models to the continuum-based PDE models, and could serve as a paradigm on extracting effective governing equations for nonlocal flocking dynamics directly from particle trajectories.

Development of Fractional Nektar Solver (F-Nekar): We developed an eigen-based algorithm for computing the fractional Laplacian defined by the eigenfunction expansion on finite 2D/3D complex domains with both homogeneous and nonhomogeneous boundary. We implemented the algorithm into spectral element Navier-Stokes equation solver Nektar and extended it to **F-Nektar**.

1. We demonstrate the excellent scalability of our algorithm on large clusters by solving diffusion problems using up to thousands of CPUs, see Figure 1.

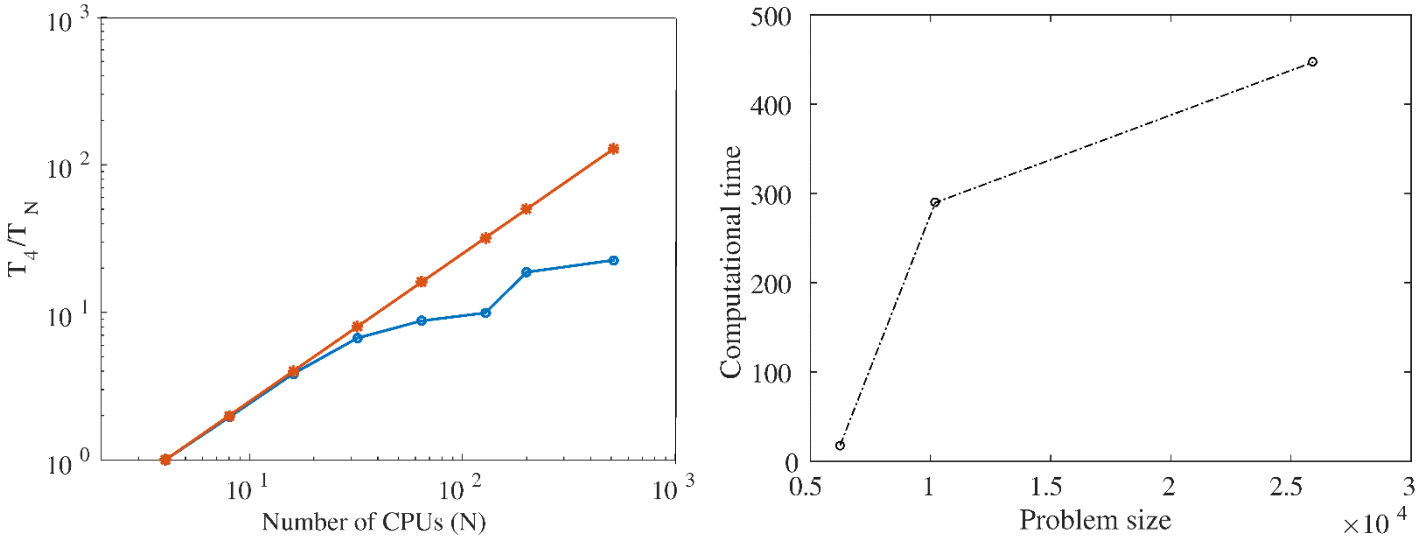

Figure 1: Left: Parallel efficiency of solving fractional diffusion equation using spectral element method with the implementations of ScaLapack routine PDSYGVX with matrix size 6241x6241. T_N - time required for solving generalized eigenvalue problem with N CPUs. Right: Computational time (s) versus matrix size using 128 CPUs.

2. To demonstrate the accuracy of this eigen-based approach, we solved the fractional diffusion equation and fractional Helmholtz equation on a 2D quadrilateral, a 3D cubic/cylindrical domain, compared the results with the contrived solutions and showed the error convergence in space, see Figure 2 for the 2D convergence test results.

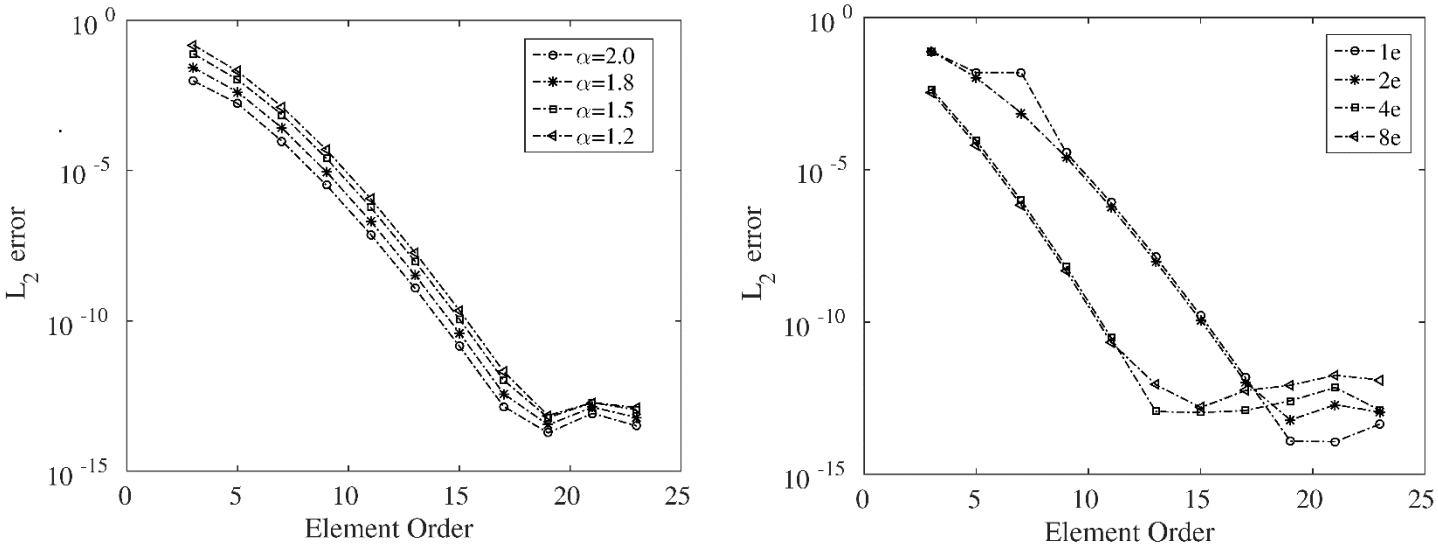

Figure 2: Convergence results for the fractional diffusion equation in 2D. Left: p-refinement, right: h-refinement.

3. We solved fractional diffusion equation on a complex 2D mesh 14641 quad elements (Hanford site). See Figure 3.

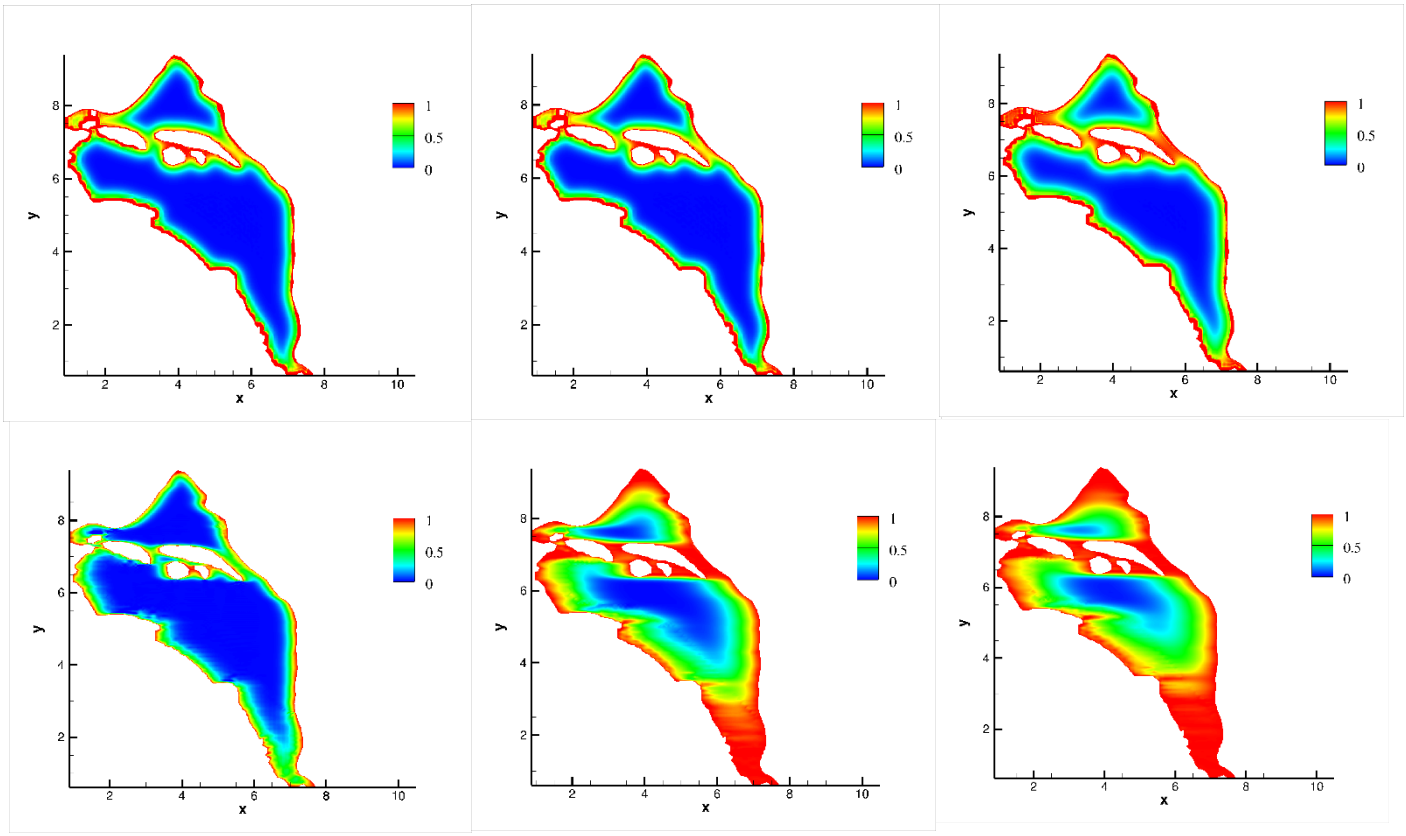

Figure 3: Fractional diffusion on 2D complex domain with Dirichlet boundary at different time. 1st row $\alpha = 1.0$; 2nd row $\alpha = 2.0$.

4. We showed that when solving eigenvalue problem with spectral element method on one single element, difference between eigenvalues from h-refinement and analytical ones are better than that between p-refinement and analytical ones. See Figure 4.

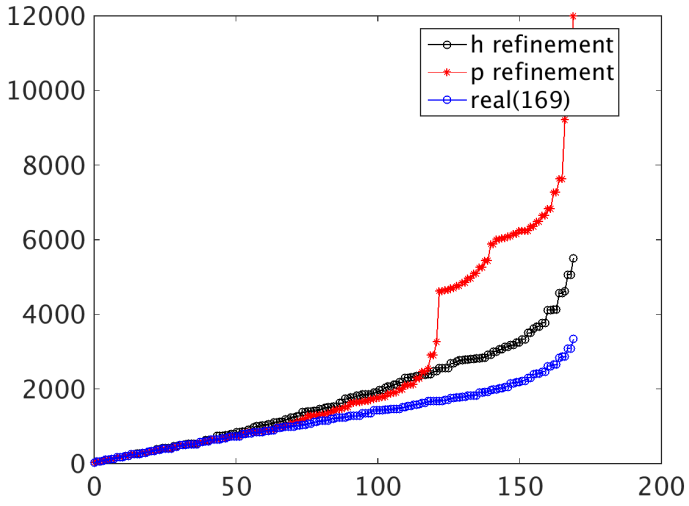

Figure 4: Comparison of eigenvalues computed from h-refinement, p-refinement and the analytical solution.

5. We are working on the improvement of the accuracy of the eigenvalues as well as conduting 3D simulation of real physical problems using the solver **F-Nektar.**

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WPI (Add-On: co-PI: Zhongqiang Zhang)

(Research Areas 2 & 4)

We focus on three projects this summer (from May 15 to July 31).

1. Efficient simulation of fractional Brownian motion and application to a nonlinear elliptic equation.
2. Fractional Schrodinger equation with fractional white noise.
3. Probabilistic numerical methods for fractional advection-diffusion-reaction equations.

Project 1.

We consider the following nonlinear elliptic equation with homogeneous Dirichlet boundary condition

$$-\Delta u(x) + f\big(u(x)\big) = \frac{\partial^d}{\partial x_1 \partial x_2 \dots \partial x_d} W_H(x), x = (x_1, x_2, \dots, x_d) \in \mathcal{D} \quad (1)$$

where $\mathcal{D} = (0,1)^d$, $W_H(x)$ is a fractional Brownian sheet on $\overline{\mathcal{D}} = [0,1]^d$. Here f is Lipschitz continuous.

- We have developed an efficient method of simulating fractional Brownian motion using its spectral representation for $d = 1$. In this case, $W_H(x)$ is the fractional Brownian motion with Hurst parameter $H \in (0, 1)$. Specifically, $W_H(x)$ is a Gaussian random process with mean 0 and covariance function $\mathbb{E}[W_H(x), W_H(y)] = \frac{1}{2}(|x|^{2H} + |y|^{2H} - |x - y|^{2H})$.

  While approximation of fractional Brownian motion usually works for H ≥ 1/2, our method works for all $H \in (0, 1)$.
- The strong convergence order (in the mean-square sense) of finite element methods plus our approximation is proved to be h^{H+1}, where h is the size of each piecewise linear elements when d = 1. When H = 0.5, our result is the same as in our previous work with Brownian motions.
- Weak convergence orders were tested, but the strong convergence order has not been implemented due to the complication of comparing numerical solutions in the same probability space. Testing strong convergence orders is still ongoing.

Project 2.

We consider the following equation

$$u_t + i\left[(-\Delta)^{\alpha/2}u + \lambda|u|^2u\right] - \beta\Delta u = f(x,t), \quad x \in (-1,1) \tag{2}$$

with homogeneous Dirichlet boundary conditions. Here the order $\alpha \in (1, 2)$ and the fractional Laplacian is defined as a singular integral operator on R,

$$(-\Delta)^{\alpha/2}u(x) = c_{d,\alpha}\int_{\mathbb{R}^d}\frac{u(x)-u(y)}{|x-y|^{d+\alpha}}dy, \quad c_{d,\alpha} = \frac{2^\alpha\Gamma\left(\frac{\alpha+d}{2}\right)}{\pi^{\frac{d}{2}}\left|\Gamma\left(-\frac{\alpha}{2}\right)\right|}.$$

We have tested two cases: 1) $f(x,t) = \sin(x)$ and 2) $f(x,t) = \dot{W}_H(t)$, where $W_H(t)$ is a fractional Brownian motion in time.

We use backward Euler scheme in time, spectral Galerkin method in space we developed in a previous MURI Add-on, and our newly developed methods of simulating fractional Brownian motion in Project 1. We discover the following facts:

When $f(x,t) = \sin(x)$, the convergence order in space is $2.5\alpha + 1$ when $\beta = 0$ and otherwise the convergence order is $2 + \alpha/2$.

When $f(x,t) = \dot{W}_H(t)$, the convergence order in time is 1 when $H \geq 1/2$. However, the order for $H < 1/2$ is not clear to us, possibly due to the low convergence order when we numerically tested the convergence $H < 1/2$.

Project 3.

We have applied the walk-on-the-sphere algorithm to solve diffusion-reaction equations with fractional Laplacian on smooth bounded domains. We are now working on the algorithm for advection-diffusion-reaction equations with fractional Laplacian and $\mu = 0$:

$$(-\Delta)^{\alpha/2}u - \beta\Delta u + \mu Du = f(x), \quad x \in \mathcal{D}.$$

Here we consider a homogeneous Dirichlet boundary condition and $\mathcal{D}$ is a smooth bounded domain and $\beta = 0$ or $\beta = 1$. This equation is written as the expectation of solutions to stochastic ordinary differential equations when the solutions do not leave the domain. The stochastic differential equations is then solved with the forward Euler scheme, with a first- order convergence.

The convergence order is dominated by the convergence of Monte Carlo methods, but the method is very robust. The method is fast when solutions at a few points are needed.

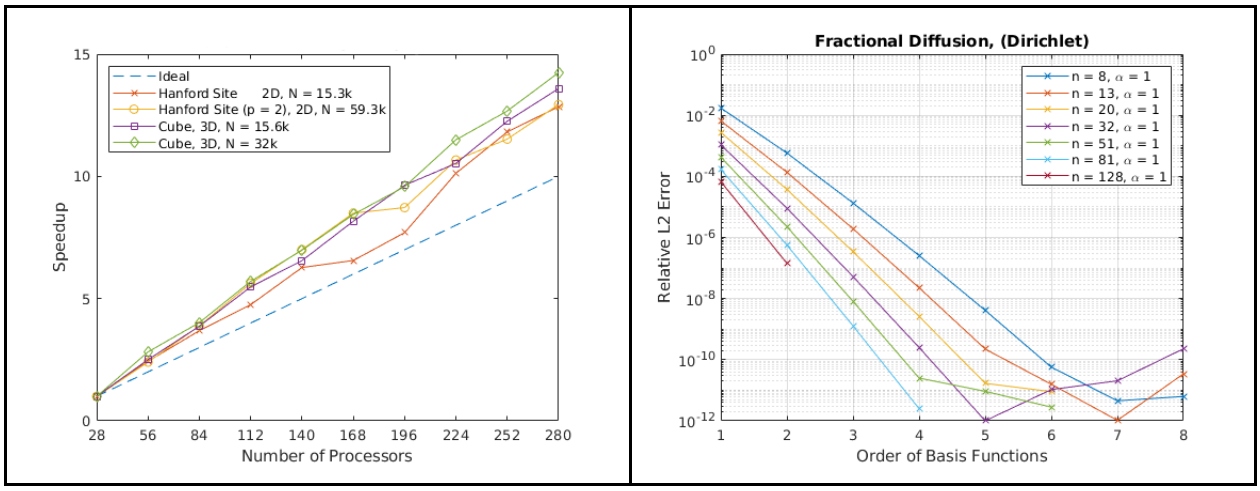
Utah (Add-On: co-PI: Robert M. Kirby)

(Research Areas 6)

Space and Time Fractional Operators in Nektar++

Maxx Carlson, Hari Sundar, Akil Narayan, Allen Sanderson and Robert M. Kirby
Scientific Computing and Imaging (SCI) Institute, University of Utah

Space-fractional differential equations: Nektar++ Space-Fractional PDE Solver via Method of Eigenfunction Expansion



At this time, we have completed the implementation of our space-fractional Laplacian extension for Netkar++. Using our highly scalable custom eigenvalue solver, we can generate the full eigenbasis for any given complex geometry for meshes with up to half a million degrees of freedom. For validation, we have tested this method of eigenfunction expansion on several geometries for both fractional diffusion and fractional Poisson and verified spectral convergence in solution error with respect to the order of the mesh's basis elements. The title figures show the parallel efficiency of the eigenvalue solver (left) and the spectral convergence of the solution error (right).

This work has generated two papers; The first paper is primarily related to the scalable eigenvalue solver and is being submitted to ICS 2020. The other paper is a joint work with our colleagues at Brown, George Karniadakis and Xiaoning Zheng. This second paper focuses more on the mathematical aspects of the solver method and will be submitted to Computer Physics Communications (CPC) journal. Scalability and performance were evaluated on University of Texas TACC's Frontera computing system.

Algorithm 1 Solver Pipeline: Fractional Poisson

1: Form standard (non-fractional) stiffness/mass matrices: K, M
2: Solve for approximate eigenpairs: Θ, Φ
3: **for** each forcing function f **do**
4: Compute FEM expansion coefficients of f: $\bar{f}$
5: Estimate spectral coefficients: $\hat{f} = \bar{f}^T M \Phi$
6: Compute solution coefficients: $\hat{u} = \Phi \Theta^{-\alpha/2} \hat{f}$
7: Evaluate FEM expansion to get approximate solution
8: **end for**

```
// Generate stiffness/mass matrices
GenGlobalMatrixEigenMM(K, ...);
GenGlobalMatrixEigenMM(M, ...);

// Solve the eigenvalue problem using EigenMM
solver.init(K, M, options);
solver.solve(&V, &lambda);

// Estimate spectral coefficients
computeInputCoefficients(fhat, fbar, M, V);

// Compute solution coefficients
computeSolutionCoefficients(uhat, V, lambda, fhat);

// Evaluate FEM expansion to get solution
evaluateSolution(u_out, uhat, V);
```

An example of the overall solution process for a fractional Poisson equation can be seen in the figures on this page. Once the eigenbasis for a given mesh is computed, the complexity for solving a space-fractional PDE is dominated by the time it takes to apply a dense N by N matrix to a vector. Since this is an O(N^2) operation, we are currently exploring techniques for reducing the complexity of applying this operator to O(NlogN). Using a hierarchical matrix compression that resembles FFT's butterfly factorization, we have achieved positive results in this direction and our next step is to implement a scalable version of the algorithm to see if our positive results hold at large scale.

The remaining work, aside from the ongoing compression project, is to prepare the space-fractional portion of the code to be merged with the time-fractional work that is being done in parallel.

Time-fractional differential equations

Fractional-order time derivatives can model delay and hysteresis-type phenomena, which cannot be captured with models involving only traditional ordinary differential equations. We focus on the Caputo-type fractional time derivative, which is more physically relevant for solving fractional differential equations than other competing time-fractional definitions.

Numerical methods for solving fractional differential equations with the Caputo derivative are challenging since the fractional operator is essentially equivalent to a convolution of the solution over the entire temporal history. After N timesteps, a standard time-stepping algorithm for further updates requires expensive and often infeasible O(N) memory storage and $O(N^2)$ computation per extra timestep.

This project focuses on development and implementation of advanced numerical methods in large-scale computing environments that require only O(log N) memory storage and O(N log N) computations per timestep for solving fractional differential equations, substantially accelerating

predictive capabilities. In particular, we concentrate our effort on implementation of these algorithms in the open-source finite element software package Nektar++.

Completed and plan: We have implemented a first-order version of the fast time-fractional differential equation (DE) solver in Nektar++. The current implementation performs fast convolution, and we demonstrate log-linear complexity in cumulative time, and logarithmic storage in the number of time steps, as shown in Figure 1 for a test problem on a system of fractional DE's. This is in contrast to more naïve algorithms that would require quadratic complexity in time and linear storage in the number of time steps. We also observe that the error committed by the algorithm does not blow up in time.

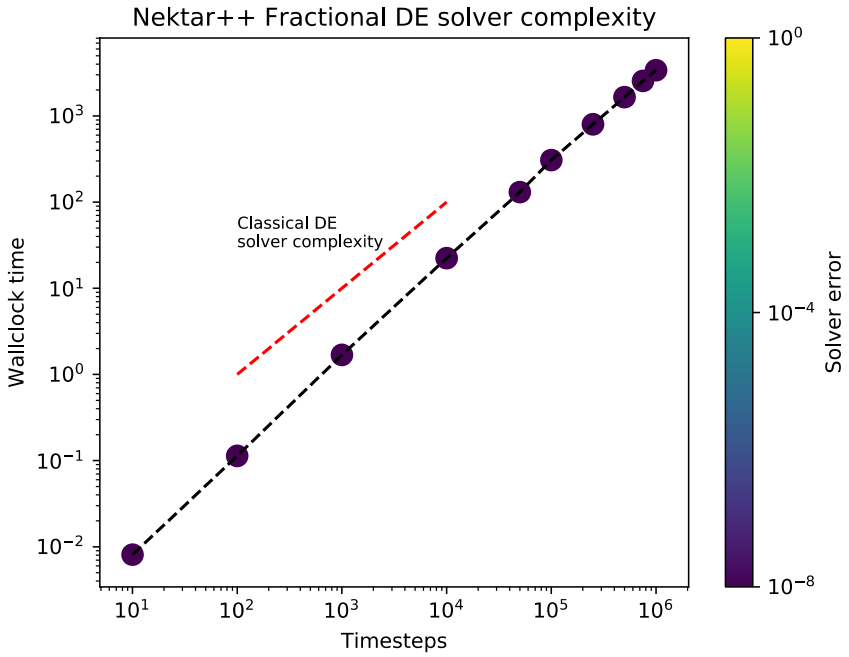


Figure 1: Computational complexity of Nektar++ Fractional DE solver.

We are currently working on generalizing the method to a high-order solver. Such a generalization is possible by using appropriate higher order exponential integrators, which are building blocks for the time-fractional solver. We currently have a Matlab template for this high-order solver that employs both multi-stage and multi-step exponential integrators to achieve high order accuracy for the fractional problem. We will work on folding these into Nektar++. Since Nektar++ already has substantial infrastructure for high-order (classical) differential equation solvers, we anticipate that this cn be completed relatively quickly.

ARO MURI # 8 Project (2015): August 2019--July 2020 Progress Report

Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications

- **George Karniadakis & Mark Ainsworth, Brown University**
- **Qiang Du, Columbia University**
- **Mohsen Zayernouri, Michigan State University**
- **Pol Spanos, Rice University**
- **Hong Wang, University of South Carolina**
- **Add-On: Robert M. Kirby (Uath)**

Background: This MURI project is the vision of a team of researchers from Brown University, Michigan State University, Columbia University, University of South Carolina, and Rice University with overlapped inerests and complementary expertise on theory, numerical methods, and applications of fractional PDEs (FPDEs). Our overarching goal is the development of a seamless integration of theory and algorithms for data-driven FPDEs, while targeting the common themes of conservation, monotonicity, adaptive refinement, and high-order accuracy in the context of simulations of multiphase flows, turbulence, fluid-structure interactions, hydrology, and solid mechanics. We envision a combined mathematical and computational framework, where the fractional operators can be constructed based on available data, hence providing model validation for the specific phenomenon but also a tailor-based simulation capability that can be scaled to real-life applications. The proposed research plan emphasizes a dynamic integration of six main research areas that form the pillars of our integrated approach:

• *Research Area 1*: Theory of non-local operators and stochastic interpretation of fractional operators.
• *Research Area 2:* Numerical solution of fractional PDEs with emphasis on variable fractional order.
• *Research Area 3:* Fast solvers for dense linear systems with linear/quasi-linear computational complexity.
• *Research Area 4:* Stochastic FPDEs and determination of the fractional order directly by available data.
• *Research Area 5:* Applications to fluid and solid mechanics, fluid-structure interactions, two-phase flows, turbulence and reactive system with front propagation.
• *Research Area 6:* High performance computing & developing opensource software for fractional problems.

MURI Objectives

- To address the common physical themes of anomalous transport, exponentially accelerated fronts, non-Markovian behavior and long-range interactions, self-similarity and scaling, singular behavior, interfaces and finite-domain decorrelation effects.
- To develop rigorous mathematical theory, algorithms and software for data-driven fractional PDEs that will provide significant breakthroughs towards modeling, analyzing and subsequently controlling complex multiscale systems characterized by the aforementioned phenomena —in a computationally scalable way.
- To demonstrate the physical relevance and effectiveness of our framework in diverse applications of interest to DoD, characterized by the common themes of conservation, monotonicity, adaptive refinement and high-order accuracy.

Status of the Project

There has been great progress in the five years on all research six areas, in recruiting excellent postdocs and PhD students, in participating in conferences with invited and contributed talks as well as on organizing mini-symposia and workshops on FPDEs. The add-on helped us to start three new areas on machine learning, fractional photonics, stochastic FPDEs, and opensource software for fractional problems. In the following, we provide a summary of progress by each co-PI. First, we provide some highlights on all our activities and then we present the report of each PI.

MURI Highlights

- More than 233 papers have been published or submitted on all six research areas of MURI.
- More than 72 invited and plenary talks by MURI personnel.
- Volume on numerical methods in Handbook of FPDEs.
- Several minisymposia and two workshops organized by MURI PIs.
- New research focusing on 2D & 3D fractional Laplacians in bounded domains with emphasis on boundary conditions and their stochastic interpretation. 11-author revised paper.
- New research focusing on machine learning, fractional photonics, stochastic fractional PDEs and opensource software enabled by the add-on funding.
- Fractional models of turbulent polymer drag reduction at high Reynolds number.
- Combine FPDE and molecular dynamics to efficiently simulate anomalous diffusive transport in heterogeneous porous materials with nanoscale pores.
- Non-local modeling of ion diffusion in battery systems & experiments.
- We discovered new fractional phase-field/non-local equations for interface problems.
- New opensource software at Brown (fractional NEKTAR), Uath (Nektar++) and MSU (FracFit).
- Developing a unified theory of fractional, nonlocal, and weighted nonlocal vector calculus.
- Physical applications of fractional models, particularly, fractional phase field crystal models.
- Theoretical formulation of a fractional subgrid-scale model for turbulent flows.
- Investigating anomalous features in materials failure, internal flows, and structural vibration.

Michigan State University: (co-PI: Mohsen Zayernouri)

(Research Areas 1, 4 & 5)

Personnel supported on the MURI grant: PhD students Mehdi Samiee, PhD student Eduardo de Moraes, PhD student Ali Akhavan-Safaei, PhD student Seyedhadi Seyedi, and MSU PI: Associate Professor Mohsen Zayernouri (PI).

Summary: The MSU team has made substantial progress on understanding anomalous features in internal flows, automatic self-singularity-capturing scheme for FDEs, phase-field based supervised machine learning for material failure, physically consistent fractional visco-elasto-plastic models with memory- and path-dependent damage, also understanding anomalous nonlinear vibration of fractional viscoelastic structures.

Highlights:

During the past year, the MSU MURI team had papers **accepted** on:

- An Integrated Sensitivity-Uncertainty Quantification Framework for Stochastic Phase-Field Modeling of Material Damage
- Data-Driven Failure Prediction in Brittle Materials: A Phase-Field Based Machine Learning Framework
- Anomalous Features in Internal Cylinder Flow Instabilities subject to Uncertain Rotational Effects

During the past year, the MSU MURI team has **published** results on:

- A Fractional Subgrid-Scale Model for Turbulent Flows: Theoretical Formulation and *a-Priori* Study
- Automatic Self-Singularity-Capturing Scheme for Fractional Differential Equations
- (A review paper) Fractional Calculus and Numerical Methods for Fractional PDEs.
- Operator-Based Uncertainty Quantification of Stochastic Fractional Partial Differential Equations

During the past year, the MSU MURI team has **submitted** papers on:

* A Thermodynamically Consistent Fractional Visco-Elasto-Plastic Model with Memory-Dependent Damage for Anomalous Materials (submitted to *CMAME*)

* Anomalous Nonlinear Vibration of Fractional Viscoelastic Structures (will be submitted to *JCP* by August 20th)

Published (& in Press) Journal Papers:

1) A. Akhavan-Safaei, S. Seyedi, M. Zayernouri (**2020**) **Anomalous Features in Internal Cylinder Flow Instabilities subject to Uncertain Rotational Effects**, *Physics of Fluid*, in Press.

2) E. de Moraes, M. Zayernouri, M. M. Meerschaert (**2020**) **An Integrated Sensitivity-Uncertainty Quantification Framework for Stochastic Phase-Field Modeling of Material Damage**, *International Journal for Numerical Methods in Engineering*, in Press.

3) E. de Moraed, H. Salehi, M. Zayernouri (**2020**) **Data-Driven Failure Prediction in Brittle Materials: A Phase-Field Based Machine Learning Framework**, *Journal of Machine Learning for Modeling and Computing*, in Press.

4) M. Samiee, A. Akhavan-Safaei, M. Zayernouri, (**2020**) ***A Fractional Subgrid-scale Model for Turbulent Flows: Theoretical Formulation and a Priori Study***, *Physics of Fluid*, 32 (5), 055102.

5) JL Suzuki, M Zayernouri (**2020**) **A Self-Singularity-Capturing Scheme for Fractional Differential Equations**, *International Journal of Computer Mathematics*, 1-32

6) E. Kharazmi, Z. Mao, G. Pang, M. Zayernouri, and G. E. Karniadakis (**2020**) **Fractional Calculus and Numerical Methods for Fractional PDEs**, *First Congress of Greek Mathematicians, Publisher: De Gruyter*.

7) E. Kharazmi and M. Zayernouri, (**2020**) **Operator-Based Uncertainty Quantification of Stochastic Fractional PDEs**, *ASME Journal on Verification, Validation, and Uncertainty Quantification, 4 (4).*

8) M. Samiee E. Kharazmi, M. Meerschaert, M. Zayernouri, (**2020**) ***A*** **Unified Petrov-Galerkin Spectral Method and Fast Solver for Distributed-Order Partial Differential Equations***, Communications on Applied Mathematics and Computation*, in Press.

9) Y. Zhou, J. Suzuki, C. Zhang, and M. Zayernouri, (**2020**) **Fast Implicit-Explicit Time-Integration of Nonlinear Fractional Differential Equations***, Journal of Applied Numerical Mathematics, Volume 156, October 2020, Pages 555-583.*
10) M. Ari, R. Teymoori-Faal, M. Zayernouri, (2019) **Vibrations Suppression of Fractionally Damped Plates using Multiple Optimal Dynamic Vibration Absorbers,** *International Journal of Computer Mathematics, 1-24.*

11) M. Samiee, M. Zayernouri, and M. M. Meerschaert, (2019) **A Unified Spectral Method for FPDEs with Two-sided Derivatives; Part I: A Fast Solver**, *Journal of Computational Physics, 385, 225-243.*

12) M. Samiee, M. Zayernouri, and M. M. Meerschaert, (2019) **A Unified Spectral Method for FPDEs with Two-sided Derivatives; Part II: Stability and Error Analysis**, *Journal of Computational Physics, 385, 244-261*

13) A. Lischke, M. Zayernouri, Z. Zhang, (2019) **Spectral and Spectral Element Methods for Fractional Advection–Diffusion–Reaction Equations**, *Handbook of Fractional Calculus with Applications, Volume 3: Numerical Methods.*

Submitted Journal Manuscripts:

14) J.L. Suzuki, Y. Zhou, M. D'Elia, M. Zayernouri (2020) **A Thermodynamically Consistent Fractional Visco-Elasto-Plastic Model with Memory-Dependent Damage for Anomalous Materials**, (submitted to *CMAME*).
15) J.L. Suzuki, P. Varghaei, E. Kharazmi, M. Zayernouri, **Anomalous Nonlinear Vibration of Fractional Viscoelastic Structures,** (to be very soon submitted to *JCP*).

Columbia University Report (co-PI: Qiang Du)

(Research Areas 1 & 5)

Progress report: August 2019-July 2020

The research team at Columbia, under the direction of Qiang Du, has actively participated in research supported by the MURI project and has sought after collaborations with other MURI team members.

Research team at Columbia:

Personnel supported on the grant at Columbia: PI Qiang Du was supported for one summer month by the grant; post-doc scholar Lorenzo Toniazzi (2019) and graduate students Kuang Huang, Hwi Lee, and Zirui Xu were partially supported for the year. Unsupported research personnel: a couple of graduate students have been collaborating on the project but they do not receive any support from this grant.

Research progress:

As outlined in the proposal, the proposed work for the Columbia team focuses on the analysis and discretization of Fractional PDEs and nonlocal integral equations. Our work has focused on the following aspects:

● **Origin of Nonlocality.**
While we focused on algorithmic development and analysis, we were also aware of important modeling issues and we studied the origin of nonlocality in a multiscale modeling context and its relations to model reduction and homogenization. Our findings were reported in [1]. A more special case study was given in [9].

● **Interpretation of nonlocal/fractional models.**
We investigated the stochastic interpretations of nonlocal-in-time diffusion models [5]. This motivated us to study more general fractional differential equations via the analysis of censored fractional derivative, and establish the well-posedness of the resulting equation and its solution behavior.

● **Nonlocal/fractional modeling.**
We have studied nonlocal smoothing of well-known models of mechanics with the goal to understand how they affect numerical methods like the SPH discretization in CFD as well as the discretization of nonlocal elasticity models. We examined in particular the nonlocal analog of the linear Stokes equations and the Navier model of linear elasticity, and linear models of linear convection, with all of them depending on the suitable definitions of the nonlocal gradient operator. The latter is a key building block for the nonlocal smoothing of traditional PDEs, as well as for nonlocal models themselves. Our finding showed that there may be intrinsic instabilities associated with some of the popular forms of the nonlocal gradient on the continuum level, thus leading to discretizations that are also prone to instabilities and lack of robustness. We proposed alternatives that can help eliminating these instabilities for some model problems. Publications related to this line of works can be found in [10, 13, 14].

We also examined the nonlocal analog of classical two point value problem and showed that one can expect second order accuracy with respect to the horizon parameter [12]. In light of possible discontinuous solutions for nonlocal diffusion models with integrable kernels, we developed hybrid continuous and discontinuous Galerkin approximations [11].

● **Algorithms for nonlocal/fractional models**.
We continued the development of asymptotically compatible discontinuous Galerkin finite element approximations and quadrature-based finite difference schemes, as well as fast spectral methods for nonlocal models [2,3,4,6,8,16,17]. We studied applications of various stable time stepping schemes to others considered nonlinear nonlocal phase field models [7]. We have also done some initial investigations

on the proper coupling of nonlocal models with local models on the continuum level using either seamless coupling approaches [15].

List of publications:

[1] Qiang Du, Bjorn Engquist and Xiaochuan Tian. Multiscale modeling, homogenization and nonlocal effects: mathematical and computational issues. Contemporary Mathematics, Celebrating 75th Anniversary of Mathematics of Computation, 754, 115-140, 2020.

[2] Qiang Du, Lili Ju and Jianfang Lu. Analysis of fully discrete approximations for dissipative systems and application to time-dependent nonlocal diffusion problems. Journal of Scientific Computing, 78:1438–1466, 2019.

[3] Qiang Du, Lili Ju and Jianfang Lu. A discontinuous Galerkin method for one-dimensional time-dependent nonlocal diffusion problems. Mathematics of Computation, 88, 123–147, 2019.

[4] Qiang Du, Yunzhe Tao, Xiaochuan Tian and Jiang Yang. Asymptotically compatible discretization of multidimensional nonlocal diffusion models and approximations of nonlocal Green's functions. IMA J. Numerical Analysis, 39:607-625, 2019.

[5] Qiang Du, Lorenzo Toniazzi, and Zhi Zhou. Stochastic representation of solution to nonlocal-in-time diffusion. Stochastic Processes and their Applications, 130, 2058-2085, 2020.

[6] Qiang Du. Nonlocal Modeling, Analysis, and Computation, volume CBMS-NSF conference series in applied mathematics 94. SIAM, 2019.

[7] Qiang Du, Lili Ju, Xiao Li, and Zhonghua Qiao. Maximum principle preserving exponential time differencing schemes for the nonlocal Allen–Cahn equation. SIAM Journal on Numerical Analysis, 57(2):875–898, 2019.

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[9] Qiang Du, Xiantao Li, and Liming Yuan. Analysis of coarse-grained lattice models and connections to nonlocal interactions, CSIAM Transaction on Applied Mathematics, 1, 155-185, 2020.

[10] Qiang Du and Xiaochuan Tian. Mathematics of smoothed particle hydrodynamics via a nonlocal stokes equation. Foundations of Computational Mathematics, 20, 801-826, 2020.

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[14] Hwi Lee and Qiang Du. Nonlocal gradient operators with a nonspherical interaction neighborhood and their applications. ESAIM: Mathematical Modelling and Numerical Analysis, 54, 105-128, 2020.

[15] Yunzhe Tao, Xiaochuan Tian and Qiang Du. Nonlocal models with heterogeneous localization and their application to seamless local-nonlocal coupling. Multiscale Modeling and Simulation, 17, 1052–1075, 2019.

[16] Xiaochuan Tian and Qiang Du. Asymptotically compatible schemes for robust discretization of parametrized problems with applications to nonlocal models. SIAM Review, 62, 199-227, 2020.

[17] Chunxiong Zheng, Qiang Du, Xiang Ma and Jiwei Zhang, Stability and error analysis for a second-order fast approximation of the local and nonlocal diffusion equations on the real line, SIAM J. Numer. Anal., 58, 1893–1917, 2020.

Recognition:
AMS fellow, 2020.
SIAM Review Digest Paper Award, 2020.

Other notation activities:
Co-chair of Machine Learning in Science and Engineering (MLSE2020, Columbia)

All products acknowledge support from ARO grant W911NF-15-1-0562.

University of South Carolina Report (co-PI: Hong Wang)

(Research Area 1, 2, 3 & 4)

Progress report: January —August 2020

The research group at University of South Carolina, under the direction of Hong Wang, has actively participated in research supported by the MURI project.
During this time period, USC research group has focused on the study of variable-order FPDEs, which were listed on many research areas of the original research tasks.

4. *Variable-order FPDEs: well-posedness, smoothness and boundary conditions (Original proposal: Research Area 1)*

   The order of FPDEs is related to the fractal dimension of the pore structure of the porous materials. As the material structure changes, the order of FPDEs should change and yield variable-order FPDEs. Moreover, FPDEs with a properly chosen variable-order naturally eliminate the nonphysical singularity of their solutions.

   In papers (7), (8) and (18), we proved well-posedness and smoothing properties of variable-order time-fractional PDEs with a time-dependent variable order alpha(t), a space-time dependent variable order alpha(x,t), and a nonlinear variable order alpha(x,t,u).

   In paper (25) we proved the well-posedness and smoothing properties of variable-order space-time fractional PDEs with a space-time dependent hidden-memory variable order. In this context, inside the fractional integral on the time interval [0,t] for any t in [0,T], the variable order alpha assumes its value alpha(s) for any s in [0,t]. The hidden memory model is physically more relevant but is mathematically more complex.

In paper (12) we proved well-posedness and smoothing property of the boundary-value problem of a variable-order space-fractional diffusion equation with a space-dependent variable order alpha(x).

In paper (5) we proved the well-posedness and smoothing property of a variably distributed-order time-fractional PDE and its numerical approximation.

5. *Numerical approximations to FPDEs (Research Area 2).*
   In paper (11) we proved optimal-order error estimates of finite element approximations to variable-order time-fractional diffusion equations with a time-dependent variable order without regularity assumptions of the solutions. We proved similar results for hidden-memory variable-order time-fractional PDEs with a time-dependent variable order.

   We proved optimal-order error estimates of numerical approximations to variable-order time-fractional PDEs with a space-time dependent variable order in paper (18) and to variable-order time-fractional PDEs with a space-time dependent hidden-memory variable order in paper (25).

6. *Development of fast numerical solvers for variable-order FPDEs (Research Area 3).*
   Because of the impact of the space or time-dependent variable order, the coefficient matrices of the numerical discretization to variable-order FPDEs do not retain Toeplitz-like structure, so the fast numerical methods for constant-order FPDEs, such as convolution quadrature and Laplace transform based sum of exponential methods, do not apply to variable-order FPDEs.

   In paper (1) we developed a binary block clustering method for variable-order time-fractional PDE that has the same computational complexity and memory requirement as the fast numerical methods for constant-order time-fractional PDEs.

   In paper (17) we developed a fast numerical method for a variable-order space-fractional diffusion equation with a space-dependent variable order alpha(x). The resulting method has O(N log N) memory requirement and O(N log^2 N) computational complexity. The fast numerical solution is proved to have the same order of accuracy as the exact numerical solution does.

7. *Stochastic FPDEs and determination of variable fractional order in variable-order FPDEs (Research Area 4).*
   As the order of FPDEs is closely related to the fractal dimension of the porous material via the Hurst index, the variable orders of FPDEs provides a feasible mean to characterize the material change of the porous media.

   In paper (16) we proved the unique identifiability of the space-dependent variable order in a variable-order space-fractional PDE. In paper (24) we proved the unique identification of a time-dependent variable order in a variable-order time-fractional diffusion equation imposed on a general multidimensional spatial domain.

In paper (9) we analyzed the well-posedness of a variable-order fractional stochastic differential equation driven by a multiplicative white noise. Based on these results we proved the strong convergence of a Euler-Maruyama scheme to the stochastic differential equation in paper (21).

In paper (26) we proved the well-posedness and regularity of an optimal control model governed by a variable-order Caputo time-fractional diffusion PDE, which is the best in the literature on the study of an optimal control of variable-order FPDEs. The key difference from the optimal control of constant-order FPDEs is that the adjoint state equation reduces to a completely different hidden-memory variable-order Riemann-Liouville time-fractional diffusion PDE. We accordingly developed and analyzed a fully-discretized finite element approximation to the optimal control model without any artificial regularity assumption of the true solution. Numerical experiments are performed to substantiate the theoretical findings.

Research publications (All acknowledged MURI support) since Jan 2020 (last report):

(1) Z.W. Fang, H.W. Sun and H. Wang, A fast method for variable-order Caputo fractional derivative with applications to time-fractional diffusion equations. Comput Math Appl 80 (2020), 1443--1458.

(2) X. Li, Z. Mao, N. Wang, F. Song, H. Wang and G.E. Karniadakis, A fast solver for spectral elements applied to fractional differential equations using hierarchical matrix approximation. Comput Methods Appl Mech Engrg 366 (2020), 113053.

(3) H. Liu, A. Cheng and H. Wang, A fast Galerkin finite element method for a space-time fractional Allen-Cahn equation. J Comput Appl Math 368 (2020), 112482.

(4) H. Wang and X. Zheng, An optimal-order error estimate of the lowest-order ELLAM-MFEM approximation to miscible displacement in three space dimensions. J Comput Math 375 (2020), 112819.

(5) Z. Yang, X. Zheng and H. Wang, A variably distributed-order time-fractional diffusion equation: analysis and approximation. Comput Methods Appl Mech Engrg 367 (2020), 113118.

(6) X. Zheng, V.J. Ervin and H. Wang, Wellposedness of the two-sided variable-coefficient Caputo flux fractional diffusion equation and error estimate of its spectral approximation. Appl Numer Math 153 (2020), 234--247.

(7) X. Zheng and H. Wang, Wellposedness and regularity of a variable-order space-time fractional diffusion equation. Analysis & Application 18 (2020), 615--638.

(8) X. Zheng, H. Wang and H. Fu, Well-posedness of fractional differential equations with variable-order Caputo-Fabrizio derivative. Chaos, Solitons & Fractals 138 (2020), 109966.

(9) X. Zhang, Z. Zhang and H. Wang, Analysis of a nonlinear variable-order fractional stochastic differential equation. Appl Math Lett 107 (2020), 106461.

(10) X. Zheng, V.J. Ervin and H. Wang, Numerical approximations for the variable coefficient fractional diffusion equations with non-smooth data. Comput Methods Appl Math (CMAM), DOI: 10.1515/cmam-2019-0038.

(11) X. Zheng and H. Wang, Optimal-order error estimates of finite element approximations to variable-order time-fractional diffusion equations without regularity assumptions of the solutions. IMA J Numer Anal, doi:10.1093/imanum/draa013.

(12) X. Zheng and H. Wang, Variable-order space-fractional diffusion equations and a variable-order modification of constant-order fractional problems. Applicable Anal, https://doi.org/10.1080/00036811.2020.1789596.

(13) X. Zheng and H. Wang, An error estimate of a numerical approximation to a hidden-memory variable-order space-time fractional diffusion equation. SIAM J Numer Anal, in press.

(14) P. Dai, J. Jia, H. Wang, Q. Wu and X. Zheng, An efficient positive-definite block-preconditioned finite volume solver for two-sided fractional diffusion equations on composite mesh, revision submitted

(15) H. Liu, X. Zheng, H. Fu and H. Wang, Analysis and efficient implementation of ADI finite volume method for Riesz space-fractional diffusion equations in two space dimensions, revision submitted.

(16) X. Zheng, Y. Li, J. Cheng and H. Wang, Uniqueness of determining the variable fractional order in the boundary-value problem of variable-order linear space-fractional diffusion equations with variable diffusivity coefficients, revision submitted.

(17) J. Jia, H. Wang and X. Zheng, A preconditioned fast finite element approximation to variable-order time-fractional diffusion equations in multiple space dimensions, submitted.

(18) B. Li, H. Wang and J. Wang, Well-posedness and numerical approximation of a fractional diffusion equation with a nonlinear variable order, submitted.

(19) H. Liu, X. Zheng, C. Chen and H. Wang, A characteristic finite element method for the time-fractional mobile/immobile advection diffusion model, submitted.

(20) Z. Yang, X. Zheng and H. Wang, An indirect collocation method for variable-order fractional wave equations on uniform or graded meshes and its optimal error estimates, submitted.

(21) Z. Yang, X. Zheng, Z. Zhang and H. Wang, Strong convergence of a Euler-Maruyama scheme to a variable-order fractional stochastic differential equation driven by a multiplicative white noise, submitted.

(22) X. Zheng, V.J. Ervin and H. Wang, Optimal Petrov-Galerkin spectral approximation method for the fractional diffusion, advection, reaction equation on a bounded interval, submitted.

(23) X. Zheng, H. Liu, H. Wang and H. Fu, Optimal-order finite element approximations to variable-coefficient two-sided space-fractional advection-reaction-diffusion equation in three space dimensions, submitted.

(24) X. Zheng and H. Wang, Uniquely identifying the variable order of time-fractional partial differential equations on general multi-dimensional domains, submitted.

(25) X. Zheng and H. Wang, A time-fractional partial differential equation with a space-time dependent hidden-memory variable order: analysis and approximation, submitted.

(26) X. Zheng and H. Wang, An optimal control of a variable-order time-fractional diffusion equation, submitted.

Invited talks by the USC team:

Conference presentations:

(19) H. Wang, "Variable-order fractional PDEs: modeling, analysis and discretization". Recent Progress in Nonlocal Modeling, Analysis, and Computation (Online Conference), Southern University of Science and Technology, Shenzhen, China 06/14--06/18, 2020.

Colloquium and seminar talks:

(26) H. Wang, "A continuous time random walk modeling of fractional diffusion partial differential equations", Ocean University of China, Qingdao, China, 1/3, 2020.

(27) H. Wang, "Fractional partial differential equations: their continuous time random walk derivation and numerical simulation", Department of Mathematics, University of Macau, Macau, 1/7, 2020.

Rice University Report (co-PI: Pol Spans)
(Research Areas 4)

Research Work on Axial vibrations of fractional rods with variable cross sections exposed to random loads

Abstract

Since the pioneering works of Nutting [1], Gemant [2] and Blair and Caffyin [3], fractional derivative models have been used for describing the behavior of visco - elastic materials. This mathematical instrument was recast in a precise theoretical framework by Bagley and Torvik [4] and is currently applied in the description materials with "memory", that is materials whose response depends upon past values of their stretching time history. A recent research endeavor was devoted to the implementation of these models in the context of continua. Beams, plates and other continua are the fundamental building blocks employed in practical engineering applications. Therefore, it is of utmost importance to develop consistent models taking advantage of this mathematical tool, as well as developing reliable solutions of the associated mathematical problems. In this context, recent results were concerned with the nonlinear vibration of beams and plates [5,6], where the authors developed Boundary Element Method – based numerical algorithms and approximate analytical solutions via the statistical linearization technique.

Those problems were concerned with the transverse vibration of continua, but no specific researches considered the axial vibration problem. In this context, the partial differential equations governing the axial vibrations of continuous elements are derived by combining the equilibrium equation along the axial direction with the material constitutive equation [7]. Specifically, the axial vibration of a rod with variable cross – section were derived by (Stevanovic) Hedrih [8]. The resulting differential equation is

$$\frac{1}{c_0^2}\frac{\partial^2}{\partial t^2}w(z,t) - \frac{1}{A(z)}\frac{\partial}{\partial z}\left[A(z)\frac{\partial}{\partial z}w(z,t)\right] - \frac{c_\alpha^2}{c_0^2}\frac{1}{A(z)}\frac{\partial}{\partial z}\left\{A(z)\ {}_0D_t^\alpha\left[\frac{\partial}{\partial z}w(z,t)\right]\right\} = \frac{1}{E_0}q(z,t),$$

which is derived by adopting the constitutive equation

$$\sigma(z,t) = E_0\varepsilon(z,t) + E_\alpha\ {}_0D_t^\alpha\varepsilon(z,t)$$

$\sigma(z,t)$ and $\varepsilon(z,t)$ being stress and strain, respectively; $A(z)$ is the rod cross-sectional area; E_0 and E_α are material properties; and $c_0^2 = E_0/\rho$ and $c_\alpha^2 = E_\alpha/\rho$, ρ being the material specific weight. The operator ${}_0D_t^\alpha$ is the fractional derivative operator and α denotes the fractional derivative order.

This is a partial fractional differential equation which is going to be studied both by analytical techniques and by numerical algorithms. The analytical technique is based on the determination of the solution via separation of variable. In this context, given the boundary conditions, the rod modes of vibration can be derived and the time variation of the mode amplitudes can be determined. Thus, the rod response in frequency domain can be calculated from the excitation power spectral density function. The reliability of this approach is assessed vis-à-vis the results of relevant Monte Carlo simulations. In this regard, the numerical algorithm used for integrating in time domain the governing equation is developed by combining the G1-algorithm used for approximating the fractional derivative with a Newmark – type integration scheme.

References

[1] P.G. Nutting, A new general law of deformation, J. Franklin Inst. 191 (1921) 679–685. https://doi.org/10.1016/S0016-0032(21)90171-6.

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V. Personnel:

H. Zhang, Graduate Student
G. Malara, Post-Graduate Fellow
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Brown University Report (PI: George Karniadakis & co-PI: Mark Ainsworth)

(Research Areas 1-6)

Brown personnel on this project, 8/1/19-7/31/20: PI George Karniadakis was supported for 0.85 months, and co-PI Mark Ainsworth for 1.1 months. Moreover, Dr. Zhiping Mao (8 months), Jinlian Ren (2 months), Shuai Jiang (0.5 months), and Lu Lu (1 month) participated as postdocs. The following PhD students were also supported by the MURI: Lu Lu (10 months), Ansel Blumers (1 month), and Liu Yang (6 months). Also, the following visiting scholars were supported by the MURI: Xiaoli Chen (1 month), Kaixuan Zhang (1 month), and Ladan Avazpour (1 month). In addition, the following people were funded from the cost-sharing account associated with this project: Zhiping Mao (1 month), Jinlian Ren (2 months), Ladan Avazpour (4 months), Xiaoli Chen (9 months), and Pavan Mehta (0.5 months).

Research at Brown U: Mark Ainsworth

During the year 2019-2020, Ainsworth's attention shifted to identifying situations in which fractional models have direct physical applications. The problem of modelling crystals was considered, in which the Phase Field Crystal Model (Elder and Grant) has gained considerable traction. Two articles were published relating to improving the classical PFC model. In particular, in [1] we showed that a Fractional Phase Field Crystal Model gives much better predictions of the grain boundary energy than the classical model as well as performing as well as the classical model for other quantities. In [2], we showed that the PFC model is able to correctly model the observed multivalued nature of the elastic constants through a structural phase transition whereas other authors have exclusively adopted a computational approach which [2] showed does not capture the correct physical behavior.

In addition, Ainsworth gave an invited talk in Singapore in which the MURI project overall was discussed along with work carried out earlier in the project on Fractional Phase Field Models. A faculty wide colloquium talk was presented at Nanyang Technological University on a similar topic.

[1] "*Fractional phase-field crystal modelling: analysis, approximation and pattern formation*", M. Ainsworth and Z. Mao, IMA Journal of Applied Mathematics, 85(2), pp. 231-262, year 2020.
We consider a fractional phase-field crystal (FPFC) model in which the classical SwiftHohenberg equation (SHE) is replaced by a fractional order SwiftHohenberg equation (FSHE) that reduces to the classical case when the fractional order =1. It is found that choosing the value of appropriately leads to FSHE giving a markedly superior fit to experimental measurements of the structure factor than obtained using the SHE (=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 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 behaviour as the SHE, which is crucial for the success of the PFC model, independently of the fractional exponent . 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. While the salient features of PFC and FPFC are identical, we expect more subtle features to differ. The prediction of grain boundary energy arising from a mismatch in orientation across a material interface is another notable success of the PFC model. The grain boundary energy can be evaluated numerically from the PFC model and compared with experimental measurements. The grain boundary energy is a derived quantity and is more sensitive to the nuances of the model. We compare the predictions obtained using the PFC and FPFC models with experimental observations of the grain boundary energy for several materials. It is observed that the FPFC model gives superior agreement with the experimental observation than those obtained using the classical PFC model, especially when the mismatch in orientation becomes larger.

[2] *"Phase field crystal based prediction of temperature and density dependence of elastic constants through a structural phase transition*", M. Ainsworth and Z. Mao, Phys. Rev. B, 100(10), pp. 104101-104112, year 2019.
Explicit, analytical forms are obtained for the elastic constants arising from the phase field crystal (PFC) model in which the dependence of the constants on proxies for the temperature and density in the PFC model is clearly exhibited. The expressions indicate that the elastic constants are multivalued in certain temperature ranges corresponding to regions where two or more phases coexist, in agreement with experimental observations. The analytical formulas for the variation of the elastic constants with density agree with those obtained using a computational approach in [Wang, Huang, and Liu, Phys. Rev. B 97, 144112 (2018)] but only in certain regimes. Specifically, if it is assumed that only the bcc state is present, then our formulas agree with the numerical results presented in [Wang, Huang, and Liu, Phys. Rev. B 97, 144112 (2018)]. In general, the bcc state is not the only phase present and, if other phases are taken into account, then the results differ in those regions where alternative states are favored energetically. Similar conclusions hold if one looks at temperature dependence instead of density variation.

Research at Brown U: George Karniadakis

A stabilized semi-implicit Fourier spectral method for nonlinear space-fractional reaction-diffusion equations [1]: The reaction-diffusion model can generate a wide variety of spatial patterns, which has been widely applied in chemistry, biology, and physics, even used to explain self-regulated pattern formation in the developing animal embryo. In this work, a second-order stabilized semi-implicit time-stepping Fourier spectral method for the reaction-diffusion systems of equations with space described by the fractional Laplacian is developed. We adopt the temporal-spatial error splitting argument to illustrate that the proposed method is stable without imposing the CFL condition, and an optimal L2-error estimate in space is proved. We also analyze the linear stability of the stabilized semi-implicit method and obtain a practical criterion to choose the time step size to guarantee the stability of the semi-implicit method. Our approach is illustrated by solving several problems of practical interest, including the fractional Allen-Cahn, Gray-Scott and FitzHugh-Nagumo models, together with an analysis of the properties of these systems in terms of the fractional power of the underlying Laplacian operator, which are quite different from the patterns of the corresponding integer-order model.

A fast solver for spectral elements applied to fractional differential equations using hierarchical matrix approximation [2]: We develop a fast solver for the spectral element method (SEM) applied to the two-sided fractional diffusion equation on uniform, geometric and graded meshes. By approximating the singular kernel with a degenerate kernel we construct a hierarchical matrix (H-matrix) to represent the stiffness matrix of the SEM and provide error estimates, which we verify numerically. We can solve efficiently the H-matrix approximation problem using a hierarchical LU (H-LU) decomposition method, which reduces the computational cost to $O(r^2 N_d \log^2 N) + O(r^3 N_d \log N)$, where r is the rank of the H-LU decomposition, Nd is the total number of degrees of freedom and N is the number of elements. However, we lose the high accuracy of the SEM. To prevent this, we solve the corresponding preconditioned system by using the H-matrix approximation problem as a preconditioner, hence, recovering the high-order accuracy of the SEM. Numerical results show that the condition number of the preconditioned system is independent of the polynomial degree P and grows with the number of elements, but at modest values of the rank R (here R is the rank of submatrices of the H-matrix approximation) it is below order 10 in our experiments, which represents a reduction of more than 11 orders of magnitude from the unpreconditioned system. This reduction is higher in the two-sided fractional derivative compared to one-sided fractional derivative. The corresponding cost is $O(r^2 N_d \log^2 N) + O(r^3 N_d \log N) + O(N_d^2)$. Moreover, by using a structured mesh (uniform or geometric mesh), we can further reduce the computational cost to $O(r^2 N_d \log^2 N) + O(r^3 N_d \log N) + O(P^2 N \log N)$ for the preconditioned system. Furthermore, we compare the present method with the adaptive cross approximation (ACA), which is kernel independent and relies on the coefficient matrix. The comparison shows that the accuracy using the present algorithm is better than the one using ACA for the H-matrix approximation problem, and furthermore, we have observed that the ACA method may fail to converge in some cases.

Potential Flow Generator with L_2 Optimal Transport Regularity for Generative Models [3]: We propose a potential flow generator with L_2 optimal transport regularity, which can be easily integrated into a wide range of generative models including different versions of GANs and flow-based models. We show the correctness and robustness of the potential flow generator in several 2D problems, and illustrate the concept of "proximity" due to the L_2 optimal transport regularity. Subsequently, we demonstrate the effectiveness of the potential flow generator in image translation

tasks with unpaired training data from the MNIST dataset and the CelebA dataset.

nPINNs: nonlocal Physics-Informed Neural Networks for a parametrized nonlocal universal Laplacian operator. Algorithms and Applications [4]: Physics-informed neural networks (PINNs) are effective in solving inverse problems based on differential and integro-differential equations with sparse, noisy, unstructured, and multifidelity data. PINNs incorporate all available information, including governing equations (reflecting physical laws), initial-boundary conditions, and observations of quantities of interest, into a loss function to be minimized, thus recasting the original problem into an optimization problem. In this paper, we extend PINNs to parameter and function inference for integral equations such as nonlocal Poisson and nonlocal turbulence models, and we refer to them as nonlocal PINNs (nPINNs). The contribution of the paper is three-fold. First, we propose a unified nonlocal Laplace operator, which converges to the classical Laplacian as one of the operator parameters, the nonlocal interaction radius δ goes to zero, and to the fractional Laplacian as δ goes to infinity. This universal operator forms a super-set of classical Laplacian and fractional Laplacian operators and, thus, has the potential to fit a broad spectrum of data sets. We provide theoretical convergence rates with respect to δ and verify them via numerical experiments. Second, we use nPINNs to estimate the two parameters δ, and α, characterizing the kernel of the unified operator. The strong non-convexity of the loss function yielding multiple (good) local minima reveals the occurrence of the operator mimicking phenomenon, that is, different pairs of estimated parameters could produce multiple solutions of comparable accuracy. Third, we propose another nonlocal operator with spatially variable order $\alpha(y)$, which is more suitable for modeling turbulent Couette flow. Our results show that nPINNs can jointly infer this function as well as δ. More importantly, these parameters exhibit a universal behavior with respect to the Reynolds number, a finding that contributes to our understanding of nonlocal interactions in wall-bounded turbulence.

A Unified Theory of Fractional, Nonlocal, and Weighted Nonlocal Vector Calculus [5]: Nonlocal and fractional models capture effects that classical (or standard) partial differential equations cannot describe; for this reason, they are suitable for a broad class of engineering and scientific applications that feature multiscale or anomalous behavior. This has driven a desire for a vector calculus based on nonlocal and fractional derivatives to derive models of, e.g., subsurface transport, turbulence, and conservation laws. In the literature, several independent definitions and theories of nonlocal and fractional vector calculus have been put forward. Some have been studied rigorously and in depth, while others have been introduced ad-hoc for specific applications. At the moment, this fragmented literature suffers from a lack of rigorous comparison and unified notation, hindering the development of nonlocal modeling. The ultimate goal of this work is to provide a new theory and to connect all the dots by defining a universal form of non-local vector calculus operators under a theory that includes, as a special case, several well-known proposals for fractional vector calculus in the limit of infinite interactions.
We show that this formulation enjoys a form of Green's identity, enabling a unified variational theory for the resulting nonlocal exterior-value problems, and is consistent with several independent results in the fractional calculus literature. The proposed unified vector calculus has the potential to go beyond the analysis of nonlocal equations by supporting new model discovery, establishing theory and interpretation for a broad class of operators and providing useful analogues of standard tools from classical vector calculus.

Convergence Analysis of The Time-Stepping Numerical Methods for Time-Fractional Nonlinear Subdiffusion Equations [6]: In 1986, Dixon and McKee developed a discrete fractional Grönwall inequality [Z. Angew. Math. Mech., 66 (1986), pp. 535–544], which can be seen as a generalization of the classical discrete Grönwall inequality. However, this generalized discrete Grönwall inequality has not been widely applied in the numerical analysis of the time-stepping methods for the time-fractional evolution equations. The main purpose of this paper is to show how to apply the generalized discrete Grönwall inequality to prove the convergence of a class of time-stepping numerical methods for time-fractional nonlinear subdiffusion equations, including the popular fractional backward difference type methods of order one and two, and the second-order fractional Crank-Nicolson type methods. We obtain the optimal L_2 error estimate in space discretization. The convergence of the fast time-stepping numerical methods is also proved in a simple manner.

Fractional Calculus and Numerical Methods for Fractional PDEs [7]: This study provides a review of the recent relevant literature and development in numerical methods for solving fractional differential equations (FDEs) with focus on high-order schemes. After an overview of classification criteria of derivatives and their definitions according to different physical backgrounds, we discuss the extension to fractional Laplacian and fractional vector calculus for the case of higher-dimensional problems in a physical domain. We present a brief summary of existing numerical methods and explain the recently developed spectral/spectral element methods with several numerical examples. We also discuss some of the recent techniques of parameter estimation in the context of fractional models.

A stabilized semi-implicit Fourier spectral method for nonlinear space-fractional reaction-diffusion equations: [8] The reaction-diffusion model can generate a wide variety of spatial patterns, which has been widely applied in chemistry, biology, and physics, even used to explain self-regulated pattern formation in the developing animal embryo. In this work, a second-order stabilized semi-implicit time-stepping Fourier spectral method for the reaction-diffusion systems of equations with space described by the fractional Laplacian is developed. We adopt the temporal-spatial error splitting argument to illustrate that the proposed method is stable without imposing the CFL condition, and an optimal L^2-error estimate in space is proved. We also analyze the linear stability of the stabilized semi-implicit method and obtain a practical criterion to choose the time step size to guarantee the stability of the semi-implicit method. Our approach is illustrated by solving several problems of practical interest, including the fractional Allen-Cahn, Gray-Scott and FitzHugh-Nagumo models, together with an analysis of the properties of these systems in terms of the fractional power of the underlying Laplacian operator, which are quite different from the patterns of the corresponding integer-order model.

An open-source parallel code for computing the spectral fractional Laplacian on 3D complex-geometry domains [9]: We present a spectral element algorithm and open source code for computing the fractional Laplacian defined by the eigenfunction expansion on finite 2D/3D complex domains with both homogeneous and nonhomogeneous boundary. We demonstrate the scalability of the spectral element algorithm on large clusters by constructing the fractional Laplacian based on computed eigenvalues and eigenfunctions using up to thousands of CPUs. To demonstrate the accuracy of this eigen-based approach for computing the factional Laplacian, we approximate the solutions of the fractional diffusion equation using the computed eigenvalues

and eigenfunctions on a 2D quadrilateral, and on a 3D cubic and cylindrical domain, and com- pare the results with the contrived solutions to demonstrate fast convergence. Subsequently, we present simulation results for a fractional diffusion equation on a hand-shaped domain discretized with 3D hexahedra, as well as on a domain constructed from the Hanford site geometry corresponding to non-zero Dirichlet boundary conditions. Finally, we apply the algorithm to solve the surface quasi-geostrophic (SQG) equation on a 2D square with periodic boundaries. Simulation results demonstrate the accuracy, efficiency, and the geometric flexibility of our algorithm and show that our algorithm can capture the subtle dynamics of anomalous diffusion modeled by the fractional Laplacian on complex-geometry domains.

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[9] M. Carlson, X. Zheng, H. Sundar, G. E. Karniadakis, R. M. Kirby, "An open-source parallel code for computing the spectral fractional Laplacian on 3D complex-geometry domains", *Computer Physics Communications*, Accepted upon Revision, 2020

Worcester Polytechnic Institute (Zhongqiang Zhang)

Error estimates of a spectral Petrov–Galerkin method for two-sided fractional reaction–diffusion equations [1]: We study regularity and the spectral method for two-sided fractional diffusion equations with a reaction term. We show that the regularity of the solution in weighted

Sobolev spaces can be greatly improved compared to that in standard Sobolev spaces. With this regularity, we prove an optimal error estimate for the spectral Petrov–Galerkin method. Numerical results are presented to verify our theoretical convergence orders.

OPTIMAL REGULARITY AND ERROR ESTIMATES OF A SPECTRAL GALERKIN METHOD FOR FRACTIONAL ADVECTION-DIFFUSION-REACTION EQUATIONS [2]: We investigate a spectral Galerkin method for the fractional advection-diffusion-reaction equations in one dimension. We first prove sharp regularity estimates of solutions in non-weighted and weighted Sobolev spaces. Then we obtain optimal convergence orders of the spectral Galerkin methods for both fractional advection-diffusion and diffusion-reaction equations. We also present an iterative solver with a quasi-optimal complexity. Numerical results are presented to verify the theoretical analysis.

ERROR ESTIMATES OF SPECTRAL GALERKIN METHODS FOR A LINEAR FRACTIONAL REACTION-DIFFUSION EQUATION [3]: We consider a fractional diffusion equation with a reaction term in one dimensional space. We first establish the regularity in weighted Sobolev spaces. Then we present an optimal error estimate for a spectral Galerkin method for the equation and a sub-optimal error estimate for a spectral Petrov-Galerkin method. Numerical results suggest that the convergence order in a weighted L_2 -norm is $2\alpha + 1$ for smooth inputs where α is the fractional order.

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[3] Z. Zhang. "Error estimates of spectral Galerkin methods for a linear fractional reaction-diffusion equation." Journal of Scientific Computing, 78:1087-1110, 2019

Utah (Add-On: co-PI: Robert M. Kirby)

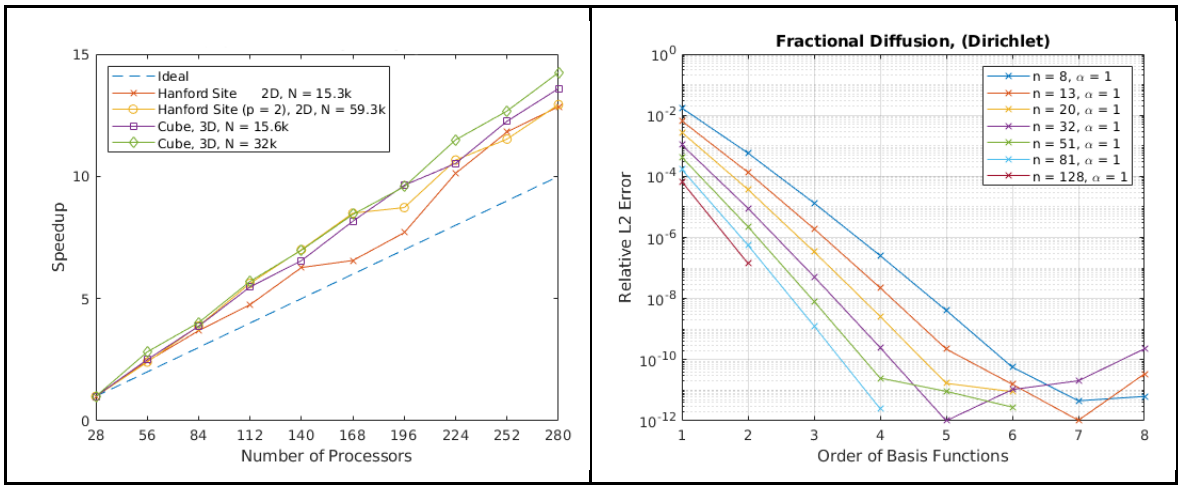
(Research Areas 6)

Space and Time Fractional Operators in Nektar++ Progress Report

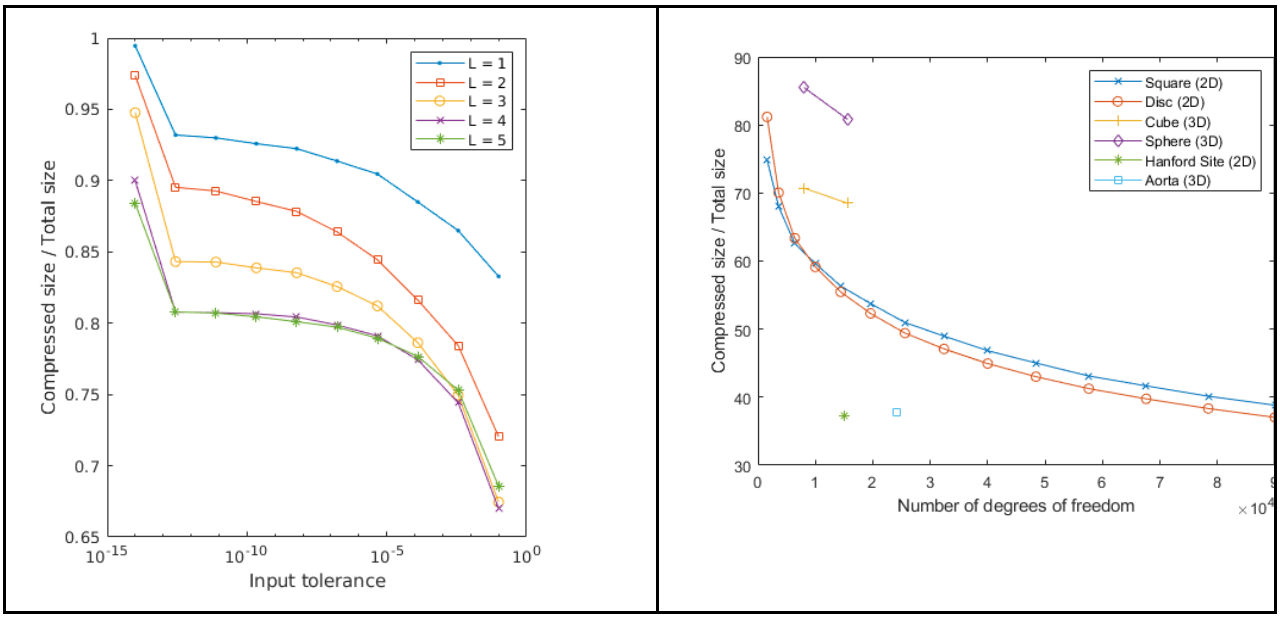
Max Carlson, Hari Sundar, Akil Narayan, Allen Sanderson and Robert M. Kirby
Scientific Computing and Imaging (SCI) Institute, University of Utah

Space-fractional differential equations

At this time we have completed the implementation of our space-fractional Laplacian extension for Netkar++. Using our highly scalable custom eigenvalue solver, we can generate the full eigenbasis for any given complex geometry for meshes with up to half a million degrees of freedom. For validation, we have tested this method of eigenfunction expansion on several geometries for both fractional diffusion and fractional Poisson and verified spectral convergence in solution error with respect to the order of the mesh's basis elements. The title figures show the parallel efficiency of the eigenvalue solver (left) and the spectral convergence of the solution error (right).



This work has generated two papers; The first paper is primarily related to the scalable eigenvalue solver and has been published at the ACM International Conference on Supercomputing (ICS 2020). The other paper is a joint work with our colleagues at Brown, George Karniadakis and Xiaoning Zheng. This second paper focuses more on the mathematical aspects of the solver method and was recently accepted for publication in the Computer Physics Communications (CPC) journal. Scalability and performance was evaluated on University of Texas TACC's Frontera computing system.



Once the eigenbasis for a given mesh is computed, the complexity for solving a space-fractional PDE is dominated by the time it takes to apply a dense N by N matrix to a vector. Since this is an $O(N^2)$ operation, we are currently exploring techniques for reducing the complexity of applying this operator to O(N log N). Since our previous report, we have experimented with various hierarchical matrix compression and developed a technique that works well for the generated eigenbasis. The figures on this page show some results from the butterfly interpolative decomposition method that we have experimented with for compressions.

We have also developed an updated interface for the Nektar++ fractional PDE solver to facilitate the merging of the space and time fractional efforts. This updated interface is also being used to develop experiments for future exploration of fractional operators as a whole.

- Max Carlson, Xiaoning Zheng, Hari Sundar, George Em Karniadakis, Robert M. Kirby, "An open-source parallel code for computing the spectral fractional Laplacian on 3D complex-geometry domains", *Computer Physics Communications*, Accepted upon Revision, 2020.
- Max Carlson, Robert M. Kirby and Hari Sundar, "A Scalable Framework from Solving Fractional Diffusion Equations", International Conference on Supercomputing (ICS) 2020, Barcelona, Spain, June 29 - July 2, 2020.

Time-fractional differential equations

We have implemented a first-order version of the fast time-fractional differential equation (DE) solver in Nektar++. Standard implementations require quadratic complexity for performing convolutions involved in time-fractional DE's. The current implementation performs fast convolution, and we demonstrate log-linear complexity in cumulative time, and logarithmic storage in the number of time steps, as shown in Figure 1 for a test problem on a system of

fractional DE's. This is in contrast to more naïve algorithms that not only require quadratic complexity in time, but also linear storage in the number of time steps. We also observe that the error committed by the algorithm does not blow up in time.

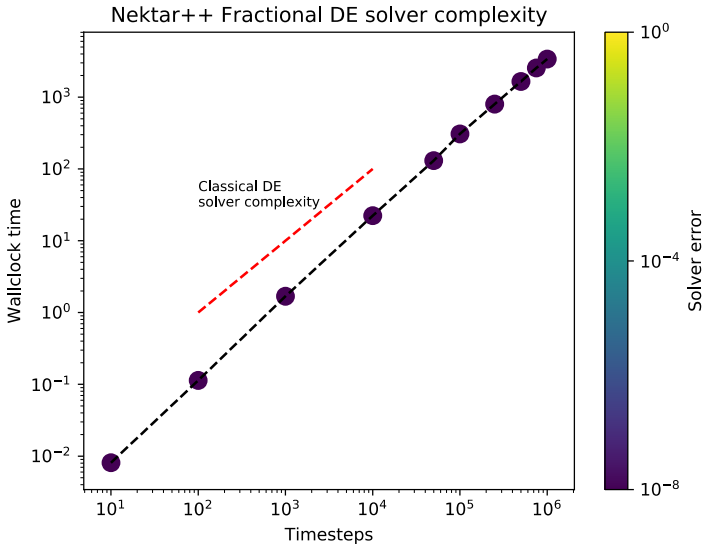


Figure 1: Computational complexity of Nektar++ Fractional DE solver.

This algorithm is currently implemented in Nektar++ with documentation, and is able to be deployed on large-scale fractional DE application problems. Current efforts are focused on combining the time-fractional DE solver with space-fractional DE methods that are developed under a parallel task in this project. Specific goals are to demonstrate the efficiency gains in Nektar++ on solving DE's that are fractional in both space and time, compared to utilizing more traditional algorithms.

ARO MURI # 8 Project (2015): August 2020--July 2021 Progress Report

Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications

- **George Karniadakis & Mark Ainsworth, Brown University**
- **Qiang Du, Columbia University**
- **Mohsen Zayernouri, Michigan State University**
- **Pol Spanos, Rice University**
- **Hong Wang, University of South Carolina**
- **Add-On: Zhen Li (Clemson University) – Guang Lin (Purdue University)**

Background: This MURI project is the vision of a team of researchers from Brown University, Michigan State University, Columbia University, University of South Carolina, and Rice University with overlapped interests and complementary expertise on theory, numerical methods, and applications of fractional PDEs (FPDEs). Our overarching goal is the development of a seamless integration of theory and algorithms for data-driven FPDEs, while targeting the common themes of conservation, monotonicity, adaptive refinement, and high-order accuracy in the context of simulations of multiphase flows, turbulence, fluid-structure interactions, hydrology, and solid mechanics. We envision a combined mathematical and computational framework, where the fractional operators can be constructed based on available data, hence providing model validation for the specific phenomenon but also a tailor-based simulation capability that can be scaled to real-life applications. The proposed research plan emphasizes a dynamic integration of six main research areas that form the pillars of our integrated approach:

• *Research Area 1*: Theory of non-local operators and stochastic interpretation of fractional operators.
• *Research Area 2:* Numerical solution of fractional PDEs with emphasis on variable fractional order.
• *Research Area 3:* Fast solvers for dense linear systems with linear/quasi-linear computational complexity.
• *Research Area 4:* Stochastic FPDEs and determination of the fractional order directly by available data.
• *Research Area 5:* Applications to fluid and solid mechanics, fluid-structure interactions, two-phase flows, turbulence and reactive system with front propagation.
• *Research Area 6:* High performance computing & developing opensource software for fractional problems.

MURI Objectives

- To address the common physical themes of anomalous transport, exponentially accelerated fronts, non-Markovian behavior and long-range interactions, self-similarity and scaling, singular behavior, interfaces and finite-domain decorrelation effects.

- To develop rigorous mathematical theory, algorithms and software for data-driven fractional PDEs that will provide significant breakthroughs towards modeling, analyzing and subsequently controlling complex multiscale systems characterized by the aforementioned phenomena —in a computationally scalable way.
- To demonstrate the physical relevance and effectiveness of our framework in diverse applications of interest to DoD, characterized by the common themes of conservation, monotonicity, adaptive refinement and high-order accuracy.

MURI Extension Tasks:
• *Task I*: Model non-local interactions in large-eddy simulations of particulate turbulent flows.

• *Task II*: Develop fractional phase field crystals models for brittle materials.

• *Task III*: Develop multi-scale stochastic phase-field models of failure in brittle materials.

• *Task IV*: Develop fractional physics-informed neural networks for high-performance engine materials.

• *Task V*: Stochastic partial differential equations with fractional operators for geotechnical engineering applications.

• *Task VI*: Model contact tracing in the COVID-19 pandemic and post-pandemic.

• *Task VII*: Develop new fractional backpropagation models for neural networks.

• *Task VIII*: Numerical analysis of algorithms for learning nonlocal-in-time dynamics.

Status of the Project
There has been great progress in the five years on all six research areas, in recruiting excellent postdocs and PhD students, in participating in conferences with invited and contributed talks as well as on organizing mini-symposia and workshops on FPDEs. The extension helped us to start new areas on machine learning and to further develop new algorithms for demanding and diverse applications. In the following, we provide a summary of progress by each co-PI. First, we provide some highlights on all our activities and then we present the report of each PI.

Interactions
To facilitate the rapid adoption of new developed models and methods and enhance team interaction and cross-institution collaborations, biweekly online meetings were held via Zoom with participants from the US Army Research Laboratory (ARL), Brown University, Clemson University and University of South Carolina. Dr. Luis Bravo, Prof. George Karniadakis, Prof. Zhen Li and Prof. Hong Wong led research teams at their respective institutions to update research progress and discuss research challenges through scheduled biweekly meetings. The ARL team was instrumental in formulating three problems of real-world application of their immediate interest, where they were equally responsible for bridging the gap between fundamental research to applied sciences. The three problems include: (1) Mission critical operations carried out in desert and arid environments often leads to deposition of sand particles in the engine, which eventually erodes the turbine blades of the jet engines. In this research direction, the research team at Clemson University alongside ARL investigated the prediction of charged particles' motion in the vicinity of solid surfaces. (2) One of open-ended questions in the turbulence community is the prediction of separated boundary layers. The prediction of which improves aircraft's overall efficiency. The

team at Brown University responded to this challenge by formulating non-local turbulence models using fractional calculus. (3) The feasibility of fractional calculus was explored for solid mechanics problems with teams at University of South Carolina jointly with ARL.

MURI Highlights

- More than 251papers have been published or submitted on all six research areas of MURI.
- More than 100 invited and plenary talks by MURI personnel.
- Volume on numerical methods in Handbook of FPDEs.
- Several mini-symposia and two workshops organized by MURI PIs.
- New research focusing on 2D & 3D fractional Laplacians in bounded domains with emphasis on boundary conditions and their stochastic interpretation. 11-author revised paper.
- New research focusing on machine learning, fractional photonics, stochastic fractional PDEs and opensource software enabled by the add-on funding.
- Fractional models of turbulent polymer drag reduction at high Reynolds number.
- Combine FPDE and molecular dynamics to efficiently simulate anomalous diffusive transport in heterogeneous porous materials with nanoscale pores.
- Non-local modeling of ion diffusion in battery systems & experiments.
- We discovered new fractional phase-field/non-local equations for interface problems.
- New opensource software at Brown (fractional NEKTAR), Uath (Nektar++) and MSU (FracFit).
- Developing a unified theory of fractional, nonlocal, and weighted nonlocal vector calculus.
- Physical applications of fractional models, particularly, fractional phase field crystal models.
- Theoretical formulation of a fractional subgrid-scale model for turbulent flows.
- Investigating anomalous features in materials failure, internal flows, and structural vibration.
- Atomistic-to-meso multi-scale data-driven graph surrogate modeling of dislocation glide.
- Data-driven fractional subgrid-scale modeling for scalar turbulence: A nonlocal LES approach.
- Data-driven failure prediction in brittle materials: A phase-field based machine learning framework.
- A thermodynamically consistent fractional visco-elasto-plastic model with memory-dependent damage for anomalous materials.
- Innovative discretization schemes for a wide class of semi-linear parabolic equations in the form of gradient flows.
- Rigorous mathematical convergence theory to the discovery of unknown dynamics through data-driven modeling
- Fractional Euler-Bernoulli and Timoshenko beam models to accurately describe the vibration of viscoelastic beams.
- A Caputo fractional derivative-based gradient descent algorithm for optimization.
- Identifiability and predictability of data-driven integer- and fractional-order epidemiological models using physics-informed neural networks.
- Efficient non-convex machine learning tools to train neural networks.

Michigan State University: (co-PI: Mohsen Zayernouri)

(Research Areas 1, 4 & 5)

(Extension Tasks I & III)

Personnel supported on the MURI grant:
Mohsen Zayenrouri, MSU-PI, 2 months
Eduardo de Moraes, PhD Student, 12 months
Mehdi Samiee, PhD Student, 7 months
Ali Akhavan-Safaei, PhD Student, 12 months
Seyed Hadi Seyedi, PhD Student, 11 months

Summary:
The MSU team has made substantial progress on understanding incompressible turbulence flows (both fluid flows and scalar turbulence), atomistic-to-meso multi-scale modeling of dislocation, self-singularity-capturing scheme for fractional models, fractional LES modeling, phase-field based supervised machine learning for material failure, thermodynamically consistent fractional visco-elasto-plastic models with memory- and path-dependent damage, also understanding anomalous nonlinear vibration of fractional viscoelastic structures.

Highlights:

During the past year, the MSU MURI team had papers accepted on:

- Atomistic-to-meso multi-scale data-driven graph surrogate modeling of dislocation glide
- Data-Driven Fractional Subgrid-scale Modeling for Scalar Turbulence: A Nonlocal LES Approach
- A self-singularity-capturing scheme for fractional differential equations
- Data-Driven Failure Prediction in Brittle Materials: A Phase-Field Based Machine Learning Framework
- A Unified Petrov–Galerkin Spectral Method and Fast Solver for Distributed-Order Partial Differential Equations
- Anomalous Nonlinear Dynamics Behavior of Fractional Viscoelastic Beams
- A thermodynamically consistent fractional visco-elasto-plastic model with memory-dependent damage for anomalous materials

Published (& in Press) Journal Papers:

[1] E. A. B. de Moraes, J. L. Suzuki, M. Zayernouri, Atomistic-to-meso multi-scale data-driven graph surrogate modeling of dislocation glide, Computational Materials Science 197, 110569 (2021)

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[8] J. L. Suzuki, E. Kharazmi, P. Varghaei, M. Naghibolhosseini, M. Zayernouri, Anomalous Nonlinear Dynamics Behavior of Fractional Viscoelastic Beams, ASME Journal of Computational and Nonlinear Dynamics

Submitted Journal Manuscripts:

- A Parallel Integrated Computational-Statistical Platform for Turbulent Transport Phenomena
- Tempered Fractional LES Modeling

Conferences/Talks:

[1] M. Zayernouri, Fractional Large Eddy Simulation (LES) Modeling for Turbulence, One Nonlocal World, Jan. 22nd, 2021

[2] E. Moraes, M. Zayernouri, Nucleation of Fractional Operators in Material Failure: A Local Nonlocal Approach, SIAM Conference on Mathematical Aspects of Material Science, Spain, May 2021.

[3] E. Moraes, M. Zayernouri, Multi-Scale Modeling of Dislocation Dynamics, 16th U.S. National Congress on Computational Mechanics, July 25-29, 2021

Columbia University Report (co-PI: Qiang Du)

(Research Areas 1 & 5)
(Extension Task VIII)

Personnel supported on the MURI grant:
Qiang Du, PI (1 mon), Hwi Lee, GRA (9 mon), Zirui Xu GRA (3 mon), Kuang Huang, GRA (0 mon)

Summary:
The research team at Columbia, under the direction of Qiang Du, has actively participated in research supported by the MURI project, focusing on the mathematical analysis and numerical computation of nonlocal and fractional models. The research resulted in publications in top applied mathematics journals like Acta Numerica and SIAM Rev, two of the journals with highest impact factors in mathematics), and invited lectures such as the plenary lecture at the SIAM Conference on the mathematical aspects of materials science (SIAM MS21).

Highlights:
We published an invited paper in **Acta Numerica** (Impact factor 8.667, highest in mathematics) to review the recent progress on the numerical solutions of nonlocal and fractional models.

One of our recent work, published in **SIAM Review** 2021 (Impact factor 8.02, second highest in mathematics) as a research spotlight article, developed innovative discretization schemes for a wide class of semi-linear parabolic equations in the form of gradient flows. One example is the nonlocal Allen-Cahn equation that has attracted much interests in the nonlocal/fractional community. Our method can preserve maximum bound principles and energy dissipation.

We had a paper published in Frac. Cal. Anal. Appl., giving stochastic interpretations to a new nonlocal/fractional dynamics that we proposed in the literature for the first time. The review commented on the paper that contains "rigor and throughout discussion", "**full of wonderful results** connecting probability theory with fractional calculus", and "a very worthy and important contribution in linking fractional calculus to the theory of Markov processes."

We also made interesting studies on nonlocal traffic flow models and numerical approximations of nonlocal conservation laws.

In addition, we also published a work to offer rigorous mathematical convergence theory to the discovery of unknown dynamics through data-driven modeling, in combination with numerical integrators such as the Linear Multistep Methods.

The PI Du also received recognition as he was awarded the **TJR Hughes Medal** by the **USACM** (US Association of Computational Mechanics) at the USNCCM 2021 for his "numerous innovative contributions to computational physics and computational fluid mechanics, and unwavering service to the scientific computing community."

Published (& in Press) Journal Papers:

[1] Q. Du, L. Ju, X. Li and Z. Qiao, Maximum bound principles for a class of semilinear parabolic equations and exponential time differencing schemes, SIAM Review, (Research Spotlight), 63, 317-359, 2021.

[2] R. Keller and Q. Du, Discovery of dynamics using linear multistep methods, SIAM J. Numer. Anal, 59, 429-455, 2021.

[3] Q. Du, J. Yang and Z. Zhou, Time-fractional Allen-Cahn equations: analysis and numerical methods, J. Sci. Comp., 85 (2), 1-30, 2020.

[4] Q. Du, L. Toniazzi and Z. Xu, Censored fractional derivative, Fract. Calc. Appl. Anal, 24 (4), 1035–1068, 2021.

[5] M. DElia, Q. Du, C. Glusa, M. Gunzburger, X. Tian and Z. Zhou, Numerical methods for nonlocal and fractional models, Acta Numerica, 29, 1-124, 2020.

Submitted Journal Manuscripts:

[1] Q. Du, T. Mengesha and X. Tian, Nonlocal criteria for compactness in the space of L^p vector fields, submitted,2020.

[2] Q. Du, X. Tian, C. Wright and Y. Yu, Nonlocal trace spaces and extension results for nonlocal calculus, submitted, 2021.

[3] Q. Du, T. Mengesha and X. Tian, Fractional Hardy-type and trace theorems for nonlocal function spaces with heterogeneous localization, submitted (under revision), 2021.

[4] X. Yu, Y. Xu and Q. Du, Asymptotically compatible approximations of linear nonlocal conservation laws with variable horizon, submitted (under revision), 2021.

[5] K. Huang and Q. Du Stability of a nonlocal traffic flow model for connected vehicles, submitted (under revision), 2020.

Conferences/Talks:

[1] Du, Top signs of nonlocal modeling, Plenary talk at the SIAM Conference on the mathematical aspects of materials science (SIAM MS21), Bilbao, Spain (online), May 2021.

[2] Du, Nonlocal conservation laws and nonlocal traffic flow models, invited lecture at the John H. Barrett Memorial Lectures, Univ of Tenn at Knoxville; May 2021

University of South Carolina Report (co-PI: Hong Wang)

(Research Area 1, 2, 3 & 4)
(Extension Task IV)

Personnel supported on the MURI grant:
Hong Wang, PI, 3 months;
Yiqun Li, female, STEM PhD student, 9 months.

Summary:
The UofSC team proved the existence, uniqueness, and smoothness of variable-order fractional wave equations (FWEs), which arise, e.g., in long term simulation of forced vibrations of viscoelastic materials when the materials may undergo fatigue and failure. However, fractional wave operators do not have the exponential decaying properties, which were fundamental in the analysis of fractional diffusion equations. We developed new techniques to make breakthrough in the analysis and simulation of variable-order FWEs.
One overarching goal of Army Research Lab (ARL) is to develop high-performance engineering materials in the evolution of highly robust and efficient propulsion systems. In particular, in collaboration with the team of Dr. Karniadakis, the lead PI of the project, and colleagues in ARL, to develop fractional Euler-Bernoulli and Timoshenko-Ehrenfest beam models to accurately simulate the vibrations of viscoelastic beams.

Highlights:

1. It is well known that a single-degree-of-freedom spring-mass system experiences resonance when the driving frequency matches the natural frequency of the system, which can be significantly reduced via damping.
2. Classical Euler-Bernoulli and Timoshenko-Ehrenfest beams have infinitely many natural frequencies, which makes it a tough task to avoid resonance in system designs and operations. Furthermore, the viscous damping mechanism cannot eliminate the resonance in these beam models.
3. We derived fractional Euler-Bernoulli and Timoshenko beam models to accurately describe the vibration of viscoelastic beams, and show that the models naturally eliminate the resonance without any artificial damping means needed.

Published (& in Press) Journal Papers:

1. Z.W. Fang, H.W. Sun, and H. Wang, A fast method for variable-order Caputo fractional derivative with applications to time-fractional diffusion equations. Comput Math Appl 80 (2020), 1443--1458.

2. H. Liu, A. Cheng, and H. Wang, A parareal finite volume method for variable-order time-fractional diffusion equations. J Sci Comput 85 (2020) Article 19.

3. H. Wang and X. Zheng, An optimal-order error estimate of the lowest-order ELLAM-MFEM approximation to miscible displacement in three space dimensions. J Comput Appl Math 375 (2020), 112819.

4. Z. Yang, X. Zheng, and H. Wang, A variably distributed-order time-fractional diffusion equation: analysis and approximation. Comput Methods Appl Mech Engrg 367 (2020), 113118.

5. X. Zheng and H. Wang, An error estimate of a numerical approximation to a hidden-memory variable-order space-time fractional diffusion equation. SIAM J Numer Anal 58 (2020), 2492--2514.

6. X. Zheng, H. Wang, and H. Fu, Well-posedness of fractional differential equations with variable-order Caputo-Fabrizio derivative. Chaos, Solitons & Fractals 138 (2020), 109966.

7. X. Zheng, Z. Zhang, and H. Wang, Analysis of a nonlinear variable-order fractional stochastic differential equation. Appl Math Lett 107 (2020), 106461.

8. J. Jia, H. Wang, and X. Zheng, A preconditioned fast finite element approximation to variable-order time-fractional diffusion equations in multiple space dimensions. Appl Numer Math 163 (2021), 15--29.

9. J. Jia, H. Wang, and X. Zheng, A fast collocation approximation to a two-sided variable-order space-fractional diffusion equation and its analysis. J Comput Appl Math 388 (2021), 113234.

10. B. Li, H. Wang, and J. Wang, Well-posedness and numerical approximation of a fractional diffusion equation with a nonlinear variable order. ESAIM: M2AN 55 (2021), 171--2021.

11. H. Liu, X. Zheng, H. Fu, and H. Wang, Analysis and efficient implementation of alternating direction implicit finite volume method for Riesz space-fractional diffusion equations in two space dimensions. Numer Meth PDEs, 37 (2021), 818—835.

12. P. Wu, Z. Yang, H. Wang, and R. Song, Time fractional stochastic differential equation driven by pure jump Levy noise. J Math Anal Appl 504 (2021), 125412.

13. S. Yang, H. Chen, V.J. Ervin, and H. Wang, Solvability and approximation of two-side conservative fractional diffusion problems with variable-coefficient based on least-squares. Appl Math Comp 406 (2021), 126229.

14. Z. Yang, X. Zheng, and H. Wang, Well-posedness and regularity of Caputo--Hadamard fractional stochastic differential equations. Zeitschrift für angewandte Mathematik und Physik 72 (2021), 141.

15. Z. Yang, X. Zheng, Z. Zhang, and H. Wang, Strong convergence of a Euler-Maruyama scheme to a variable-order fractional stochastic differential equation driven by a multiplicative white noise. Chaos, Solitons & Fractals 142 (2021), 110392.

16. X. Zheng, V.J. Ervin, and H. Wang, Optimal Petrov-Galerkin spectral approximation method for the fractional diffusion, advection, reaction equation on a bounded interval. J Sci Comput 86 (2021), Article 29.

17. X. Zheng, Y. Li, J. Cheng, and H. Wang, Uniqueness of determining the variable fractional order in the boundary-value problem of variable-order linear space-fractional diffusion equations with variable diffusivity coefficients. J Inv Illposed P 29 (2021), 219--231.

18. X. Zheng, H. Liu, H. Wang, and H. Fu, Optimal-order finite element approximations to variable-coefficient two-sided space-fractional advection-reaction-diffusion equation in three space dimensions. Appl Numer Math 161 (2021), 1--12.

19. X. Zheng and H. Wang, Analysis and numerical approximation to time-fractional diffusion equation with a general time-dependent variable order. Nonlinear Dyn 104 (2021), 4203--4219.

20. X. Zheng and H. Wang, A hidden-memory variable-order time-fractional optimal control model: analysis and approximation. SIAM J. Control Optim. 59 (2021), 1851--1880.

21. X. Zheng and H. Wang, The unique identification of variable-order fractional wave equations. Zeitschrift f\"{u}r angewandte Mathematik und Physik (ZAMP) 72 (2021), 100, https://doi.org/10.1007/s00033-021-01476-z.

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23. P. Dai, J. Jia, H. Wang, Q. Wu, and X. Zheng, An efficient positive-definite block-preconditioned finite volume solver for two-sided fractional diffusion equations on composite mesh. Numer Linear Algebra Appl, (published online March 19, 2021), https://doi.org/10.1002/nla.2372.

24. Z. Yang, X. Zheng, and H. Wang, An indirect collocation method for variable-order fractional wave equations on uniform or graded meshes and its optimal error estimates. Int J Comput Math, https://doi.org/10.1080/00207160.2021.1895987.

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27. X. Zheng and H. Wang, Uniquely identifying the variable order of time-fractional partial differential equations on general multi-dimensional domains. Inv Problem Sci Engrg (published online Nov 20, 2020), https://doi.org/10.1080/17415977.2020.1849182.

Conferences/Talks:

1. Hidden-memory variable-order time-fractional PDEs. The Fourth Conference on Numerical Methods for Fractional-Derivative Problems (Online Conference), Beijing, China, 10/22--10/24, 2020.
2. `On mathematical models by (variable-order) time-fractional PDEs" (online presentation). School of Mathematics, Ocean University of China, Qingdao, China, 11/11, 2020.
3. Variable-order time-fractional diffusion partial differential equations (online presentation). School of Mathematical Sciences, Huaqiao University, Quanzhou, China, 12/30, 2020.
4. Analysis and approximation to variable-order fractional PDEs. Minisymposium on Nonlocal Models in Computational Mechanics: Challenges and Applications, WCCM-ECCOMAS Congress 2020 & 14th WCCM Virtual Congress}, Paris, 01/11--01/15, 2021.
5. Analysis and discretization of an optimal control problem constrained by a variable-order time-fractional PDE. Model Learning and Optimization for Nonlocal and Fractional Equations, SIAM Conference on Computational Science and Engineering (CSE21) (online conference), 3/1--3/5, 2021.
6. Modeling and Simulation of continuous time random walk and variable-order time-fractional PDEs (online presentation), Anomalous Relaxation and Diffusion Study Group, Center for Advanced Imaging, University of Queensland, Austrilia, 4/1, 2021.
7. Modeling, analysis, and simulation of variable-order time-fractional partial differential equations. Nonlocal Model: Theory and Computation (Online Conference), Wuhan, China, 4/15--4/18, 2021.

Rice University Report (co-PI: Pol Spans)

(Research Areas 4)
(Extension Tasks V)

Personnel:

Pol Spanos
Giovanni Malara
Beatrice Pomaro
Hansou Zhoui

Research Work on Axial vibrations of fractional rods with variable cross sections exposed to random loads

Report

The activity has dealt with the problem of computing efficiently the nonlinear response of a rod involving a fractional constitutive model, and exposed to random excitation. The constitutive model is a three-parameter model comprising, an instant elasticity modulus, a prolonged elasticity modulus, and a relaxation parameter. The nonlinear term is a linear-plus-cubic force of the Winkler kind. The resulting nonlinear fractional partial differential equation governing the rod displacement has no known exact solution. Thus, the research has been directed towards proposing an approximate analytical solution by relying on the statistical linearization technique. Further, it has developed a Boundary Element Method (BEM)-based approach to estimate numerically the rod response statistics. The statistical linearization solution has been obtained by representing the rod displacement as the superposition of linear modes of vibration having time-dependent coefficients. In this context, it has been shown that the equation governing the time variation of the mode coefficients is a nonlinear fractional ordinary differential equation, whose solution is computed by a surrogate linear system identified by minimizing the response error between the linear system and the nonlinear one in a mean square sense. Relevant Monte Carlo studies showed that the proposed analytical solution is in a good agreement with data obtained by the numerical (BEM) approach. Such an approach was shown to be effective also in other problems pertaining to the vibration of continua, such as beam and plate vibration [1–3], as well as in problems involving the fractional Laplacian operator [4,5].

The mathematical model of the axial rod vibration was developed by considering a rod with variable cross-section $A(x)$, density ρ, and length L excited by a random load $q(x,t)$. The stress-strain relationship describing the material constitutive behaviour is given by the equation [6–10]

$$\sigma(x,t) = E_0\varepsilon(x,t) + E_\alpha\ {}_0D_t^\alpha\varepsilon(x,t), \tag{1}$$

where $\sigma(x,t)$ and $\varepsilon(x,t)$ denote stress and strain, respectively; E_0 and E_α are instant, and prolonged elasticity moduli, respectively; and α is the relaxation parameter ranging in the interval $0 < \alpha < 1$. The strain along the rod axis is related to the rod longitudinal displacement $u(x,t)$ by the equation

$$\varepsilon(x,t) = \frac{\partial u(x,t)}{\partial x}. \tag{2}$$

The rod is exposed to a linear-plus-cubic nonlinear load of the Winkler kind as considered by Cveticanin and Uzelac [11]. In this framework, the longitudinal vibration of the rod is governed by the equation

$$\frac{1}{c_0^2}\frac{\partial^2 u(x,u)}{\partial t^2} - \frac{1}{A(x)}\frac{\partial}{\partial x}\left[A(x)\frac{\partial u(x,t)}{\partial x}\right] - \frac{c_\alpha^2}{c_0^2}\frac{1}{A(x)}\frac{\partial}{\partial x}\left[A(x)\ {}_0D_t^\alpha\left[\frac{\partial u(x,t)}{\partial x}\right]\right] + \frac{c_1}{c_0^2}u(x,t) + \frac{c_3}{c_0^2}u^3(x,t) = \frac{1}{E_0}q(x,t), \tag{3}$$

which is a nonlinear fractional partial differential equation, with $c_0^2 = E_0/\rho$ and $c_\alpha^2 = E_\alpha/\rho$. The first two terms in the left-hand side of eq. (3) are inertia and restoring forces appearing also in the case of the classical stress-strain relationship. The third quantity relates to the fractional derivative operator in eq. (1). In this regard, it is seen that, by setting the fractional derivative order $\alpha = 0$, a purely elastic model is obtained. The last two quantities are Winkler-kind loads with characteristic parameters c_1 and c_3.

The load $q(x,t)$ is of a separable kind. That is

$$q(x,t) = p(x)f(t), \tag{4}$$

where $p(x)$ is a deterministic function representing the space-wise distribution of the load, and $f(t)$ is a random time-dependent process.

Malara et al. [12] developed the approximate analytical solution and a numerical scheme for determining the system response statistics. The results shown in the following figures show that the response statistics are well estimated and that also the response frequency content is captured quite well irrespective of the fractional derivative order. The figures are reproduced from Ref. [12].

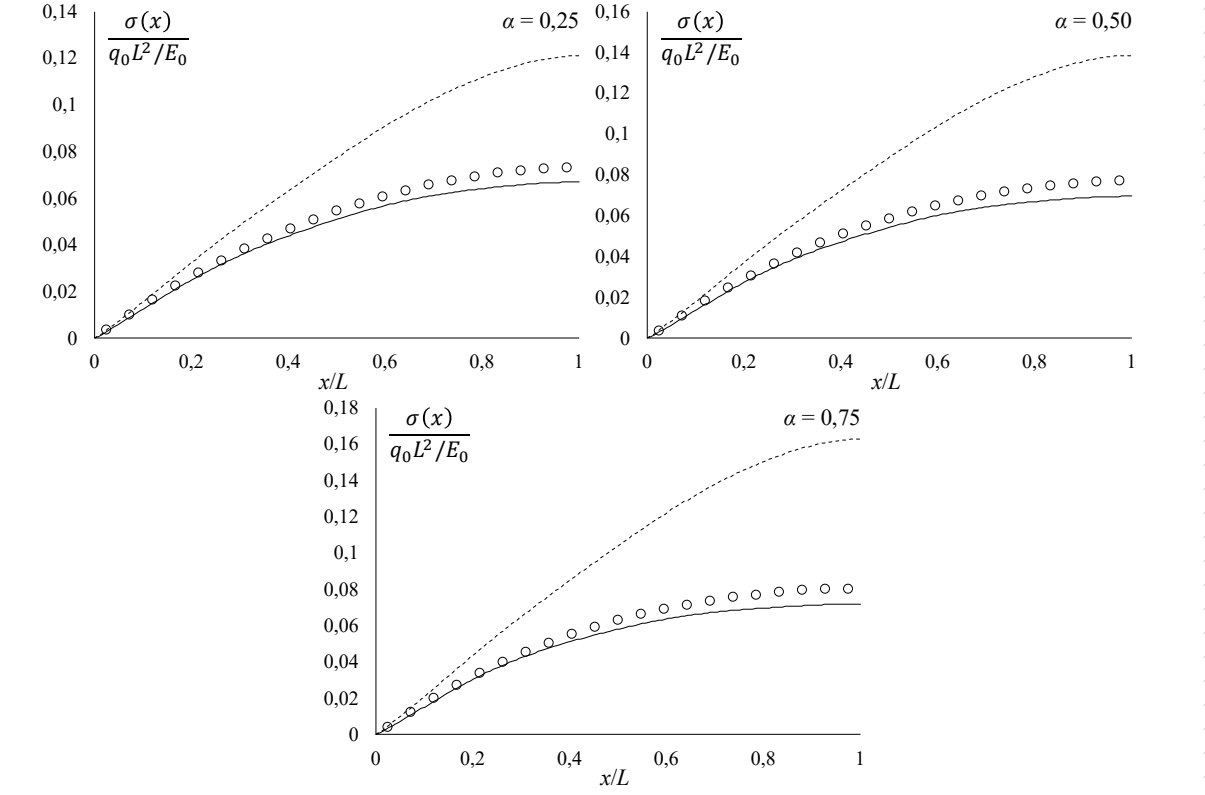

Figure 1. Response standard deviation of a fixed-free rod with fractional derivative orders: α = 0,25 (top left panel), α = 0,50 (top right panel); α = 0,75 (bottom). Continuous lines: statistical linearization solutions; circles: BEM solutions; dotted lines: analytical solutions of associated fractional linear problem obtained by neglecting the Winkler-kind force.

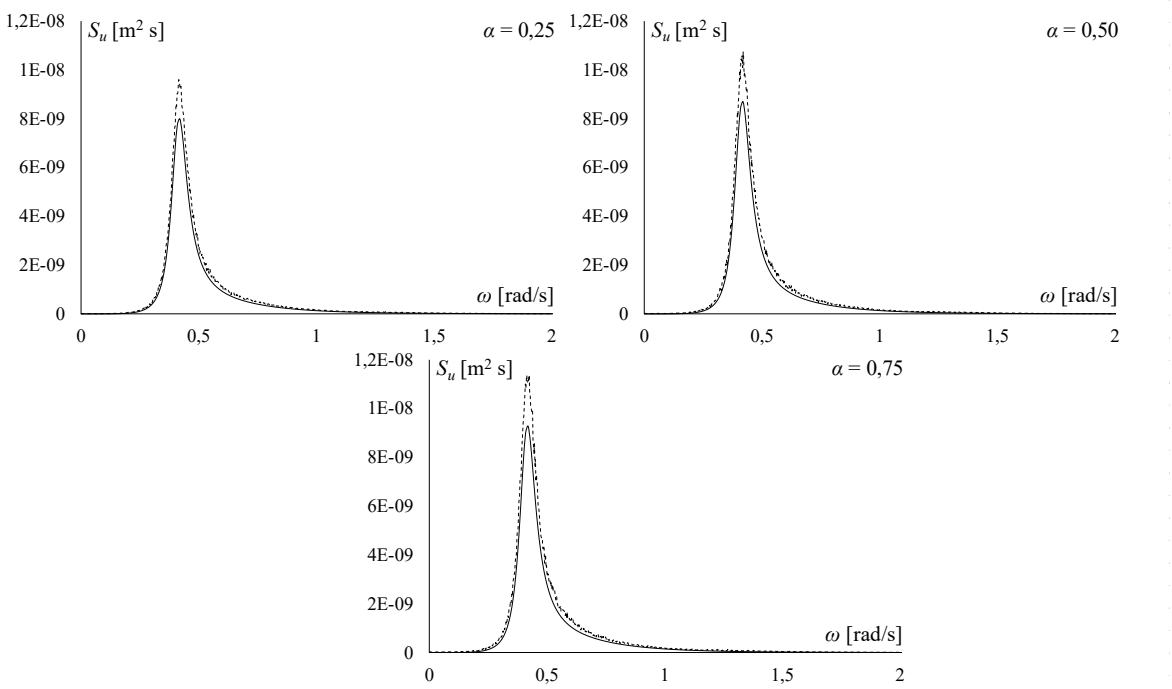

Figure 2. Power spectral density function of the rod displacement at $x = L$ calculated for various fractional derivative orders α. Continuous lines: statistical linearization solutions; dotted lines: BEM solutions.

Currently, application of the developed approach is explored towards other germane problems such as shear beams often considered in modeling seismic engineering and geotechnical engineering affine to the ARO mission.

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Brown University Report (PI: George Karniadakis & co-PI: Mark Ainsworth)

(Research Areas 1-6)
(Extension Tasks II, VI & VII)

Brown personnel on this project: 8/1/20-7/31/21

- George Karnaidakis, PI - 1.6 months
- Mark Ainsworth, co-PI - 1.45 months
- Jerome Darbon, co-PI - 1 month
- Martin Maxey, co-PI - 0.5 months
- Yeongjong Shin, co-PI - 3 months
- Ameya Jagtap, Postdoc - 3.5 months
- Shuai Jiang, Postdoc - 2.6 months
- Ehsan Kharazmi - 9 months
- Lu Lu - 1 month
- Zhiping Mao - 2 months
- Pavan Pranjivan Mehta - 1 month
- Mehdi Samiee - 1 month

- Sumit Vashishtha - 3 months
- Zhicheng Wang - 3.5 months

Research at Brown U: Mark Ainsworth

Summary: Ainsworth worked with a post-doctoral assistant, Shuai Jiang, towards developing efficient high order methods for the approximation of fractional order PDEs on general polygonal domains. This resulted in one completed paper [2] and another paper in preparation. Ainsworth also initiated new work with a visiting scholar from Germany (supported by a prestigious Fullbright Fellowship) on the topic of fractional diffusion on graphs and networks.

Highlights:
[1] shows how fractional order models are able to provide superior predictions of the grain boundary energy of crystalline material than the classical (integer order) phase field crystal approach.

Description of the Research
In **[1]**, we consider a fractional phase-field crystal (FPFC) model in which the classical Swift–Hohenberg equation (SHE) is replaced by a fractional order Swift–Hohenberg equation (FSHE) that reduces to the classical case when the fractional order β=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 (β=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 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. While the salient features of PFC and FPFC are identical, we expect more subtle features to differ. The prediction of grain boundary energy arising from a mismatch in orientation across a material interface is another notable success of the PFC model. The grain boundary energy can be evaluated numerically from the PFC model and compared with experimental measurements. The grain boundary energy is a derived quantity and is more sensitive to the nuances of the model. We compare the predictions obtained using the PFC and FPFC models with experimental observations of the grain boundary energy for several materials. It is observed that the FPFC model gives superior agreement with the experimental observation than those obtained using the classical PFC model, especially when the mismatch in orientation becomes larger.

In **[2]**, a systematic approach to building preconditioners for meshes of tensor product elements equipped only with uniform preconditioners for lower dimensional simplices is presented. The resulting preconditioners are uniform with respect to polynomial order p and mesh size h, and can be implemented efficiently by exploiting the structure of the preconditioners on the lower dimensional elements. We also develop an approach for constructing substructuring, or static condensation type, preconditioning schemes, again, only using knowledge of effective

preconditioners for the lower order simplicial elements. Numerical examples are presented illustrating the performance of the preconditioner on prisms, and challenging hybrid meshes consisting of both quadrilaterals and triangles. This work paves the way for an article (with Shuai Jiang, in preparation) in which we develop efficient hp-finite element methods for approximating fractional PDEs on general polygonal domains. In particular, the solution of the resulting, singularly perturbed elliptic systems is tackled using the work developed in [2].

Published/Submitted Journal Papers:

[1] Fractional phase-field crystal modelling: analysis, approximation and pattern formation, Mark Ainsworth, Zhiping Mao IMA Journal of Applied Mathematics, Volume 85, Pages 231–262, 2020 https://doi.org/10.1093/imamat/hxaa004

[2] A SYSTEMATIC APPROACH TO CONSTRUCTING PRECONDITIONERS FOR THE MASS MATRIX ON TENSOR PRODUCT ELEMENTS, Mark Ainsworth & Shuai Jiang, SIAM J. Sci. Comp. (submitted).

Conferences/Talks:

Ainsworth presented a plenary talk on "Fractional Order Modelling of Crystalline Structures" at The 50th John H. Barrett Memorial Lectures A^3N^2M: Approximation, Applications, and Analysis of Nonlocal, Nonlinear Models, May 17 – 19, 2021. University of Tennessee, TN.
The support of ARO through the MURI was acknowledged at the start of the presentation.

Research at Brown U: George Karniadakis

A Caputo fractional derivative-based algorithm for optimization [1]: We propose a novel Caputo fractional derivative-based optimization algorithm. Upon defining the Caputo fractional gradient with respect to the Cartesian coordinate, we present a generic Caputo fractional gradient descent (CFGD) method. We prove that the CFGD yields the steepest descent direction of a locally smoothed objective function. The generic CFGD requires three parameters to be specified, and a choice of the parameters yields a version of CFGD. We propose three versions -- non-adaptive, adaptive terminal and adaptive order. By focusing on quadratic objective functions, we provide a convergence analysis. We prove that the non-adaptive CFGD converges to a Tikhonov regularized solution. For the two adaptive versions, we derive error bounds, which show convergence to integer-order stationary point under some conditions. We derive an explicit formula of CFGD for quadratic functions. We computationally found that the adaptive terminal (AT) CFGD mitigates the dependence on the condition number in the rate of convergence and results in significant acceleration over gradient descent (GD). For non-quadratic functions, we develop an efficient implementation of CFGD using the Gauss-Jacobi quadrature, whose computational cost is approximately proportional to the number of the quadrature points and the cost of GD. Our numerical examples show that AT-CFGD results in acceleration over GD, even when a small number of the Gauss-Jacobi quadrature points (including a single point) is used.

Identifiability and predictability of integer- and fractional-order epidemiological models using physics-informed neural networks [2]: We analyze a plurality of epidemiological models through the lens of physics-informed neural networks (PINNs) that enable us to identify multiple time-dependent parameters and to discover new data-driven fractional differential operators. In particular, we consider several variations of the classical susceptible-infectious-removed (SIR) model by introducing more compartments and delay in the dynamics described by integer-order, fractional-order, and time-delay models. We report the results for the spread of COVID-19 in New York City, Rhode Island and Michigan states, and Italy, by simultaneously inferring the unknown parameters and the unobserved dynamics. For integer-order and time-delay models, we fit the available data by identifying time-dependent parameters, which are represented by neural networks (NNs). In contrast, for fractional differential models, we fit the data by determining different time-dependent derivative orders for each compartment, which we represent by NNs. We investigate the structural and practical identifiability of these unknown functions for different datasets, and quantify the uncertainty associated with NNs and with control measures in forecasting the pandemic.

Modeling non-local interactions in turbulent flows using Fractional gradients [3]: It is a well-known fact that Turbulence exhibits non-locality, however, modeling has largely received local treatment. Through our research we discovered, in fact, there is a duality in turbulence, implying there is an amalgamation of both local and non-local regions. We further showed a variable-order Caputo Fractional gradient can address this duality where it can transition seamlessly from local to non-local regimes, thereby a most generally applicable model structure. The effect of pressure gradients further complicates the problem, especially in separated flows, which has been a long standing problem in the turbulence modelling community. Thus, in this work we investigate the role of pressure coupled with Reynolds number effects for adverse pressure gradient boundary layers, including modelling of the recirculation bubble. Upon the formulation of one- and two-sided models using Caputo fractional gradients, we found that only the two-sided model leads to physical solutions. This is not a surprise as non-locality at a given point is an aggregate effect of all directions and the two-sided model addresses this very fact. Thus the predictive nature of this formulation presents a model free of ad-hoc tuning coefficients thereby providing the basis for a robust engineering tool.

Theory and simulation of electrokinetic fluctuations in electrolyte solutions at the mesoscale [4]: Electrolyte solutions play an important role in energy storage devices, whose performance highly relies on the electrokinetic processes at sub-micron scales.\ Although fluctuations and stochastic features become more critical at small scales, the long-range Coulomb interactions pose a particular challenge for both theoretical analysis and simulation of fluid systems with fluctuating hydrodynamic and electrostatic interactions. Here, we present a theoretical framework based on the Landau-Lifshitz theory to derive closed-form expressions of fluctuation correlations in electrolyte solutions, indicating significantly different decorrelation processes of ionic concentration fluctuations from hydrodynamic fluctuations, which provides insights for understanding transport phenomena of coupled fluctuating hydrodynamics and electrokinetics. Furthermore, we simulate fluctuating electrokinetic systems using both molecular dynamics (MD) with explicit ions and mesoscopic charged dissipative particle dynamics (cDPD) with semi-implicit ions, from which we identify that the spatial probability density functions of local charge density follow Gamma distribution at sub-nanometer scale (i.e., 0.3 nm) and converge to Gaussian

distribution above nanometer scales (i.e., 1.55 nm), indicating the existence of a lower limit of length scale for mesoscale models using Gaussian fluctuations. The temporal correlation functions of both hydrodynamic and electrokinetic fluctuations are computed from all-atom MD and mesoscale cDPD simulations, showing a good agreement with the theoretical predictions based on the linearized fluctuating hydrodynamics theory.

Fractional Buffer Layers: Absorbing Boundary Conditions for Wave Propagation [5]: We develop fractional buffer layers (FBLs) to absorb propagating waves without reflection in bounded domains. Our formulation is based on variable-order spatial fractional derivatives. We select a proper variable-order function so that dissipation is induced to absorb the coming waves in the buffer layers attached to the domain. In particular, we first design proper FBsL for the one-dimensional one-way and two-way wave propagation. Then, we extend our formulation to two-dimensional problems, where we introduce a consistent variable-order fractional wave equation. In each case, we obtain the fully discretized equations by employing a spectral collocation method in space and Crank-Nicolson or Adams-Bashforth method in time. We compare our results with the perfectly matched layer (PML) method and show the effectiveness of FBL in accurately suppressing any erroneously reflected waves, including corner reflections in two-dimensional rectangular domains. FBLs can be used in conjunction with any discretization method appropriate for fractional operators describing wave propagation in bounded or truncated domains.

An integrated framework for building trustworthy data-driven epidemiological models: Application to the COVID-19 outbreak in New York City [6]: Epidemiological models can provide the dynamic evolution of a pandemic but they are based on many assumptions and parameters that have to be adjusted over the time when the pandemic lasts. However, often the available data are not sufficient to identify the model parameters and hence infer the unobserved dynamics. Here, we develop a general framework for building a trustworthy data-driven epidemiological model, consisting of a workflow that integrates data acquisition and event timeline, model development, identifiability analysis, sensitivity analysis, model calibration, model robustness analysis, and forecasting with uncertainties in different scenarios. In particular, we apply this framework to propose a modified susceptible–exposed–infectious–recovered (SEIR) model, including new compartments and model vaccination in order to forecast the transmission dynamics of COVID-19 in New York City (NYC). We find that we can uniquely estimate the model parameters and accurately predict the daily new infection cases, hospitalizations, and deaths, in agreement with the available data from NYC's government's website. In addition, we employ the calibrated data-driven model to study the effects of vaccination and timing of reopening indoor dining in NYC.

Solving Inverse Stochastic Problems from Discrete Particle Observations Using the Fokker--Planck Equation and Physics-Informed Neural Networks [7]: The Fokker-Planck (FP) equation governing the evolution of the probability density function (PDF) is applicable to many disciplines, but it requires specification of the coefficients for each case, which can be functions of space-time and not just constants and hence require the development of a data-driven modeling approach. When the data available is directly on the PDF, there exist methods for inverse problems that can be employed to infer the coefficients and thus determine the FP equation and subsequently obtain its solution. Herein, we address a more realistic scenario, where only sparse data are given

on the particles' positions at a few time instants, which are not sufficient to accurately construct directly the PDF even at those times from existing methods, e.g., kernel estimation algorithms. To this end, we develop a general framework based on physics-informed neural networks (PINNs) that introduces a new loss function using the Kullback--Leibler divergence to connect the stochastic samples with the FP equation to simultaneously learn the equation and infer the multidimensional PDF at all times. In particular, we consider two types of inverse problems, type I, where the FP equation is known but the initial PDF is unknown, and type II, in which, in addition to the unknown initial PDF, the drift and diffusion terms are also unknown. In both cases, we investigate problems with either Brownian or Lévy noise or a combination of both. We demonstrate the new PINN framework in detail in the one-dimensional (1D) case, but we also provide results for up to five dimensions demonstrating that we can infer both the FP equation and dynamics simultaneously at all times with high accuracy using only very few discrete observations of the particles.

B-PINNs: Bayesian physics-informed neural networks for forward and inverse PDE problems with noisy data [8]: We propose a Bayesian physics-informed neural network (B-PINN) to solve both forward and inverse nonlinear problems described by partial differential equations (PDEs) and noisy data. In this Bayesian framework, the Bayesian neural network (BNN) combined with a PINN for PDEs serves as the prior while the Hamiltonian Monte Carlo (HMC) or the variational inference (VI) could serve as an estimator of the posterior. B-PINNs make use of both physical laws and scattered noisy measurements to provide predictions and quantify the aleatoric uncertainty arising from the noisy data in the Bayesian framework. Compared with PINNs, in addition to uncertainty quantification, B-PINNs obtain more accurate predictions in scenarios with large noise due to their capability of avoiding overfitting. We conduct a systematic comparison between the two different approaches for the B-PINNs posterior estimation (i.e., HMC or VI), along with dropout used for quantifying uncertainty in deep neural networks. Our experiments show that HMC is more suitable than VI with mean field Gaussian approximation for the B-PINNs posterior estimation, while dropout employed in PINNs can hardly provide accurate predictions with reasonable uncertainty. Finally, we replace the BNN in the prior with a truncated Karhunen-Loève (KL) expansion combined with HMC or a deep normalizing flow (DNF) model as posterior estimators. The KL is as accurate as BNN and much faster but this framework cannot be easily extended to high-dimensional problems unlike the BNN based framework.

Published/Submitted Journal Papers:

[1] Shin, Yeonjong, Jérôme Darbon, and George Em Karniadakis. "A Caputo fractional derivative-based algorithm for optimization." arXiv preprint arXiv:2104.02259 (2021).

[2] E. Kharazmi, M. Cai, X. Zheng, Z. Zhang, G. Lin, and G. E. Karniadakis, “Identifiability and predictability of integer- and fractional-order epidemiological models using physics-informed neural networks.” Submitted to Nature Journal of Computational Science.

[3] Mehta, P. P., Karniadakis, G. and Bravo, L. 2021. Fractional Reynolds-averaged Navier Stokes equations (f-RANS) for modeling of separated boundary layers. In APS Division of Fluid Dynamics Meeting Abstracts (submitted).

[4] Deng, M., Tushar, F., Bravo, L., Ghoshal, A., Karniadakis, G. and Li, Z., 2021. Theory and simulation of electrokinetic fluctuations in electrolyte solutions at the mesoscale. arXiv preprint arXiv:2107.05733.

[5] Cai, M., Kharazmi, E., Li, C. and Karniadakis, G.E., 2021. Fractional Buffer Layers: Absorbing Boundary Conditions for Wave Propagation. Submitted to Communications in Computational Physics.

[6] Zhang, S., Ponce, J., Zhang, Z., Lin, G. and Karniadakis, G.E., 2021. An integrated framework for building trustworthy data-driven epidemiological models: Application to the COVID-19 outbreak in New York City. PLOS Computational Biology, in press.

[7] Chen, X., Yang, L., Duan, J. and Karniadakis, G.E., 2021. Solving Inverse Stochastic Problems from Discrete Particle Observations Using the Fokker--Planck Equation and Physics-Informed Neural Networks. SIAM Journal on Scientific Computing, 43(3), pp.B811-B830.

[8] L. Yang, X. Meng, G. E. Karniadakis, "B-PINNs: Bayesian physics-informed neural networks for forward and inverse PDE problems with noisy data", Journal of Computational Physics, Volume 425, (2021), 109913

Conferences/Talks:

[1] E. Kharazmi, G. E. Karniadakis. Data-Driven Physics-Informed Frameworks for Stochastic Fractional PDEs. The 1st Online Conference on Nonlinear Dynamics and Complexity, 2020.

[2] E. Kharazmi, G. E. Karniadakis. fVPINN: Variational Physics-Informed Neural Networks for Fractional Differential Equations. SIAM Conference on Mathematical Aspects of Material Science.

Awards: George Karniadakis received the SIAM/ACM Prize in Computational Science and Engineering (2021) for advancing spectral elements, reduced-order modeling, uncertainty quantification, dissipative particle dynamics, fractional PDEs, and scientific machine learning, while pushing applications to extreme computational scales and mentoring many leaders.

Clemson University (Add-On: co-PI: Zhen Li)

(Extension Task I)

Personnel supported on the MURI grant:

- Zhen Li, PI, 1 month funded.
- Faisal Tushar, PhD student, 7 months funded.
- Ali Mohammadi, Master's student, 2 months funded.

Summary: Electrolyte solutions consisting of a polarized solvent and ionic species are extremely important in a wide range of fields including chemical physics, biology, and geochemistry. They are also of interest in engineering physics, such as aggregation and dispersion of charged liquid particles present in aerospace systems. The performance of an electrolyte solution highly relies on the electrokinetic processes at sub-micron scales. Although fluctuations and stochastic features become more critical at small scales, the long-range Coulomb interactions pose a particular challenge for both theoretical analysis and simulation of fluid systems with fluctuating hydrodynamic and electrostatic interactions. We developed a theoretical framework based on the Landau-Lifshitz theory to derive closed-form expressions of fluctuation correlations in electrolyte solutions, indicating significantly different decorrelation processes of ionic concentration fluctuations from hydrodynamic fluctuations, which provides insights for understanding transport phenomena of coupled fluctuating hydrodynamics and electrokinetics. Furthermore, we simulated fluctuating electrokinetic systems using both molecular dynamics with explicit ions and mesoscopic charged dissipative particle dynamics with semi-implicit ions, from which we identify that the spatial probability density functions of local charge density follow Gamma distribution at sub-nanometer scale and converge to Gaussian distribution above nanometer scales, indicating the existence of a lower limit of length scale for mesoscale models using Gaussian fluctuations. The temporal correlation functions of both hydrodynamic and electrokinetic fluctuations are computed from all-atom molecular dynamics and mesoscale charged dissipative particle dynamics simulations, showing a good agreement with the theoretical predictions based on the linearized fluctuating hydrodynamics theory.

Highlights: This research work developed a new linearized theory based on the Landau-Lifshitz fluctuating hydrodynamics model for coupled hydrodynamic and electrokinetic fluctuations, and results in closed-form expressions of fluctuation correlations in electrolyte solutions. The theoretical predictions based on linear response theory in terms of temporal correlation functions (hydrodynamics and charge) as well as the vast differences in decay time, i.e., varying by a few orders of magnitude, were validated by numerical experiments using both molecular dynamics with explicit ions and mesoscopic charged dissipative particle dynamics with semi-implicit ions, showing a great agreement between theoretical predictions and numerical results. The theoretical results indicate a significantly different decorrelation process of ionic concentration fluctuations from the hydrodynamic fluctuations when the fluid system is close to thermodynamic equilibrium, which provides new insights for understanding transport phenomena of coupled fluctuating hydrodynamics and electro-kinetics.

Submitted Journal Manuscripts:

- Mingge Deng, Faisal Tushar, Luis Bravo, Anindya Ghoshal, George Karniadakis and Zhen Li. *Theory and simulation of electrokinetic fluctuations in electrolyte solutions at the mesoscale*. Journal of Fluid Mechanics, 2021 (under review).

Conferences/Talks:

- Zhen Li, invited talk: *Non-Markovian coarse-grained models of polymeric fluids derived via the Mori-Zwanzig formalism*, CECAM Flagship Workshop of Multiscale simulations of soft matter: New method developments and mathematical foundations, October 02, 2020.

- Zhen Li, oral talk: *Active-learning methods applied to multiscale modeling of viscoelastic flows*, SIAM Conference on Computational Science and Engineering (CSE21), March 4, 2021.

Purdue University (Add-On: co-PI: Guang Lin)

(Extension Task VI)

Personnel supported on the MURI grant:
G. Lin, PI, one month summer salary funded.
Z. Zhang, postdoc, 2 months, C.Moya, postdoc, 6 months funded.
3 STEM graduate students: W. Deng, H. Zheng, J. Zhang, graduate students, 2 months summer funded

Summary:
In this project, an integrated framework for building trustworthy data-driven epidemiological models was developed. This developed framework was employed to study the COVID-19 outbreak in New York City.
This general framework for building a trustworthy data-driven epidemiological model consists of a workflow that integrates data acquisition and event timeline, model development, identifiability analysis, sensitivity analysis, model calibration, model robustness analysis, and forecasting with uncertainties in different scenarios. In particular, we apply this framework to propose a modified susceptible–exposed–infectious–recovered (SEIR) model, including new compartments and model vaccination in order to forecast the transmission dynamics of COVID-19 in New York City (NYC). We find that we can uniquely estimate the model parameters and accurately predict the daily new infection cases, hospitalizations, and deaths, in agreement with the available data from NYC's government's website. In addition, we employ the calibrated data-driven model to study the effects of vaccination and timing of reopening indoor dining in NYC.
In addition, we analyze a plurality of epidemiological models through the lens of physics-informed neural networks (PINNs) that enable us to identify multiple time-dependent parameters and to discover new data-driven fractional differential operators. In particular, we consider several variations of the classical susceptible-infectious-removed (SIR) model by introducing more compartments and delay in the dynamics described by integer-order, fractional-order, and time-delay models. We report the results for the spread of COVID-19 in New York City, Rhode Island and Michigan states, and Italy, by simultaneously inferring the unknown parameters and the unobserved dynamics. For integer-order and time-delay models, we fit the available data by identifying time-dependent parameters, which are represented by neural networks (NNs). In contrast, for fractional differential models, we fit the data by determining different time-dependent derivative orders for each compartment, which we represent by NNs. We investigate the identifiability of these unknown functions for different datasets, and quantify the uncertainty associated with NNs and with control measures in forecasting the pandemic.
Moreover, we developed efficient non-convex machine learning tools via replica exchange stochastic gradient Markov Chain Monte Carlo to train neural networks. Replica exchange Monte Carlo (reMC), also known as parallel tempering, is an important technique for accelerating the convergence of the conventional Markov Chain Monte Carlo (MCMC) algorithms. However, such

a method requires the evaluation of the energy function based on the full dataset and is not scalable to big data. The naive implementation of reMC in mini-batch settings introduces large biases, which cannot be directly extended to the stochastic gradient MCMC (SGMCMC), the standard sampling method for simulating from deep neural networks (DNNs). In this paper, we propose an adaptive replica exchange SGMCMC (reSGMCMC) to automatically correct the bias and study the corresponding properties. The analysis implies an acceleration accuracy trade-off in the numerical discretization of a Markov jump process in a stochastic environment. Empirically, we test the algorithm through extensive experiments on various setups and obtain the state-of-the-art results on CIFAR10, CIFAR100, and SVHN in both supervised learning and semi-supervised learning tasks.

Highlights:

1. Developed a general framework for building a trustworthy data-driven epidemiological model
2. Investigated the identifiability and predictability of integer- and fractional-order epidemiological models using physics-informed neural networks
3. Developed efficient non-convex machine learning tools via replica exchange stochastic gradient Markov Chain Monte Carlo to train neural networks

Published (& in Press) Journal Papers:

1. Sheng Zhang, Joan Ponce, Zhen Zhang, Guang Lin, George Karniadakis, An integrated framework for building trustworthy data-driven epidemiological models: Application to the COVID-19 outbreak in New York City, PLOS Computational Biology, in press. https://www.medrxiv.org/content/10.1101/2021.02.22.21252255v1

2. Y. Wang, W. Deng, G. Lin. Bayesian Sparse Learning with Preconditioned Stochastic Gradient MCMC and its Applications. Journal of Computational Physics. 432(5):110134, 2021. https://doi.org/10.1016/j.jcp.2021.110134

3. Y. Wang, W. Deng, G. Lin. An Adaptive Hessian Approximated Stochastic Gradient MCMC Method. Journal of Computational Physics. 432(5):110150, 2021. https://doi.org/10.1016/j.jcp.2021.110150

4. W. Deng, Q. Feng, G. Karagiannis, G. Lin, F. Liang. Accelerating Convergence of Replica Exchange Stochastic Gradient MCMC via Variance Reduction. The 9th International Conference on Learning Representations (ICLR 2021).
5. W. Deng, Q. Feng*, L. Gao*, F. Liang, G. Lin. Non-convex Learning via Replica Exchange Stochastic Gradient MCMC. The 37th International Conference on Machine Learning (ICML 2020).
6. W. Deng, G. Lin, F. Liang. A Contour Stochastic Gradient Langevin Dynamics Algorithm for Simulations of Multi-modal Distributions. The 34th Conference on Neural Information Processing Systems (NeurIPS 2020)

Submitted Journal Manuscripts:

1. Ehsan Kharazmi, Min Cai, Xiaoning Zheng, Guang Lin, George Karniadakis, Identifiability and predictability of integer- and fractional-order epidemiological models using physics-informed neural networks, Nature Computational Science, in review.

Conferences/Talks:

1. Invited talk on predicting the COVID-19 pandemic with uncertainties using trustworthy data-driven epidemiological models at Society for Mathematical Biology Annual Meeting, June 13-17, 2021, (virtual meeting).
2. Invited talk at Numerical Analysis Seminar, University of Iowa, Mar. 23, 2021.
3. Invited talk at Center for Computational and Applied Mathematics Seminar, Mar. 15, 2021.
4. Invited talk at SIAM Conference on Computational Science and Engineering, Feb. 15, 2021.

ARO MURI # 8 Project (2015): August 2021--July 2022
Progress Report
Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications

- **George Karniadakis & Mark Ainsworth, Brown University**
- **Qiang Du, Columbia University**
- **Mohsen Zayernouri, Michigan State University**
- **Pol Spanos, Rice University**
- **Hong Wang, University of South Carolina**
- **Add-On: Zhen Li (Clemson University) – Guang Lin (Purdue University)**

Background: This MURI project is the vision of a team of researchers from Brown University, Michigan State University, Columbia University, University of South Carolina, and Rice University with overlapped interests and complementary expertise on theory, numerical methods, and applications of fractional PDEs (FPDEs). Our overarching goal is the development of a seamless integration of theory and algorithms for data-driven FPDEs, while targeting the common themes of conservation, monotonicity, adaptive refinement, and high-order accuracy in the context of simulations of multiphase flows, turbulence, fluid-structure interactions, hydrology, and solid mechanics. We envision a combined mathematical and computational framework, where the fractional operators can be constructed based on available data, hence providing model validation for the specific phenomenon but also a tailor-based simulation capability that can be scaled to real-life applications. The proposed research plan emphasizes a dynamic integration of six main research areas that form the pillars of our integrated approach:

• *Research Area 1*: Theory of non-local operators and stochastic interpretation of fractional operators.
• *Research Area 2:* Numerical solution of fractional PDEs with emphasis on variable fractional order.
• *Research Area 3:* Fast solvers for dense linear systems with linear/quasi-linear computational complexity.
• *Research Area 4:* Stochastic FPDEs and determination of the fractional order directly by available data.
• *Research Area 5:* Applications to fluid and solid mechanics, fluid-structure interactions, two-phase flows, turbulence and reactive system with front propagation.
• *Research Area 6:* High performance computing & developing opensource software for fractional problems.

MURI Objectives

- To address the common physical themes of anomalous transport, exponentially accelerated fronts, non-Markovian behavior and long-range interactions, self-similarity and scaling, singular behavior, interfaces and finite-domain decorrelation effects.
- To develop rigorous mathematical theory, algorithms and software for data-driven fractional PDEs that will provide significant breakthroughs towards modeling, analyzing and subsequently controlling complex multiscale systems characterized by the aforementioned phenomena —in a computationally scalable way.
- To demonstrate the physical relevance and effectiveness of our framework in diverse applications of interest to DoD, characterized by the common themes of conservation, monotonicity, adaptive refinement and high-order accuracy.

MURI Extension Tasks:

• *Task I*: Model non-local interactions in large-eddy simulations of particulate turbulent flows.

• *Task II*: Develop fractional phase field crystals models for brittle materials.

• *Task III*: Develop multi-scale stochastic phase-field models of failure in brittle materials.

• *Task IV*: Develop fractional physics-informed neural networks for high-performance engine materials.

• *Task V*: Stochastic partial differential equations with fractional operators for geotechnical engineering applications.

• *Task VI*: Model contact tracing in the COVID-19 pandemic and post-pandemic.

• *Task VII*: Develop new fractional backpropagation models for neural networks.

• *Task VIII*: Numerical analysis of algorithms for learning nonlocal-in-time dynamics.

Status of the Project

There has been great progress in the five years on all six research areas, in recruiting excellent postdocs and PhD students, in participating in conferences with invited and contributed talks as well as on organizing mini-symposia and workshops on FPDEs. The extension helped us to start new areas on machine learning and to further develop new algorithms for demanding and diverse applications. In the following, we provide a summary of progress by each co-PI. First, we provide some highlights on all our activities and then we present the report of each PI.

Interactions

To facilitate the rapid adoption of new developed models and methods and enhance team interaction and cross-institution collaborations, biweekly online meetings were held via Zoom with participants from the US Army Research Laboratory (ARL), Brown University, Clemson University and University of South Carolina. Dr. Luis Bravo, Prof. George Karniadakis, Prof. Zhen Li and Prof. Hong Wong led research teams at their respective institutions to update research progress and discuss research challenges through scheduled biweekly meetings. The ARL team was instrumental in formulating three problems of real-world application of their immediate interest, where they were equally responsible for bridging the gap between fundamental research to applied sciences. The three problems include: (1) Mission critical operations carried out in desert and arid environments often leads to deposition of sand particles in the engine, which eventually erodes the turbine blades of the jet engines. In this research direction, the research team at Clemson

University alongside ARL investigated the prediction of charged particles' motion in the vicinity of solid surfaces. (2) One of open-ended questions in the turbulence community is the prediction of separated boundary layers. The prediction of which improves aircraft's overall efficiency. The team at Brown University responded to this challenge by formulating non-local turbulence models using fractional calculus. (3) The feasibility of fractional calculus was explored for solid mechanics problems with teams at University of South Carolina jointly with ARL.

MURI Highlights

- More than 288papers have been published or submitted on all six research areas of MURI.
- More than 100 invited and plenary talks by MURI personnel.
- Volume on numerical methods in Handbook of FPDEs.
- Several mini-symposia and two workshops organized by MURI PIs.
- New research focusing on 2D & 3D fractional Laplacians in bounded domains with emphasis on boundary conditions and their stochastic interpretation. 11-author revised paper.
- New research focusing on machine learning, fractional photonics, stochastic fractional PDEs and opensource software enabled by the add-on funding.
- Fractional models of turbulent polymer drag reduction at high Reynolds number.
- Combine FPDE and molecular dynamics to efficiently simulate anomalous diffusive transport in heterogeneous porous materials with nanoscale pores.
- Non-local modeling of ion diffusion in battery systems & experiments.
- We discovered new fractional phase-field/non-local equations for interface problems.
- New opensource software at Brown (fractional NEKTAR), Uath (Nektar++) and MSU (FracFit).
- Developing a unified theory of fractional, nonlocal, and weighted nonlocal vector calculus.
- Physical applications of fractional models, particularly, fractional phase field crystal models.
- Theoretical formulation of a fractional subgrid-scale model for turbulent flows.
- Investigating anomalous features in materials failure, internal flows, and structural vibration.
- Atomistic-to-meso multi-scale data-driven graph surrogate modeling of dislocation glide.
- Data-driven fractional subgrid-scale modeling for scalar turbulence: A nonlocal LES approach.
- Data-driven failure prediction in brittle materials: A phase-field based machine learning framework.
- A thermodynamically consistent fractional visco-elasto-plastic model with memory-dependent damage for anomalous materials.
- Innovative discretization schemes for a wide class of semi-linear parabolic equations in the form of gradient flows.
- Rigorous mathematical convergence theory to the discovery of unknown dynamics through data-driven modeling
- Fractional Euler-Bernoulli and Timoshenko beam models to accurately describe the vibration of viscoelastic beams.
- A Caputo fractional derivative-based gradient descent algorithm for optimization.

- Identifiability and predictability of data-driven integer- and fractional-order epidemiological models using physics-informed neural networks.
- Efficient non-convex machine learning tools to train neural networks.

Michigan State University: (co-PI: Mohsen Zayernouri)
(Research Areas 1, 4 & 5)
(Extension Tasks I & III)

Personnel supported on the MURI grant:
Mohsen Zayenrouri, MSU-PI, 2 months
Eduardo de Moraes, PhD Student, 12 months
Mehdi Samiee, PhD Student, 7 months
Ali Akhavan-Safaei, PhD Student, 12 months
Seyed Hadi Seyedi, PhD Student, 11 months

Dynamic Nonlocal Passive Scalar Subgrid-Scale Turbulence Modeling [1]: Extensive experimental evidence highlights that scalar turbulence exhibits anomalous diffusion and stronger intermittency levels at small scales compared to that in fluid turbulence. This renders the corresponding subgrid-scale dynamics modeling for scalar turbulence a greater challenge to date. We develop a new large eddy simulation (LES) paradigm for efficiently and dynamically nonlocal LES modeling of the scalar turbulence. To this end, we formulate the underlying nonlocal model starting from the filtered Boltzmann kinetic transport equation, where the divergence of subgrid-scale scalar fluxes emerges as a fractional-order Laplacian term in the filtered advection-diffusion model, coding the corresponding supper-diffusive nature of scalar turbulence. Subsequently, we develop a robust data-driven algorithm for estimation of the fractional (non-integer) Laplacian exponent, where we on-the-fly calculate the corresponding model coefficient employing a new dynamic procedure. Our a priori tests show that our new dynamically nonlocal LES paradigm provides better agreements with the ground-truth filtered DNS data in comparison to the conventional static and dynamic Prandtl-Smagorisnky models. Moreover, in order to analyze the numerical stability and assessing the model's performance, we carry out a comprehensive a posteriori tests. They unanimously illustrate that our new model considerably outperforms other existing functional models, correctly predicting the backscattering phenomena at the same time and providing higher correlations at small-to-large filter sizes. We conclude that our proposed nonlocal subgrid-scale model for scalar turbulence is amenable for coarse LES and VLES frameworks even with strong anisotropies, applicable to environmental applications.

A Data-Driven Dynamic Nonlocal Subgrid-Scale Model for Turbulent Flows [2]: We developed a novel autonomously dynamic nonlocal turbulence model for the large and very large eddy simulation (LES, VLES) of the homogeneous isotropic turbulent flows (HIT). The model is based on a generalized (integer-to-noninteger) order Laplacian of the filtered velocity field, and a novel dynamic model has been formulated to avoid the need for tuning the model constant. Three data-driven approaches were introduced for the determination of the fractional-order to have a model which is totally free of any tuning parameter. Our analysis includes both the a priori and the a posteriori tests. In the former test, using a high-fidelity and well-resolved dataset from direct

numerical simulations (DNS), we computed the correlation coefficients for the stress components of the subgrid-scale (SGS) stress tensor and the one we get directly from the DNS results. Moreover, we compared the probability density function of the ensemble averaged SGS forces for different filter sizes. In the latter, we employed our new model along with other conventional models including static and dynamic Smagorinsky into our pseudo-spectral solver and tested the final predicted quantities. The results of the newly developed model exhibit an expressive agreement with the ground-truth DNS results in all components of the SGS stress and forces. Also, the model exhibits promising results in the VLES region as well as the LES region, which could be remarkably important for the cost-efficient nonlocal turbulence modelings e.g., in meteorological and environmental applications.

A Nonlocal Spectral Transfer Model and New Scaling Law for Scalar Turbulence [3]: In this study, we revisit the spectral transfer model for the turbulent intensity in the passive scalar transport (under large-scale anisotropic forcing), and a subsequent modification to the scaling of scalar variance cascade is presented. From the modified spectral transfer model, we obtain a revised scalar transport model using fractional-order Laplacian operator that facilitates the robust inclusion of the nonlocal effects originated from large-scale anisotropy transferred across the multitude of scales in the turbulent cascade. We provide an a priori estimate for the nonlocal model based on the scaling analysis of scalar spectrum, and later examine our developed model through direct numerical simulation. We present a detailed analysis on the evolution of the scalar variance, high-order statistics of scalar gradient, and important two-point statistical metrics of the turbulent transport to make a comprehensive comparison between the nonlocal model and its standard version. Finally, we present an analysis that seamlessly reconciles the similarities between the developed model with the fractional-order subgrid-scale scalar flux model for the large-eddy simulation (Akhavan-Safaei et al. 2021) when the filter scale approaches the dissipative scales of turbulent transport. In order to perform this task, we employ a Gaussian process regression model to predict the model coefficient for the fractional-order subgrid model.

Data-Driven Fractional Subgrid-scale Modeling for Scalar Turbulence: A Nonlocal LES Approach [4]: Filtering the passive scalar transport equation in the large-eddy simulation (LES) of turbulent transport gives rise to the closure term corresponding to the unresolved scalar ux. Understanding and respecting the statistical features of subgrid-scale (SGS) flux is a crucial point in robustness and predictability of the LES. In this work, we investigate the intrinsic nonlocal behavior of the SGS passive scalar flux through studying its two-point statistics obtained from the filtered direct numerical simulation (DNS) data for passive scalar transport in homogeneous isotropic turbulence (HIT). Presence of long-range correlations in true SGS scalar flux urges to go beyond the conventional local closure modeling approaches that fail to predict the non-Gaussian statistical features of turbulent transport in passive scalars. Here, we propose an appropriate statistical model for microscopic SGS motions by taking into account the filtered Boltzmann transport equation (FBTE) for passive scalar. In FBTE, we approximate the filtered equilibrium distribution with an α-stable Levy distribution that essentially incorporates a power-law behavior to resemble the observed nonlocal statistics of SGS scalar ux. Generic ensemble-averaging of such FBTE lets us formulate a continuum level closure model for the SGS scalar flux appearing in terms of fractional-order Laplacian that is inherently nonlocal. Through a data-driven approach, we infer the optimal version of our SGS model using the high-fidelity data for the two-point correlation function between the SGS scalar flux and filtered scalar gradient, and sparse linear regression. In

an a priori test, the optimal fractional-order model yields a promising performance in reproducing the probability distribution function (PDF) of the SGS dissipation of the filtered scalar variance compared to its true PDF obtained from the filtered DNS data.

Tempered Fractional LES Modeling [5]: The presence of nonlocal interactions and intermittent signals in the homogeneous isotropic turbulence grant multi-point statistical functions a key role in formulating a new generation of large-eddy simulation (LES) models of higher fidelity. We establish a tempered fractional order modeling framework for developing nonlocal LES subgrid-scale models, starting from the kinetic transport. We employ a tempered Levy-stable distribution to represent the source of turbulent effects at the kinetic level, and we rigorously show that the corresponding turbulence closure term emerges as the tempered fractional Laplacian,$(\Delta + \lambda)^{\alpha}$ (o), for $\alpha \in (0,1)$. 1o, $\alpha \neq 1/2$, and $\lambda > 0$ in the filtered Navier-Stokes equations. Moreover, we prove the frame invariant properties of the proposed model, complying with the subgrid-scale stresses. To characterize the optimum values of model parameters and infer the enhanced efficiency of the tempered fractional subgrid-scale model, we develop a robust algorithm, involving two-point structure functions and conventional correlation coefficients. In an a priori statistical study, we evaluate the capabilities of the developed model in fulfilling the closed essential requirements, obtained for a weaker sense of the ideal LES model (Meneveau 1994). Finally, the model undergoes the a posteriori analysis to ensure the numerical stability and pragmatic efficiency of the model.

Fractional Modeling in Action: A Survey of Nonlocal Models for Subsurface Transport, Turbulent Flows, and Anomalous Materials [6]: Modeling of phenomena such as anomalous transport via fractional-order differential equations has been established as an effective alternative to partial differential equations, due to the inherent ability to describe large-scale behavior with greater efficiency than fully resolved classical models. In this review article, we first provide a broad overview of fractional-order derivatives with a clear emphasis on the stochastic processes that underlie their use. We then survey three exemplary application areas-subsurface transport, turbulence, and anomalous materials – in which fractional-order differential equations provide accurate and predictive models. For each area, we report on the evidence of anomalous behavior that justifies the use of fractional-order models, and survey both foundational models as well as more expressive state-of-the-art models. We also propose avenues for future research, including more advanced and physically sound models, as well as tools for calibration and discovery of fractional-order models.

A Data-Driven Memory-Dependent Modeling Framework for Anomalous Rheology: Application to Urinary Bladder Tissue [7]: We introduce a data-driven fractional modeling framework for complex materials, and particularly bio-tissues. From multi-step relaxation experiments of distinct anatomical locations of porcine urinary bladder, we identify an anomalous relaxation character, with two power-law-like behaviors for short/long times, and nonlinearity for strains greater than 25%. The first component of our framework is an existence study, to determine admissible fractional viscoelastic models that qualitatively describe linear relaxation. After the linear viscoelastic model is selected, the second stage adds large-strain effects to the framework through a fractional quasi-linear viscoelastic approach for the nonlinear elastic response of the bio-tissue of interest. From single-step relaxation data of the urinary bladder, a fractional Maxwell model captures both short/long-term behaviors with two fractional orders, being the most suitable

model for small strains at the first stage. For the second stage, multi-step relaxation data under large strains were employed to calibrate a four-parameter fractional quasi-linear viscoelastic model, that combines a Scott-Blair relaxation function and an exponential instantaneous stress response, to describe the elastin/collagen phases of bladder rheology. Our obtained results demonstrate that the employed fractional quasi-linear model, with a single fractional order in the range $a = 0.25–0.30$, is suitable for the porcine urinary bladder, producing errors below 2% without need for recalibration over subsequent applied strains. We conclude that fractional models are attractive tools to capture the bladder tissue behavior under small-to-large strains and multiple time scales, therefore being potential alternatives to describe multiple stages of bladder functionality.

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[1] Hadi Seyedi, S., A. Akhavan-Safaei, and M. Zayernouri. "Dynamic Nonlocal Passive Scalar Subgrid-Scale Turbulence Modeling." arXiv e-prints (2022): arXiv-2203

[2] Seyedi, S. H., and M. Zayernouri. "A data-driven dynamic nonlocal subgrid-scale model for turbulent flows." Physics of Fluids 34, no. 3 (2022): 035104

[3] Akhavan-Safaei, A., and M. Zayernouri. "A nonlocal spectral transfer model and new scaling law for scalar turbulence." arXiv preprint arXiv:2111.06540 (2021).

[4] Akhavan-Safaei, A., M. Samiee, and M. Zayernouri. "Data-driven fractional subgrid-scale modeling for scalar turbulence: A nonlocal LES approach." Journal of Computational Physics 446 (2021): 110571

[5] Samiee, M., A. Akhavan-Safaei, and M. Zayernouri. "Tempered fractional LES modeling." Journal of Fluid Mechanics 932 (2022)

[6] D'Elia, M., M. Gulian, J. Suzuki, and M. Zayernouri. "Fractional Modeling in Action: A Survey of Nonlocal Models for Subsurface Transport, Turbulent Flows, and Anomalous Materials." (2021)

[7] Suzuki, J. L., T. G. Tuttle, S. Roccabianca, and M. Zayernouri. "A data-driven memory-dependent modeling framework for anomalous rheology: Application to urinary bladder tissue." Fractal and Fractional 5, no. 4 (2021): 223

Columbia University Report (co-PI: Qiang Du)

(Research Areas 1 & 5)
(Extension Task VIII)

Personnel supported on the MURI grant:
Qiang Du, PI (1 mon), Hwi Lee, GRA (9 mon), Zirui Xu GRA (3 mon), Kuang Huang, GRA (0 mon)

Censored stable subordinators and fractional derivatives [1]: Based on the popular Caputo fractional derivative of order β in $(0, 1)$, we define the censored fractional derivative on the positive half-line R_+. This derivative proves to be the Feller generator of the censored (or resurrected) decreasing β-stable process in R_+. We provide a series representation for the inverse of this censored fractional derivative, which we use to study general censored initial value problems. We are then able to prove that this censored process hits the boundary in a finite time τ_inf, whose expectation is proportional to that of the first passage time of the β-stable subordinator. We also show that the censored relaxation equation is solved by the Laplace transform of τ_inf. This relaxation solution proves to be a completely monotone series, with algebraic decay one order faster than its Caputo counterpart, leading, surprisingly, to a new regime of fractional relaxation models. Lastly, we discuss how this work identifies a new sub-diffusion model.

Second order accurate Dirichlet boundary conditions for linear nonlocal diffusion problems [2]: We present an approach to handle Dirichlet type nonlocal boundary conditions for nonlocal diffusion models with a finite range of nonlocal interactions. Our approach utilizes a linear extrapolation of prescribed boundary data. A novelty is, instead of using local gradients of the boundary data that are not available a priori, we incorporate nonlocal gradient operators into the formulation to generalize the finite differences-based methods which are pervasive in literature; our particular choice of the nonlocal gradient operators is based on the interplay between a constant kernel function and the geometry of nonlocal interaction neighborhoods. Such an approach can be potentially useful to address similar issues in peridynamics, smoothed particle hydrodynamics and other nonlocal models. We first show the well-posedness of the newly formulated nonlocal problems and then analyze their asymptotic convergence to the local limit as the nonlocality parameter shrinks to zero. We justify the second order localization rate, which is the optimal order attainable in the absence of physical boundaries.

Nonlocal diffusion models with consistent local and fractional limits [3]: For some spatially nonlocal diffusion models with a finite range of nonlocal interactions measured by a positive parameter δ, we review their formulation defined on a bounded domain subject to various conditions that correspond to some inhomogeneous data. We consider their consistency to similar inhomogeneous boundary value problems of classical partial differential equation (PDE) models as the nonlocal interaction kernel gets localized in the local $\delta --> 0$ limit, and at the same time, for rescaled fractional type kernels, to corresponding inhomogeneous nonlocal boundary value problems of fractional equations in the global $\delta --> \inf $ limit. Such discussions help to delineate issues related to nonlocal problems defined on a bounded domain with inhomogeneous data.

Nonlocal Trace Spaces and Extension Results for Nonlocal Calculus [4]: For a given Lipschitz domain Ω, it is a classical result that the trace space of $W^{1,p}(\Omega)$ is $W^{1-1/p, p}(∂\Omega)$, namely any $W^{1,p}(\Omega)$ function has a well-defined $W^{1-1/p, p}(∂\Omega)$ trace on its codimension-1 boundary $∂(\Omega)$ and any $W^{1-1/p, p}(∂\Omega)$ function on $∂\Omega$ can be extended to a $W^{1,p}(\Omega)$ function. Recently, [26] characterizes the trace space for nonlocal Dirichlet problems involving integrodifferential operators with infinite interaction ranges, where the boundary datum is provided on the whole complement of the given domain $R^d \ \Omega$. In this work, we study function spaces for nonlocal Dirichlet problems with a finite range of nonlocal interactions, which naturally serves a bridging role between the classical local PDE problem and the nonlocal problem with infinite interaction ranges. For these nonlocal Dirichlet problems, the boundary conditions are normally imposed on a region with finite thickness volume which lies outside of the domain. We introduce a function space on the volumetric boundary region that serves as a trace space for these nonlocal problems and study the related extension results. Moreover, we discuss the consistency of the new nonlocal trace space with the classical $W^{1-1/p, p}(∂\Omega)$, space as the size of nonlocal interaction tends to zero. In making this connection, we conduct an investigation on the relations between nonlocal interactions on a larger domain and the induced interactions on its subdomain. The various forms of trace, embedding and extension theorems may then be viewed as consequences in different scaling limits.

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[1] Du, Q., L. Toniazzi, and Z. Xu. "Censored stable subordinators and fractional derivatives." Fractional Calculus and Applied Analysis 24, no. 4 (2021): 1035-1068

[2] Lee, H., and Q. Du. "Second order accurate Dirichlet boundary conditions for linear nonlocal diffusion problems." arXiv preprint arXiv:2108.11817 (2021).

[3] Du, Q., X. Tian, and Z. Zhou. "Nonlocal diffusion models with consistent local and fractional limits." arXiv preprint arXiv:2203.00167 (2022)

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University of South Carolina Report (co-PI: Hong Wang)

(Research Area 1, 2, 3 & 4)
(Extension Task IV)

Personnel supported on the MURI grant:
Hong Wang, PI, 3 months;
Yiqun Li, female, STEM PhD student, 9 months.

Published (& in Press) Journal Papers:

1. J. Jia, X. Zheng, and H. Wang, Numerical discretization and fast approximation of a variably distributed-order fractional wave equation. ESAIM:M2AN 55 (2021) 2211-2232. https://doi.org/10.1051/m2an/2021045
2. J. Jia, X. Zheng, and H. Wang, Analysis and fast approximation of a steady-state spatially-dependent distributed-order space-fractional diffusion equation. Fract Calc & Appl Anal 24 (2021), 1477--1506, DOI: 10.1515/fca-2021-0062
3. R.L. Du, Z.Z. Sun, and H. Wang, Temporal second-order finite difference schemes for variable-order time-fractional wave equations. SIAM J Numer Anal 60 (2022), 104-132. https://doi.org/10.1137/19M1301230.
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6. J. Jia, H. Wang, and X. Zheng, Numerical analysis of a fast finite element method for a hidden-memory variable-order time-fractional diffusion equation. J Sci Comput 91 (2022), Article 54. https://doi.org/10.1007/s10915-022-01820-z
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12. X. Zheng, H. Wang, and X. Guo, Analysis of a time-fractional substantial diffusion equation of variable order. Fractal Fract. 2022, 6, 114. https://doi.org/10.3390/fractalfract60201
13. X. Zheng and H. Wang, A time-stepping finite element method for a time-fractional partial differential equation of hidden-memory space-time variable order. Electronic Transactions on Numerical Analysis 55 (2022), 652-670.

Brown University Report (PI: George Karniadakis & co-PI: Mark Ainsworth)

(Research Areas 1-6)
(Extension Tasks II, VI & VII)

Brown personnel on this project:

Name	Role	8/1/21-5/31/22
Karniadakis, George	PI	1.00
Maxey, Martin	Co-I	0.50
Shin, Yeonjong	Co-I	1.00
Liu, Sicheng	Grad Student	4.00
Zhang, Zhen	Grad Student	4.00
Zou, Zongren	Grad Student	4.00
Jagtap, Ameya	Postdoc	7.00
Kharazmi, Ehsan	Postdoc	1.00
Nath, Kamaljyoti	Postdoc	6.00
Shekarpaz, Simin	Postdoc	2.00
Shukla, Khemraj	Postdoc	2.50

Honors and Awards (Karniadakis)

1. **SIAM/ACM Computational Science and Engineering Award, 2021**
2. **Elected to the National Academy of Engineering, 2022**
3. **Vannevar Bush Faculty Fellowship, 2022**

Research at Brown U: George Karniadakis

Theory and simulation of electrokinetic fluctuations in electrolyte solutions at the mesoscale [1]: Electrolyte solutions play an important role in energy storage devices, whose performance relies heavily on the electrokinetic processes at sub-micron scales. Although fluctuations and stochastic features become more critical at small scales, the long-range Coulomb interactions pose a particular challenge for both theoretical analysis and simulation of fluid systems with fluctuating hydrodynamic and electrostatic interactions. Here, we present a theoretical framework based on the Landau–Lifshitz theory to derive closed-form expressions for fluctuation correlations in electrolyte solutions, indicating significantly different decorrelation processes of ionic concentration fluctuations from hydrodynamic fluctuations, which provides insights for understanding transport phenomena of coupled fluctuating hydrodynamics and electrokinetics. Furthermore, we simulate fluctuating electrokinetic systems using both molecular dynamics (MD) with explicit ions and mesoscopic charged dissipative particle dynamics (cDPD) with semi-

implicit ions, from which we identify that the spatial probability density functions of local charge density follow a gamma distribution at sub-nanometre scale (i.e. 0.3 nm) and converge to a Gaussian distribution above nanometre scales (i.e. 1.55 nm), indicating the existence of a lower limit of length scale for mesoscale models using Gaussian fluctuations. The temporal correlation functions of both hydrodynamic and electrokinetic fluctuations are computed from all-atom MD and mesoscale cDPD simulations, showing good agreement with the theoretical predictions based on the linearized fluctuating hydrodynamics theory.

Bayesian Physics-Informed Neural Networks for real-world nonlinear dynamical systems [2]: Understanding real-world dynamical phenomena remains a challenging task. Across various scientific disciplines, machine learning has advanced as the go-to technology to analyze nonlinear dynamical systems, identify patterns in big data, and make decision around them. Neural networks are now consistently used as universal function approximators for data with underlying mechanisms that are incompletely understood or exceedingly complex. However, neural networks alone ignore the fundamental laws of physics and often fail to make plausible predictions. Here we integrate data, physics, and uncertainties by combining neural networks, physics-informed modeling, and Bayesian inference to improve the predictive potential of traditional neural network models. We embed the physical model of a damped harmonic oscillator into a fully-connected feedforward neural network to explore a simple and illustrative model system, the outbreak dynamics of COVID-19. Our Physics-Informed Neural Networks can seamlessly integrate data and physics, robustly solve forward and inverse problems, and perform well for both interpolation and extrapolation, even for a small amount of noisy and incomplete data. At only minor additional cost, they can self-adaptively learn the weighting between data and physics. Combined with Bayesian Neural Networks, they can serve as priors in a Bayesian Inference, and provide credible intervals for uncertainty quantification. Our study reveals the inherent advantages and disadvantages of Neural Networks, Bayesian Inference, and a combination of both and provides valuable guidelines for model selection. While we have only demonstrated these different approaches for the simple model problem of a seasonal endemic infectious disease, we anticipate that the underlying concepts and trends generalize to more complex disease conditions and, more broadly, to a wide variety of nonlinear dynamical systems.

DynG2G: An Efficient Stochastic Graph Embedding Method for Temporal Graphs [3]: Dynamic graph embedding has gained great attention recently due to its capability of learning low-dimensional and meaningful graph representations for complex temporal graphs with high accuracy. However, recent advances mostly focus on learning node embeddings as deterministic "vectors" for static graphs, hence disregarding the key graph temporal dynamics and the evolving uncertainties associated with node embedding in the latent space. In this work, we propose an efficient stochastic dynamic graph embedding method (DynG2G) that applies an inductive feedforward encoder trained with node triplet energy-based ranking loss. Every node per timestamp is encoded as a time-dependent probabilistic multivariate Gaussian distribution in the latent space, and, hence, we are able to quantify the node embedding uncertainty on-the-fly. We have considered eight different benchmarks that represent diversity in size (from 96 nodes to 87 626 and from 13 398 edges to 4 870 863) as well as diversity in dynamics, from slowly changing temporal evolution to rapidly varying multirate dynamics. We demonstrate through extensive experiments based on these eight dynamic graph benchmarks that DynG2G achieves new state-of-the-art performance in capturing the underlying temporal node embeddings. We also demonstrate

that DynG2G can simultaneously predict the evolving node embedding uncertainty, which plays a crucial role in quantifying the intrinsic dimensionality of the dynamical system over time. In particular, we obtain a “universal” relation of the optimal embedding dimension, L_o , versus the effective dimensionality of uncertainty, D_u , and infer that $L_o=D_u$ for all cases. This, in turn, implies that the uncertainty quantification approach we employ in the DynG2G algorithm correctly captures the intrinsic dimensionality of the dynamics of such evolving graphs despite the diverse nature and composition of the graphs at each timestamp. In addition, this $L_0 - D_u$ correlation provides a clear path to selecting adaptively the optimum embedding size at each timestamp by setting $L \ge D_u$.

Convergence analysis of the time-stepping numerical methods for time-fractional nonlinear subdiffusion equations [4]: In 1986, Dixon and McKee developed a discrete fractional Gr¨onwall inequality [Z. Angew. Math. Mech., 66 (1986), pp. 535–544], which can be seen as a generalization of the classical discrete Gr¨onwall inequality. However, this generalized discrete Gr¨onwall inequality and its variant [SIAM J. Numer. Anal., 57 (2019), pp. 1524–1544] have not been widely applied in the numerical analysis of the time-stepping methods for the time-fractional evolution equations. The main purpose of this paper is to show how to apply the generalized discrete Gr¨onwall inequality to prove the convergence of a class of time-stepping numerical methods for time-fractional nonlinear subdiffusion equations, including the popular fractional backward difference type methods of order one and two, and the fractional Crank-Nicolson type methods. We obtain the optimal L 2 error estimate in space discretization for multi-dimensional problems. The convergence of the fast time-stepping numerical methods is also proved in a simple manner. The present work unifies the convergence analysis of several existing time-stepping schemes. Numerical examples are provided to verify the effectiveness of the present method.

Fluid-structure interactions in a flexible pipe conveying two-phase flow [5]: We present three-dimensional direct numerical simulation (DNS) results of a horizontal flexible pipe conveying two-phase incompressible flow at moderate Reynolds numbers (400 ∼ 700). We find that the Reynolds number (Re) and the void fraction (α) essentially determine the onset of self sustained oscillations in the two-fluid/pipe system. We employ a phase-field formulation to solve the Navier-Stokes coupled with the Cahn-Hilliard equation and the structure equation in an arbitrary Lagrangian Eulerian (ALE) framework. A spectral/hp element method is adopted for the fluid solver and a Galerkin method for the structure solver. We construct stability diagrams showing the transitions between different states of the two-fluid/pipe system. Specifically, we focus on the transition from a stable state to a planar oscillatory state and also to an out-of-plane oscillatory state as a function of four non-dimensional parameters, the Reynolds number Re, the void fraction α, the fluid-tension parameter Ip, and the averaged flow velocity U. By comparing simulation results with those for a pipe conveying single-phase flow under similar conditions, we find that the two-fluid/pipe system loses stability at a lower Reynolds number. We also find that, under similar Re, Ip, and U, at values of void fraction $\alpha \in 0.6 \sim 0.8$, corresponding to the slug/churn flow regimes, the pipe experiences the largest vibrations, which is consistent with previous experimental and theoretical studies. We also perform a spectral analysis and identify the different excited modes,which are found to vary depending on the values of the void fraction α.

An open-source parallel code for computing the spectral fractional Laplacian on 3D complex geometry domains [6]: We present a spectral element algorithm and open-source code for

computing the fractional Laplacian defined by the eigenfunction expansion on finite 2D/3D complex domains with both homogeneous and nonhomogeneous boundaries. We demonstrate the scalability of the spectral element algorithm on large clusters by constructing the fractional Laplacian based on computed eigenvalues and eigenfunctions using up to thousands of CPUs. To demonstrate the accuracy of this eigen-based approach for computing the factional Laplacian, we approximate the solutions of the fractional diffusion equation using the computed eigenvalues and eigenfunctions on a 2D quadrilateral, and on a 3D cubic and cylindrical domain, and compare the results with the contrived solutions to demonstrate fast convergence. Subsequently, we present simulation results for a fractional diffusion equation on a hand-shaped domain discretized with 3D hexahedra, as well as on a domain constructed from the Hanford site geometry corresponding to nonzero Dirichlet boundary conditions. Finally, we apply the algorithm to solve the surface quasi-geostrophic (SQG) equation on a 2D square with periodic boundaries. Simulation results demonstrate the accuracy, efficiency, and geometric flexibility of our algorithm and that our algorithm can capture the subtle dynamics of anomalous diffusion modeled by the fractional Laplacian on complex geometry domains. The included open-source code is the first of its kind.

Published/Submitted Journal Papers:

[1] Deng, M., F. Tushar, L. Bravo, A. Ghoshal, G. Karniadakis, and Zhen Li. "Theory and simulation of electrokinetic fluctuations in electrolyte solutions at the mesoscale." Journal of Fluid Mechanics 942 (2022).

[2] Linka, K, A. Schafer, X. Meng, Z. Zou, G. E. Karniadakis, and Ellen Kuhl. "Bayesian Physics-Informed Neural Networks for real-world nonlinear dynamical systems." arXiv preprint arXiv:2205.08304 (2022).

[3] Xu, M., A. V. Singh, and G. E. Karniadakis. "DynG2G: An Efficient Stochastic Graph Embedding Method for Temporal Graphs." IEEE Transactions on Neural Networks and Learning Systems (2022).

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Purdue University (Add-On: co-PI: Guang Lin)

(Extension Task VI)

Personnel supported on the MURI grant:
G. Lin, PI, one month summer salary funded.
Z. Zhang, postdoc, 2 months, C.Moya, postdoc, 6 months funded.
3 STEM graduate students: W. Deng, H. Zheng, J. Zhang, graduate students, 2 months summer funded

Block triangular preconditioning for stochastic Galerkin method [1]: In this paper, we develop a new block triangular preconditioner for solving partial differential equations with random coefficients. We prove spectral bounds for the preconditioned system. Several numerical examples are provided to demonstrate the efficiency of this preconditioner, especially for stochastic problems with large variance.

A consistent and conservative Phase-Field method for multiphase incompressible flows [2]: In the present study, a consistent and conservative Phase-Field method, including both the model and scheme, is developed for multiphase flows with an arbitrary number of immiscible and incompressible fluid phases. The consistency of mass conservation and the consistency of mass and momentum transport are implemented to address the issue of physically coupling the Phase-Field equation, which locates different phases, to the hydrodynamics. These two consistency conditions, as illustrated, provide the "optimal" coupling because (i) the new momentum equation resulting from them is Galilean invariant and implies the kinetic energy conservation, regardless of the details of the Phase-Field equation, and (ii) failures of satisfying the second law of thermodynamics or the consistency of reduction of the multiphase flow model only result from the same failures of the Phase-Field equation but are not due to the new momentum equation. Physical interpretation of the consistency conditions and their formulations are first provided, and general formulations that are obtained from the consistency conditions and independent of the interpretation of the velocity are summarized. Then, the present consistent and conservative multiphase flow model is completed by selecting a reduction consistent Phase-Field equation. Several novel techniques are developed to inherit the physical properties of the multiphase flows after discretization, including the gradient-based phase selection procedure, the momentum conservative method for the surface force, and the general theorems to preserve the consistency conditions on the discrete level. Equipped with those novel techniques, a consistent and conservative scheme for the present multiphase flow model is developed and analyzed. The scheme satisfies the consistency conditions, conserves the mass and momentum, and assures the summation of the volume fractions to be unity, on the fully discrete level and for an arbitrary number of phases. All those properties are numerically validated. Numerical applications demonstrate that the present model and scheme are robust and effective in studying complicated multiphase dynamics, especially for those with large-density ratios.

AMS-Net: Adaptive Multiscale Sparse Neural Network with Interpretable Basis Expansion for Multiphase Flow Problems [3]: In this work, we propose an adaptive sparse learning algorithm that can be applied to learn the physical processes and obtain a sparse representation of the solution given a large snapshot space. Assume that there is a rich class of precomputed basis functions that can be used to approximate the quantity of interest. For instance, in the simulation of multiscale flow system, one can adopt mixed multiscale methods to compute velocity bases from local problems and apply the proper orthogonal decomposition (POD) method to construct bases for the saturation equation. We then design a neural network architecture to learn the coefficients of solutions in the spaces which are spanned by these basis functions. The information of the basis functions are incorporated in the loss function, which minimizes the differences between the downscaled reduced order solutions and reference solutions at multiple time steps. The network contains multiple submodules and the solutions at different time steps can be learned simultaneously. We propose some strategies in the learning framework to identify important degrees of freedom. To find a sparse solution representation, a soft thresholding operator is applied to enforce the sparsity of the output coefficient vectors of the neural network. To avoid over-simplification and enrich the approximation space, some degrees of freedom can be added back to the system through a greedy algorithm. In both scenarios, that is, removing and adding degrees of freedoms, the corresponding network connections are pruned or reactivated guided by the magnitude of the solution coefficients obtained from the network outputs. The proposed adaptive learning process are applied to some toy case examples to demonstrate that it can achieve a good basis selection and accurate approximation. More numerical tests are successfully performed on two-phase multiscale flow problems to show the capability and interpretability of the proposed method on complicated applications.

Special Issue: Geostatistics and Machine Learning [4]: Recent years have seen a steady growth in the number of papers that apply machine learning methods to problems in the earth sciences. Although they have different origins, machine learning and geostatistics share concepts and methods. For example, the kriging formalism can be cast in the machine learning framework of Gaussian process regression. Machine learning, with its focus on algorithms and ability to seek, identify, and exploit hidden structures in big data sets, is providing new tools for exploration and prediction in the earth sciences. Geostatistics, on the other hand, offers interpretable models of spatial (and spatiotemporal) dependence. This special issue on Geostatistics and Machine Learning aims to investigate applications of machine learning methods as well as hybrid approaches combining machine learning and geostatistics which advance our understanding and predictive ability of spatial processes.

A consistent and conservative Phase-Field model for thermo-gas-liquid-solid flows including liquid-solid phase change [5]: In the present study, a consistent and conservative Phase-Field model is developed to study thermogas-liquid-solid flows with liquid-solid phase change. The proposed model is derived with the help of the consistency conditions and exactly reduces to the consistent and conservative Phase-Field method for incompressible two-phase flows, the fictitious domain Brinkman penalization (FD/BP) method for fluidstructure interactions, and the Phase-Field model of solidification of pure material. It honors the mass conservation, defines the volume fractions of individual phases unambiguously, and therefore captures the volume change due to phase change. The momentum is conserved when the solid phase is absent, but it changes when the solid phase appears due to the no-slip condition at the solid boundary. The proposed model

also conserves the energy, preserves the temperature equilibrium, and is Galilean invariant. A novel continuous surface tension force to confine its contribution at the gas-liquid interface and a drag force modified from the Carman-Kozeny equation to reduce solid velocity to zero are proposed. The issue of initiating phase change in the original Phase-Field model of solidification is addressed by physically modifying the interpolation function. The corresponding consistent scheme is developed to solve the model, and the numerical results agree well with the analytical solutions and the existing experimental and numerical data. Two challenging problems having a wide range of material properties and complex dynamics are conducted to demonstrate the capability of the proposed model.

Flow-driven spectral chaos (FSC) method for long-time integration of second-order stochastic dynamical systems [6]: For decades, uncertainty quantification techniques based on the spectral approach have been demonstrated to be computationally more efficient than the Monte Carlo method for a wide variety of problems, particularly when the dimensionality of the probability space is relatively low. The time-dependent generalized polynomial chaos (TD-gPC) is one such technique that uses an evolving orthogonal basis to better represent the stochastic part of the solution space in time. In this paper, we present a new numerical method that uses the concept of enriched stochastic flow maps to track the evolution of the stochastic part of the solution space in time. The computational cost of this proposed flow-driven stochastic chaos (FSC) method is an order of magnitude lower than TD-gPC for comparable solution accuracy. This gain in computational cost is realized because, unlike most existing methods, the number of basis vectors required to track the stochastic part of the solution space, and consequently the computational cost associated with the solution of the resulting system of equations, does not depend upon the dimensionality of the probability space. Four representative numerical examples are presented to demonstrate the performance of the FSC method for long-time integration of second-order stochastic dynamical systems in the context of stochastic dynamics of structures.

A consistent and conservative volume distribution algorithm and its applications to multiphase flows using Phase-Field models [7]: In the present study, the multiphase volume distribution problem, where there can be an arbitrary number of phases, is addressed using a consistent and conservative volume distribution algorithm. The proposed algorithm satisfies the summation constraint, the conservation constraint, and the consistency of reduction. The first application of the volume distribution algorithm is to determine the Lagrange multipliers in multiphase Phase-Field models that enforce the mass conservation, and a multiphase conservative Allen-Cahn model that satisfies the consistency of reduction is developed. A corresponding consistent and conservative numerical scheme is developed for the model. The multiphase conservative Allen-Cahn model has a better ability than the multiphase Cahn-Hilliard model to preserve underresolved structures. The second application is to develop a numerical procedure, called the boundedness mapping, to map the order parameters, obtained numerically from a multiphase model, into their physical interval, and at the same time to preserve the physical properties of the order parameters. Along with the consistent and conservative schemes for the multiphase Phase-Field models, the numerical solutions of the order parameters are reduction consistent, conservative, and bounded, which are theoretically analyzed and numerically validated. Then, the multiphase Phase-Field models are coupled with the momentum equation by satisfying the consistency of mass conservation and the consistency of mass and momentum transport, thanks to the consistent formulation. It is demonstrated that the proposed model and scheme converge to

the sharp-interface solution and are capable of capturing the complicated multiphase dynamics even when there is a large density and/or viscosity ratio.

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Supported by OSD/ARO/MURI on “Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics and Applications (W911NF-15-1-0562)”

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