Grünwald-Letnikov operators for fractional relaxation in Havriliak-Negami models ☆

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Abstract

Several classes of differential and integral operators of non integer order have been proposed in the past to model systems exhibiting anomalous and hereditary properties. A wide range of complex and heterogeneous systems are described in terms of laws of Havriliak-Negami type involving a special fractional relaxation whose behaviour in the time-domain can not be represented by any of the existing operators. In this work we introduce new integral and differential operators for the description of Havriliak-Negami models in the time-domain. In particular we propose a formulation of Grünwald-Letnikov type which turns out to be effective not only to provide a theoretical characterization of the operators associated to Havriliak-Negami systems but also for computational purposes. We study some properties of the new operators and, by means of some numerical experiments, we present their use in practical computation and we show the superiority with respect to the few other approaches previously proposed in literature.

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1. Introduction

Integral and differential operators of non integer order attract ever growing interest motivated by the large extent of applications in which they are fruitfully employed; models based on fractional integrals or fractional derivatives are indeed effective to describe complex phenomena in a variety of fields ranging from biochemistry to control theory, engineering, mechanics, physics and so on.

Alongside Riemann-Liouville operators, which are the basis of the fractional calculus, new specific fractional operators (e.g., of Caputo, Erdélyi-Kober, Marchaud, Riesz and Weyl type [1, 2, 3, 4]) have been introduced with the aim of describing, in the most appropriate way, systems and models for which traditional operators are not sufficiently satisfactory.

New operators are usually proposed on the basis of theoretical considerations but in same cases specific operators are introduced from experimental observations after measuring, in the frequency domain, the response of a system to some external excitations and matching the experimental data to a theoretical model.

For several years only very simple models have been considered and the Debye model [5] has been the most popular because of the possibility of describing the corresponding action in the time domain by means of ordinary differential equations.

Experimental observations on the asymmetry and broadness of the dielectric dispersion in some polymers [6] led, in 1967, to the formulation of the Havriliak-Negami (HN) model which is obtained by inserting two independent real powers in the classical Debye model.

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Empirical laws of HN type, which are recognized as manifestation of simultaneous nonlocality and nonlinearity [7, 8] in the response of disordered materials and heterogeneous systems, are nowadays applied in physics [9, 10], in mechanical engineering [11], in the analysis of electric circuits [12] and, in particular, to describe dielectrics properties of dispersive and disordered media [13, 14, 15].

A major issue with the HN model, which has so far mainly studied in the frequency domain, is the absence of a formal representation in the time domain. Some noticeable efforts have been made to formulate new operators as combination of classic fractional derivatives [16, 17, 18] or to introduce specific convolution operators [19, 20, 21] (see also [22] for applications in fractional Poisson processes). Anyway, as a consequence of the non-linearity in the frequency domain, the corresponding integral and differential operators in the time domain are still not completely known in an explicit way [23].

The aim of this work is to contribute to fill this gap by introducing and investigating new integral and differential operators for the description of HN models in the time domain. In particular, we propose an approach based on fractional differences [24] which can be considered as the natural generalization of Grünwald-Letnikov (GL) operators, a class of operators widely used in fractional calculus.

The importance of GL operators is not only for historical and theoretical reasons but it is also related to the possibility of direct application in numerical computation since, in a straightforward way, they also provide a discretization scheme. The generalization to HN models is done on the basis of the work of Lubich [25, 26] on quadrature rules for convolution integrals.

This paper is organized as follows. In Section 2 we review some basic definitions and properties and in Section 3, after introducing the HN model, we discuss the problem of its formulation in the time-domain in terms of fractional operators. We hence derive, in Section 4, integrals and derivatives of GL type for operators of HN type and we study some of their main properties. Numerical experiments are presented in Section 5 and some final remarks conclude the paper.

2. Integrals and derivatives of fractional order

Several types of integral and differential operators of non-integer order have been proposed and investigated in the past. From an historical point of view, the origins of the fractional calculus are strictly related to the *Riemann-Liouville* (RL) integral of real order $\alpha > 0$

$$J_{t_0}^{\alpha} y(t) = \frac{1}{\Gamma(\alpha)} \int_{t_0}^{t} (t-u)^{\alpha-1} y(u) du, \quad t \in [t_0, T], \tag{1}$$

where $\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt$ is the Euler gamma function and $y \in L^1([t_0, T])$. We refer to the reviews [27, 28] for historical notes on fractional calculus and to [29, 30, 31, 32, 33] for introductory material.

The left-inverse of the fractional integral (1) is the RL fractional derivative

$$D_{t_0}^{\alpha} y(t) \equiv D^m J_{t_0}^{m-\alpha} y(t) = \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dt^m} \int_{t_0}^{t} (t-u)^{m-\alpha-1} y(u) du,$$

where $m = \lceil \alpha \rceil$ is the smallest integer such that $m > \alpha$ and D^m and d^m/dt^m denote standard derivatives of integer order; the absolute continuity of y is required for the existence of $D_{t_0}^{\alpha} y(t)$ [29].

Some other fractional operators have been introduced for practical reasons or for describing specific phenomena in a more detailed way. For instance, the *Caputo* derivative, which allows to couple fractional differential equations with standard initial conditions of Cauchy type is defined, for m-times absolutely continuous functions, as

$$^{C}D_{t_0}^{\alpha} y(t) \equiv J_{t_0}^{m-\alpha} D^m y(t) = \frac{1}{\Gamma(m-\alpha)} \int_{t_0}^{t} (t-u)^{m-\alpha-1} y^{(m)}(u) du$$

and it is strictly related to the RL derivative by means of the relationship

$$ {}^{C}D^{\alpha}_{t_0} y(t) = D^{\alpha}_{t_0}\left(y(t) - \sum_{k=0}^{m-1} \frac{(t-t_0)^k}{k!} y^{(k)}(t_0) \right). \tag{2} $$

Alternative definitions of integral and derivatives of fractional order are provided by means of GL operators which are based on the classic representation of the integer order derivative D^m as the limit of finite differences

$$ D^m y(t) = \lim_{h\to 0} \frac{1}{h^m} \sum_{k=0}^{m} (-1)^k \binom{m}{k} y(t-kh), \quad t \in (t_0, T], \tag{3} $$

where, as usual, the binomial coefficients are

$$ \binom{m}{k} = \frac{m(m-1)\cdots(m-k+1)}{k!} = \frac{m!}{k!(m-k)!}. \tag{4} $$

To extend the derivative (3) to any fractional order α, the function $y(t)$ must be defined on the whole half-line $(-\infty, T]$; to deal with functions defined on a finite interval $[t_0, T]$ it is usually assumed that $y(t)$ vanishes for $t < t_0$ [30, 24]. Moreover, the generalization of binomial coefficients to any real α, with $\alpha \notin \{0, -1, -2, -3, \dots\}$, is obtained by replacing in (4) the factorial with the gamma function. After introducing, for shortness, the coefficients

$$ \omega_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}, \quad \binom{\alpha}{k} = \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)}, \tag{5} $$

which can be evaluated in a recursive way according to

$$ \omega_0^{(\alpha)} = 1, \quad \omega_k^{(\alpha)} = \left(1 - \frac{\alpha+1}{k}\right) \omega_{k-1}^{(\alpha)}, \tag{6} $$

we are able to present GL derivatives and GL integrals in a rather compact notation.

Definition 1. Let $\alpha > 0$ and $y \in \mathcal{C}^m\big([t_0, T]\big)$, $m = \lceil \alpha \rceil$. For any $t \in (t_0, T]$ the GL derivative of fractional order α is

$$ \widetilde{D}^{\alpha}_{t_0} y(t) = \lim_{h\to 0} \frac{1}{h^\alpha} \sum_{k=0}^{\infty} \omega_k^{(\alpha)} y(t-kh). \tag{7} $$

Definition 2. Let $\alpha > 0$ and $y \in \mathcal{C}^0\big([t_0, T]\big)$. For any $t \in (t_0, T]$ the GL integral of fractional order α is

$$ \widetilde{J}^{\alpha}_{t_0} y(t) = \lim_{h\to 0} h^\alpha \sum_{k=0}^{\infty} \omega_k^{(-\alpha)} y(t-kh). \tag{8} $$

Derivatives and integrals of GL type are useful also for practical computation. By fixing h and truncating the series in (7) and/or (8) after the first $K = \lceil (t-t_0)/h \rceil$ terms, it is indeed possible to numerically approximate the corresponding RL operators with an error proportional to h [34, 35]. Thanks to the equivalence (2), a similar approximation also applies to the Caputo derivative.

To review the main properties of GL operators we refer, for instance, to [29, 36, 24]. Moreover, the following properties (which will be used later on in this paper) hold.

Proposition 1. *Let* $0 < \alpha < 1$. *Then*

1. $\omega_0^{(\alpha)} = 1$ *and* $\omega_k^{(\alpha)} \le 0$ *for any* $k \ge 1$;
2. $\big|\omega_{k+1}^{(\alpha)}\big| < \big|\omega_k^{(\alpha)}\big| < \omega_0^{(\alpha)}$, $k \ge 1$;

3. $\sum_{k=0}^{\infty} \omega_k^{(\alpha)} = 0$.

Proposition 2. *Let $-1 < \alpha < 0$. Then*

1. $\omega_0^{(\alpha)} = 1$ *and* $\omega_k^{(\alpha)} \geq 0$ *for any* $k \geq 1$*;*
2. $\omega_{k+1}^{(\alpha)} < \omega_k^{(\alpha)} < \omega_0^{(\alpha)}$, $k \geq 1$*;*
3. $\sum_{k=0}^{\infty} \omega_k^{(\alpha)} = +\infty$.

3. The Havriliak-Negami model and operational representation

3.1. The Havriliak-Negami model

Relaxation processes are often investigated on the basis of experimental observations in the frequency domain. The response $Y(s)$ of a system forced by some external excitation $F(s)$ is observed at different frequencies and the parameters of a constitutive law $H(s) \approx Y(s)/F(s)$ are found by matching the experimental data to some theoretical model described by the function $H(s)$.

For several years the model involving the simple rational function $H(s) = 1/(s+\lambda)$, proposed in 1912 by the physicist Peter Debye [5], has been considered suitable to describe relaxation processes in a large variety of fields.

More accurate investigations, together with the improvement of the measurement precision, have shown that models based on pure "Debye relaxation" are often not completely satisfactory, especially in the presence of hereditary phenomena in which the memory of the excitation is not instantaneously lost [37]. It is nowadays well-accepted, for instance, that in amorphous polymers near glassy phase transition [38] and in biological tissues [39] the induced electric polarization differs in a substantial way from the Debye model which is not capable to take in account the nonlocality and nonlinearity of complex and disordered systems [7, 8].

More involved functions are therefore employed to better fit experimental data and take into account hereditary effects; in particular, in the Havriliak-Negami model [6]

$$H_{\alpha,\gamma}(s;\lambda) = \frac{1}{\left(s^\alpha + \lambda\right)^\gamma}, \tag{9}$$

the relaxation is stretched by inserting two non integer powers in the basic Debye function. The real constant λ is related to the relaxation time and therefore it is assumed $\lambda > 0$. The problem of identifying the admissible range for the parameters α and γ has been often discussed in literature. Although the restriction $0 < \alpha, \gamma \leq 1$ is usually assumed, in [40] the HN model has been extended to $0 < \alpha, \alpha\gamma \leq 1$ and the complete monotonicity of the corresponding relaxation function (an essential condition for the physical admissibility [41]) has been proved in [42, 43]. However, since in this paper we are interested in a presentation at a more general mathematical level, when possible we will just assume $\lambda \geq 0$ and $\alpha, \gamma > 0$.

Unlike Debye relaxation, whose formulation in the time-domain in terms of integral and differential operators is well-established, the description of Havriliak-Negami relaxation is more difficult and not completely investigated [23].

3.2. Integral operator for Havriliak-Negami relaxation

It is a well known result (see, for instance [43, 44]) that the Laplace transform pair for $H_{\alpha,\gamma}(s;\lambda)$ is

$$\frac{1}{\left(s^\alpha + \lambda\right)^\gamma} \div e^{\gamma}_{\alpha,\alpha\gamma}(t;-\lambda), \tag{10}$$

where

$$e^{\gamma}_{\alpha,\beta}(t;\lambda) = t^{\beta-1}E^{\gamma}_{\alpha,\beta}(t^{\alpha}\lambda)$$

is a generalization of the three parameter Mittag-Leffler (ML) function [44]

$$E^{\gamma}_{\alpha,\beta}(z) = \frac{1}{\Gamma(\gamma)}\sum_{k=0}^{\infty}\frac{\Gamma(\gamma+k)z^k}{k!\Gamma(\alpha k+\beta)} \tag{11}$$

which is often referred to as the Prabhakar function [21].

For $\alpha,\beta > 0$, $\gamma,\lambda \in \mathbb{R}$ and $f \in L^1([t_0,T])$ a multiparameter operator of convolution type with kernel of Prabhakar type

$$\mathbf{E}^{\gamma}_{\alpha,\beta,\lambda,t_0+}f(t) = \int_{t_0}^{t} e^{\gamma}_{\alpha,\beta}(t-\tau;\lambda)f(\tau)\,d\tau, \quad t \in (t_0,T], \tag{12}$$

has been introduced and investigated in [19, 20, 21]. It has been proved, for instance, that $\mathbf{E}^{\gamma}_{\alpha,\beta,\lambda,t_0+}$ is a bounded operator both in the space of Lebesgue measurable functions and in the space of continuous functions [20].

The multiparameter operator (12) is useful to study HN relaxations in the time-domain. By inversion of the Laplace transform, it is indeed immediate from (10) to verify the correspondence between the frequency domain input-output relationship

$$Y(s) = H_{\alpha,\gamma}(s;\lambda)F(s), \quad s \in \mathbb{C}$$

and its time domain representation

$$y(t) = \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,t_0+}f(t), \quad t > t_0.$$

This observation thus justifies the introduction of the following specific integral for describing HN relaxations in the time-domain.

Definition 3 (HN integral). Let $\alpha,\gamma > 0$, $\lambda \geq 0$ and $y \in L^1([t_0,T])$. For any $t \in [t_0,T]$ the HN integral of order (α,γ) is

$$J^{\alpha,\gamma}_{t_0,\lambda}y(t) \equiv \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,t_0+}y(t) = \int_{t_0}^{t} e^{\gamma}_{\alpha,\alpha\gamma}(t-\tau;-\lambda)y(\tau)\,d\tau. \tag{13}$$

The HN integral (13) generalizes in a straightforward way the RL integral; indeed, since for $\gamma = 1$ and $\lambda = 0$ it is $e^{1}_{\alpha,\beta}(t;0) = t^{\beta-1}/\Gamma(\beta)$, we can easily verify that $J^{\alpha,1}_{t_0,0} = J^{\alpha}_{t_0}$, with $J^{\alpha}_{t_0}$ the RL integral (1). The following properties of the HN integral $J^{\alpha,\gamma}_{t_0,\lambda}$ can be proved.

Proposition 3. *Let $\alpha,\gamma > 0$ and $\lambda \geq 0$. Then for any $t > t_0$ and $\mu > 0$*

1. $J^{\alpha,\gamma}_{t_0,\lambda}\frac{1}{\Gamma(\mu)}(t-t_0)^{\mu-1} = e^{\gamma}_{\alpha,\alpha\gamma+\mu}(t-t_0;-\lambda)$;
2. $J^{\alpha,\gamma}_{t_0,\lambda}1 = e^{\gamma}_{\alpha,\alpha\gamma+1}(t-t_0;-\lambda)$

Proof. For the proof of point 1. we refer to [21]; point 2. is a direct consequence of point 1. when $\mu = 1$. □

3.3. Derivative operator for Havriliak-Negami relaxation

The left inversion of $\mathbf{E}^{\gamma}_{\alpha,\beta,\lambda,t_0+}$ has been discussed in [19, 20] with the introduction of the derivative

$$\mathbf{D}^{\gamma}_{\alpha,\beta,\lambda,t_0+} = \frac{d^m}{dt^m}\mathbf{E}^{-\gamma}_{\alpha,m-\beta,\lambda,t_0+}, \quad m = \lceil\beta\rceil\,.$$

This inversion allows us to introduce a derivative corresponding to the HN integral (13). From now on, we will adopt the convention that $m = \lceil\alpha\gamma\rceil$.

Definition 4 (HN derivative). Let $\alpha, \gamma > 0$, $\lambda \geq 0$ and $y \in L^1([t_0, T])$. For any $t \in [t_0, T]$ the HN derivative of order (α, γ) is

$$D^{\alpha,\gamma}_{t_0,\lambda} y(t) \equiv \frac{d^m}{dt^m} \mathbf{E}^{-\gamma}_{\alpha,m-\alpha\gamma,-\lambda,t_0+} y(t) = \frac{d^m}{dt^m} \int_{t_0}^{t} e^{-\gamma}_{\alpha,m-\alpha\gamma}(t-\tau;-\lambda) y(\tau)\, d\tau. \tag{14}$$

Also in this case, it is straightforward to verify the correspondence between RL and HN derivatives when $\gamma = 1$ and $\lambda = 0$; indeed, it is $D^{\alpha,1}_{t_0,0} = D^{\alpha}_{t_0}$. We also observe the following property of the HN derivative $D^{\alpha,\gamma}_{t_0,\lambda}$.

Proposition 4. *Let $\alpha, \gamma > 0$, $\lambda \geq 0$ and $\mu > -1$. Then*

$$D^{\alpha,\gamma}_{t_0,\lambda} \frac{(t-t_0)^{\mu}}{\Gamma(\mu+1)} = e^{-\gamma}_{\alpha,\mu-\alpha\gamma+1}(t-t_0;-\lambda) - \varphi_{\mu}(t-t_0),$$

where

$$\varphi_{\mu}(t) = \frac{1}{\Gamma(-\gamma)} \sum_{k \in \mathcal{K}_{\mu}} \frac{\Gamma(-\gamma+k)(-\lambda)^k t^{-\alpha\gamma+\alpha k+\mu}}{\Gamma(-\alpha\gamma+\alpha k+\mu+1)}$$

and $\mathcal{K}_{\mu} = \left\{ k \in \mathbb{N} \,:\, k > \gamma - \frac{\mu}{\alpha} \wedge m - \alpha\gamma + \alpha k + \mu \in \mathbb{N} \right\}$.

Proof. From (14) and by using the expansion (11) we have

$$\begin{aligned} D^{\alpha,\gamma}_{t_0,\lambda}(t-t_0)^{\mu} &= \frac{d^m}{dt^m} \sum_{k=0}^{\infty} \frac{\Gamma(-\gamma+k)(-\lambda)^k}{\Gamma(-\gamma)\Gamma(\alpha k+m-\alpha\gamma)} \int_{t_0}^{t} (t-\tau)^{m-\alpha\gamma+\alpha k-1} (\tau-t_0)^{\mu}\, d\tau \\ &= \sum_{k=0}^{\infty} \frac{\Gamma(\mu+1)\Gamma(-\gamma+k)(-\lambda)^k}{\Gamma(-\gamma)\Gamma(\alpha k+m-\alpha\gamma+\mu+1)} \frac{d^m}{dt^m} (t-t_0)^{m-\alpha\gamma+\alpha k+\mu}. \end{aligned}$$

When $k \notin \mathcal{K}_{\mu}$ it is $m - \alpha\gamma + \alpha k + \mu \notin \mathbb{N}$ or $m < m - \alpha\gamma + \alpha k + \mu$ and hence

$$\frac{d^m}{dt^m} (t-t_0)^{m-\alpha\gamma+\alpha k+\mu} = \frac{\Gamma(m-\alpha\gamma+\alpha k+\mu+1)}{\Gamma(-\alpha\gamma+\alpha k+\mu+1)} (t-t_0)^{-\alpha\gamma+\alpha k+\mu};$$

when $k \in \mathcal{K}_{\mu}$ the above derivative is the integer order derivative of a polynomial and, since the order of the derivative is greater than the degree of the polynomial, the corresponding term vanishes and can be eliminated from the summation. The proof then easily follows. □

By following the same approach proposed in [19], a regularization of the HN derivative (14) in the sense of the Caputo derivative can be introduced by means of

$${}^{C}D^{\alpha,\gamma}_{t_0,\lambda} y(t) \equiv \mathbf{E}^{-\gamma}_{\alpha,m-\alpha\gamma,-\lambda,t_0+} \frac{d^m}{dt^m} y(t) = \int_{t_0}^{t} e^{-\gamma}_{\alpha,m-\alpha\gamma}(t-\tau;-\lambda) y^{(m)}(\tau)\, d\tau$$

and it is possible to prove [19] the relationship with the standard HN derivative (14)

$${}^{C}D^{\alpha,\gamma}_{t_0,\lambda} y(t) = D^{\alpha,\gamma}_{t_0,\lambda} \left(y(t) - \sum_{k=0}^{m-1} \frac{(t-t_0)^k}{k!} y^{(k)}(t_0) \right). \tag{15}$$

As in the case of RL fractional derivatives, the HN derivative of a constant is not necessarily zero. We are indeed able to provide the following results whose proofs are immediate consequences of Proposition 4 and equation (15).

Corollary 5. *Let $\alpha > 0$, $0 < \gamma < 1/\alpha$ and $\lambda \geq 0$. Then*

1. $D^{\alpha,\gamma}_{t_0,\lambda} 1 = e^{-\gamma}_{\alpha,1-\alpha\gamma}(t-t_0;-\lambda)$ *;*

2. ${}^{C}D^{\alpha,\gamma}_{t_0,\lambda} 1 = 0$.

Very often in literature the derivative of HN type is denoted by means of the symbol $\bigl(D^{\alpha}_{t_0} + \lambda\bigr)^{\gamma}$ which do not correspond to any well established definition and it is usually indicated as the fractional pseudo-derivative of HN type. In [16] Nigmatullin and Ryabov expressed $\bigl(D^{\alpha}_{0} + \lambda\bigr)^{\gamma}$ as the combination of exponential and RL derivative operators

$$\bigl(D^{\alpha}_{0} + \lambda\bigr)^{\gamma} = \exp\left(-\frac{\lambda t}{\alpha} D^{1-\alpha}_{0}\right) D^{\alpha\gamma}_{0} \exp\left(\frac{\lambda t}{\alpha} D^{1-\alpha}_{0}\right),$$

thus providing an useful tool for studying the HN relaxation under a theoretical point of view. Other authors [17, 45] proposed to expand $\bigl(D^{\alpha}_{t_0} + \lambda\bigr)^{\gamma}$ as the infinite binomial series of fractional derivatives

$$\bigl(D^{\alpha}_{t_0} + \lambda\bigr)^{\gamma} = \sum_{k=0}^{\infty} \binom{\gamma}{k} \lambda^k D^{\alpha(\gamma-k)}_{t_0}, \tag{16}$$

and the main interest for this approach is in the possibility of truncating the series and using (16) for numerical simulations [13]; the problem of establishing the number of terms in the truncated series which are necessary to obtain a given accuracy on a interval $[t_0, T]$ is however not completely solved.

It is immediate to show the equivalence between (16) and the HN derivative of Definition 4. Indeed, starting from (14) and by using (11), we can see that

$$\begin{aligned} D^{\alpha,\gamma}_{t_0,\lambda} y(t) &= \frac{1}{\Gamma(-\gamma)} \sum_{k=0}^{\infty} \frac{\Gamma(-\gamma+k)(-\lambda)^k}{\Gamma(k+1)} \frac{d^m}{dt^m} \int_{t_0}^{t} \frac{(t-\tau)^{m-\alpha\gamma+\alpha k}}{\Gamma(\alpha k + m - \alpha\gamma)} y(\tau)\, d\tau \\ &= \sum_{k=0}^{\infty} \binom{\gamma}{k} \lambda^k D^m J^{m-\alpha(\gamma-k)}_{t_0} y(t) = \sum_{k=0}^{\infty} \binom{\gamma}{k} \lambda^k D^{\alpha(\gamma-k)}_{t_0}. \end{aligned}$$

4. GL operators for HN relaxation

Definitions 3 and 4 for integrals and derivatives of HN type ground on convolution integrals whose kernel is the three parameter ML function (11).

As studied in [46, 47], the evaluation of this function is not a simple task and the kernel in (13) and (14) can be treated just in an approximated way.

It is, therefore, preferable to find alternative definitions for representing HN relaxation laws in the time-domain. In particular, we are interested in finding definitions of GL type, based on fractional differences, which could be profitably exploited both for theoretical and computational purposes.

To this aim we must first recall the theory developed by Lubich [25, 26] and concerning the discretization of convolution integrals.

4.1. Lubich's convolution quadratures

Let us consider a convolution integral

$$y(t) = \int_{t_0}^{t} g(t-\tau) f(\tau)\, d\tau \tag{17}$$

and a classic k-step linear multistep method (LMM)

$$\sum_{j=0}^{k} \alpha_j y_{n+j-k} = h \sum_{j=0}^{k} \beta_j f(t_{n+j-k}, y_{n+j-k}),$$

whose generating function is

$$\delta(\xi) = \frac{\alpha_0 \xi^k + \cdots + \alpha_{k-1}\xi + \alpha_k}{\beta_0 \xi^k + \cdots + \beta_{k-1}\xi + \beta_k}.$$

In [25, 26] it has been shown that it is possible to generalize a LMM in order to derive a quadrature rule

$$y_n = \sum_{k=0}^{n} G_k f(t_n - kh) \tag{18}$$

for the discretization of the convolution integral (17). The main feature of this approach is that the weights G_k are derived by combining the Laplace transform $G(s)$ of the kernel $g(t)$ in (17) and the generating function $\delta(\xi)$ of the LMM. The following assumptions are however necessary:

H1 $G(s)$ is analytic and bounded by $|G(s)| \le M|s|^{-\mu}$, for some real $\mu > 0$ and $M < \infty$, in a sector $\Sigma_{\varphi,c} = \left\{ s \in \mathbb{C} \,:\, |\arg(s-c)| < \pi - \varphi \right\}$, where $\varphi < \frac{\pi}{2}$ and $c \in \mathbb{R}$;

H2 the LMM is consistent of order p, $A(\theta)$-stable (i.e., its stability domain $S = \mathbb{C} \backslash \{\delta(\xi)\,;\, |\xi| < 1\}$ contains the wedge $\{z \in \mathbb{C} \,:\, |\arg(-z)| < \theta\}$) for $\theta > \varphi$, and the generating function $\delta(\xi)$ is analytic and without zeros in a neighbourhood of $|\xi| \le 1$ (except for a zero at $\xi = 1$).

Given on $[t_0, t]$ an equispaced grid $t_n = t_0 + nh$ with step-size $h > 0$, the convolution integral (17) can be approximated by means of the convolution quadrature (18) with weights G_n given by the coefficients in the power series of

$$G\left(\frac{\delta(\xi)}{h}\right) = \sum_{k=0}^{\infty} G_k \xi^k \tag{19}$$

(we refer again to [25, 26] for major details).

Under suitable conditions on the smoothness of $f(t)$, it is possible to prove that convolution quadratures of this kind preserve the same order of convergence of the underlying LMM. In particular for first order methods, which (as we will see) are of interest in this work, we can provide the following result which is an immediate consequence of Theorem 3.1 in [25].

Theorem 6. *Let $f \in \mathcal{C}^1([0,T])$ and assume that H1 and H2 hold. If the underlying LMM method is convergent of the first order, then*

$$\left| y(t_n) - y_n \right| \le C t_n^{\mu-1} h \big(|f(0)| + t_n \max_{0 \le t \le t_n} |f'(t)| \big)$$

for a constant C independent of h. Consequently, it is

$$\lim_{h \to 0} \sum_{k=0}^{\infty} G_k f(t - kh) = \int_{t_0}^{t} g(t-\tau) f(\tau)\, d\tau. \tag{20}$$

A special case is the backward Euler method, one of the most simple first order LMMs satisfying the assumption H2; its generating function is $\delta(\xi) = 1 - \xi$. When applied to discretize RL integrals (1), i.e. when $G(s) = \mathcal{L}\big(t^{\alpha-1}/\Gamma(\alpha); s\big) = s^{-\alpha}$, the weights in the corresponding convolution quadrature (18) are the coefficients in the power series of $G((1-\xi)/h) = h^{\alpha}(1-\xi)^{-\alpha}$ and it is immediate to verify that they are the coefficients of the GL integral (8). We refer to [34] for a detailed analysis concerning the use of these quadrature rules in fractional calculus.

GL operators (7) and (8) can be therefore considered as a special case of the theory devised in [25, 26] and, indeed, their first order convergence as $h \to 0$ is a direct consequence of Theorem 6.

4.2. Application to HN relaxation law

The approach described in the previous subsection not only allows to device the discretization scheme (18) but it also provides the alternative representation (20) for the integral (17).

It appears therefore highly promising for introducing an explicit representation, in the time-domain, of HN operators whose analytic knowledge is mainly restricted to the frequency domain (indeed, the Laplace transform (9) of the kernel of (13) and (14) is much more simple than the kernel $e^{\gamma}_{\alpha,\alpha\gamma}(t;-\lambda)$ itself).

For real and positive λ it is immediate to verify that the region of analyticity of the HN function (9) is the whole complex plane (except for a branch-cut on the negative real axis) when $0<\alpha<1$ and the sector $|\arg(s)|<\pi/\alpha$ otherwise. The assumption H1 is, thus, satisfied whenever $0<\alpha<2$.

To generalize the backward Euler method, whose generating function is $\delta(\xi)=1-\xi$, we consider the function

$$H_{\alpha,\gamma}\left(\frac{\delta(\xi)}{h};\lambda\right)=\frac{h^{\alpha\gamma}}{(1+h^{\alpha}\lambda)^{\gamma}}\hat{H}_{\alpha,\gamma}(\xi;h^{\alpha}\lambda),$$

with

$$\hat{H}_{\alpha,\gamma}(\xi;z)=\left(\frac{(1-\xi)^{\alpha}+z}{1+z}\right)^{-\gamma}.$$

The main issue to derive quadrature rules of type (18), and hence representations of type (20), is the evaluation of the coefficients $w_k^{(\gamma)}$ in the power series

$$\hat{H}_{\alpha,\gamma}(\xi;h^{\alpha}\lambda)=\sum_{k=0}^{\infty}w_k^{(\gamma)}\xi^k \tag{21}$$

(for notational convenience, in $w_k^{(\gamma)}$ we have highlighted only the dependence on γ; however, we point out that coefficients $w_k^{(\gamma)}$ depend also on α, λ and h).

In [26] after representing each coefficient of (19) in terms of Cauchy integrals, it was proposed their approximation by means of a quadrature rule on a circular contour around the origin. This method is highly efficient to numerically evaluate the coefficients in (21) in an accurate and fast way. Anyway, it does not provide any explicit representation of the weights $w_k^{(\gamma)}$ which is instead necessary in order to define and study the operators (25) and (26) from a theoretical point of view.

For this reason we use an alternative approach which is based on the Miller's formula. This is an old but effective tool for recursively evaluating the coefficients of a formal power series (FPS) raised to any power and it is based on the following result [48, Theorem 1.6c].

Theorem 7. *Let $\varphi(\xi)=1+\sum_{n=1}^{\infty}a_n\xi^n$ be a FPS. Then for any $\beta\in\mathbb{C}$,*

$$\big(\varphi(\xi)\big)^{\beta}=\sum_{n=0}^{\infty}v_n^{(\beta)}\xi^n,$$

where coefficients $v_n^{(\beta)}$ are recursively evaluated as

$$v_0^{(\beta)}=1,\quad v_n^{(\beta)}=\sum_{j=1}^{n}\left(\frac{(\beta+1)j}{n}-1\right)a_jv_{n-j}^{(\beta)}.$$

By means of Theorem 7 we are now able to provide an analytic representation of the coefficients in the expansion of $\hat{H}_{\alpha,\gamma}(\xi;h^{\alpha}\lambda)$.

Proposition 8. *Let $\alpha, \gamma > 0$, $\lambda \geq 0$. The coefficients $w_k^{(\gamma)}$ in the expansion (21) of $\hat{H}_{\alpha,\gamma}(\xi; h^\alpha \lambda)$ are*

$$w_0^{(\gamma)} = 1, \quad w_k^{(\gamma)} = \sum_{j=1}^{k} \left(\frac{(1-\gamma)j}{k} - 1 \right) \frac{\omega_j^{(\alpha)}}{1 + h^\alpha \lambda} w_{k-j}^{(\gamma)}, \tag{22}$$

where $\omega_j^{(\alpha)}$ are the generalized binomial coefficients (5).

Proof. After expanding $(1-\xi)^\alpha$ by means of the binomial series with coefficients $\omega_n^{(\alpha)}$, and since $\omega_0^{(\alpha)} = 1$, we can rewrite $\hat{H}_{\alpha,\gamma}(\xi; h^\alpha \lambda)$ as

$$\hat{H}_{\alpha,\gamma}(\xi; h^\alpha \lambda) = \left(1 + \sum_{n=1}^{\infty} \frac{\omega_n^{(\alpha)}}{1 + h^\alpha \lambda} \xi^n \right)^{-\gamma}$$

and the application of the Miller's formula of Theorem 7, for the negative power $-\gamma$, allows to conclude the proof. □

Thanks to the following result it is possible to verify that the $w_k^{(\gamma)}$'s generalize the coefficients (5) of classical GL operators.

Proposition 9. *Let $\alpha > 0$, $\lambda = 0$ and $h > 0$. Then for any $k = 0, 1, 2, \ldots$ it is $w_k^{(1)} = \omega_k^{(-\alpha)}$ and $w_k^{(-1)} = \omega_k^{(\alpha)}$.*

Proof. Since for $k = 0$ the proof is obvious we consider $k > 0$. When $\gamma = 1$ we observe that

$$w_k^{(1)} = \sum_{j=1}^{k} -\omega_j^{(\alpha)} w_{k-j}^{(1)}$$

and, since $\omega_k^{(\alpha)}$ are the coefficients in the power series $1 + \omega_1^{(\alpha)}\xi + \omega_2^{(\alpha)}\xi^2 + \ldots$ corresponding to $(1-\xi)^\alpha$, the proof follows by inversion of the series. When $\gamma = -1$ it is

$$w_k^{(-1)} = \sum_{j=1}^{k} \left(\frac{2j}{k} - 1 \right) \omega_j^{(\alpha)} w_{k-j}^{(-1)}$$

from which we obtain

$$\sum_{j=0}^{k} j \omega_j^{(\alpha)} w_{k-j}^{(-1)} = \sum_{j=0}^{k} (k-j) \omega_j^{(\alpha)} w_{k-j}^{(-1)}. \tag{23}$$

Denoted with $w(\xi)$ the power series with coefficients $w_j^{(-1)}$, we observe that for any $k > 0$ the left hand side of (23) gives the coefficients of $\xi w(\xi) \frac{d}{d\xi}(1-\xi)^\alpha$ while the right hand side gives the coefficients of $\xi(1-\xi)^\alpha \frac{d}{d\xi} w(\xi)$. As a consequence it is $\frac{d}{d\xi}\left(w(\xi) - (1-\xi)^\alpha\right) = 0$ and therefore all the coefficients of $w(\xi)$ and $(1-\xi)^\alpha$ coincides for $k > 0$. □

Let us introduce now the weights

$$W_k^{(\gamma)} = \frac{h^{\alpha\gamma}}{(1 + h^\alpha \lambda)^\gamma} w_k^{(\gamma)} \tag{24}$$

which are obviously the coefficients in the expansion of $H_{\alpha,\gamma}\left(\delta(\xi)/h; \lambda\right)$. The following properties can be verified in immediate way.

Proposition 10. *For any $\alpha, \gamma > 0$, $\lambda \geq 0$, $m > \alpha\gamma$ and $k = 0, 1, \ldots$ it is*

$$\lim_{h \to 0} W_k^{(\gamma)} = 0, \quad \lim_{h \to 0} W_k^{(-\gamma)} = +\infty, \quad \lim_{h \to 0} h^m W_k^{(-\gamma)} = 0.$$

The weights $W_k^{(\gamma)}$ are clearly the coefficients of the quadrature rule (18) when applied to convolution integrals of HN type according to the theory recalled in Subsection 4.1. Thanks to (20) and Proposition 10 we can now introduce new specific operators of GL type for HN relaxation processes.

Definition 5. Let $\alpha, \gamma > 0$, $\lambda \geq 0$ and $y \in \mathcal{C}\bigl([t_0, T]\bigr)$. For any $t \in (t_0, T]$ the HN integral of GL type is

$$\widetilde{J}_{t_0,\lambda}^{\alpha,\gamma} y(t) = \lim_{h \to 0} \sum_{k=0}^{\infty} W_k^{(\gamma)} y(t - kh). \tag{25}$$

Definition 6. Let $\alpha, \gamma > 0$, $\lambda \geq 0$ and $y \in \mathcal{C}^m\bigl([t_0, T]\bigr)$, $m = \lceil \alpha\gamma \rceil$. For any $t \in (t_0, T]$ the HN derivative of GL type is

$$\widetilde{D}_{t_0,\lambda}^{\alpha,\gamma} y(t) = \lim_{h \to 0} \sum_{k=0}^{\infty} W_k^{(-\gamma)} y(t - kh). \tag{26}$$

It is possible to prove the equivalence between the HN integral of GL type (25) and the original HN integral (13).

Theorem 11. *Let $0 < \alpha < 2$, $\gamma > 0$, $\lambda \geq 0$ and $y \in \mathcal{C}^0([t_0, T])$. Then for any $t \in (t_0, T]$ it is $\widetilde{J}_{t_0,\lambda}^{\alpha,\gamma} y(t) = J_{t_0,\lambda}^{\alpha,\gamma} y(t)$.*

Proof. It is immediate that (25) is the convolution quadrature (18) applied to $H_{\alpha,\gamma}(s; \lambda)$ when using the generating function $\delta(\xi) = 1 - \xi$ corresponding to the backward Euler method. The proof therefore is a consequence of the last part of Theorem 6 (the restriction on α is due to the region of analyticity of $H_{\alpha,\gamma}(s; \lambda)$). □

The proof of the corresponding equivalence for the HN derivative is less direct.

Theorem 12. *Let $0 < \alpha < 2$, $\gamma > 0$, $\lambda \geq 0$ and $y \in \mathcal{C}^m([t_0, T])$, with $m = \lceil \alpha\gamma \rceil$. Then for any $t \in (t_0, T]$ it is $\widetilde{D}_{t_0,\lambda}^{\alpha,\gamma} y(t) = D_{t_0,\lambda}^{\alpha,\gamma} y(t)$.*

Proof. Let us consider $\mathbf{E}_{\alpha,m-\alpha\gamma,-\lambda,t_0+}^{-\gamma} y(t)$ which can be expressed in terms of the convolution integral (17) with kernel $e_{\alpha,m-\alpha\gamma}^{-\gamma}(t; -\lambda)$, whose Laplace transform is $(s^\alpha + \lambda)^\gamma / s^m$. The coefficients of the quadrature rule (18) generalizing the backward Euler method (i.e., with $\delta(\xi) = 1 - \xi$) to this integral are therefore obtained from the series expansion

$$\frac{\left(\left(\frac{1-\xi}{h}\right)^\alpha + \lambda\right)^\gamma}{\dfrac{(1-\xi)^m}{h^m}} = \frac{h^m}{(1-\xi)^m} \cdot \frac{((1-\xi)^\alpha + h^\alpha \lambda)^\gamma}{h^{\alpha\gamma}} = h^m \sum_{k=0}^{\infty} U_k \xi^k.$$

Denote with $A_k^{(m)}$ and $W_j^{(-\gamma)}$ the coefficients in the expansion of $(1-\xi)^{-m}$ and $\left((1-\xi)^\alpha + h^\alpha \lambda\right)^\gamma / h^{\alpha\gamma}$ respectively. It is immediate to see that

$$A_k^{(m)} = \binom{k+m-1}{m-1}$$

and $W_k^{(-\gamma)}$ are obtained from (24), with γ replaced by $-\gamma$, again from the application of the Miller's formula. Thanks to Theorem 6 it is therefore

$$\mathbf{E}_{\alpha,m-\alpha\gamma,-\lambda,t_0+}^{-\gamma} y(t) = \lim_{h \to 0} \sum_{k=0}^{\infty} U_k y(t - hk),$$

with

$$U_k = \sum_{j=0}^{k} A_{k-j}^{(m)} W_j^{(-\gamma)}$$

and hence, from (14), we have

$$D_{t_0,\lambda}^{\alpha,\gamma} y(t) = \lim_{\tau \to 0} \frac{1}{\tau^m} \sum_{\ell=0}^{m} (-1)^\ell \binom{m}{\ell} \cdot \lim_{h \to 0} h^m \sum_{k=0}^{\infty} U_k y(t - \ell\tau - kh).$$

Thus, by putting $\tau = h$ we obtain

$$\begin{aligned} D_{t_0,\lambda}^{\alpha,\gamma} y(t) &= \lim_{h \to 0} \sum_{\ell=0}^{m} \sum_{k=0}^{\infty} (-1)^\ell \binom{m}{\ell} U_k y(t - (\ell + k)h) \\ &= \lim_{h \to 0} \sum_{k=0}^{\infty} F_k y(t - kh), \end{aligned}$$

where a simple manipulation allows to verify that

$$F_k = \sum_{j=0}^{k} C_{k,j} W_j^{(-\gamma)}$$

and

$$C_{k,j} = \sum_{\ell=0}^{\min\{m,k-j\}} (-1)^\ell \binom{m}{\ell} \binom{k-j-\ell+m-1}{m-1}.$$

Since $C_{k,j} = 0$ when $k \neq j$ and $C_{k,j} = 1$ when $k = j$, it is $F_k = W_k^{(-\gamma)}$ from which the proof follows. □

As observed in [25], the weights $W_k^{(\gamma)}$ approximate the inverse Laplace transform of the kernel $H_{\alpha,\gamma}(s;\lambda)$ at $t = hk$, i.e. the Prabhakar function $e_{\alpha,\alpha\gamma}^{\gamma}(hk;-\lambda)$. By means of the following result, we are able to prove that the weights $W_k^{(\gamma)}$ preserve, for the same range of parameters α and γ [43, 42], the positivity and monotonicity of $e_{\alpha,\alpha\gamma}^{\gamma}(t;-\lambda)$. This result appears of interest since validates the robustness of the approach discussed in this work.

Proposition 13. *Let $0 < \alpha < 1$, $\lambda > 0$. Then for any $h > 0$ and $k = 0, 1, 2, \ldots$ it is*

1. $W_k^{(\gamma)} > 0$, *for* $\gamma > 0$;
2. $W_{k+1}^{(\gamma)} > W_k^{(\gamma)}$, *for* $0 < \gamma \leq 1/\alpha$.

Proof. Because of (24), it is sufficient to prove the Proposition for the $w_k^{(\gamma)}$'s. For point 1. we first observe that $1 + h^\alpha\lambda > 0$ and, thanks to Proposition 1, $\omega_j^{(\alpha)} < 0$, for $j \geq 1$. The proof thus follows from (22) by induction on k since for any $\gamma > 0$ and $j = 1, \ldots, k$ it is $(1-\gamma)j/k - 1 \leq 0$. For point (2) we preliminary observe that

$$w_1^{(\gamma)} = \frac{\alpha\gamma}{1 + h^\alpha\lambda} < 1 = w_0^{(\gamma)}$$

and, again by induction on k, we assume $w_{j+1}^{(\gamma)} > w_j^{(\gamma)}$ for any $j = 0, 1, \ldots, k-1$. It is hence immediate to observe from (22) that

$$w_{k+1}^{(\gamma)} = \frac{-\gamma\omega_{k+1}^{(\alpha)}}{(1 + h^\alpha\lambda)^\gamma} + \sum_{j=1}^{k} \left(\frac{(1-\gamma)j}{k+1} - 1 \right) \frac{\omega_j^{(\alpha)} w_{k+1-j}^{(\gamma)}}{(1 + h^\alpha\lambda)^\gamma} > \sum_{j=1}^{k} \left(\frac{(1-\gamma)j}{k+1} - 1 \right) \frac{\omega_j^{(\alpha)}}{(1 + h^\alpha\lambda)^\gamma} w_{k+j}^{(\gamma)} = w_k^{(\gamma)}$$

which allows us to conclude the proof. □

Table 1: Errors E_h and EOC=$\log_2(E_h/E_{h/2})$ in $J^{\alpha,\gamma}_{t_0,\lambda}1$ at $t = 2.0$.

	$\alpha = 0.5$ $\gamma = 0.9$ $\lambda = 1.0$		$\alpha = 0.8$ $\gamma = 1.2$ $\lambda = 2.0$		$\alpha = 0.9$ $\gamma = 0.9$ $\lambda = 1.0$	
h	Error	EOC	Error	EOC	Error	EOC
2^{-6}	$4.91(-4)$		$2.14(-5)$		$4.94(-4)$	
2^{-7}	$2.47(-4)$	0.989	$1.09(-5)$	0.973	$2.51(-4)$	0.973
2^{-8}	$1.24(-4)$	0.999	$5.35(-6)$	1.026	$1.26(-4)$	1.001
2^{-9}	$6.18(-5)$	1.000	$2.65(-6)$	1.013	$6.28(-5)$	1.001
2^{-10}	$3.09(-5)$	0.999	$1.33(-6)$	0.997	$3.15(-5)$	0.997
2^{-11}	$1.55(-5)$	0.999	$6.64(-7)$	0.998	$1.57(-5)$	0.998
2^{-12}	$7.74(-6)$	1.000	$3.32(-7)$	1.002	$7.87(-6)$	1.000

Table 2: Errors E_h and EOC=$\log_2(E_h/E_{h/2})$ in $J^{\alpha,\gamma}_{t_0,\lambda}t^\mu/\Gamma(\mu)$ at $t = 2.0$ for $\mu = 1.6$

	$\alpha = 0.5$ $\gamma = 0.9$ $\lambda = 1.0$		$\alpha = 0.8$ $\gamma = 1.2$ $\lambda = 2.0$		$\alpha = 0.9$ $\gamma = 0.9$ $\lambda = 1.0$	
h	Error	EOC	Error	EOC	Error	EOC
2^{-6}	$4.62(-4)$		$8.96(-5)$		$7.73(-4)$	
2^{-7}	$2.35(-4)$	0.975	$4.71(-5)$	0.928	$3.96(-4)$	0.963
2^{-8}	$1.19(-4)$	0.987	$2.40(-5)$	0.970	$2.00(-4)$	0.985
2^{-9}	$5.97(-5)$	0.992	$1.22(-5)$	0.980	$1.01(-4)$	0.990
2^{-10}	$3.00(-5)$	0.994	$6.17(-6)$	0.983	$5.07(-5)$	0.992
2^{-11}	$1.50(-5)$	0.996	$3.11(-6)$	0.989	$2.54(-5)$	0.995
2^{-12}	$7.53(-6)$	0.998	$1.56(-6)$	0.994	$1.27(-5)$	0.997

5. Numerical experiments

The aim of the subsequent experiments is to assess the efficacy of the GL operator (25) when employed, as a computational method, in order to numerically approximate HN integrals (13) after fixing the step-size h and truncating the series in (25) at $K = \lceil (t - t_0)/h \rceil$; from Theorem 6 an error proportional to h is expected.

All the experiments are carried out in Matlab, version 7.8.0.347, on a computer equipped with the Intel Core i3-2365M processor running at 1.47 GHz under the Windows 10 operating system.

In the first experiment we consider the HN integral of the constant function $f(t) \equiv 1$; as stated by Proposition 3, the exact integral is $e^{\gamma}_{\alpha,\alpha\gamma+1}(t-t_0; -\lambda)$ and this reference value can be evaluated, with an accuracy close to the machine precision, by means of the algorithm presented in [46].

The results obtained, at $t = 2.0$, and for various values of α, γ and λ are presented in Table 1 where, for a decreasing sequence of the step-size h, we report the error E_h and the estimated order of convergence (EOC) evaluated as $\log_2(E_h/E_{h/2})$. As we can clearly see the first order of convergence predicted by Theorem 6 is achieved.

The same experiment is hence repeated for the integration of the function $f(t) = t^\mu/\Gamma(\mu)$ for $\mu = 1.6$ (see Table 2) and for $\mu = 2.0$ (see Table 3). Also in this case the theoretical predictions of Theorem 6 are verified, thus indicating the suitability of (25) not only for defining specific HN operators in the time-domain but also for numerical purposes.

To test the performance we propose now the comparison with the only existing alternative method consisting in truncating the series (16) after a certain number K of terms and discretizing the fractional derivatives $D^{\alpha(\gamma-k)}_{t_0}$ (for consistence, the classical GL scheme is used).

The accuracy of this approach (which has been proposed in [13]) strongly depends on the number of terms in the truncated series (16). In our experiments we have considered the minimum numbers K for which it is obtained an error close to the error produced from the method discussed in this paper.

The results of this comparison are presented in Figure 1 where, for $\alpha = 0.5$, $\gamma = 0.9$ and

Table 3: Errors E_h and EOC=$\log_2(E_h/E_{h/2})$ in $J^{\alpha,\gamma}_{t_0,\lambda} t^\mu/\Gamma(\mu)$ at $t = 2.0$ for $\mu = 2.0$

	$\alpha = 0.5$ $\gamma = 0.9$ $\lambda = 1.0$		$\alpha = 0.8$ $\gamma = 1.2$ $\lambda = 2.0$		$\alpha = 0.9$ $\gamma = 0.9$ $\lambda = 1.0$	
h	Error	EOC	Error	EOC	Error	EOC
2^{-6}	$9.48(-4)$		$5.22(-4)$		$1.90(-3)$	
2^{-7}	$4.75(-4)$	0.998	$2.62(-4)$	0.993	$9.53(-4)$	0.994
2^{-8}	$2.38(-4)$	0.999	$1.31(-4)$	1.000	$4.77(-4)$	0.999
2^{-9}	$1.19(-4)$	1.000	$6.55(-5)$	1.000	$2.38(-4)$	0.999
2^{-10}	$5.94(-5)$	1.000	$3.28(-5)$	0.999	$1.19(-4)$	0.999
2^{-11}	$2.97(-5)$	1.000	$1.64(-5)$	1.000	$5.97(-5)$	1.000
2^{-12}	$1.49(-5)$	1.000	$8.20(-6)$	1.000	$2.98(-5)$	1.000

$\lambda = 1.0$, we have considered the approximation at $t = 2.0$ of $J^{\alpha,\gamma}_{t_0,\lambda} t^\mu/\Gamma(\mu)$ for $\mu = 1.6$; the CPU time against the error is plotted in correspondence of the same first 5 values of the step-size h used in Tables 1-3.

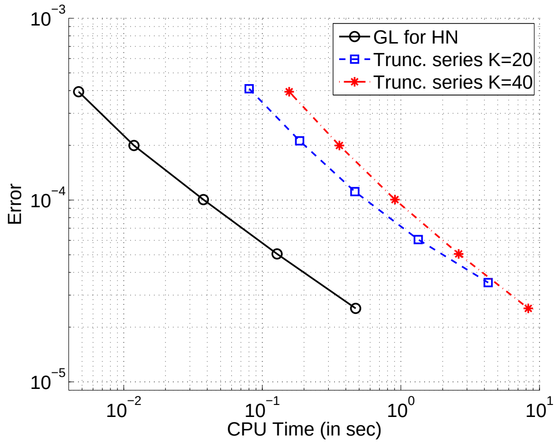

Figure 1: Comparison, at $t = 2.0$, of the scheme (25) with the truncated (after K terms) series (16) for $J^{\alpha,\gamma}_{t_0,\lambda} t^\mu/\Gamma(\mu)$ with $\mu = 1.6$; here $\alpha = 0.5$, $\gamma = 0.9$ and $\lambda = 1$.

As we can clearly see, in order to produce acceptable errors the method based on truncating the series (16) demands for an exceedingly higher CPU time with respect to the approach under investigation (denoted as “GL for HN” in the plot).

Most importantly, the number K of summands to consider in (16) in order to obtain a given error depends on the parameters α and γ of the HN operator (as well as on the width of the integration interval), as we can infer from Figure 2, where the same experiment has been repeated for $\alpha = 0.9$, $\gamma = 0.9$ and $\lambda = 1$.

This dependence is a major drawback when using the truncation of the series (16); indeed, not only the computational time varies with different parameters α and γ (while this does not happens with the method discussed in this paper) but it is also extremely difficult to estimate the proper number of terms necessary to achieve a prescribed accuracy.

In order to present a slightly more involved experiment, we finally consider the function $\cos(t)$. As we can see from Figure 3 the HN integral of this function tends to the RL integral when $\gamma \to 1$ and $\lambda \to 0$ (the value $\alpha = 0.8$ has been considered).

In this case we are not able to provide the exact HN integral. Thus, as reference solution we use the one obtained with the same approach proposed in this paper but with a smaller step-size.

Also in this case, as shown in Figure 4, the approximation of the HN integral by means of the GL operators involves a lower computational time with respect to the use of the truncation of the series (16).

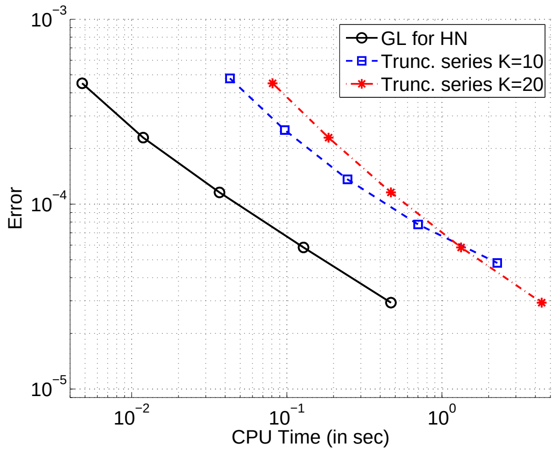

Figure 2: Comparison, at $t = 2.0$, of the scheme (25) with the truncated (after K terms) series (16) for $J^{\alpha,\gamma}_{t_0,\lambda} t^{\mu}/\Gamma(\mu)$ with $\mu = 1.6$; here $\alpha = 0.9$, $\gamma = 0.9$ and $\lambda = 1$.

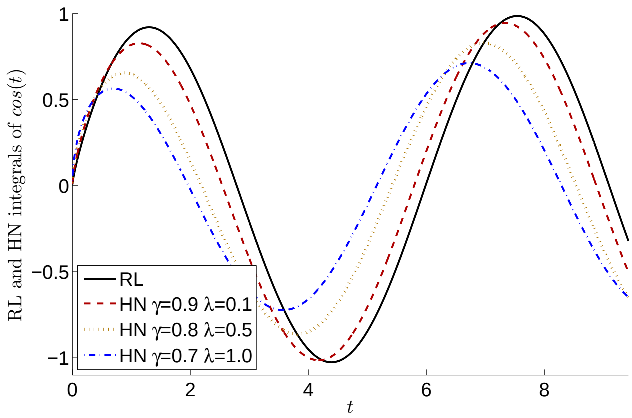

Figure 3: Comparison, for $\alpha = 0.8$, of RL and HN integrals of $\cos(t)$

6. Concluding remarks

In this paper we have discussed fractional operators describing the time relaxation in systems governed by HN laws and we have introduced and studied new integral and differential operators of GL type whose corresponding weights are provided in an explicit way. Some of their properties have been investigated and their use for numerical computation has been tested.

We have also shown the better performance of this approach with respect to the only method available in literature and consisting in truncating a series representation and discretizing the resulting fractional derivatives by means of the standard GL scheme.

With the aim of employing the proposed approach in applicative fields, as for instance in computational electromagnetism for wave propagation in complex media such as biological tissues, a future research will concern operators based on higher order LMMs together with suitable short-memory implementations capable of preserving the quality of the approximation and reducing the computational effort; in this respect, recent methods [49] based on rational approximations of the generating function appear particularly promising.

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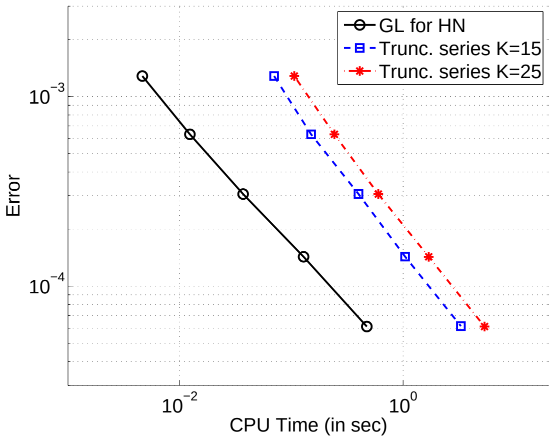

Figure 4: Comparison, at $t = 2.0$, of the scheme (25) with the truncated (after K terms) series (16) for $J^{\alpha,\gamma}_{t_0,\lambda} \cos(t)$; here $\alpha = 0.8$, $\gamma = 0.9$ and $\lambda = 1$.

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