Inverse Problems for Anomalous Diffusion Processes

Diane Guignard (University of Ottawa),
Barbara Kaltenbacher (University of Klagenfurt),
William Rundell (Texas A&M University)

May 8 - May 13, 2022

1 Overview of the Field

The roots of the modern theory of diffusion processes are to be found in the early decades of the nineteenth century. The work of Fourier in formulating his famous heat equation comes to mind. Fourier's arguments were from a macroscopic viewpoint but from a particle-diffusion perspective, the first systematic study was by two Scottish scientists: the chemist Thomas Graham and the botanist Robert Brown. Einstein's 1905 paper on the topic provided the now generally accepted explanation for Brownian motion and had far-reaching consequences for physics. There are two key pieces to this work: first, the assumption that a change in the direction of motion of a particle is random and that the mean-squared displacement over many changes is proportional to time; second, he combined this with the Boltzmann distribution for a system in thermal equilibrium to get a value on the proportionality, the "diffusivity" D in $\langle x^2\rangle = 2Dt,\ D = \frac{RT}{6N\pi\eta a}$ where T is the temperature, R the universal gas constant, N is Avogadro's number and $\gamma = 6\pi\eta a$ where a is the particle radius and η the viscosity. In the same year, the first dialogues about "random walk" models based on the ideas of Lord Rayleigh some 20 years previous began.

The heat equation can be derived from such a model based on equal step lengths in equal time intervals with the coupling between time and space $dt \propto dx^2$ given by the diffusion constant. Indeed, the time and space steps can be drawn from a probability density functions $p(t)$ and $\psi(x)$ – provided that the mean of $p(t)$ and the variance of $\psi(x)$ are finite. Therefore, classical Brownian motion can be viewed as a random walk in which the dynamics is governed by an uncorrelated, Markovian, Gaussian stochastic process. On the other hand, when the random walk involves correlations, non-Gaussian statistics or a non-Markovian process (for example, due to "memory" effects) the diffusion equation will fail to describe the macroscopic limit. These considerations lead to so-called "anomalous diffusion" processes and the physically-motivated examples are numerous.

Issue with the fixed paradigms of Brownian motion should not lie only with the underlying assumptions; we should ask if the outcomes of the model are satisfactory from a physical perspective. Rayleigh's observation that in Brownian motion the particles have a high probability of being near their starting position can be seen in terms of the probability density function given by the Gaussian; a relatively slow diffusion initially but a very rapid decay of the plume in space. It has certainly been observed that many processes exhibit a very different effect.

If we break the above assumptions by either $p(t) \propto t^{-1-\alpha}$ for $0 < \alpha < 1$ or $\psi(x) \propto x^{-2-\beta}$ for $1 < \beta < 2$, then the model no longer generates classical differential equations but ones with fractional derivatives. These can be described as an operator product of an integer order derivative and an Abel fractional integral – another 1820's idea.

Partial differential equations remain the lingua franca of the physical sciences and we want to ensure any model will have such a translation. In the case of a time fractional derivative, the diffusion equation becomes $\partial_t^\alpha u - \triangle u = f$ and the governing function is no longer the exponential of the parabolic form, but a Mittag-Leffler function $E_{\alpha,\beta}(z)$. Such *sub-diffusion* equations have very different properties. The most basic of these is perhaps the nonlocality of the operator. The fractional derivative's value at time t depends on all previous values of the solution - a striking example of the non-Markovian behaviour of the model. Moreover, the long term decay of their solution is only linear in time and they have very limited smoothing behaviour in terms of the initial data and f – again in sharp contrast to the classical parabolic case. Needless to say, their analysis is correspondingly more complex. However, this slow decay can be a substantial advantage in inversion and many extremely (exponentially) ill-conditioned inverse problems become less so (polynomial) under the subdiffusion paradigm. This comes at a price. Numerical methods are needed to obtain computable approximations of the solutions which can be used, for instance, to determine if a mathematical model is accurately describing the underlying physical phenomena. Due to the complexity of problems involving fractional operators, new and often clever methods must be used to obtain efficient and reliable approximations.

A similar effect occurs in wave equations under damping. Incorporating a classical first order time derivative simulating velocity, the exponential decay of the solution makes it difficult to extract information from anything but very small times. Under fractional damping, the decay is only linear and vastly changes an inverse problem designed to recover important coefficients in the equation from time-trace data.

In the superdiffusion case, where we incorporate a spatial fractional derivative, the situation is even more complex and, unlike the subdiffusion case which is now becoming well-understood, remains more of an enigma. We should remark here that there are many definitions of fractional operators in space - in particular of elliptic operators. These include the "fractional Laplacian of order β" which in $\mathbb{R}^d$ can be viewed as that pseudo differential operator whose Fourier transform has symbol ξ^β or in a bounded domain Ω as that operator with the same eigenfunctions as $-\triangle$ but with eigenvalues raised to the power β. These have a rich mathematical theory but their direct connection to a physical process is more tenuous. On the other hand, they have useful mathematical properties that simulate many of the desired physical properties.

In both the sub and super-diffusion cases, there is the question of obtaining effective numerical methods as the parabolic paradigm no longer holds and the spatial effects involve the entire region. Again, the situation is that much has been done but there is even more to do especially in the super-diffusion models, and this aspect will be a central part of our workshop.

2 Objectives of the Workshop

The primary interest of the organisers was, on the one hand, the analysis of inverse problems for partial differential equations and on the other hand, the development and analysis of numerical methods for solving the underlying equations.

Of particular interest are reaction diffusion equations either of subdiffusion type $\partial u_t^\alpha - Lu = f(x,t,u)$ or containing a space fractional operator L^β as in $\partial u_t^\alpha - L^\beta u = f(x,t,u)$. These can be single equations or coupled systems and there may be unknown coefficients appearing in the elliptic operator or its fractional substitute, as well as in the nonlinear term $f(x,t,u)$. Such equations in classical derivative form have formed the basis of chemical reactions, combustion, mathematical ecology and epidemiology, just to name a few application areas. In each case, there is a considerable rationale for the inclusion of non-Markovian models and their differential equation counterparts. Materials with memory require such a mechanism: many biologists and epidemiologists have pointed out that species rarely diffuse with a Brownian-type motion and they have to incorporate "long space step" jumps in the model. This is precisely what fractional operators provide. All of the above mentioned applications have conditions under which the forced, classical exponential decaying solutions no longer capture the dynamics and their replacement with nonlocal operators provide a more realistic physical model.

Inverse problems play a major role in all of the above. Indeed, the central issue with complex epidemic modelling is the recovery of the various rate constants under high noise measurements and it is clear that such finite dimensional parameter identification problems are vastly more simple and model-restrictive than the more universal approach of treating the unknowns as functions in a prescribed class.

In recent years, the development of numerical methods for problems involving fractional operators has made considerable strides in reducing the computational cost of previous methods. This is especially true for the case of direct or forward problems. For instance, borrowing tools traditionally used in the context of parametric PDEs, the reduced basis method has been recently considered to efficiently approximate the solution of fractional diffusion problems. Computational methods for inverse problems, where recovery of the unknowns is frequently done by iterative methods, is more challenging. The strategy of using as much of the information as possible from previous iteration steps can make a significant difference yet is a considerable challenge from both an algorithmic and a convergence analysis perspective. Moreover, the performance of such methods in the context of ill-posed inverse problems is still to be explored. This aspect was seen as one of the main goals of this workshop.

Another goal was to seek the group's interest in tackling partial differential operators with space fractional derivatives of Riemann-Liouville or Caputo type rather than as "fractional powers" of existing classical elliptic operators – the so-called *superdiffusion* case. The rationale for this is a closer connection to the underlying physics and models based on the probabilistic approach noted in the overview section. The difficulties here are considerable from both an analysis and a numerical perspective. Many of the PDE results in standard use either don't hold or do so in restricted sense, or are simply unknown. The same can be said to some extent about the functional analysis of these operators and, compared to other definitions, there are significantly less numerical algorithms available with provable convergence properties. The blend of participants we had invited are ideally suited to making substantial progress on this problem.

While each of the organisers have research areas grounded in partial differential equations, they do so from slightly different perspectives that will be valuable for the proposed meeting.

Diane Guignard is a classically trained numerical analyst specialising in adaptive algorithms and both linear and nonlinear reduced models for PDEs. Barbara Kaltenbacher and William Rundell have worked in PDE inverse problems for their entire career: the former is an expert in regularisation techniques, the latter has taken a mathematical physics perspective. Both Kaltenbacher and Rundell have a long individual history of meeting organisation as well as in collaboration. They also have collaborated in many research papers central to the workshop topic.

3 Recent Developments and Open Problems

The first discussion session in the afternoon of Monday, May 9 was very lively and ran well over the allocated time (it was the last session of the day). There was general consensus that the traditional fractional powers of an operator had seen an enormous success from both a numerical and inverse problems perspective. There was also the sense that the area has become perhaps over-saturated and new directions are needed. To be avoided are trends in "artificial" new definitions of fractional operators; research needs to be tied more strongly to physical applications. Ricardo Nochetto and Andrea Bonito who have been at the forefront of current research in numerical methods for some time were very much in agreement with this consensus as was Masahiro Yamamoto representing a more theoretical viewpoint. Specific topics such as fractional partial differential equations with space-dependent fractional power or with different type of boundary conditions (other than homogeneous Dirichlet boundary condition), as well as fully nonlinear fractional partial differential equations were touched on during this discussion. Again, all participants of this session agreed that physical motivations for studying such problems, even if interesting by themselves from a mathematical point of view, are needed.

A second discussion round in the morning of Thursday, May 12 (chaired by Masahiro Yamamoto and Bangti Jin) dealt with similar questions as the first one, but putting more emphasis on time fractional models. Concerning the analysis, it was once more emphasized that fully nonlinear fractional partial differential equations are a still largely unexplored field with many crucial mathematical challenges and interesting applications. Also the importance of physically sound modeling was addressed - in particular in view of a certain trend to just "fractionalizing" classical models without caring about a justification that threatens the image of fractional calculus in the scientific community. In the numerics of fractional PDEs, many new approaches have been developed recently, including time adaptivity or structure and asymptotic preserving methods. However, the tools for analyzing these methods are to some extent still missing. The development of these tools is one of the key open tasks in this area and will certainly benefit from the interaction between numerics oriented researchers and people with expertise on the analytical side of fractional calculus. Finally, joining the space and the time fractional world - which was one of the main motivations of this workshop - remains an important and worthwhile aim.

4 Presentation Highlights

Juan Pablo Borthagaray: *Linear and quasi-linear fractional operators in Lipschitz domains: regularity and approximation*

In this talk, we discuss the formulation, regularity, and finite element approximation of linear and quasi-linear fractional-order operators in bounded, Lipschitz domains. We emphasize recent results about Besov regularity, a priori error estimates in quasi-uniform and graded meshes, and local error estimates for linear problems.

Abner Salgado: *Time fractional gradient flows, theory and numerics*

We consider a so-called time fractional gradient flow: an evolution equation aimed at the minimization of a convex and l.s.c. energy, but where the evolution has memory effects. This memory is characterized by the fact that the negative of the (sub)gradient of the energy equals the so-called Caputo derivative of the state. We introduce a notion of "energy solutions" for which we refine the proofs of existence, uniqueness, and certain regularizing effects provided in [Li and Liu,SINUM 2019]. This is done by generalizing, to non-uniform time steps the "deconvolution" schemes of [Li and Liu, SINUM 2019], and developing a sort of "fractional minimizing movements" scheme. We provide an a priori error estimate that seems optimal in light of the regularizing effects proved above. We also develop an a posteriori error estimate, in the spirit of [Nochetto, Savare, Verdi, CPAM 2000] and show its reliability.
This is joint work with Wenbo Li (UTK).

Andrea Bonito: (tutorial talk) *The Dunford-Taylor Method and Fractional Diffusion*

In the first part of the talk, we review numerical algorithms for the approximation of fractional elliptic operators with a particular attention on their analysis and implementations. Our main emphasis is on methods using the Dunford-Taylor representations of fractional diffusion problems, but other methods are discussed as well. The Dunford-Taylor representation consists of an improper integral, which is approximated an exponentially convergent sinc quadrature method. In turn, the integrand at each quadrature point is approximated using a standard finite element method. The method is easily parallelizable and consists of a straightforward modification of standard finite element methods for reaction-diffusion problems.

In the second part of the talk, we propose numerical methods for the discretization of the surface-quasi geostrophic (SQG) system. The latter is a nonlinear partial differential system of equations coupling transport and fractional diffusion phenomena. The time discretization consists of an explicit strong-stability-preserving three-stage Runge-Kutta method while a flux-corrected-transport method while the space discretization is based on the Dunford-Taylor representations discussed earlier. In the so-called inviscid case, we show that the resulting scheme satisfies a discrete maximum principle property under a standard CFL condition and observe, in practice, its second-order accuracy in space. The algorithm successfully approximates several benchmarks with sharp transitions (frontogenesis) and fine structures typical of SQG flows. In addition, theoretical Kolmogorov energy decay rates are observed on a freely decaying atmospheric turbulence simulation.

Bangti Jin: (tutorial talk) *Tutorial on Recent Advances on Inverse Problems for Time-Fractional Diffusion*

Diffusion type models involving a fractional-order derivative in time have received a lot of attention in the physical and engineering communities during the last few decades, due to their extraordinary capabilities for accurately describing anomalous transport processes. There have also been intensive research activities on inverse problems for such models, starting from the pioneering works of Cheng, Nakagawa, Yamamoto and Yamazaki (Inverse Problems, 2009). In this tutorial talk, I will describe basic facts about the direct problem of the canonical mathematical model and discuss some recent advances on related inverse problems. I will mainly discuss three classes of model inverse problems, i.e., backward problem, order determination and inverse coefficient problems, and describe representative recent results, the idea of proofs and some outstanding issues.

Eric Soccorsi: *Inverse coefficient problem for time fractional diffusion equations*

Let Ω be a bounded domain of $\mathbb{R}^d$, $d \geq 2$, with $C^{1,1,}$ boundary $\partial\Omega$. We consider an initial boundary value problem for a fractional diffusion equation on $\Omega \times (0,T)$, $T > 0$, with time-fractional Caputo derivative of order $\alpha \in (0,1) \cup (1,2)$. We prove that two out the three time-independent coefficients ρ (density), a (conductivity) and q (potential) appearing in the equation $\rho(x)\partial_t^\alpha u(x,t) + \nabla \cdot (a(x)\nabla u(x,t)) + q(x)u(x,t) = 0$ are recovered simultaneously from measurements of the solutions on a subset of $\partial\Omega$ at fixed time $T_0 \in (0,T)$.

Vanja Nikolic: *Time-fractional Moore–Gibson–Thompson equations*

In this talk, we will present several time-fractional generalizations of the JordanMooreGibsonThompson (JMGT) equations in nonlinear acoustics. Following the procedure described in Jordan (2014), these time-fractional acoustic equations are derived from four fractional versions of the MaxwellCattaneo law in Compte and Metzler (1997). Additionally to presenting the local well-posedness results, we will also discuss their limiting behavior as the fractional order tends to one, leading to the classical third order in time (J)MGT equation. The talk is based on joint work with Barbara Kaltenbacher (University of Klagenfurt).

Yikan Liu: *Unique determination of orders and parameters in multi-term time-fractional diffusion equations by inexact data*

As the most significant difference from parabolic equations, the asymptotic behavior of solutions to time-fractional evolution equations is dominated by the fractional orders, whose unique determination has been frequently investigated in literature. Unlike all existing results, in this talk we explain the uniqueness of orders and parameters (up to a multiplier for the latter) only by the inexact data near $t = 0$ at a single point. Moreover, we discover special conditions on unknown initial values for the coincidence of observation data. As a byproduct, we can even conclude the uniqueness for initial values or source terms by the same data. The proof relies on the asymptotic expansion after taking the Laplace transform and the completeness of generalized eigenfunctions.

Guanglian Li: *Wavelet-based Edge Multiscale Parareal Algorithm for subdiffusionequations with heterogeneous coefficients in a large time domain*

I will present in this talk the Wavelet-based Edge Multiscale Parareal (WEMP) Algorithm recently proposed in [Li and Hu, *J. Comput. Phys.*, 2021] to efficiently solve subdiffusion equations with hetero-geneous coefficients in long time. This algorithm combines the advantages of multiscale methods thatcan effectively deal with heterogeneity in the spatial domain, and the strength of parareal algorithms forspeeding up time evolution problems when sufficient processors are available. Compared with the previ-ous work for parabolic problem, the main challenge in both the analysis and simulation arises from thenonlocality of the fractional derivative. To conquer this obstacle, an auxiliary problem is constructed oneach coarse temporal subdomain to uncouple the temporal variable completely. In this manner, the ap-proximation properties of the correction operator is proved. In addition, a new summation of exponentialsums is derived to generate single-step time stepping scheme, with the number of terms of $\mathcal{O}(|\log \tau_f|)$ independent of final time. Here, τ_f is the fine-scale time step size. We derive the convergence rateof this algorithm in terms of the mesh size in the spatial domain, the level parameter used in the multi-scale method, the coarse-scale time step size and the fine-scale time step size. Several numerical tests arepresented to demonstrate the performance of our algorithm, which verify our theoretical results perfectly.

Matti Lassas: *Geometric inverse problems for the fractional diffusion equation*

Given a connected compact Riemannian manifold (M,g) without boundary, $dimM \geq 2$, we consider a spacetime fractional diffusion equation with an interior source that is supported on an open subset V of the manifold. The time-fractional part of the equation is given by the Caputo derivative of order $\alpha \in (0,1]$, and the space fractional part by $(-\Delta_g)^\beta$, where $\beta \in (0,1]$ and Δ_g is the Laplace–Beltrami operator on the manifold. The case $\alpha = \beta = 1$, which corresponds to the standard heat equation on the manifold, is an important special case. We construct a specific source such that measuring the evolution of the corresponding solution on V determines the manifold up to a Riemannian isometry.

Olena Burkovska: *Identifying the fractional power and extent of interactions in nonlocal models*

Nonlocal operators of fractional type are a popular modeling choice for applications that do not adhere to classical diffusive behavior; however, one major challenge in nonlocal simulations is the selection of model parameters. In this talk we propose an optimization-based approach to parameter identification for fractional models with an optional truncation radius. We formulate the inference problem as an optimal control problem where the objective is to minimize the discrepancy between observed data and an approximate solution of the model, and the control variables are the fractional order and the truncation length. For the numerical solution of the minimization problem we propose a gradient-based approach, where we enhance the numerical performance by an approximation of the bilinear form of the state equation and its derivative with respect to the fractional order. We present several numerical tests in one and two dimensions that illustrate the theoretical results and show the robustness and applicability of our method. This work is in collaboration with M. D'Elia and C. Glusa.

Tram Thi Ngoc Nguyen: *From neural-network-based learning to discretization of inverse problems*

We investigate the problem of learning an unknown nonlinearity in parameter-dependent PDEs. The nonlinearity is represented via a neural network of an unknown state. The learning-informed PDE model has three unknowns: physical parameter, state and nonlinearity. We propose an all-at-once approach to the minimization problem. (Joint work: Martin Holler, Christian Aarset)

More generally, the representation via neural networks can be realized as a discretization scheme. We study convergence of Tikhonov and Landweber methods for the discretized inverse problems, and prove convergence when the discretization error approaches zero. (Joint work: Barbara Kaltenbacher)

Ekaterina Sherina: *Quantitative optical coherence elastography*

Elastography is an imaging modality which can map the biomechanical properties of a given sample, and is interested in identifying the spatial distribution and values of its biomechanical parameters. It is typically implemented as an add-on, e.g. to ultrasound, magnetic resonance imaging, optical coherence tomography (OCT) etc. In this work, we consider optical coherence elastography (OCE), which is a promising emerging research field but still lacking high precision and reproducibility. We aim at a quantitative multi-faceted analysis of key factors such as data quality and properties of reconstruction methods required for the successful application of quantitative elastography. Mathematically, we deal with two inverse problems in OCE - a reconstruction of the mechanical displacement and a reconstruction of the Young's modulus (stiffness) from OCT data of a sample which undergoes a static compression. In this work, we propose, analyse and compare three reconstruction methods for the Young's modulus: uniaxial analysis, strain map based reconstruction facilitating a particle tracking improved optical flow (EOFM), and a novel image-based inverse reconstruction method (IIM). The quality of the proposed reconstruction methods with respect to samples of different mechanical properties is investigated by comparing their performance on twelve silicone elastomer phantoms with inclusions of varying size and stiffness.

Andrea Aspri: *Phase-field approaches for reconstruction of elastic cavities*

In this talk I will present some recent results on geometrical inverse problems related to the shape reconstruction of cavities and inclusions in a bounded linear isotropic medium by means of boundary measurements. We adopt the point of view of the optimal control, that is we rephrase the inverse problems as a minimization procedure where the goal is to minimize, in the class of Lipschitz domains, a mis-fit boundary functional or an energy-type functional with the addition of a regularization term which penalizes the perimeter of the cavity/inclusion to be reconstructed. The optimization problem is addressed by a phase-field approach, approximating the perimeter functional with a Modica-Mortola relaxation.

This is a joint work with E. Beretta, C. Cavaterra, E. Rocca and M. Verani.