

Innovations in fractional calculus and applications to functional and biological materials









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> Jan Hesthaven EPFL, Switzerland

George Karniadakis
Brown University, United States

Ignacio Pagonabarraga University of Barcelona, Spain

Igor Podlubny
Technical University of Kosice, Slovakia

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1. Description

Fractional partial differential equations (FPDEs) are emerging as a powerful tool for modeling challenging multiscale phenomena including microstructure in materials, overlapping microscopic and macroscopic scales, anomalous transport, and long-range time memory or spatial interactions. Furthermore, fractional calculus is an excellent framework for modelling nonconventional fractal and non-local media, opening valuable prospects on future engineered materials. Compared to integer-order PDEs, the fractional order of the derivatives in FPDEs may be a function of space and time or even a distribution, opening up great opportunities for modeling and simulation of multi-physics phenomena, e.g. seamless transition from wave propagation to diffusion, or from local to non-local dynamics. In addition, data-driven fractional differential operators may be constructed to fit data from a particular experiment or specific phenomenon, including the effect of uncertainties, in which the fractional orders are determined directly from the data, and introducing nonlinearities leading to more complex operators, with one or more fractional orders, capable to model less typical phenomena (such as, for instance, wave propagation in heterogeneous systems). Similarly, in imaging applications the variable and even distributed fractional order that may change in space offer great flexibility that can be used to suppress noise while preserving edge

In short, FPDEs lead to a paradigm shift, according to which data-driven fractional operators may be constructed to model a specific phenomenon instead of the current practice of tweaking free parameters that multiply pre-set integer-order differential operators. Also important is that the misspecification of physical models using integer order derivatives leads to a variable coefficient fit (struggling to fit the data at each location, for example) whereas it was shown in the literature that the "correct" fractional order model can fit all the data with a constant coefficient model.

The main reasons that FPDE modeling has not been used extensively so far is that FPDEs are non-unique and that they are quite expensive to solve numerically as they typically generate dense linear algebraic systems due to the nonlocality of fractional differential operators. Furthermore, FPDEs present additional mathematical and numerical difficulties, which are not encountered in the context of integer-order PDEs.

This workshop will focus on the use of fractional calculus in different areas of materials, addressing multiscale structure, porous media, crack propagation, visco-elasto-plasticity, wave propagation, non-local continua, dynamic fracture in brittle and quasi-brittle solids, etc. We will invite researchers who work on multiscale modeling of materials as well as applied mathematicians who have made significant progress in advancing the fundamentals of FPDEs.

2. Program

Day 1 - Wednesday September 13th 2023

- 09:00 to 09:10 Welcome by Sara Bonella, CECAM Deputy Director & Aude Merola, CECAM Event Manager
- 09:10 to 09:20 Introduction by Hollie Pietsch, US Army DEVCOM-Atlantic
- 09:20 to 09:30 Introduction by George Karniadakis, co-organiser
- 09:30 to 09:40 Introduction by Igor Podlubny, co-organiser

SESSION 1 - Chair: Igor Podlubny

• 09:40 to 10:20 - Gareth McKinley

Compact and accurate descriptions of complex fluids and soft solids using fractional differential and integral equations

• 10:20 to 11:00 - Sverre Holm

Fractional derivatives appear wherever there are power laws in physics

- 11:00 to 11:30 Coffee break
- 11:30 to 12:10 Yuriy Povstenko Fractional nonlocal elasticity
- 12:10 to 12:50 Karabi Biswas

Fabrication of fractional capacitor: Journey from capacitive probe dipped in liquid media to solid state analog circuit element

• 12:50 to 14:00 - Lunch

SESSION 2 - Chair: George Karniadakis

• 14:00 to 14:40 - Hong Wang

A fractional mean-field control (fMFC) for accidental contaminant spill and its remediation, and for detecting damage in visco-elasto-plastic structure and optimal sensor placement

• 14:40 to 15:20 - Teodor Atanackovic

Compartmental models with general fractional derivatives: Motivation and some results

• 15:20 to 16:00 - Yue Yu

Learning nonlocal constitutive laws via invariant neural operators

- 16:00 to 16:30 Coffee break
- 16:30 to 17:10 Francesco Mainardi

Wright functions of the second kind in fractional diffusion processes

• 17:10 to 17:50 - Massimiliano Zingales

Anomalous poromechanical coupling for the analysis of meniscal tissue

- 17:50 to 18:30 Discussion
- 18:30 to 19:30 Poster session & aperitif

Day 2 - Thursday September 14th 2023

SESSION 3 - Chair Gareth Mckinley

09:00 to 09:40 - Kurt Kremer
 Challenges and opportunities in polymer / soft matter science: A multiscale computational view

09:40 to 10:20 - Blas M. Vinagre
 Soft robotics & fractional calculus. A convenient marriage

- 10:20 to 10:50 Coffee break
- 10:50 to 11:30 Mohsen Zayernouri
 Anomalous advection-diffusion modeling in fluids and aging materials
- 11:30 to 12:10 Mark Ainsworth
 Robust solvers for fractional PDEs on polygonal domains
- 12:10 to 12:50 **Kai Diethelm**Efficient handling of fractional order material laws in finite element simulations
- 12:50 to 14:00 Lunch

SESSION 4 - Chair: YangQuan Chen

- 14:00 to 14:40 Christoph Schwab
 Exponential convergence of hp FEM for spectral fractional diffusion in polygons
- 14:40 to 15:20 Jie Shen
 Efficient space-time Petrov-Galerkin method for fractional PDEs
- 15:20 to 16:00 Qiang Du Nonlocal calculus with heterogeneous localization
- 16:00 to 16:30 Coffee break
- 16:30 to 17:10 **Changpin Li**Fractional partial differential equations for ultra-slow diffusion: Analysis and computation
- 17:10 to 17:30 Katarzyna Ryszewska
 Regularity of weak solutions to parabolic-type problems with distributed order timefractional derivative
- 17:30 to 17:50 Adam Kubica
 A self-similar solution to time-fractional Stefan problem
- 17:50 to 18:30 Discussion
- 19:30 to 00:00 Social dinner

Day 3 - Friday September 15th 2023

SESSION 5 - Chairs: Igor Podlubny & George Karniadakis

09:00 to 09:40 - Ralf Metzler
 Long-range correlated processes: Confinement & heterogeneity

09:40 to 10:20 - YangQuan Chen Two triangles: complexity / inverse power law / fractional calculus & fractional calculus / renormalization group / machine learning (FC-RG-ML)

- 10:20 to 10:50 Coffee break
- 10:50 to 11:30 Yuri Luchko
 Basic properties and some applications of the general fractional integrals and derivatives with the sonin kernels
- 11:30 to 11:50 **Ling Guo** TBA
- 11:50 to 12:20 **Anindya Ghoshal** TBA
- 12:20 to 12:50 Discussion
- 12:50 to 13:00 Closing Word

3. Abstracts

A fractional mean-field control (fMFC) for accidental contaminant spill and its remediation, and for detecting damage in visco-elasto-plastic structure and optimal sensor placement Hong Wang

University of South Carolina, United States

Contamination of groundwater supplies by hazardous organic, inorganic, or radioactive contaminants introduced to the environment from accidental spill, terrorist attack or even war crime imposes severe threat to the world. These incidents may lead to tragedy to the society and require urgent treatment to ensure the safety of groundwater supplies to the public. The goal of this research is to control the transport and remediation of the contaminant with minimal transportation cost so that the contaminant does not pollute groundwater supply zone. Note that the dynamic behavior of the transport is hardly influenced by individual particles but is determined by the aggregate behavior of particles. Hence, MFC is well suited and provides a powerful modeling tool, in which integer-order constraining PDEs are typically used. But subsurface porous media are generally heterogeneous and of fractal nature, through which the contaminant transport is anomalous and exhibits highly skewed power-law decaying tails. Integer-order advection-diffusion transport PDEs, which are characterized by Gaussian fundamental solutions, fail to accurately describe contaminant transport in heterogeneous media. In contrast, fractional PDEs, characterized by highly skewed power-law decaying fundamental solutions, accurately model contaminant transport and remediation in heterogeneous media.

We develop an fMFC to optimize the transport and remediation of the spilled contaminant with minimal transportation cost to ensure that the contaminant does not pollute the groundwater supply zone to ensure the safe groundwater supply to the public. These are verified by preliminary numerical experiments.

In the second application we develop an fMFC for damage detection of visco-elasto-plastic structure. The presence of damage in engineering structures may significantly deteriorate their mechanical properties, leading to tragic consequences. Detecting structural damage improves safety, extends serviceability and operating limits, and reduces maintenance costs. Modern engineering materials, e.g., composite, piezoelectric, or soft materials, polymers, natural and synthetic bio-tissues, are widely used due to their high strength, low weight, good fatigue and corrosion resistance. They inherit restorative elastic solid behavior and internally dissipative fluid behavior, have characteristics of time-dependent stress or strain response, and exhibit power-law memory effects in terms of relaxation or creep in time. Further, long term vibrations may cause structural damages, which are initiated at micro scales through the development of micro cracks and bond breakage and propagate to macro scales that eventually lead to material failure. Mathematically, this leads to the change of fractal dimension of the materials, leading to variable-order fractional PDEs.

We develop an fMFC constrained by variable-order fractional PDEs and equipped with shape or topological optimization for detecting damage in visco-elasto-plastic engineering structures that leverage changes in a structure's inherent frequencies, allowing for accurate detection and characterization of damage in complicated engineering structures to be successfully modeled with realistic model sizes, using the time history of dynamic responses of the structure measures at minimal number of locations. The fMFC provides advantages over traditional nondestructive tests in that (i) it detects many types of damage, (ii) it does not require prior knowledge of the location of the damage as well as the easy accessibility of the portion of the structure being inspected, and (iii) it provides both local and global information on the structural strength and damage.

We further study optimal placement of the sensor locations in engineering structures, which provides the best measurements that ensures the best performance of the fMFC in damage detection, through the Kolmogorov N-width.

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A self-similar solution to time-fractional Stefan problem Adam Kubica

Warsaw University of Technology, Poland

We derive the fractional version of one-phase one-dimensional Stefan model, where we assume that the diffusive flux is given by the time-fractional Riemann-Liouville derivative, i.e. we impose the memory effect in the examined model. Furthermore, we find a self-similar solution to this problem. It is a joint work with Katarzyna Ryszewska.

Anomalous advection-diffusion modeling in fluids and aging materials Mohsen Zayernouri

Michigan State University, United States

The presence and evolution of defects that appear in the manufacturing process play a vital role in the failure mechanisms of aging materials. Particularly, the collective behavior of dislocation advection-diffusion dynamics at the mesoscale leads to avalanche, strain bursts, intermittent energy spikes, and nonlocal interactions producing anomalous features across different time- and length-scales, directly affecting plasticity, void and crack nucleation. Discrete Dislocation Dynamics (DDD) simulations are often used at the meso-level, but the cost and complexity increase dramatically with simulation time. To further understand how the anomalous features propagate to the continuum, we develop a probabilistic model for dislocation motion constructed from the position statistics obtained from DDD simulations. We obtain the continuous limit of discrete dislocation dynamics through a Probability Density Function (PDF) for the dislocation motion and propose a nonlocal transport model for the PDF. We develop a machine-learning framework to learn the parameters of the nonlocal operator with a power-law kernel, connecting the anomalous nature of DDD to the origin of its corresponding nonlocal operator at the continuum, facilitating the integration of dislocation dynamics into multi-scale, long-time material failure simulations.

Moreover, the transport phenomena occurring in the microstructure of functional and biological materials can emerge as memory-dependent and nonlocal. For instance, in the transport of scalar spices, the delineation of coherent structures/motions, being spatially spotty, giving rise to interestingly anomalous spatio-temporal fluctuating signals. The statistical anomalies in such stochastic fields

emerge as: sharp peaks, heavy-skirts of power-law form, long-range correlations, and skewed distributions, which scientifically manifest the non-Markovian/non-Fickian nature of the underlying transport phenomena at small scales. Such physical-statistical evidence highlights that 'nonlocal features' and 'global inertial interactions' cannot be ruled out in physics of anomalous advection-diffusion processes. We establish a new foundation through filtering the Boltzmann kinetic transport equations. Next, we model the corresponding equilibrium distribution functions with *stable heavy-tailed* distributions to address and incorporate the anomalous features at small scales. Finally, we derive a new class of *fractional-order and tempered Laplacian models* for the divergence of subgrid-scale stresses, naturally emerging as the underlying subgrid-scale (SGS) models.

Anomalous poromechanical coupling for the analysis of meniscal tissue Massimiliano Zingales, Emanuela Bologna

Università degli Studi di Palermo, Italy

Menisci are C-shaped fibrocartilaginous tissues located between femoral condoles and tibia. They play a crucial role in proprioception, joint lubrication, and nutrition of articular cartilage, as well as absorbing shock and distributing loads evenly, cooperating with tendons and protecting knee joint against damage caused by hyperextension and hyperflexion Complete or partial loss of a meniscus can have detrimental effects on knee, leading to serious long-term consequences. For this reason, several studies have been conducted to formulate menisci mechanical behavior, but this is extremely challenging due to their complex in-homogeneous micro-structure and lack of complete experimental characterization of material properties. Indeed, a diffusion phenomenon explains how interstitial fluid moves through interconnected pores in the solid matrix of the menisci. According to this, a considerable number of studies have been conducted on poromechanical models to describe diffusion phenomenon on meniscus assuming linear poroelasticity which combines Hooke's law to describe the linear deformation of porous solid, and Darcy's law to describe flow in a porous medium. This approach, however, does not account for the marked hereditariness provided by meniscal tissues as well as on the non-fickian diffusion due to the microstructure.

In recent years, the Fick and/or Darcy transport equations were also modified using fractional calculus to introduce the memory effect induced by interaction between fluid particles and pore structure of elastic medium.

This study introduces a novel poromechanical coupling among the fluid diffusion and the mechanical characterization of the meniscal tissue with the aid of fractional-order hereditariness. In this framework structure-function relationships and prediction of the stress/strain state by biomechanical simulations may be assessed for different kind of load conditions.

[1] F. Amiri, E. Bologna, G. Nuzzo, L. Moroni, M. Zingales, Numer. Methods. Biomed. Eng. (2023) [2] E. Bologna, F. Graziano, L. Deseri, M. Zingales, Int J Non Linear Mech, 115, 61 (2019)

Basic properties and some applications of the general fractional integrals and derivatives with the Sonin kernels

Yuri Luchko

Berliner Hochschule für Technik, Germany

In this talk, some recent results regarding the general fractional integrals and derivatives with the Sonin kernels are presented. We discuss the first and the second fundamental theorems of Fractional Calculus for the general fractional derivatives of arbitrary order, for the regularized general fractional derivatives of arbitrary order, and for the sequential general fractional derivatives. As an application of these results, the generalized convolution Taylor formulas and the generalized convolution Taylor series with the coefficients and remainders in terms of the general fractional derivatives and the regularized general fractional derivatives are deduced.

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- [3] Y. Luchko, Symmetry, 13, 755 (2021)
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Challenges and opportunities in polymer / soft matter science: A multiscale computational view

Kurt Kremer

Max Planck Institute for Polymer Research, Germany

Characteristic features that come with the softness of Soft Matter are large conformational fluctuations, slow dynamics, and susceptibility to small molecular stimuli. That is a point where generic physical concepts meet the consequences of chemically detailed interactions. This interplay makes soft matter so versatile and interesting. Furthermore, almost all soft matter materials/systems are not in thermodynamic equilibrium. They are either stuck in a metastable state or permanently driven, i.e., they consume and dissipate energy. We thus have to arrive at structure-process-property relations. The talk will review a few characteristic examples such as the role of topology conservation in polymer melts or properties so called smart polymers, where such effects lead to physically and/or chemically interesting phenomena. Starting from these examples challenges and perspectives will be shortly discussed.

Compact and accurate descriptions of complex fluids and soft solids using fractional differential and integral equations

Gareth McKinley, Bavand Keshavarz, Joshua Rathinaraj MIT, United States

Many soft materials including foods, consumer products, biopolymer gels & associative polymer networks are characterized by multi-scale microstructures and exhibit power-law responses in canonical rheological experiments such as Small Amplitude Oscillatory Shear (SAOS) and creep. Even in the linear limit of small deformations it is difficult to describe the material response of such systems quantitatively within the classical framework of springs and dashpots - which give rise universally to Maxwell-Debye exponential responses. Instead, empirical functions and subjective metrics such as 'firmness', 'thickness' etc. are often used to describe and compare material responses. Scott Blair argued that such measures are best thought of as 'quasi-properties' that capture a snapshot of the underlying dynamical processes in these complex materials. The language of fractional differential equations and the concept of a 'spring-pot' element provides a useful framework that is especially well suited for modeling and quantifying the rheological response of power-law-like viscoelastic materials characterized by very broad relaxation spectra. We illustrate the general utility of this approach by outlining fractional differential forms of the Maxwell, Kelvin-Voigt and Zener models and using these models to quantify linear viscoelastic responses of a range of soft materials including gluten and milk protein gels, cheese, skin, and soft tissue, filled polymer melts, hydrogen-bonded biopolymer networks, pastes, foods as well as complex interfaces. The fractional exponents that characterize the dynamic material response can also be connected directly with scaling exponents from microstructural models such as the Soft Glassy Rheology (SGR) model and the fractal dimensions of the underlying network. This fractional framework can also be readily extended to the nonlinear domain by generating a corresponding continuous relaxation spectrum in terms of the Mittag-Leffler function and combining this fractional relaxation kernel with nonlinear strain damping into a frame-indifferent generalization of the Boltzmann integral theory of viscoelasticity. Using this integral fractional framework and carefully considering the asymptotic limits of small and large deformation rates we develop general expressions for the rate-dependent viscosity of a complex fluid. This analysis also provides a systematic understanding of why familiar rheological heuristics such as the "Cox-Merz rule" and the "Gleissle mirror relation" [1] work so well for many (but not all) complex fluids.

Compartmental models with general fractional derivatives: Motivation and some results

Teodor Atanackovic

Serbian Academy of Sciences, Serbia

We present formulation of two compartmental pharmacokinetic model with General fractional derivatives of distributed order. The model is applied to the study the release of antibiotic gentamicin in poly(vinylalcohol)/gentamicin (PVA/Gent) hydrogel aimed for wound dressing in medical treatment of deep chronical wounds. The advantage of this model is the existence of new parameters in the definition of fractional derivative, as compared with classical fractional compartmental models. This enables the better approximation of the measured values of gentamicin concentration.

Efficient handling of fractional order material laws in finite element simulations Kai Diethelm¹. André Schmidt²

¹Technical University of Applied Sciences Würzburg-Schweinfurt, Germany

The Finite Element Method is a well-established technique for simulating the behavior of objects under mechanical loads. Inside of a standard mathematical framework, it requires to solve the equations that describe the material laws of the object under consideration at a potentially very large number of points in the body. For classical (memory-free) material laws such as, e.g., Hooke's law, this is an elementary matter. However, many materials of current interest like biological tissue, polymers, etc. exhibit a behavior governed by fractional order models, i.e., models that possess memory. The necessity to handle this memory of the material imposes challenges in a number of respects; specifically, typical approaches increase (in comparison to corresponding methods for classical memory-free material laws)

- 1. the run time of the material law simulation algorithms,
- 2. the memory requirements of these software routines, and
- 3. the software engineering complexity of integrating the codes into existing general FE software packages.

In this talk, we will discuss alternative approaches for implementing the material laws and integrating them into FE packages that are efficient in all three respects in the sense that they asymptotically (i.e., when a large number of time steps is taken in the simulation) do not have a higher complexity than typical algorithms for memory-free materials. Our main tools in the development of these algorithms will be so-called diffusive representations of fractional integral operators, classical numerical integration theory, and the concept of sum-of-exponentials approximation schemes. This allows us to establish an abstract setting that automatically ensures the desired efficiency and yet provides a great deal of freedom for the concrete implementation. How this freedom can be best used to achieve the highest possible efficiency is a topic of ongoing investigations.

The work described in this talk is performed within a joint project with André Schmidt (Institute of Nonlinear Mechanics, Universität Stuttgart). This project is supported by the German Federal Ministry of Education and Research (BMBF) under Grant 05M22WHA.

Efficient space-time Petrov-Galerkin method for fractional PDEs JIE SHEN

Eastern Institute of Technology, Ningbo, and Purdue University, China

There are two main difficulties for numerical solution of fractional differential equations: (i) fractional derivatives are non-local operators; and (ii) Solutions of fractional PDEs exhibit weakly singular behaviors at the endpoints or initial time so a usual (local or global) polynomial based numerical method is not effective.

The aim of this talk is to present two classes of basic functions for the discretization of the time fractional derivative that allow us to construct space-time Petrov-Galerkin methods which overcome the above two difficulties in a quite general setting.

We consider numerical solution for a class of time fractional PDEs.

Exponential convergence of hp FEM for spectral fractional diffusion in polygons

Christoph Schwab¹, Lehel Banjai², Markus Melenk³

¹ETH Zurich, Switzerland

²Heriot-Watt University, Edinburgh, United Kingdom

³Technische Universität Wien, Austria

We report recent results from [2, 3] and [1]. For the spectral fractional diffusion operator L^s of order 2s, $s \in (0, 1)$, in bounded, curvilinear polygonal domains $\Omega \subset \mathbb{R}^2$, we prove exponential convergence of two classes of hp FE discretizations under the assumption of analytic data (coefficients and source terms, without any boundary compatibility), in the natural fractional Sobolev norm $H^s(\Omega)$. The first hp discretization is based on writing the solution as a conormal derivative of a 2+1-dimensional local, linear elliptic boundary value problem, going back to Caffarelli, Sylvestre and Stinga. To this degenerate, local 2nd order divergence-form PDE an hp-FE discretization with exponential convergence from [1] is applied. A diagonalization in the extended variable reduces the numerical approximation of the inverse of the spectral fractional diffusion operator to the numerical approximation of a system of local, decoupled, second order reaction-diffusion equations in Ω .

²Universität Stuttgart, Germany

Leveraging results on robust exponential convergence of hp-FEM for second order, linear reaction diffusion boundary value problems in Ω , exponential convergence rates for solutions $u \in H^s(\Omega)$ of $L^s u = f$ follow. Key ingredient in this hp-FEM is boundary fitted meshes with geometric mesh refinement towards $\partial\Omega$.

The second discretization is based on exponentially convergent numerical sinc quadrature approximations of the Balakrishnan integral representation of L^{-s} combined with hp-FE discretizations of a decoupled system of local, linear, singularly perturbed reaction-diffusion equations in Ω . The present analysis for either approach extends to (polygonal subsets M of) analytic, compact 2-manifolds M, parametrized by a global, analytic chart χ with polygonal Euclidean parameter domain $\Omega \subset \mathbb{R}^2$.

Numerical experiments with the code NGSOLVE of J. Schoberl (Vienna) [9, 10] for model problems in nonconvex polygonal domains and with incompatible data confirm the theoretical results.

Exponentially small bounds on Kolmogorov *n*-widths of solution sets for spectral fractional diffusion in curvilinear polygons and for analytic source terms are deduced, which imply exponential convergence of MOR and RB approaches as in [4, 5].

Related work includes an hp-FE analysis of the integral fractional Laplacean [8, 7, 6].

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- [2] L. Banjai, J. Melenk, R. Nochetto, E. Otárola, A. Salgado, C. Schwab, Found. Comput. Math., 19, 901 (2018)
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- [10] J. Schoberl. C++11 Implementation of Finite Elements in NGSolve (2014)

Fabrication of fractional capacitor: Journey from capacitive probe dipped in liquid media to solid state analog circuit element Karabi Biswas

Indian Institute of Technology Kharagpur, India

TBA

Fractional derivatives appear wherever there are power laws in physics Sverre Holm

University of Oslo, Norway

Power laws in time and frequency appear in fields such as linear viscoelasticity and acoustics, viscous boundary layer problems, and dielectrics. As power laws in time and frequency are related by the Fourier transform, and also to fractional derivatives, this is consistent with fractional derivatives in the fundamental descriptions. Examples here include power-law frequency dependent attenuation in ultrasound, elastography and sediment acoustics. In turbulence problems there is usually dependence of the square root of frequency which hints at a half order fractional derivative in time. In viscous boundary problems there is a viscodynamic operator in the Biot poroviscoelastic theory which may be formulated with a fractional pseudo-differential operator. The Curie-von Schweidler power law and the Kohlrausch stretched exponential temporal responses of non-ideal capacitors can also be shown to relate to among others the Cole-Cole power-law dielectric model.

Fractional nonlocal elasticity Yuriv Povstenko

Jan Dlugosz University, Poland

In nonlocal elasticity, integral stress constitutive equation takes into account interatomic long-range forces and reduces to the classical theory of elasticity in the long-wave-length limit and to the atomic lattice theory in the short-wave-length limit. We propose the new nonlocal elasticity theory with the weight function in the stress constitutive equation being the Green function of the Cauchy problem for the fractional diffusion equation. The proposed theory can be used for better matching the theory of elasticity and the atomic lattice theory. Several examples are solved in the framework of the proposed approach.

Fractional partial differential equations for ultra-slow diffusion: Analysis and computation

Changpin Li

Shanghai University, China

The known ultra-slow diffusion indicates that the diffusion rate is algebraic in the sense of logarithmic function. Such a kind of diffusions is often modeled by the fractional Hadamard derivatives. In this talk, we first introduce the various kinds of numerical algorithms for Caputo-Hadamard derivatives. Then we apply the derived algorithms to long term integration of the typical fractional differential equations, such as the fractional Lorenz system, the Bagley-Torvik system, and the fractional Allen-Cahn equation, with Caputo-Hadamard derivatives. Last, we theoretically and numerically study the finite blow-up solutions of the semi-linear fractional partial differential equations with Caputo-Hadamard derivatives.

Learning nonlocal constitutive laws via invariant neural operators Yue Yu

Lehigh University, United States

Neural operators, which emerge as implicit solution operators of hidden governing equations, have recently become popular tools for learning responses of complex real-world physical systems. Nevertheless, the majority of neural operator applications has thus far been data-driven, which neglects the intrinsic preservation of fundamental physical laws in data.

In this work, we introduce a novel integral neural operator architecture, to learn a nonlocal constitutive law from data. As such, the neural operator provides a forward model in the form of state-based peridynamics, with fundamental conservation and momentum balance laws automatically guaranteed. As applications, we demonstrate the expressivity and efficacy of our model in learning complex material behaviors from both synthetic and experimental datasets, and show that, by using neural networks to capture the complex responses while automatically satisfying essential physical laws, our learned neural operator achieves improved accuracy and efficiency from the baseline peridynamics models.

Long-range correlated processes: Confinement & heterogeneity Ralf Metzler

University of Potsdam, Germany

Stochastic processes driven by Gaussian yet power-law correlated noise, such as Mandelbrot's fractional Brownian motion (FBM) represent a quite ubiquitous effective description of the dynamics in a range of complex systems, e.g., for the motion of tracers in viscoelastic environments, in "rough" financial data, or for the persistent motion of animals. FBM is an ergodic yet strongly non-Markovian process, with often surprising behavior. In this talk I will briefly introduce these processes and demonstrate that in strong confinement their probability density may assume non-Boltzmannian, multimodal stationary shapes, while in soft external potentials no steady state exists. An application of this effect to brain fibre growth is discussed. In heterogeneous environments the memory correlations of a diffusing test particle may become a (random or deterministic) function of time or space. For these cases I will introduce "doubly-stochastic" extensions such as FBM with random scaling exponent, memory-multimodal FBM, and FBM with a "diffusing diffusivity".

Nonlocal calculus with heterogeneous localization Qiang Du

Columbia University, United States

We discuss the need for a nonlocal calculus for problems on bounded domains involving finite-range nonlocal interactions with heterogeneous localization. The subject is motivated by applications from various disciplines. We show how they can lead to well-posed nonlocal problems with local boundary conditions that enjoy good mathematical properties. We also discuss how to design reliable and robust schemes for their discretization. Future development and applications will also be addressed.

Regularity of weak solutions to parabolic-type problems with distributed order time-fractional derivative Katarzyna Ryszewska

Warsaw University of Technology, Poland

TBA

Robust solvers for fractional PDEs on polygonal domains

Mark Ainsworth¹, Shuai Jiang²

¹Brown University, United States

²Sandia National Laboratory, United States

The numerical discretization of fractional PDEs on polygonal domains is often achieved using an integer order in one additional space dimension. This avoids the need to deal with non-local and fractional order operators directly but comes at the price of having to deal with a degenerate elliptic PDE. Examples include the Caffarelli-Silvestre formulation or methods based on Balakrishnan formulae. The additional space dimension often results in a system of coupled algebraic systems that are singularly perturbed, and which becomes highly ill-conditioned as the discretization is refined. We outline recent work in this direction that results in simple and effective preconditioners.

Soft robotics & fractional calculus. A convenient marriage

Blas M. Vinagre, Inés Tejado, Andrés Serrano University of Extremadura, Spain

Soft robotics is a step forward in the adventure of technology for imitating nature by creating machines that, like the biological ones, are soft, elastic, compliant and can have a high number, ideally infinite, degrees of freedom, properties that will allow them to perform, safely, complex tasks in complex and changing environments. It is still in the cradle and demands huge research in areas like materials science and engineering, mathematical modeling of dynamical behavior, and control. In many cases, the materials have viscous and rheological properties ruling their dynamics, and the robots move into environments which shares the same or similar properties, a fertilized land to farm with the tools of fractional calculus. This talk explores the possible uses of fractional calculus in soft robotics, for modeling and control the robots, and providing, at the same time, a more precise idea of their interaction with the environment.

Two triangles: complexity / inverse power law / fractional calculus & fractional calculus / renormalization group / machine learning (FC-RG-ML) YangQuan Chen

University of California Merced, United States

In the 1st part of this talk, I will introduce a triangle that connects "complexity", "inverse power law" (IPL) and "fractional calculus" (FC). The key message is that to better understand complexity one has to use FC. Based on this foundation, in the 2nd part of this talk, I will mainly discuss how FC, renormalization group (RG) theory and machine learning (ML) are connected. FC has been shown to help us better understand complex systems, improve the processing of complex signals, enhance the control of complex networks, increase optimization performance, and even extend the enabling of the potential for creativity. RG allows one to investigate the changes of a dynamical system at different scales.

Although extensive research has been carried out on the three topics separately, few studies have investigated the association triangle between the FC, RG, and ML. In the FC and RG, scaling laws reveal the complexity of the phenomena discussed. It is emphasized that the FC's and RG's critical connection is the form of inverse power laws (IPL), and the IPL index provides a measure of the level of complexity. For FC and ML, the critical connections in big data, wherein variability, optimization, and non-local models are described. In the end, the association between the RG and ML is also explained. The mutual information, feature extraction, and locality are also discussed. Many of the cross-sectional studies suggest a connection between the RG and ML. It is shown that the new triangle between FC, RG, and ML, forms a stool on which the foundation to complexity science might comfortably sit for a wide range of future research topics. For example, we should look into "complexity-informed machine learning".

[1] H. Niu, Y. Chen, B. West, Entropy, 23, 297 (2021)

Wright functions of the second kind in fractional diffusion processes Francesco Mainardi

University of Bologna (Retired), Italy

In the framework of higher transcendental functions, the Wright functions of the second kind have increased their relevance resulting from their applications in probability theory and, in particular, in fractional diffusion processes. We first start with the analytical properties of the classical Wright functions of which we distinguish two kinds. We then justify the relevance of the Wright functions of the second kind as fundamental solutions of the time-fractional diffusion-wave equations.

We think that this approach is the most accessible one for describing the transition from sub diffusion processes to wave propagation.

4. Participant list

Organizers

Hesthaven, Jan
EPFL, Switzerland
Karniadakis, George
Brown University, United States
Pagonabarraga, Ignacio
University of Barcelona, Spain
Podlubny, Igor
Technical University of Kosice, Slovakia

On-site participants

Ainsworth, Mark - Brown University, United States

Atanackovic, Teodor - Serbian Academy of Sciences, Serbia

Chen. Yangguan - University of California Merced, United States

Diethelm, Kai - Technical University of Applied Sciences Würzburg-Schweinfurt, Germany

Du, Qiang - Columbia University, United States

Guo, Ling - Shanghai Normal University, China

Holm, Sverre - University of Oslo, Norway

Kremer, Kurt - Max Planck Institute for Polymer Research, Germany

Kubica, Adam - Warsaw University of Technology, Poland

Li, Changpin - Shanghai University, China

Luchko, Yuri - Berliner Hochschule für Technik, Germany

Mainardi, Francesco - University of Bologna, Italy

Marynets, Kateryna - TU Delft, Netherlands

Mckinley, Gareth - MIT, Cambridge, United States

Metzler, Ralf - University of Potsdam, Germany

Pantova, Dona - TU Delft, Netherlands

Pawlak, Karolina - Warsaw University of Technology, Poland

Povstenko, Yuriy - Jan Dlugosz University, Poland

Ryszewska, Katarzyna - Warsaw University of Technology, Poland

Saberi, Mehdi - EPFL, Switzerland

Schwab, Christoph - ETH Zurich, Switzerland

Shen, Jie - Eastern Institute of Technology, Ningbo, China & Purdue University, United States

Vinagre, Blas M. - University of Extremadura, Spain

Wang, Hong - University of South Carolina, United States

Yu, Yue - Lehigh University, United States

Zayernouri, Mohsen - Michigan State University, United States

On-line participants

Biswas, Karabi - Indian Institute of Technology Kharagpur, India Ghoshal, Anindya - U.S. Army Research Laboratory, United States Knap, Jaroslaw - U.S. Army Research Laboratory, United States Pietsch, Hollie - US Army DEVCOM-Atlantic, United Kingdom Zingales, Massimiliano - Università degli Studi di Palermo, Italy