

Fractional Prabhakar derivative and applications in anomalous dielectrics: a numerical approach.*

Roberto Garrappa¹ and Guido Maione²

¹ Dipartimento di Matematica, Università degli Studi di Bari,
Via E. Orabona 6, 70125 Bari, Italy
`roberto.garrappa@uniba.it`

² Dipartimento di Ingegneria Elettrica e dell'Informazione, Politecnico di Bari,
Via E. Orabona 6, 70125 Bari, Italy
`guido.maione@poliba.it`

Abstract. Fractional integrals and derivatives based on the Prabhakar function are useful to describe anomalous dielectric properties of materials whose behaviour obeys to the Havriliak-Negami model. In this work some formulas for defining these operators are described and investigated. A numerical method of product-integration type for solving differential equations with the Prabhakar derivative is derived and its convergence properties are studied. Some numerical experiments are presented to validate the theoretical results.

Keywords: Havriliak-Negami model, fractional derivative, Prabhakar function, numerical method, product integration

1 Introduction

Complex systems in different areas, such as chemistry, electromagnetism, mechanics, optics and so on, are modelled by means of integral and differential operators of integer or fractional order. Since fractional derivatives and fractional integrals allow to describe anomalous phenomena in a more accurate way, their use for the description of real-life problems is gaining an increasing popularity.

In more recent years, an accurate analysis of experimental data has highlighted the existence of situations in which classical operators of integer or fractional order are no more sufficient to fit data in a satisfactory way and more involved operators have been introduced.

This is the case of the dielectric properties of Havriliak-Negami type observed in some polymers [10] whose mathematical description in the time-domain is characterized in terms of the so-called Prabhakar integrals and derivatives [17, 6].

* Work supported by the Cost Action CA15225. Preprint of the paper published in: Garrappa R., Maione G. *Fractional Prabhakar derivative and applications in anomalous dielectrics: a numerical approach*. Chapter book in "Theory and Applications of Non-Integer Order Systems" (editors: Babiari, A., Czornik, A., Klamka, J., Niezabitowski, M.), Springer 2017, 429-439 ISBN: 978-3-319-45474-0

This work reviews the available formulas for defining fractional operators of Prabhakar type involved in the description of Havriliak-Negami models and proposes a numerical method, of product-integration type, for solving the resulting fractional differential equations.

This paper is organized as follows: in Section 2 the Prabhakar function is introduced and its main properties are illustrated. Section 3 discusses the applications of the Prabhakar function in modelling some anomalous dielectrics in the Havriliak-Negami model and describes the operators involved in the time-domain representation. Section 4 introduces a product-integration formula for the discretization of these operators and analyses its convergence properties. In Section 5 we present some numerical experiments assessing the effectiveness of the proposed approach and validating the theoretical results and we conclude the paper with some concluding remarks in Section 6.

2 The Prabhakar function

The Mittag-Leffler (ML) function is a special function playing a key role in fractional calculus. After the introduction in 1902 of a one parameter version [14], the generalization to two parameters

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad z \in \mathbb{C}, \quad (1)$$

was proposed few years later [20]. In 1971, the Indian mathematician Tialk Raj Prabhakar introduced a three parameter generalization of the ML function [17]

$$E_{\alpha,\beta}^{\gamma}(z) = \frac{1}{\Gamma(\gamma)} \sum_{k=0}^{\infty} \frac{\Gamma(\gamma + k) z^k}{k! \Gamma(\alpha k + \beta)}, \quad z \in \mathbb{C}, \quad (2)$$

and studied integral equations of convolution type with $E_{\alpha,\beta}^{\gamma}(z)$ in the kernel.

This function can be defined also for complex parameters α, β and γ under the restriction $\Re\alpha > 0$ and it is an entire function of order $(\Re\alpha)^{-1}$. It is, moreover, a generalization of (1) since $E_{\alpha,\beta}^1(z) = E_{\alpha,\beta}(z)$. Nowadays, $E_{\alpha,\beta}^{\gamma}(z)$ is commonly known as the three parameter ML function or Prabhakar function.

The Prabhakar function (2) provides an explicit formulation of the derivatives of the standard ML function (1) since for any $k \in \mathbb{N}$ it is $D^k E_{\alpha,\beta}(z) = k! E_{\alpha,\alpha k + \beta}^{k+1}(z)$ (we refer to the monograph [9] for a comprehensive analysis of the ML functions).

In applications it is usually used a further generalization of (2) given by

$$e_{\alpha,\beta}^{\gamma}(t; \lambda) = t^{\beta-1} E_{\alpha,\beta}^{\gamma}(t^{\alpha} \lambda), \quad (3)$$

where $\lambda \in \mathbb{C}$ is a parameter and $t > 0$ the independent real variable. For the practical computation of $e_{\alpha,\beta}^{\gamma}(t; \lambda)$ formulas (2-3) can be used only for t very

close to the origin. An asymptotic expansion holding for large values of t has been derived in [13] for real and negative λ according to

$$e_{\alpha,\beta}^{\gamma}(t; \lambda) = \begin{cases} t^{\beta-\alpha\gamma-1} \sum_{k=0}^{\infty} \binom{-\gamma}{k} \frac{t^{-\alpha k} |\lambda|^{\gamma-k}}{\Gamma(\beta - \alpha k - \alpha\gamma)} & \text{if } \beta \neq \alpha\gamma \\ \sum_{k=1}^{\infty} \binom{-\gamma}{k} \frac{t^{-\alpha k - 1} |\lambda|^{\gamma-k}}{\Gamma(-\alpha k)} & \text{if } \beta \neq \alpha\gamma . \end{cases}$$

For values of t in a intermediate range both asymptotic expansions (for large and small values) usually fail to provide acceptable results. For this reason a method based on the numerical inversion of the Laplace transform (LT) has been presented in [7]. This method, which allows to compute the Prabhakar function in an accurate way, presents some advantages because the LT of (3) is much more simple than the function itself. One can indeed verify that the following LT pair holds [17, 9]

$$e_{\alpha,\beta}^{\gamma}(t; \lambda) \doteq \frac{s^{\alpha\gamma-\beta}}{(s^{\alpha} - \lambda)^{\gamma}}, \quad \Re(s) > 0, \quad |\lambda s^{-\alpha}| < 1 .$$

By using the LT, it is also simple to verify that the integral of the Prabhakar function is

$$\int_0^t e_{\alpha,\beta}^{\gamma}(u; \lambda) du = e_{\alpha,\beta+1}^{\gamma}(t; \lambda) \quad (4)$$

and a term by term derivation of the series in (2) allows to compute

$$\frac{d}{dt} e_{\alpha,\beta}^{\gamma}(t; \lambda) = e_{\alpha,\beta-1}^{\gamma}(t; \lambda) . \quad (5)$$

3 Anomalous dielectrics and the Prabhakar derivative

In recent years, applications of the Prabhakar function have been recognized in several fields, ranging from astronomy [1] to physics [18], quantum mechanics [3] and so on. One of the most interesting applications is however related to the description of the relaxation properties of anomalous dielectric materials.

In 1967 a new model of dielectric relaxation, known as Havriliak-Negami (HN), was proposed [10] with the aim of describing in a more realistic way non-typical behaviours experimentally observed in certain classes of polymers. The complex susceptibility of the HN model (formulated in the frequency domain) is

$$\hat{\chi}(\omega) = \frac{1}{(1 + (i\omega\tau)^{\alpha})^{\gamma}},$$

where τ is the relaxation time and α and γ two real parameters accounting respectively for the asymmetry in the shape of the permittivity spectrum and the broadness of the response. Usually it is assumed $0 < \alpha, \gamma < 1$, although in [13, 11] the extension to $0 < \alpha, \alpha\gamma < 1$ has been also considered.

The HN model generalizes and extends the more familiar Debye and Cole-Cole models for which, however, it is also available a representation in the time-domain by means of differential operators of integer and fractional order. Finding differential operators for the HN model is instead less immediate and the research in this field is still at a very early stage.

From a formal point of view, the relationship in the frequency-domain

$$\hat{y}(\omega) = \hat{\chi}(\omega)\hat{f}(\omega)$$

(in dielectric applications \hat{y} is the polarization and \hat{f} the electric field) is formulated in the time-domain as

$$({}_0D_t^\alpha + \lambda)^\gamma y(t) = \frac{1}{\tau^{\alpha\gamma}} f(t) ,$$

where $\lambda = \tau^{-\alpha}$ and $({}_0D_t^\alpha + \lambda)^\gamma$ is just a symbol to denote the fractional pseudo-differential operator resulting from the Fourier inversion of $((i\omega)^\alpha + \lambda)^\gamma$.

Over the years some attempts have been made to provide robust and practical characterizations of $({}_0D_t^\alpha + \lambda)^\gamma$. In [15] it was derived

$$({}_0D_t^\alpha + \lambda)^\gamma = \exp\left(-\frac{t\lambda}{\alpha} {}_0D_t^{1-\alpha}\right) {}_0D_t^{\alpha\gamma} \exp\left(\frac{t\lambda}{\alpha} {}_0D_t^{1-\alpha}\right) ,$$

where the exponential of the Riemann-Liouville (RL) derivative ${}_0D_t^{1-\alpha}$ must be intended in terms of a series representation; the expansion

$$({}_0D_t^\alpha + \tau^{-\alpha})^\gamma = \sum_{k=0}^{\infty} \binom{\gamma}{k} \lambda^k {}_0D_t^{\alpha(\gamma-k)} ;$$

was instead considered in [16, 19] and successively used for numerical simulations in [2]. In both approaches, however, the criteria for truncating the series in order to achieve a given accuracy are not completely clear.

Recently, Garra et al. [6] worked on the integral representation obtained by inversion of the Laplace transform and proposed the following characterization

$$({}_0D_t^\alpha + \lambda)^\gamma y(t) = \frac{d}{dt} \int_{t_0}^t e_{\alpha,1-\alpha\gamma}^{-\gamma}(t-\tau; -\lambda) y(\tau) d\tau , \quad (6)$$

where $e_{\alpha,1-\alpha\gamma}^{-\gamma}(t-\tau; -\lambda)$ is the Prabhakar function introduced in the previous section. A regularization in the Caputo sense has also been introduced in [6] according to

$$({}_0^C D_t^\alpha + \lambda)^\gamma y(t) = \int_0^t e_{\alpha,1-\alpha\gamma}^{-\gamma}(t-\tau; -\lambda) y'(\tau) d\tau , \quad (7)$$

and it has been shown that (7) is related to (6) by the relationship

$$({}_0^C D_t^\alpha + \lambda)^\gamma y(t) = ({}_0D_t^\alpha + \lambda)^\gamma (y(t) - y(0)) . \quad (8)$$

The derivatives (6) and (7) are clearly generalizations of the classical fractional derivatives of RL and Caputo type. Indeed, since by the Euler's reflection formula $1/\Gamma(-1) = 0$, it is immediate to verify that $e_{\alpha,1-\alpha}^{-1}(t; 0) = t^{1-\alpha}/\Gamma(1-\alpha)$ and hence when $\gamma = 1$ and $\lambda = 0$ the derivative (6) coincides with the RL derivative and (7) with the fractional Caputo derivative.

An integral operator $({}_0J_t^\alpha + \lambda)^\gamma$ inverting the derivative (6) has been also considered in [6] as

$$({}_0J_t^\alpha + \lambda)^\gamma f(t) = \int_0^t e_{\alpha,\alpha\gamma}^\gamma(t-u; -\lambda) f(u) du , \quad (9)$$

thus generalizing the classical RL integral of order α when $\gamma = 1$ and $\lambda = 0$.

More recently, a further formulation of $({}_0D_t^\alpha + \lambda)^\gamma$ has been proposed in terms of fractional differences of Grünwald-Letnikov type [8]

$$({}_0D_t^\alpha + \lambda)^\gamma y(t) = \lim_{h \rightarrow 0} \frac{(1 + h^\alpha \lambda)^\gamma}{h^{\alpha\gamma}} \sum_{k=0}^{\infty} \Omega_k^{(\alpha,\gamma)} y(t - kh) , \quad (10)$$

where

$$\Omega_0^{(\alpha,\gamma)} = 1, \quad \Omega_k^{(\alpha,\gamma)} = \frac{1}{1 + h^\alpha \lambda} \sum_{j=1}^k (-1)^j \binom{\alpha}{j} \left(\frac{(1 + \gamma)j}{k} - 1 \right) \Omega_{k-j}^{(\alpha,\gamma)} .$$

4 A product integration rule

Let us consider the initial value problem for the pseudo fractional differential equation of Havriliak-Negami type

$$\begin{cases} ({}_0^C D_t^\alpha + \lambda)^\gamma y(t) = f(t, y(t)) \\ y(0) = y_0 \end{cases} , \quad (11)$$

where $f(t, y)$ is assumed Lipschitz continuous with respect to the second argument. The non-linearity in (11) is motivated by the fact that, in the dielectric applications the right side f is the electric field which, by the Maxwell equations, itself depends on the polarization y . Thanks to (9), the above fractional pseudo-differential equation can be reformulated in the integral form

$$y(t) = y_0 + ({}_0J_t^\alpha + \lambda)^\gamma f(t, y(t)) .$$

In order to numerically approximate the solution of (11) we consider a grid-mesh $t_j = jh$, with a constant step-size $h > 0$. After rewriting, at $t = t_n$, the above integral equation in the piece-wise form

$$y_n = y_0 + \sum_{j=1}^n \int_{t_{j-1}}^{t_j} e_{\alpha,\alpha\gamma}^\gamma(t_n - u; -\lambda) f(u, y(u)) du ,$$

the vector field $f(u, y(u))$ is approximate, on each interval $[t_{j-1}, t_j]$, by interpolating polynomials and the resulting integrals are evaluated in an exact way. This technique, which is named as product-integration, has been firstly proposed in [21] for the numerical solution of weakly singular Volterra integral equations and hence successfully applied to fractional differential equations [4].

The simplest method of this type is obtained by considering the constant approximation $f(u, y(u)) \equiv f(t_j, y_j)$ on each interval $[t_{j-1}, t_j]$. Since it is

$$\int_{t_{j-1}}^{t_j} e^{\gamma_{\alpha, \alpha\gamma}}(t_n - u; -\lambda) du = \int_{t_{j-1}}^{t_n} e^{\gamma_{\alpha, \alpha\gamma}}(t_n - u; -\lambda) du - \int_{t_j}^{t_n} e^{\gamma_{\alpha, \alpha\gamma}}(t_n - u; -\lambda) du ,$$

by applying (4) we obtain

$$\int_{t_{j-1}}^{t_j} e^{\gamma_{\alpha, \alpha\gamma}}(t_n - u; -\lambda) du = e^{\gamma_{\alpha, \alpha\gamma+1}}(t_n - t_{j-1}; -\lambda) - e^{\gamma_{\alpha, \alpha\gamma+1}}(t_n - t_j; -\lambda)$$

and, since $e^{\gamma_{\alpha, \alpha\gamma+1}}(t_n - t_j; -\lambda) = h^{\alpha\gamma} e^{\gamma_{\alpha, \alpha\gamma+1}}(n - j; -h^\alpha \lambda)$, the corresponding numerical scheme, which can be considered as a generalization of the implicit Euler method, reads as

$$y_n = y_0 + h^{\alpha\gamma} \sum_{j=1}^n w_{n-j}^{\alpha, \gamma} f(t_j, y_j) , \quad (12)$$

where

$$w_n^{\alpha, \gamma} = e^{\gamma_{\alpha, \alpha\gamma+1}}(n + 1; -h^\alpha \lambda) - e^{\gamma_{\alpha, \alpha\gamma+1}}(n; -h^\alpha \lambda) . \quad (13)$$

In the following we will assume that the exact solution of (11) admits an asymptotic expansion in mixed powers of integer order and fractional order, i.e.

$$y(t) = y_0 + \sum_{j=1}^{\infty} c_j t^j + \sum_{j=1}^{\infty} d_j t^{\alpha\gamma j} \quad (14)$$

for some sequences of real coefficients c_j and d_j . To the best of authors' knowledge, there exist no theoretical results on this subject; anyway, the assumption (14) appears reasonable and by no means restrictive since it is congruent with the asymptotic expansion of the solution of simpler weakly singular convolution integral equations (e.g., see [12]).

Theorem 1. *Let $0 < \alpha, \alpha\gamma < 1$, $\lambda > 0$ and assume that the solution $y(t)$ of (11) admits the expansion (14). For any $h > 0$ there exist two positive constants C_1 and C_2 (which do not depend on h) such that*

$$|y(t_n) - y_n| \leq C_1 h + C_2 t_n^{\alpha\gamma-1} h^{1+\alpha\gamma} .$$

Proof. The proof will follow very closely the proof of Theorem 2.1 in [5]. After writing, at $t = t_n$, the exact solution of (11) as

$$y(t_n) = y_0 + h^{\alpha\gamma} \sum_{j=1}^n w_{n-j}^{\alpha, \gamma} f(t_j, y(t_j)) + R_n , \quad (15)$$

where R_n is the quadrature error

$$R_n = \sum_{j=1}^n \int_{t_{j-1}}^{t_j} e_{\alpha, \alpha\gamma}^{\gamma}(t_n - u; -\lambda) (f(u, y(u)) - f(t_j, y(t_j))) du ,$$

we subtract (12) from (15) and, thanks to the Lipschitzianity of f , for a constant $L > 0$ it is

$$|y(t_n) - y_n| < |R_n| + L \sum_{j=1}^n |w_{n-j}^{\alpha, \gamma}| \cdot |y(t_j) - y_j| .$$

We put $M_1 = \sup_{0 < t < T} E_{\alpha, \alpha\gamma}^{\gamma}(-t^{\alpha}\lambda)$ (the Prabhakar function is indeed bounded [17]) and by using again the Lipschitzianity of f we obtain

$$|R_n| \leq M_1 L \sum_{j=1}^n \int_{t_{j-1}}^{t_j} (t_n - u)^{\alpha\gamma-1} |y(u) - y(t_j)| du ,$$

Note now that $w_1^{\alpha, \gamma} = E_{\alpha, \alpha\gamma}^{\gamma}(-\lambda)$ while for $n > 1$ the Taylor expansion, together with (5), immediately leads to

$$w_n^{\alpha, \gamma} = e_{\alpha, \alpha\gamma}(n + 1 - v; -h^{\alpha}\lambda), \quad v \in [0, 1]$$

and hence

$$w_n^{\alpha, \gamma} \leq M_1 \frac{(n + 1 - v)^{\alpha\gamma-1}}{\Gamma(\alpha\gamma)} < M_1 \frac{n^{\alpha\gamma-1}}{\Gamma(\alpha\gamma)}$$

from which we infer

$$|y(t_n) - y_n| < |R_n| + M_1 L \sum_{j=1}^n (n - j)^{\alpha\gamma} |y(t_j) - y_j| .$$

Since $\alpha\gamma < 1$ and the expansion (14), close to the origin it is $|y(u) - y(t_j)| \leq M_2 h^{\alpha\gamma}$; away from the origin $y(u)$ is instead smooth and, by the remainder of the polynomial interpolation, it is $|y(u) - y(t_j)| \leq M_3 h$. Therefore, given $r \in \mathbb{N}$ such that $y(u)$ can be assumed non smooth for $u \leq t_r$ and smooth elsewhere, we have

$$\begin{aligned} |R_n| &\leq M_1 L \left(M_2 h^{\alpha\gamma} \sum_{j=1}^{r-1} \int_{t_{j-1}}^{t_j} (t_n - u)^{\alpha\gamma-1} du + M_3 h \sum_{j=r}^n \int_{t_{j-1}}^{t_j} (t_n - u)^{\alpha\gamma-1} du \right) \\ &\leq M_4 h^{1+\alpha\gamma} t_n^{\alpha\gamma-1} + M_5 h , \end{aligned}$$

and the proof follows in the same way as the proof of Theorem 2.1 in [5]. \square

An explicit counterpart of the method (12) can be devised by using in each interval $[t_{j-1}, t_j]$ the approximation $f(u, y(u)) \equiv f(t_{j-1}, y_{j-1})$. The resulting method is

$$y_n = y_0 + h^{\alpha\gamma} \sum_{j=0}^{n-1} w_{n-j-1}^{\alpha, \gamma} f(t_j, y_j) \quad (16)$$

and convergence properties can be proved in a similar way as in Theorem 1.

5 Numerical experiments

To numerically test the product integration method devised in Section 4, we first consider the linear test equation

$$({}_0^C D_t^\alpha + \lambda)^\gamma y(t) = -2y(t) + \cos(2\pi t), \quad y(0) = 1. \quad (17)$$

Since the exact solution is not known in an analytical form, for reference we will use the solution obtained by truncating the Grünwald-Letnikov formula (10) with a smaller step-size h . Thanks to the first order convergence of this method [8], it can be considered accurate enough to be used for reference. For some parameters α , γ and λ the solution of this problem is presented in Figure 1 (all the experiments are made by using Matlab and the Prabhakar function for the weights of the rule is evaluated by means of the `ml.m` code devised in [7]).

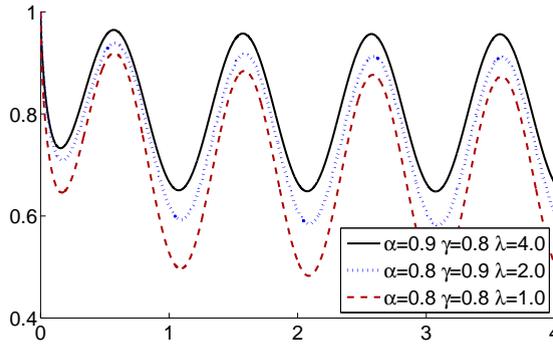


Fig. 1. Solution of the problem (17) for some values of α , γ and λ .

In Table 1 we report the error $E_h = |y(t_n) - y_n|$ and the estimated order of convergence (EOC) evaluated as $\log_2(E_h/E_{h/2})$ resulting from the application of the product-integration method described in Section 4. As we can readily observe, convergence of the first order is clearly achieved, thus confirming the theoretical findings of Theorem 1.

For a second test problem we consider the nonlinear equation

$$({}_0^C D_t^\alpha + \lambda)^\gamma y(t) = t^2 - (y(t))^2, \quad y(0) = 1, \quad (18)$$

whose solutions are shown in Figure 2.

Also in this case the theoretical results on the first order convergence are confirmed by the numerical experiments as reported in Table 2, thus validating the effectiveness of the approach proposed in this work.

h	$\alpha = 0.9 \quad \gamma = 0.8$ $\lambda = 4.0$		$\alpha = 0.8 \quad \gamma = 0.9$ $\lambda = 2.0$		$\alpha = 0.8 \quad \gamma = 0.8$ $\lambda = 1.0$	
	Error	EOC	Error	EOC	Error	EOC
2^{-5}	4.01×10^{-3}		4.08×10^{-3}		3.57×10^{-3}	
2^{-6}	2.02×10^{-3}	0.987	2.04×10^{-3}	0.999	1.73×10^{-3}	1.049
2^{-7}	1.01×10^{-3}	1.000	1.01×10^{-3}	1.008	8.35×10^{-4}	1.047
2^{-8}	5.04×10^{-4}	1.004	5.04×10^{-4}	1.009	4.06×10^{-4}	1.039
2^{-9}	2.51×10^{-4}	1.005	2.51×10^{-4}	1.008	1.99×10^{-4}	1.030
2^{-10}	1.25×10^{-4}	1.004	1.25×10^{-4}	1.006	9.80×10^{-5}	1.022

Table 1. Errors and EOC for problem (17) at $t = 4.0$.

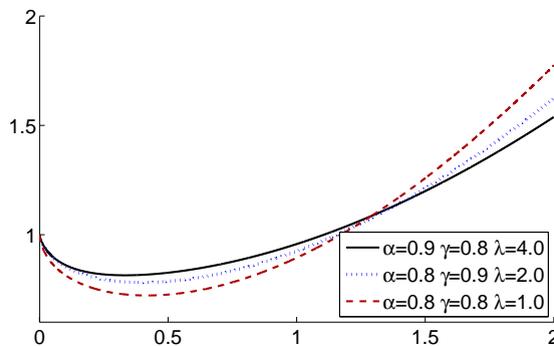


Fig. 2. Solution of the problem (18) for some values of α , γ and λ .

6 Concluding remarks

In this paper we have discussed the problem of numerically solving differential equations with Prabhakar derivatives; problems of this kind arise in the simulation of anomalous relaxation properties in Havriliak-Negami models.

We have devised a product-integration rule with weights expressed in terms of the Prabhakar function and studied the convergence properties. By means of some numerical experiments the effectiveness of the proposed approach has been illustrated. As far as we know, this is one of the very few methods available for solving problems of this kind.

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h	$\alpha = 0.9 \quad \gamma = 0.8$ $\lambda = 4.0$		$\alpha = 0.8 \quad \gamma = 0.9$ $\lambda = 2.0$		$\alpha = 0.8 \quad \gamma = 0.8$ $\lambda = 1.0$	
	Error	EOC	Error	EOC	Error	EOC
2^{-5}	6.79×10^{-3}		7.09×10^{-3}		6.62×10^{-3}	
2^{-6}	3.52×10^{-3}	0.947	3.64×10^{-3}	0.961	3.39×10^{-3}	0.965
2^{-7}	1.80×10^{-3}	0.968	1.85×10^{-3}	0.976	1.72×10^{-3}	0.978
2^{-8}	9.12×10^{-4}	0.981	9.34×10^{-4}	0.986	8.70×10^{-4}	0.986
2^{-9}	4.60×10^{-4}	0.989	4.70×10^{-4}	0.992	4.37×10^{-4}	0.991
2^{-10}	2.31×10^{-4}	0.993	2.36×10^{-4}	0.995	2.20×10^{-4}	0.994

Table 2. Errors and EOC for problem (18) at $t = 2.0$.

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