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Editorial

Special Issue on "Fractional PDEs: Theory, Numerics, and Applications"

Fractional Partial Differential Equations (FPDEs) are emerging as a powerful tool for modeling challenging multiscale phenomena including overlapping microscopic and macroscopic scales, anomalous transport, and long-range temporal or spatial interactions. The fractional order may be a function of *space–time* or even be a *distribution*, opening up tremendous opportunities for modeling and simulation of multiphysics phenomena, e.g. seamless transition from wave propagation to diffusion, or from local to non-local dynamics. It is even possible to construct *data-driven fractional differential operators* that 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. In other words, a *new* (and simple) data assimilation paradigm can be formulated to determine the fractional order (or possibly a distribution) by taking into account a diverse set of sources of information, including available experimental data albeit of variable fidelity.

Researchers who are new to the field of FPDEs wonder as to when "to think fractionally?" and in which areas factional modeling may be useful. Fractional modeling is effective in systems with self-similarity and scale-invariance, systems characterized by non-Markovian behavior and long-range interactions or power laws as well as for lossy or disordered media. In applications such as anomalous diffusion or propagation through random media, in turbulence, in porous and granular media and sediment transport, in biophysics and cell migration, in crack propagation, in viscoplastic materials, etc., we encounter processes that are perhaps best described by time- or space-fractional derivatives.

In the context of computational physics, even classical long-standing issues of monotonicity, boundary conditions, anisotropy, and limited regularity, typical of problems involving interfaces, e.g. multiphase flows and fluid–structure-interactions, can be re-formulated and re-interpreted in terms of fractional derivatives as well as probabilistically. Examples include the classical second Stokes flow problem of vorticity diffusion, which can be reformulated as "half-order" advection equation with a transport velocity proportional to the square-root of viscosity. Another example involves Lévy flights that can explain super-diffusion and acceleration of steep fronts in reaction–diffusion systems.

Fractional calculus (FC) is of course not new, initiated in 1665 in a letter of L'Hospital to Leibnitz requesting clarification on the meaning of the half derivative of the function $f(x) = x$. Later, Leibnitz, Liouville (1834) and Riemann (1892) developed the basic mathematical ideas, and subsequently, FC was brought to the attention of the engineering community by Heaviside in the 1890s. However, until the end of the previous century only isolated efforts were undertaken on the theoretical or application side. Hence, it is reasonable to wonder why fractional calculus was not adopted much earlier by the computational science community. This is a difficult question to answer but two reasons that fractional modeling has not been used extensively so far is that FPDEs are non-unique, and that they are quite expensive to solve numerically. We believe, however, that both issues can be effectively addressed in the near-future, especially at this juncture, as the first is closely related to availability of (big) data, while the second to advanced discretizations and solvers. In both areas, there has been impressive progress during the last three decades.

The number of papers on FC that have been published since 1985 is increasing exponentially, and so is the number of scientific fields affected by FC and FPDEs. For example, according to the Web of Science, in 1985 there were only 14 fields affected by the FC and FPDEs while at the present time, there are ten times more, see Fig. 1. Hence, the current number – 145 fields in the Web of Science – means that now FC and FPDEs affect all fields of science and engineering as the Web of Science lists currently exactly 145 fields/categories.

With this ever-expanding range of applications and models based on fractional calculus comes a need for the development of *rigorous* theory and corresponding *robust*, *accurate* and *efficient* computational methods for approximating the solutions of FPDEs. On the theoretical side, the well-posedness of *ad hoc* fractional reformulations of conservation laws is in doubt. Even basic questions, e.g. what are the proper boundary conditions for non-local problems, is a complex and generally open problem. Moreover, non-local features and the singular kernels involved in fractional operators give rise to significant computational challenges to the extent that current numerical methods for fractional modeling in *three-dimensions* and for *long-time integration* become prohibitively expensive. Accordingly, new research is needed on two main fronts: fast linear

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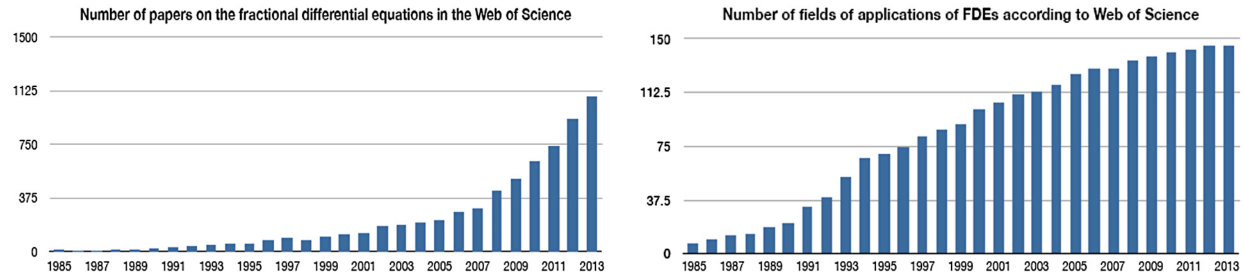

Fig. 1. Data from the Web of Science (March 2015): Left – number of papers on the fractional differential equations per year. Right – number of fields of applications of fractional differential equations per year.

solvers based on rigorous information-based complexity bounds; and, *adaptive grid-refinement* based on *a posteriori* error estimators. In conservation laws, correct prediction of the propagation of steep fronts requires *conservative* numerical schemes. In addition, by employing fractional Laplacians or fractional convective derivatives, future research has the potential to resolve issues of *monotonicity* arising in high-order discretization methods in the presence of non-smooth solutions.

The 31 papers collected in this special issue address most of the aforementioned issues and provide the foundation for further developments on all aspects of fractional modeling going forward. The idea for the special JCP volume was born on June 3–5, 2013 in Newport, RI, USA where George Em Karniadakis and Jan S. Hesthaven organized the "*International Symposium on FPDEs: Theory, Numerics, and Applications*", the first such conference in USA. It was supported by the US Army Research Office, the US Air Force Office of Scientific Research and the Department of Energy through a PNNL special fund. The papers of this special volume are not proceedings of the conference, yet the objectives and the themes are the same. Moreover, several of the invited speakers are contributors to this issue, including Igor Podlubny, the co-editor, who was an invited speaker at the Newport conference. What makes this special issue unique and different than previous special issues (see Refs. [1–11]) is the focus of all papers on the fundamental open issues of FPDEs. To the best of our knowledge, this is also the largest collection of FPDE papers in a single volume. The five special issues published in various journals cites in the references have covered either very special topics, e.g. in signal processing, in control, etc. or they contain a mix of applications, fractional ODEs and fractional PDEs.

We have organized this volume into different thematic units, starting from theoretical topics, and continuing with numerical methods, first for time-fractional PDEs, and subsequently for space- (and space-/time-) fractional PDES. We then present papers on fast solvers, and we conclude with novel applications of FPDEs to computational physics. In the following, we provide a few more details that will help the reader navigate through this extensive collection of novel and timely research in this very active research area.

Theory: There are seven contributions in this section. The first paper introduces the concept of the fractional derivative and provides two criteria required for an operator to be classified as a fractional derivative. The next two papers present advances on tempered fractional calculus and tempered stable processes, focusing on the underlying stochastic dynamics that allows useful probabilistic interpretations, especially in the context of bounded domains. The fourth paper introduces the concept of the neutral-fractional PDE where the fractional order is the same for all time- or space-derivatives. In the case of the wave equation, solutions of the neutral-fractional equation can be interpreted as damped waves with constant propagation velocities. The next paper introduces a discrete time random walk that can also be used to model anomalous diffusion in an external force field and provides the foundation for a novel numerical method. The sixth paper focuses on the monotonicity of the Prabhakar function, which is a three-parameter extension of the classic Mittag–Leffler function with important applications in modeling the physics of dielectrics. The final paper presents explicit and approximate solutions of the nonlinear fractional KdV–Burgers equation with time–space-fractional derivatives, in the form of rapidly convergent series with easily computable components.

Time-fractional derivatives: The next unit on PDEs with time-fractional derivatives has nine contributions. The first one addresses the fundamental question of how to approximate the left- and right-derivative numerically and the relationship between them. The second paper generalizes the time-fractional telegraph equation using the concept of a derivative of fractional variable order and presents analysis and numerical results. The next paper solves the time-fractional Schrödinger equation through Krylov projection methods, enabled by expressing the solution in terms of the Mittag–Leffler function. The fourth contribution focuses on shooting problems for final value problems of fractional order and proposes new algorithmic strategies for improving the efficiency of such methods. The next three papers present spectral discretizations of the time-fractional derivative. First, a spectral-tau algorithm is discussed for time-fractional diffusion-wave equations. In the next two papers, a multi-domain spectral method is developed and implemented in the context of parareal formalism that allows parallel-in-time solution. The eighth paper of this section presents a second-order accurate method for variable-order time-fractional derivative, which can be exploited in diverse physical and biological applications where rates of change of the quantity of interest may depend on space and/or time. The final paper presents an analysis of error bounds due to time-stepping for fractional diffusion problems with non-smooth initial data, using the discontinuous Galerkin method.

Space-fractional derivatives: This section on PDEs with space-fractional and possibly space- and time-fractional derivatives has eight contributions. The first paper discusses high-order accurate methods for the representation of the Riesz derivative and its application to fractional reaction–diffusion problems. The next contribution develops an energy conservative scheme for solving the fractional Schrödinger equation, again based on the Riesz derivative. In the third paper, emphasis is on the development of alternating direction methods for the two-dimensional fractional FitzHugh–Nagumo equation, used to describe the dynamics of electric potentials in the cardiac tissue. In the fourth paper, finite difference/finite element methods for two-dimensional Bloch–Torrey equations are discussed, encompassing a problem that is fractional in both space and time. The fifth contribution explores the use of radial basis functions to the space-fractional advection–dispersion equation, and the sixth paper proposes an iterative scheme for solving fractional differential equations with applications to diffusion in heterogeneous media. The seventh paper introduces a spectral collocation method for fractional PDE, including nonlinear problems with variable coefficients. The final contribution proposes *a posteriori* error analysis for the adaptive solution of fractional Laplacian by extension.

Fast solvers: This section on efficient solution of the full linear systems resulting from discretization of FPDEs has two contributions. The first paper discusses the structure of the linear systems arising from a finite difference approximation of space-fractional diffusion problem and explores this to devise efficient solvers for the linear systems. In the second paper, a new matrix-based method for the rapid solution of the discrete systems arriving from discretizing fractional PDE is proposed, relying on reducing the problem to a Sylvester equation.

Applications: The final section of this special issue on applications of FPDEs has five contributions. The first paper discusses the development and analysis of solitary patterns in time-fractional models while the second contribution demonstrates the use of a fractional model of damage and fatigue in materials. In the third paper, the authors present dispersive transport of charge carriers in disordered nanostructured materials while in the fourth paper the propagation of fronts in sub-diffusive media is studied. The last contribution explores the use of fractional models in the context of image registration using a variational formulation.

Finally, we would like to thank all the authors and the referees for their contributions to this special issue as well as the Editor-in-Chief, Gretar Tryggvason, who gave us this opportunity.

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