NUMERICAL FRACTIONAL DIFFUSION: A PDE APPROACH, INTEGRAL FORMULATION, EXTENSIONS AND APPLICATIONS

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By now it is clear that computational science is one of the bases, together with theory and experiments, of scientific inquiry. A carefully crafted computational model/experiment can replace a very expensive or unrealizable experimental setting, and it can give new insight into the theoretical developments of a specific discipline. Discussions about computer aided simulation and high performance computing are recurring themes in science. But, are these computational models a faithful representation of the underlying physical processes? How can we make sure that the results obtained by the computer are meaningful? The answer to these questions is, evidently, not a simple one. Even if we, for the time being, assume that the computer is always right, we still might obtain meaningless results simply because the model that we are using does not describe the process of our interest. How to detect this kind of errors is a question for the specialists in the physical sciences and so I will discuss it no more.

In the discussion above, a big assumption was made: the computer is right. But, how can we guarantee that? Even more, we may ask, How can we get the best possible answer with the least possible amount of effort? A quest for the answer to these and many related questions is the underlying reason for numerical analysis, which is the analysis of computational schemes. It offers us, in short, a solid mathematical background that describes to what extent the computer's output approximates the process of interest.

In general, my research concentrates on the numerical analysis of partial differential equations (PDE), in particular on fractional diffusion. Diffusion is the tendency of a substance to evenly spread into an available space, and is one of the most common physical processes. The classical models of diffusion lead to well known models and even better studied equations. However, in recent times, it has become evident that many of the assumptions that lead to these models are not always satisfactory or not even realistic at all. Consequently, different models of diffusion have been proposed, fractional diffusion being one of them.

Inspired by a novel result from PDE [4], in our research we have made a decisive advance in the numerical solution and analysis of fractional diffusion, a relatively new but rapidly growing area of research. Although its mathematical analysis is highly nontrivial, the computational implementation of such method is done using standard components of numerical analysis; see [7, 8, 11, 13]. This is the main advantage of our scheme, since the approaches advocated in the literature require special attention due to the mathematical difficulties inherent to fractional diffusion; see [15] for a discussion.

The mathematical structure of fractional diffusion is shared by a wide class of mathematical objects: *nonlocal operators*. These objects have a strong connection with real-world problems, since they constitute a fundamental part of the modeling and simulation of complex phenomena. Their applications are vast, and span control theory, finance, electromagnetic fluids, image processing, materials science, optimization, porous media flow, turbulence, continuum field theories and others. We will be concerned with applications in image processing and optimal control of PDE; see [1] for preliminary results in control theory. From this it is evident that the particular type of mathematical object appearing in applications can widely vary and that a unified analysis might be well beyond our reach. A more modest, but nevertheless quite ambitious, goal is to develop a computational analysis that is representative of a particular class: fractional diffusion.

In mathematical terms, exploiting the *cylindrical* extension proposed and investigated by X. Cabré and J. Tan [3] and Capella, Dávila, Dupaigne and Sire [6], in turn inspired in a work of L. Caffarelli and L. Silvestre [4], we have replaced the (intricate) integral formulation of a problem involving the *fractional Laplacian* $(-\Delta)^s u = f$ in Ω, $0 < s < 1$, by the (local) elliptic PDE

$$\operatorname{div}(y^\alpha \nabla U) = 0 \quad \text{in} \quad \Omega \times (0, \infty) \quad (\alpha = 1 - 2s), \tag{1}$$

with variable coefficient y^α (which either degenerates or blows up) in one higher dimension y; f enters as a natural boundary condition at $y = 0$. In [11], we have proposed a simple strategy to find the solution of the fractional Laplace problem in general bounded polyhedral domains Ω of $\mathbb{R}^d$. Moreover, we have derived a quasi-optimal a priori error analysis, in the context of weighted Sobolev spaces, valid for tensor product elements which may be graded in Ω and exhibit a large aspect ratio in y (anisotropy) to fit the behavior of $U(x, y)$ with $x \in \Omega$, $y > 0$.

Upon realizing that the weight y^α belongs to the class A_2 of Muckenhoupt weights, in [14] we have been able to extend the interpolation theory of [11] to a general one in a Muckenhoupt weighted Sobolev space setting. This is of interest not only for the solution of problem (1) but also for that of nonuniformly elliptic problems in general. This brings to numerical analysis techniques and methods developed within harmonic analysis to deal with, for instance, maximal functions, Calderon Zygmund operators and weighted norm inequalities. This might serve as a starting point for the numerical analysis on homogeneous spaces [9].

The main advantage of the algorithm proposed in [11] is that we are solving the local problem (1) instead of dealing with the nonlocal operator $(-\Delta)^s$. However, this comes at the expense of incorporating one more dimension to the problem, thus raising the question of how computationally efficient this approach is. The development of an efficient computational technique for the solution of problem (1) has been the subject of [7]: *multilevel methods*. We have designed a multilevel method with line smoothers in the y direction, which reveals a competitive performance in terms of computational cost.

In contrast to [2] and [10], our approach seems to be flexible enough to study other problems with fractional diffusion in space. As a natural extension of the elliptic case studied in [11], we have designed and analyzed solution techniques for evolution equations with *fractional diffusion* and *fractional time derivative* [13]. In this paper, the fractional time derivative, in the sense of Caputo, is discretized by a first order scheme and analyzed in a general Hilbert space setting. We have also derived discrete stability estimates which yield a novel energy estimate for evolution problems with fractional time derivative.

As an application and extension of the a priori theory developed in [11], we have designed and studied solution techniques for a linear-quadratic optimal control problem involving fractional powers of elliptic operators in a bounded domain [1]. We have derived a priori error estimates for the optimal control and state for two discretization approaches: one that is semi-discrete, where the control is not discretized, and the other one is a fully discrete via the discretization of the control. This is the first work addressing the the numerical approximation of an optimal control problem involving fractional powers of elliptic operators.

Future work

A posteriori error estimators. Given that the coefficient y^α in the equation (1) is singular, we cannot proceed with the usual residual based techniques. Moreover, preliminary studies with alternative approaches show that, since this problem has a preferred direction, anisotropic error estimators and mesh refinement procedures must be developed and analyzed. This is of value not only for this problem, but in general for anisotropic problems, as such tools are not available in the literature. Numerical results show a competitive performance of our methods; see for preliminary results [8]. This is the first step to do adaptivity, which is the study of iterative improvement based on a posteriori estimators.

The obstacle problem. Another application of [11] is the obstacle problem for fractional diffusion both elliptic and parabolic. The elliptic case can be written in complementarity form for the fractional Laplacian: $u \geq \varphi$, $(-\Delta)^s u \geq 0$ and $(u - \varphi)(-\Delta)^s u = 0$. This leads to studying a thin obstacle problem for the nonuniformly elliptic PDE (1) [5]. These type of problems arise, for instance, in financial mathematics as a pricing model for American options, and are thus of increasing interest [16]. The function u represents the rational price of a perpetual American option where the assets prices are modeled by a Levy process, and the payoff function is φ. For non perpetual options, a parabolic obstacle problem must be considered [16]. For some preliminaries results in the elliptic case, we refer to the submiited article [12].

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