Causal generalized functions in geophysical and environmental modelling

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Abstract. Geophysical exploration often uses energy sources of impulsive type (explosives, air gun, etc.), and the constitutive laws (either mechanical or electromagnetic) of geo-materials should take into account the "memory" of the system with a cause-effect relationship expressed by a time convolution (in particular, by a fractional differential equation). Therefore, causal generalized functions (i.e., distributions with support in the positive real semi-axis) play a major role in this kind of modelling, and also allow us to simplify the mathematical treatment in virtue of the higher level of abstraction in comparison with functions of classical analysis. This scientific paradigm has been successfully applied to seismic exploration (viscoelasticity), reservoir engineering (poroelasticity), and environmental geophysics (modelling of ground-penetrating radar). It is reasonable to expect other similar applications of fractional calculus to earth sciences, and especially to geophysical fluid dynamics (parameterization of turbulence in meteorology and oceanography), hydrology (identification of the instantaneous unit hydrograph), and to ecology and climatology (relationship between forests and greenhouse gases).

Key words convolution, fractional derivatives, visco-poro-elasticity, ground-penetrating radar, geo-physical fluid dynamics, ecology, climatology.

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Introduction

The basic equations of geophysical modelling may be broadly classified into two main categories: balance equations and constitutive assumptions. The former rely on first principles and hence are hardly questionable. The latter have to describe the peculiar properties of the various materials and therefore leave more freedom to the mathematical modeller, who may also choose which phenomena and which scales he wants to focus on.

A constitutive equation often expresses a local, linear and time-invariant relationship between a cause and an effect. In this case, by Riesz representation theorem, a convolution equation arises; moreover, the convolution kernel must be causal, i.e., zero-valued for negative times. In other words, such a cause-effect relationship satisfies Boltzmann's superposition principle [14].

In geophysics, energy sources are often of an impulsive nature (e. g., explosives and airguns in seismic prospecting); therefore, singular distributions like Dirac's delta come into play in addition to classical smooth functions [19].

One aim of the present paper is to support the view that "where there is a convolution, there is an opportunity for fractional calculus". In Section 1, a short heuristic summary of fractional calculus is presented, with emphasis on causal distributions. Section 2 contains a brief review of some topics in geophysics and environmental sciences where fractional calculus has found either explicit (time-domain) or implicit (frequency-domain) applications. Finally, Section 3 points out some problems in the geosciences where fractional calculus should possibly play an important role, although few related papers (if any) refer to it, since the main relationship used in these studies is a convolution equation.

1 A glance on fractional calculus

1.1 Gelfand-Shilov distributions

The one-parameter family of Gelfand-Shilov distributions G_{α} , with $\alpha \in \mathbb{R}$, is defined by:

$$G_{0} = \delta$$

$$G_{\nu}[t] = \frac{1}{\Gamma[\nu]} t^{\nu-1} \theta[t] \qquad \nu > 0$$

$$G_{-n} = \partial^{n} \delta \qquad n = 1, 2, \dots$$

$$G_{-\nu} = \partial^{n} G_{\epsilon} \qquad \nu = n - \epsilon, \ 0 < \epsilon < 1, \ n = 1, 2, \dots$$

where δ is Dirac's delta distribution, θ is Heaviside unit-step function, and Γ is Euler's Gamma function. Its main property is that it constitutes a one-parameter group with respect to convolution:

$$G_{\alpha} * G_{\beta} = G_{\alpha+\beta} \qquad \qquad \alpha, \, \beta \in \mathbb{R} \,.$$

1.2 Iterated and fractional integrals

The iterated integral

$$\left(\int^{n} f\right)[t] := \int_{-\infty}^{t} \mathrm{d}t_{1} \int_{-\infty}^{t_{1}} \mathrm{d}t_{2} \dots \int_{-\infty}^{t_{n-1}} \mathrm{d}t_{n} f[t_{n}]$$

satisfies the Cauchy-Dirichlet formula

$$\int^n = G_n *$$

This motivativates the following definition of, and notation for, the Gelfand-Shilov fractional integral:

$$\int_{\mathrm{GS}}^{\nu} := G_{\nu} * \qquad \nu \in \mathbb{R}$$

On the other hand, the classical definition of the fractional integral may be written as [16]

$$\left(\int_{\mathrm{cl}}^{\nu} f \right) [t] := \frac{1}{\Gamma[\nu]} \int_{0}^{t} \mathrm{d}\tau \, (t-\tau)^{\nu-1} \, f[\tau]$$

and the relationship between the two definitions is given by

$$\int_{\rm GS}^{\nu} (f\,\theta) = \theta \int_{\rm cl}^{\nu} f \,,$$

where f is an ordinary function.

1.3 Fractional derivatives

Several definitions of fractional derivatives are possible, such as [16]:

$$\begin{array}{lll} \partial^{\nu}_{\mathrm{GS}} & := & G_{-\nu} * & \nu \in \mathbb{R} & (\mathsf{Gelfand-Shilov}) \\ \partial^{\nu}_{\mathrm{LR}} & := & \partial^{n} \int_{\mathrm{cl}}^{n-\nu} & 0 \leq n-1 < \nu < n & (\mathsf{Liouville-Riemann}) \\ \partial^{\nu}_{\mathrm{CM}} & := & \int_{\mathrm{cl}}^{n-\nu} \partial^{n} & 0 \leq n-1 < \nu < n & (\mathsf{Caputo-Mainardi}) \end{array}$$

Taking into account the group property of Gelfand-Shilov distributions, we see that:

$$\partial^{\alpha}_{\mathrm{GS}} \circ \partial^{\beta}_{\mathrm{GS}} = \partial^{\alpha+\beta}_{\mathrm{GS}} \qquad \partial^{\nu}_{\mathrm{GS}} \circ \int^{\nu}_{\mathrm{GS}} = \int^{\nu}_{\mathrm{GS}} \circ \partial^{\nu}_{\mathrm{GS}} = \mathrm{identity} \;.$$

Hence, for causal distributions, the (fractional) derivative is really the "inverse operation" of the (fractional) integral, and we have $\partial_{GS}^{\nu} = f_{GS}^{-\nu}$.

In the following we shall mainly rely on Gelfand-Shilov fractional derivatives, and simply write ∂^{α} for ∂^{α}_{GS} .

2 Classical geophysical applications

2.1 Ground-penetrating radar (electromagnetism)

The mathematical modelling of electromagnetic waves in complex materials is a research field of high and growing interest in connection with smart materials [11]. In geophysics, this topic is mainly studied in connection with ground-penetrating radar (GPR), which is a relatively easy-to-use and unexpensive prospecting tool with high resolution (see Figs. 1 and 2). Its penetration depth may reach a few thousands of meters in the Anctarctic ice, but also be limited to few centimeters in a soil saturated with brine. A typical order of magnitude for GPR penetration depth is 10 meters, which makes GPR mainly used in geotechnical and environmental studies. This clarifies the importance of accurately modelling the electromagnetic energy loss in the soil and the subsoil. Essentially, this is achieved through a suitable constitutive law relating the electrical displacement field \underline{D} to the electrical intensity field \underline{E} . One such



Figure 1: Data acquisition with ground-penetrating radar.

model goes back to K. S. Cole and R. H. Cole in the forties, and it is still the object of fruitful analysis [2]. Its 3-D anisotropic formulation in time domain may be written as

$$(\underline{\underline{\alpha}}_{\underline{0}} + \underline{\underline{\alpha}}_{\underline{1}} \partial_t^{\alpha}) \underline{\underline{D}} = (\underline{\underline{\beta}}_{\underline{=0}} + \underline{\underline{\beta}}_{\underline{=1}} \partial_t^{\beta}) \underline{\underline{E}} , \qquad (1)$$

where $\alpha = \beta$ for thermodynamic reasons, and twice underlined quantities are 3×3 matrices. This equation may be solved for the electric displacement <u>D</u>:

$$\underline{D} = \partial_t \underline{\varepsilon} * \underline{E} \; ;$$

where

$$\partial_{t} \underline{\underline{\varepsilon}} = (\theta \exp_{\nu, -\underline{\alpha}_{1}^{-1} \underline{\alpha}_{0}}) * (G_{0} \underline{\underline{\beta}}_{\underline{=}0} + G_{-\alpha} \underline{\underline{\beta}}_{1})$$

$$\exp_{\nu, a}[t] = t^{\nu - 1} \operatorname{E}_{\nu, \nu}[a t^{\nu}]$$

$$\operatorname{E}_{\alpha, \beta}[z] = \sum_{k=0}^{\infty} \frac{z^{k}}{\Gamma[\alpha k + \beta]}$$
(Mittag-Leffler function)
(2)

We see from equation (1) that fractional calculus has a crucial role to play in GPR modelling.



Figure 2: Example of radargram showing reflection hyperbolas due to buried pipes.

2.2 Seismic prospecting (viscoelasticity)

Seismic prospecting consists in probing the earth with acoustic signals generated by impulsive sources (airguns in the sea, explosives or hammers for land surveys) or by oscillating forcing tools as with the Vibroseis system for land exploration (see Fig. 3). Penetration depth for exploration purposes may reach several kilometers, which (together with good resolution properties) makes seismics the most important technology for oil and gas exploration. The seismograms registered by geophones or by hydrophones are then processed to give a *seismic section*, which yields a more or less accurate image of the subsoil (see Fig. 4). Direct seismic modelling may greatly improve seismic data processing and interpretation by producing synthetic data, compatible with the assumed geologic structure, to be compared with measured data. Moreover, inverse seismic modelling leads to parameter estimation, which is often even more important than imaging. In both direct and inverse modelling one needs to take into account energy dissipation, especially when Amplitude Variation with Offset (AVO) is concerned. To this purpose, a viscoelastic constitutive assumption is to be preferred to a purely elastic one.

The general theory of viscoelaticity, based on the assumption that the stress-strain relationship satisfies Boltzmann's superposition principle, is nowadays a mature mathematical field [10]. But, for the purposes of numerical modelling, one has still to choose a specific convolution kernel, which is not obvious [6]. Experimental studies indicate that the quality factor Q of harmonic modes should be (almost) constant over a wide range of frequencies [15]. Such a behaviour may be obtained from the constitutive law either through a combination of exponential functions [15], or by using fractional calculus ([4], [5]). The advantage of the latter approach stays in the lesser number of parameters involved in the relaxation function, which makes a big difference especially in view of inverse modelling.

2.3 Reservoir engineering (poroelasticity)

One often thinks to porous media as continuos materials with isolated cavities, and this is indeed correct in some cases (see Fig. 5, left); for example, pumice contains isolated pores that resulted from gas bubbles in the molten volcanic rock from which it originated. But voids in sedimentary rocks of interest to the oil industry are interconnected (see Fig. 5, right), so that hydrocarbons can migrate through a



Figure 3: Schematic view of data acquisition in seismic prospecting.



Figure 4: Example of interpreted seismic section resulting from seismic data processing.





Figure 5: Cavities in porous media may be either isolated (left) or interconnected (right). The latter situation is by far more important in geophysics.

carrier bed from kerogen-rich source rocks (shales or limestones) to a sandstone reservoir rock. Since reservoir engineers are highly concerned with pore pressure prediction, pertinent seismic models must be poro(visco)elastic and, as such, include pore pressure p together with its "dual" kinematic quantity ζ , which is related to the fluid dilatation and has been called *increment of fluid content* [6].

Fractional calculus has been applied to this kind of problems, although often inadvertently, at least since the early sixties. For example, Marcel Biot (who has been recognized as the principal creator of poroelasticity) relates the strain-like quantity γ_z to the stress-like quantity τ_{xy} in the frequency domain through the equation (cf. [3, eq. (6.7)])

$$\gamma_z = \frac{1}{a \, p^s} \, \tau_{xy} \, , \qquad \qquad 0 < s < 1 \, ,$$

where a is a constant and $p = i \omega$, whose time-domain counterpart is

$$\tau_{xy} = a \,\partial_t^s \gamma_z$$

More recently, Hanyga has extended and deepened this approach by using Liouville-Riemann fractional derivatives and their discretized counterpart, the Grünwald-Letnikov derivatives, which are most suited for finite-difference numerical modelling [13].

3 Prospective geophysical applications

3.1 Meteorology and oceanography (geophysical fluid dynamics)

It is well known that the constitutive equation for a linear isotropic *solid* relates the stress T to the pressure p = -tr T and the strain E through [12]

$$\mathbf{T} = -p\,\mathbf{I} + 2\mu\,\left(\mathbf{E} - \frac{1}{3}\,(\mathrm{tr}\,\mathbf{E})\,\mathbf{I}\right)\,,\tag{3}$$

where μ is the shear modulus.

Likewise, the constitutive equation for a Newtonian *fluid* may be written as

$$\mathbf{T} = -p\,\mathbf{I} + 2\eta\,\partial_t\,\left(\mathbf{E} - \frac{1}{3}\,(\mathrm{tr}\,\mathbf{E})\,\mathbf{I}\right) \,, \tag{4}$$

where η is a constant viscosity ([1], [8], [17]). Since viscous dissipation is best taken into account by memory effects that may be described through a convolution integral, the last equation should be profitably generalized into the constitutive law for an elastic fluid:

$$\mathbf{T} = -p\,\mathbf{I} + 2\eta_{\text{fun}} * \partial_t^2 \left(\mathbf{E} - \frac{1}{3} \left(\operatorname{tr} \mathbf{E} \right) \mathbf{I} \right) , \qquad (5)$$

where viscosity is now represented by the time-dependent function η_{fun} . As a simple special case, we may take $\eta_{\text{fun}} = \eta t_0^{\alpha-1} G_{2-\alpha}$ and hence (5) becomes

$$\mathbf{T} = -p\,\mathbf{I} + 2\eta\,t_0^{\alpha-1}\,\partial_t^\alpha\,\left(\mathbf{E} - \frac{1}{3}\,(\mathrm{tr}\,\mathbf{E})\,\mathbf{I}\right)\,,\tag{6}$$

which gives back (3) and (4) as special cases. Inserting (6) into the momentum balance equation

$$\operatorname{div} \mathbf{T} + \mathbf{f} = \rho \, \frac{\mathrm{D} \mathbf{v}}{\mathrm{D} t}$$

and using the incompressibility condition div $\mathbf{v} = 0$ yields the *fractional Navier-Stokes equations*

$$\rho \frac{\mathrm{D}\mathbf{v}}{\mathrm{D}t} = \mathbf{f} - \nabla p + \eta t_0^{\epsilon} \partial_t^{\epsilon} \Delta \mathbf{v}$$

where $\epsilon = \alpha - 1$. It is tempting to speculate that this equation may describe turbulence more accurately than classical Navier-Stokes equations, and constitute the starting point for developing a more reliable formulation of geophysical fluid dynamics.

3.2 Hydrology (unit hydrograph)

A typical problem in surface hydrology is that of evaluating the rainfall-unoff relationship (see Fig. 6). One of the most useful approches is through the *instantaneous unit hydrograph* IUH, which gives the runoff q when convolved with the rainfall p [18]:

$$\begin{array}{rll} \mathsf{runoff} & \mathsf{rainfall} \\ \downarrow & \downarrow \\ q &= \mathsf{IUH} & * p \end{array}$$

A "classical" example of IUH is

$$\mathsf{IUH} = \frac{k_1 \, k_2}{k_2 - k_1} \left(\exp[k_2 \, t] - \exp[k_1 \, t] \right) \,. \tag{7}$$

Higher flexibility should come from a "fractional" IUH like

$$\mathsf{IUH} = \frac{k_1 k_2}{k_2 - k_1} \left(\exp_{\nu, k_2}[t] - \exp_{\nu, k_1}[t] \right) \,. \tag{8}$$

Expression (7) is the solution of a linear ordinary differential equation with constant coefficients; likewise, expression (8) is related to a fractional differential equation. Two requirements restrict the choice of the IUH ansatz: the IUH must always be positive, and its integral with respect to time must give 1. The parameters must be suitably chosen to fulfill the first requirement, while the second is assured by the normalization constant.



Figure 6: A schematic representation of the main components of the hydrologic cycle.

3.3 Ecology and climatology (greenhouse gases vs. deforestation)

A presently much debated question in climate dynamics pertains the role of greenhouse gases in the global atmospheric warming and, specifically, the possibility that deforestation may act as a triggering factor of an irreversible climate change (see Fig. 7). Some pertinent contributions have been recently given by Eshleman [9], who proposes a simple linear response model to describe the flux of nitrate from a forested watershed subjected to a large-scale disturbance of vegetation:

$$N[t] = B + \int_0^t \mathrm{d}\tau \, U[t-\tau] \, D[\tau] \; ,$$

where N is the nitrogen export from watershed, U is the unit nitrogen-export response function, D is the proportion of forested watershed disturbed, and B is the baseline nitrogen export from watershed in the absence of disturbance. In practice, a discretized version of this equation is used in [9], where the discrete unit response is estimated for a specific watershed by a method very similar to that implemented in [7]. Moreover, Eshleman has proposed to extend this approach to the study of the carbon budget using data from satellite remote sensing (http://al.umces.edu/ fiscus/research/nasa-prop-final.doc).

It is likely that these experimental studies would greatly benefit from an analytical model using, for the unit nitrogen-export response function, an ansatz similar to the Cole-Cole function (2). Such an approach would yield further insight into the polluting effects of deforestation, elucidating the main qualitative features of the phenomenon and allowing for an appreciation of parameter sensitivity; general properties valid for all watersheds might be obtained.

Conclusions

Convolution has an important role in geophysical modelling, in that any cause-effect relationship can be described by a convolution, if the system is time invariant and linear.



Figure 7: Fire in the Amazonian equatorial rainforest.

Specifically, constitutive laws expressed by linear fractional differential equations are able to account for phenomena intermediate between diffusion and propagation. Moreover, the fractional-calculus approach requires fewer phenomenological parameters than its traditional competitors, which is a substantial advantage especially in inverse problems.

Since fractional derivatives and integrals are linear operators, it is not clear whether fractional calculus will play a crucial role in the modelling of nonlinear systems as well. But there are good reasons to favor an affirmative answer: (i) after all, integer-order derivatives and integrals are linear operators and yet are ubiquitous in nonlinear analysis; (ii) the most interesting systems are both nonlinear and dissipative, and fractional calculus is most suitable to describe dissipation through memory effects.

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