Computational Methods in Applied Mathematics
Vol. 14 (2014), No. 1, pp. 55–70

Doi: 10.1515/cmam-2013-0022

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High Order Numerical Methods for Fractional Terminal Value Problems

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Abstract — In this paper we present a shooting algorithm to solve fractional terminal (or boundary) value problems. We provide a convergence analysis of the numerical method, derived based upon properties of the equation being solved and without the need to impose smoothness conditions on the solution. The work is a sequel to our recent investigation where we constructed a nonpolynomial collocation method for the approximation of the solution to fractional initial value problems. Here we show that the method can be adapted for the effective approximation of the solution of terminal value problems. Moreover, we compare the efficiency of this numerical scheme against other existing methods.

2010 Mathematical subject classification: Primary 65L05; secondary 34A08, 26Axx.

Keywords: Fractional Calculus, Caputo Derivative, Boundary Value Problem, Nonpolynomial Collocation Method, Shooting Method.

1. Introduction

Fractional Calculus is a topic of rapidly growing interest. Numerous applications motivate the analysis and numerical approximation of solutions of differential equations of noninteger order. In this paper, we concentrate on equations that use the Caputo fractional derivative which is widely applied modelling physical and biological processes such as, for example, modelling of the mechanical properties of materials [2, 28], modelling of the behaviour of viscoelastic and viscoplastic materials under external influences [9, 10, 19], signal processing [21], diffusion problems [22], mathematical models in finance [26, 27], bioengineering [18, 20], among other (see also the books [4, 24, 25]). We recognise that there are several other (non-equivalent) definitions of the fractional derivative and, as is usual in this field, our approach would need to be adapted for a different definition.

We aim to construct reliable numerical schemes for the approximation of solutions to fractional boundary value problems (FBVPs) of order α, $0 < \alpha < 1$, with a reasonable

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convergence order. We focus on problems of the form

$$D_*^\alpha y(t) = f(t, y(t)), \quad t \in (0, T], \tag{1}$$
$$y(a) = y_a, \tag{2}$$

where $0 < a < T$, f is a continuous function and D_*^α denotes the Caputo differential operator of order $\alpha \notin \mathbb{N}$, defined by

$$D_*^\alpha y(t) := D^\alpha (y - T[y])(t)$$

(see [2]), where $T[y]$ is the Taylor polynomial of degree $\lfloor \alpha \rfloor$ for y, centered at 0, and D^α is the Riemann–Liouville fractional derivative of order α,

$$D^\alpha := D^{\lceil \alpha \rceil} J^{\lceil \alpha \rceil - \alpha}$$

(see [25]), with J^β being the Riemann–Liouville integral operator,

$$J^\beta y(t) := \frac{1}{\Gamma(\beta)} \int_0^t (t-s)^{\beta-1} y(s) ds,$$

and $D^{\lceil \alpha \rceil}$ is the classical integer order derivative, where $\lceil \alpha \rceil$ is the smallest integer greater or equal to α.

The case where $a = 0$, that is, the case where (1)–(2) is an initial value problem, has been studied extensively (see for example [3, 5, 7, 8, 12, 13, 23] and the references therein). Here we are only concerned with the case where $a \neq 0$, that is, the case where (1)–(2) is a terminal (or boundary) value problem, and we will seek solutions of this problem over a finite interval $[0, T]$ where $0 < a < T$.

In [14], the authors considered the case where $a \neq 0$ and they proved that the boundary value problem (1)–(2) is equivalent to a Fredholm integral equation and has a unique continuous solution on $[0, a]$.

Lemma 1. *Consider the terminal value problem* (1)–(2)*. If the function f is continuous on $[0, T]$ and satisfies a Lipschitz condition with Lipschitz constant $L > 0$ with respect to its second argument, where L is such that $\frac{2La^\alpha}{\Gamma(\alpha+1)} < 1$, then the terminal value problem* (1)–(2) *is equivalent to the integral equation*

$$y(t) = y(a) + \frac{1}{\Gamma(\alpha)} \int_0^a \left((t-s)^{\alpha-1} \chi_{[0,t]} - (a-s)^{\alpha-1} \right) f(s, y(s)) ds, \tag{3}$$

where $\chi_{[0,t]}$ is the indicator function of the interval $[0, t]$.

Furthermore the terminal value problem (1)–(2) *has a unique solution $y(t)$ for $t \in [0, a]$.*

On the other hand, in [16] the authors proved that, under the assumptions of Lemma 1, the problem (1)–(2) is stable in the sense that small perturbations of the given parameters, namely of the boundary condition, of the order of the derivative and of the right-hand side function, will produce small changes in the solution. This, together with the existence and uniqueness result means that the terminal value problem (1)–(2) is a well posed problem.

From Lemma 1 it follows that the terminal value problem (1)–(2) coincides with a unique initial condition:

$$y_0 = y(0) = y(a) - \frac{1}{\Gamma(\alpha)} \int_0^a (a-s)^{\alpha-1} f(s, y(s)) ds. \tag{4}$$

Then having proved the existence of $y(0)$, existence and uniqueness results for $t > a$ are inherited from the corresponding initial value problem theory.

In [14] the authors also proposed a simple shooting method to approximate the solution of (1)–(2). In order to do that, they considered the initial value problem

$$D_*^\alpha y(t) = f(t, y(t)), \quad t \in (0, T], \tag{5}$$

$$y(0) = y_0, \tag{6}$$

and for a certain value of y_0, they determined its numerical solution using standard initial value problem solvers. Then they used an iterative scheme to find the appropriate y_0, for which the solution of the initial value problem passes through the point (a, y_a). As can be seen in that paper, the convergence order of the schemes is the same as the convergence order of the initial value problem solvers, which can be relatively low if the solutions of the problems are nonsmooth, a feature that is highly probable in the fractional setting.

Hence, in this paper, we consider the initial value problem solver proposed in [17]. The paper is organised in the following way: in Section 2 we outline the numerical method used to approximate the solution of (1)–(2), in the case where $a = 0$ and then we describe the algorithm used to approximate the solution of (1)–(2), in the case where $a > 0$. In Section 3, we provide a convergence analysis for the initial value problem solver and finally, in Section 4 we illustrate the performance of the algorithm by considering some numerical examples. We also compare this method with other methods existing in the literature, in terms of convergence order, absolute errors and computational time. We end with some conclusions and plans for future work.

2. The Numerical Method

One of the known properties of fractional differential equations is that we cannot expect a solution to be smooth even if the right-hand side function f is smooth. For example, the non-differentiable function $y(x) = x^{1/2}$ is the unique solution of the initial value problem

$$D^{1/2} y(t) = \Gamma\left(\frac{3}{2}\right), \quad y(0) = 0.$$

The numerical method proposed in [17] is based on the following result concerning the form of the solution of a fractional differential equation (see [4]).

Lemma 2. *Consider the terminal value problem* (1)–(2)*, with f a continuous function on $[0, T]$ and satisfying a Lipschitz condition with respect to its second argument and with the Lipschitz constant $L > 0$ defined as in Lemma 1. If $\alpha = \frac{p}{q}$, where $p \geqslant 1$ and $q \geqslant 2$ are two relatively prime integers and if the right-hand side function f can be written in the form $f(t, y(t)) = \overline{f}(t^{1/q}, y(t))$, where $\overline{f}$ is analytic in a neighbourhood of $(0, y_0)$, with y_0 given by* (4)*, then the unique solution of the problem* (5)–(6) *can be represented in terms of powers of $t^{1/q}$: $y(t) = \sum_{i=0}^{\infty} a_i t^{i/q}$, $t \in [0, r)$, where the a_i are constants.*

Proof. From Lemma 1 the terminal value problem (1)–(2) has a unique solution $y(t)$ for $t \in [0, T]$ and then applying [4, Lemma 6.32] to the initial value problem

$$\begin{aligned} D_*^\alpha y(t) &= f(t, y(t)), \quad t \in (0, T], \\ y(0) &= y(a) - \frac{1}{\Gamma(\alpha)} \int_0^a (a - s)^{\alpha - 1} f(s, y(s)) ds, \end{aligned}$$

the result follows. □

This means that, assuming that the solution of (1)–(2) exists and is unique, then we can always write it as a sum $y = y_1 + y_2$ where, for a fixed integer m, $y_1 \in C^m([0,T])$ is the smooth part of the solution (made up of the integer powers of t), and y_2 is the nonsmooth part.

The numerical method proposed in [17] can be summarised in the following way:

Consider a partition of the interval $[0,T]$, the interval where the solution is sought,

$$\Delta_h = \{t_i = i\,h : i = 0, 1, \dots, N\},$$

into N subintervals of equal size $h = T/N$, $\sigma_0 = [0, t_1]$ and $\sigma_i = (t_i, t_{i+1}]$, $i = 1, 2, \dots, N-1$. At each one of these subintervals we define ℓ collocation points $t_{ik} = t_i + c_k\, h$, $k = 1, 2, \dots, \ell$, where $c_k \in [0, 1]$.

Consider the finite dimensional space V_m^α, with dimension $\ell = \#V_m^\alpha$, of nonpolynomial functions defined by

$$V_m^\alpha = \text{span}\{t^{i+j\alpha} : i, j \in \mathbb{N}_0 \text{ such that } i + j\alpha < m\},$$

where $m \in \mathbb{N}$ is a fixed parameter.

The above notation may be simplified introducing the index set

$$W_{\alpha,m} = \{i + j\alpha : i, j \in \mathbb{N}_0 \text{ such that } i + j\alpha < m\} = \{\nu_k : k = 1, \dots, \ell\}.$$

Using this notation we can write V_m^α as

$$V_m^\alpha = \text{span}\{t^{\nu_k} : k = 1, \dots, \ell\}.$$

Define the set

$$V_{h,m}^\alpha = \{v : v|_{\sigma_i} \in V_m^\alpha,\ i = 0, 1, \dots, N-1\}.$$

We will then seek a function $u \in V_{h,m}^\alpha$ such that u satisfies (5)–(6) at the chosen collocation points, or equivalently, the following Volterra integral equation (for details of this equivalence see, for example [4]):

$$u(t_{ik}) = y_0 + \frac{1}{\Gamma(\alpha)} \int_0^{t_{ik}} (t_{ik} - s)^{\alpha-1} f(s, u(s)) ds, \quad i = 0, 1, \dots, N-1,\ k = 1, 2, \dots, \ell. \quad (7)$$

Introducing the projection operator $P_h : C([0,T]) \to V_{h,m}^\alpha$, defined by (see [1])

$$(P_h g)(s) = \sum_{k=1}^{\ell} L_{ik}(s) g(t_{ik}), \quad s \in \sigma_i,$$

where the Lagrange functions $L_{ik} \in V_m^\alpha$ are defined by

$$L_{ik}(s) = \sum_{p=1}^{\ell} \beta_{pk}^i t^{\nu_p}, \quad i = 0, 1, \dots, N-1,\ k = 1, \dots, \ell, \quad (8)$$

and the coefficients $[\beta_{pk}^i]_{p=1,\dots,\ell}$ may be determined by solving the $(\ell \times \ell)$ linear system of equations $L_{ik}(t_{ij}) = \delta_{jk}$, $k, j = 1, \dots, \ell$, an approximation of $f(s, u(s))$, on each of the subintervals σ_i, $i = 0, 1, \dots, N-1$, may be given by

$$f(s, u(s)) \approx (P_h f)(s) = \sum_{k=1}^{\ell} L_{ik}(s) f(t_{ik}, u(t_{ik})). \quad (9)$$

For $s \in [t_i, t_{ik}]$, $i = 0, 1, \ldots, N-1$, $k = 1, \ldots, \ell$, we use

$$f(s, u(s)) \approx P_h(f)(s) = \sum_{\gamma=1}^{\ell} L_{i\gamma}^k(s) f(t_i + hc_\gamma c_k, u(t_i + hc_\gamma c_k)), \tag{10}$$

where $L_{i\gamma}^k$, $i = 0, 1, \ldots, N-1$, $k = 1, \ldots, \ell$, $\gamma = 1, \ldots, \ell$ are the Lagrange functions associated with the points $t_i + hc_\gamma c_k$, defined similarly to (8).

Substituting (9) and (10) in (7), we obtain the following approximation of $u(t_{ik})$:

$$\begin{aligned}
\hat{u}(t_{ik}) &= y_0 + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{i-1} \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} \int_{t_j}^{t_{j+1}} (t_{ik} - s)^{\alpha-1} s^{\nu_p} ds \beta_{\gamma p}^i f(t_{j\gamma}, \hat{u}(t_{j\gamma})) \\
&\quad + \frac{1}{\Gamma(\alpha)} \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} \int_{t_i}^{t_{ik}} (t_{ik} - s)^{\alpha-1} s^{\nu_p} ds \beta_{\gamma p}^{ik} f(t_i + hc_k c_\gamma, \hat{u}(t_i + hc_k c_\gamma)) \\
&= y_0 + \sum_{j=0}^{i-1} \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} w_{ik}^{j,p} \beta_{\gamma p}^j f(t_{j\gamma}, \hat{u}(t_j + hc_\gamma)) \\
&\quad + \sum_{\gamma=1}^{\ell} \sum_{p=1}^{\ell} w_{ik}^{i,p} \beta_{\gamma p}^{ik} f(t_i + hc_k c_\gamma, \hat{u}(t_i + hc_k c_\gamma)), \quad i = 0, 1, \ldots, N-1,\ k = 1, \ldots, \ell,
\end{aligned} \tag{11}$$

where

$$\begin{aligned}
w_{ik}^{j,p} &= \frac{1}{\Gamma(\alpha)} \int_{t_j}^{t_{j+1}} (t_{ik} - s)^{\alpha-1} s^{\nu_p} ds, \quad j < i, \\
w_{ik}^{i,p} &= \frac{1}{\Gamma(\alpha)} \int_{t_i}^{t_{ik}} (t_{ik} - s)^{\alpha-1} s^{\nu_p} ds, \quad i = 0, 1, \ldots, N-1,\ k = 1, \ldots, \ell.
\end{aligned}$$

After solving (11) an approximation to the solution of (5)–(6) will be given by

$$y(s) \approx \sum_{k=1}^{\ell} y_{jk} L_{jk}(s), \quad s \in \sigma_j,\ j = 0, 1, \ldots, N-1,$$

where $y_{jk} = \hat{u}(t_{jk})$.

In [17], we proved the convergence of the method in the linear case. In that proof we did not need to impose any smoothness conditions on the solution of our problem in order to obtain the optimal order of convergence m, a fact that brings a great advantage over some other numerical methods. In the following section we extend this result to the nonlinear case, but first, we describe the algorithm to solve (1)–(2). This is a standard shooting algorithm, as was already presented in [14] but using different initial value problem solvers. First we consider the initial value problem (5)–(6) for a certain value of y_0. Next we determine its numerical solution using the collocation method presented above. Then we use an iterative scheme to find the appropriate y_0, for which the solution of the initial value problem passes through the point (a, y_a).

To be precise, assume that we can find a y_{01} and a y_{02}, such that the solutions of (5)–(6), which we will denote by y_1 and y_2 respectively, satisfy

$$y_1(a) > y_a, \quad y_2(a) < y_a.$$

Therefore, and because the solution of this kind of problem depends continuously on the initial value (see [16]), we are able to find the value $y_0 \in (y_{01}, y_{02})$ for which the solution of the initial value problem satisfies (2). This can be achieved to any required degree of accuracy by using, for example, the bisection method.

3. Convergence Analysis

In this section a convergence analysis for the numerical scheme (11) applied to the nonlinear initial value problem (5)–(6), with f satisfying the assumptions of Lemma 2, will be provided.

In what follows, for each vector $x = [x_1, \ldots, x_N]^T \in \mathbb{R}^N$ we denote

$$\|x\| = \|x\|_\infty = \max_{i=1,\ldots,N} \{|x_i|\}$$

and $\|f\|_\sigma = \max_{s\in\sigma} |f(s)|$, for a continuous function f.

In order to analyse the error associated with the approximation $\hat{u}$ of the solution of equation (5)–(6) we consider the equality

$$y(t) - \hat{u}(t) = e(t) + \hat{e}(t), \quad t \in [0, T],$$

where

$$e(t) = y(t) - u(t), \quad \hat{e}(t) = u(t) - \hat{u}(t). \tag{12}$$

For each $i = 0, 1, \ldots, N-1$ let us define the vectors

$$\mathbf{e}_i = [e(t_{i1}), e(t_{i2}), \ldots, e(t_{il})]^T, \quad \hat{\mathbf{e}}_i = [\hat{e}(t_{i1}), \hat{e}(t_{i2}), \ldots, \hat{e}(t_{il})]^T.$$

Now we will estimate $e(t)$ and $\hat{e}(t)$.

For the error analysis we will need the following two auxiliary lemmas from [1] and [11], respectively:

Lemma 3. *Let L_{ik} be the Lagrange functions defined by (8). There exists a positive constant c such that*

$$\|L_{ik}\|_{\sigma_i} \leqslant c, \quad k = 1, \ldots, \ell. \tag{13}$$

Furthermore, for $f = f_1 + f_2$, where $f_1 \in C^m([0,T])$ and $f_2 \in V_m^\alpha$, we have

$$\|f - P_h f\|_{\sigma_i} \leqslant \bar{c} h^m \|f_1^{(m)}\|_{\sigma_i},$$

for some positive constant $\bar{c}$.

Lemma 4. *Let x_i, $0 \leqslant i \leqslant N$, be a sequence of non-negative real numbers satisfying*

$$x_i \leqslant \psi_i + M h^{1-\beta} \sum_{j=0}^{i-1} \frac{x_j}{(i-j)^\beta}, \quad 0 \leqslant i \leqslant N, \tag{14}$$

where $0 < \beta < 1$, $M > 0$ is bounded independently of h, and ψ_i, $0 \leqslant i \leqslant N$, is a monotonic increasing sequence of non-negative real numbers. Then

$$x_i \leqslant \psi_i E_{1-\beta}(M\Gamma(1-\beta)(ih)^{1-\beta}), \quad 0 \leqslant i \leqslant N,$$

where $E_\alpha(x) = \sum_{k=0}^{+\infty} \frac{x^k}{\Gamma(\alpha k+1)}$ denotes the Mittag-Leffler function of order α.

We start by obtaining estimates for the norms of the vectors $\mathbf{e}_i$.

The function f is a continuous function so the solution of the initial value problem (5)–(6) satisfies the following Volterra integral equation of the second kind:

$$y(t) = y_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} f(s, y(s)) ds.$$

Therefore, the error $e(t)$ at $t = t_{ik}$, $i = 0, 1, \ldots, N-1$, $k = 1, 2, \ldots, \ell$ satisfies

$$e(t_{ik}) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{ik}} (t_{ik}-s)^{\alpha-1} \big(f(s, y(s)) - f(s, u(s))\big) ds.$$

Since the function $f(s, y)$ satisfies a Lipschitz condition, with respect to the second variable, it follows that

$$|e(t_{ik})| \leqslant \frac{L}{\Gamma(\alpha)} \Big(\sum_{j=0}^{i-1} \|y-u\|_{\sigma_j} \int_{t_j}^{t_{j+1}} (t_{ik}-s)^{\alpha-1} ds + \|y-u\|_{\sigma_i} \int_{t_i}^{t_{ik}} (t_{ik}-s)^{\alpha-1} ds \Big).$$

By a similar analysis made in [17] we have that the errors $\mathbf{e}_i$ and $\|y-u\|_{\sigma_i}$ satisfy the following inequalities:

$$\|\mathbf{e}_i\|_\infty \leqslant C_0 h^m, \tag{15}$$

$$\|y-u\|_{\sigma_i} \leqslant C_1 h^m + C_2 \|\mathbf{e}_i\|_\infty, \quad i = 0, 1, \ldots, N-1. \tag{16}$$

From (15) and (16) we obtain

$$\|y-u\|_{\sigma_i} \leqslant C_3\, h^m. \tag{17}$$

Next we obtain estimates for the norm of the $\hat{\mathbf{e}}_i$ (cf. (12)).

From equations (7) and (11), the error $\hat{e}(t)$ at $t = t_{ik}$, $i = 0, 1, \ldots, N-1$, $k = 1, \ldots, \ell$, is given by

$$\begin{aligned}
\hat{e}(t_{ik}) = u(t_{ik}) - \hat{u}(t_{ik}) &= \frac{1}{\Gamma(\alpha)} \Big(\int_0^{t_i} (t_{ik}-s)^{\alpha-1} \big(f(s, u(s)) - P_h f(s, \hat{u}(s))\big) ds \\
&\quad + \int_{t_i}^{t_{ik}} (t_{ik}-s)^{\alpha-1} \big(f(s, u(s)) - P_h f(s, \hat{u}(s))\big) ds \Big) \\
&= \frac{1}{\Gamma(\alpha)} \Big(\int_0^{t_i} (t_{ik}-s)^{\alpha-1} \big(f(s, u(s)) - P_h f(s, u(s))\big) ds \\
&\quad + \int_{t_i}^{t_{ik}} (t_{ik}-s)^{\alpha-1} \big(f(s, u(s)) - P_h f(s, u(s))\big) ds \\
&\quad + \int_0^{t_i} (t_{ik}-s)^{\alpha-1} \big(P_h f(s, u(s)) - P_h f(s, \hat{u}(s))\big) ds \\
&\quad + \int_{t_i}^{t_{ik}} (t_{ik}-s)^{\alpha-1} \big(P_h f(s, u(s)) - P_h f(s, \hat{u}(s))\big) ds \Big).
\end{aligned}$$

From Lemma 2, $f(t, u)$ can be written in the form of a convergent power series

$$f(t, u) = \sum_{j,k=0}^{\infty} f_{jk} t^j u^k. \tag{18}$$

On the other hand, $u \in V_m^\alpha$ which implies $u(t) = \sum_{\gamma=0}^{\ell} t^{\nu_\gamma}$ and from (18) we obtain

$$f(t,u) = \sum_{j,k=0}^{\infty} f_{jk} t^j \Big(\sum_{\gamma=0}^{\ell} t^{\nu_\gamma} \Big)^k. \tag{19}$$

Therefore from (19) we can conclude that, given $m \in \mathbb{N}$ and $\alpha \in (0,1)$, the function $f(t,u)$ can be written as

$$f(t,u(t)) = u_1(t) + u_2(t),$$

with $u_1 \in C^m([0,T])$ and $u_2 \in V_m^\alpha$.

Hence, taking Lemma 3 into account we obtain a bound for $\|f(s,u(s)) - P_h f(s,u(s))\|_{\sigma_i}$, $i = 0,1,\dots,N-1$:

$$\big\|f(s,u(s)) - P_h f(s,u(s))\big\|_{\sigma_i} \leqslant C_4 h^m \|u_1^{(m)}\|_{\sigma_i} \leqslant C_5 h^m, \quad i = 0,1,\dots,N-1. \tag{20}$$

Taking the modulus and using (20), we obtain, for $i = 0,1,\dots,N-1$, $k = 1,2,\dots,\ell$,

$$\begin{aligned} |\hat{e}(t_{ik})| \leqslant \frac{1}{\Gamma(\alpha)} \Big(C_5 h^m \frac{t_{ik}^\alpha}{\alpha} + \sum_{j=0}^{i-1} \int_{t_j}^{t_{j+1}} (t_{ik}-s)^{\alpha-1} \big\|P_h f(s,u(s)) - P_h f(s,\hat{u}(s))\big\|_{\sigma_j} ds \\ + \int_{t_i}^{t_{ik}} (t_{ik}-s)^{\alpha-1} \big\|P_h f(s,u(s)) - P_h f(s,\hat{u}(s))\big\|_{\sigma_i} ds \Big). \end{aligned} \tag{21}$$

Since, by definition,

$$P_h f(s,u(s)) = \sum_{k=1}^{\ell} L_{ik}(s) f(t_{ik}, u(t_{ik})), \quad P_h f(s,\hat{u}(s)) = \sum_{k=1}^{\ell} L_{ik}(s) f(t_{ik}, \hat{u}(t_{ik})),$$

for $s \in \sigma_i$, and f satisfies a Lipschitz condition, with respect to the second variable, we obtain

$$\big\|P_h f(s,u(s)) - P_h f(s,\hat{u}(s))\big\|_{\sigma_i} \leqslant L \sum_{k=1}^{\ell} \|L_{ik}\|_{\sigma_i} |u(t_{ik}) - \hat{u}(t_{ik})|.$$

Using the fact that the Lagrange functions L_{ik} are uniformly bounded (cf. (13) of Lemma 3) we obtain

$$\big\|P_h f(s,u(s)) - P_h f(s,\hat{u}(s))\big\|_{\sigma_i} \leqslant L\,c \sum_{k=1}^{\ell} |u(t_{ik}) - \hat{u}(t_{ik})| = L\,c \sum_{k=1}^{\ell} |\hat{e}(t_{ik})| \leqslant L\,c\,\ell \|\hat{\mathbf{e}}_i\|. \tag{22}$$

Using estimate (22) on (21) and the fact that

$$\int_{t_j}^{t_{j+1}} (t_{ik}-s)^{\alpha-1} ds \leqslant D h^\alpha (i-j)^{\alpha-1}, \quad j < i,\ i = 0,1,\dots,N-1,\ k = 1,\dots,\ell,$$

for some positive constant D, it follows that

$$\|\hat{\mathbf{e}}_i\| \leqslant C_6 h^m + C_7 h^\alpha \sum_{j=0}^{i-1} (i-j)^{\alpha-1} \|\hat{\mathbf{e}}_j\| + C_8 h^\alpha \|\hat{\mathbf{e}}_i\|,$$

where $C_6 = \frac{C_5 T^\alpha}{\Gamma(\alpha)\alpha}$, $C_7 = \frac{L\,c\,D\,\ell}{\Gamma(\alpha)}$ and $C_8 = \frac{L\,c\,\ell}{\alpha\Gamma(\alpha)}$.

Under the condition $(1 - C_8 h^\alpha) > 0$, which certainly holds for sufficiently small $h > 0$, we conclude that

$$\|\hat{\mathbf{e}}_i\| \leqslant C_9 h^m + C_9 h^\alpha \sum_{j=0}^{i-1} (i-j)^{\alpha-1} \|\hat{\mathbf{e}}_j\|,$$

with $C_9 = \max\{C_6/C_8, C_7/C_8\}$. Now applying the standard weakly singular Gronwall inequality (14) from Lemma 4 leads to the following result:

$$\|\hat{\mathbf{e}}_i\| \leqslant C_{10} h^m. \tag{23}$$

We can now draw the following conclusions about the error $\|u - \hat{u}\|_{\sigma_i}$, $i = 0, 1, \ldots, N-1$. Since $u, \hat{u} \in V_m^\alpha$, it follows that, for $t \in \sigma_i$,

$$u(t) - \hat{u}(t) = \sum_{k=1}^{\ell} L_{ik}(t) \big(u(t_{ik}) - \hat{u}(t_{ik}) \big) = \sum_{k=1}^{\ell} L_{ik}(t) \hat{e}(t_{ik}),$$

which leads to

$$\|u - \hat{u}\|_{\sigma_i} \leqslant \ell c \|\hat{\mathbf{e}}_i\|,$$

where c is the positive constant defined in Lemma 3. Hence from (23), we obtain, for $i = 0, 1, \ldots, N-1$,

$$\|u - \hat{u}\|_{\sigma_i} \leqslant C\, h^m. \tag{24}$$

Having obtained upper bounds for the errors $\|y - u\|_{\sigma_i}$ and $\|u - \hat{u}\|_{\sigma_i}$, $i = 0, 1, \ldots, N-1$, we can now conclude about the error $\|y - u\|_{[0,T]}$.

Theorem 5. *Let y be the continuous solution of the initial value problem* (5)–(6) *and $\hat{u} \in V_m^\alpha$ the solution of the discretised collocation equation* (11)*. Then, for sufficiently small h, there exists a positive constant C independent of h, such that, for all collocation parameters $\{c_j\}$ with $0 \leqslant c_1 < c_2 < \cdots < c_m \leqslant 1$, we have*

$$\|y - \hat{u}\| = \max_{0 \leqslant i \leqslant N-1} \|y - \hat{u}\|_{\sigma_i} \leqslant C\, h^m. \tag{25}$$

Proof. We start by noting that $\|y - u\|_{[0,T]} = \max_{0 \leqslant i \leqslant N-1} \|y - u\|_{\sigma_i}$ and $\|y - u\|_{\sigma_i} \leqslant \|y - u\|_{\sigma_i} + \|u - \hat{u}\|_{\sigma_i}$. Therefore, the result (25) follows from (17) and (24). □

4. Numerical Examples

In this section we consider examples to illustrate the performance and feasibility of the proposed method. All the numerical experiments have been coded in Mathematica and run on a personal computer with processor Intel(R) Core(TM) i5, 2.4 GHz under operating system Microsoft Windows 7 Home Premium.

First we consider a linear terminal value problem given by

$$\begin{aligned} &D_*^{1/2} y(t) = -\frac{1}{4} t^{3/2} + \frac{3\sqrt{\pi}}{4} t + \frac{1}{4} y = f(t, y), \quad t \in (0, a], \\ &y_a = \frac{1}{2\sqrt{2}}, \quad a = \frac{1}{2}, \end{aligned} \tag{26}$$

	Collocation parameters			
	Radau points		Gauss points	
h	E_h	EOC	E_h	EOC
1/20	$1.20 \cdot 10^{-2}$	—	$6.90 \cdot 10^{-3}$	—
1/40	$4.23 \cdot 10^{-3}$	1.50	$2.47 \cdot 10^{-3}$	1.48
1/80	$1.50 \cdot 10^{-3}$	1.50	$8.84 \cdot 10^{-4}$	1.49
1/160	$5.30 \cdot 10^{-4}$	1.50	$3.15 \cdot 10^{-4}$	1.49
1/320	$1.87 \cdot 10^{-4}$	1.50	$1.11 \cdot 10^{-4}$	1.49

Table 1. Example (26): Maximum of errors at the mesh points and experimental order of convergence (EOC).

	Collocation parameters			
	Radau points		Gauss points	
h	ε_h	EOC	ε_h	EOC
1/20	$7.75 \cdot 10^{-4}$	—	$4.78 \cdot 10^{-4}$	—
1/40	$2.78 \cdot 10^{-4}$	1.48	$1.28 \cdot 10^{-4}$	1.90
1/80	$9.92 \cdot 10^{-5}$	1.48	$3.72 \cdot 10^{-5}$	1.78
1/160	$3.53 \cdot 10^{-5}$	1.49	$1.55 \cdot 10^{-5}$	1.26
1/320	$1.26 \cdot 10^{-5}$	1.49	$6.09 \cdot 10^{-6}$	1.35

Table 2. Example (26): Maximum of errors at the collocation points and experimental order of convergence (EOC).

whose analytical solution is given by $y(t) = t^{3/2}$. Note that in this case the solution and the fractional derivative $D^\alpha y$ are not smooth at the origin.

The approximate solution of (26) is computed by the shooting algorithm based on the bisection method, where successive approximations for y_0 are computed until the distance between the two last approximations does not exceed a given tolerance ε. In our numerical experiments we used $\varepsilon = 10^{-10}$. In order to evaluate $y(a)$ we use the nonpolynomial collocation method presented in Section 2.

We will consider $m = 1$, obtaining in this way a numerical scheme with the lowest possible convergence order provided by the nonpolynomial collocation method, and we compare the numerical results with the ones obtained with two other known numerical methods. In the numerical experiments presented in Table 1 we have used the nonpolynomial collocation method on the space $V_{h,1}^{1/2}$, $h = \frac{a}{N}$, for several values of N and with the following choice for the collocation parameters:

- Radau points: $c_1 = \frac{1}{3}$ and $c_2 = 1$,
- Gauss points: $c_1 = \frac{3-\sqrt{3}}{6}$ and $c_2 = \frac{3+\sqrt{3}}{6}$.

The maximum of the errors at the collocation points, $\varepsilon_h = \max_{1 \leqslant i \leqslant N,\, j=1,2} |u_h(t_{ij}) - y(t_{ij})|$, and mesh points, $E_h = \max_{1 \leqslant i \leqslant N} |u_h(t_i) - y(t_i)|$, and the experimental orders of convergence are presented in Tables 1 and 2 for a sequence of values of the stepsize h and for both choices of collocations parameters.

The results presented in Table 3 are computed using the Adams method (AM) [8] and the fractional backward difference method (FBDM) [3] to solve the initial value problems. It

	Method used to solve the IVP			
	AM		FBDM	
h	E_h	EOC	E_h	EOC
1/20	$3.33 \cdot 10^{-3}$	—	$7.92 \cdot 10^{-3}$	—
1/40	$1.15 \cdot 10^{-3}$	1.53	$3.00 \cdot 10^{-3}$	1.40
1/80	$3.99 \cdot 10^{-4}$	1.53	$1.11 \cdot 10^{-3}$	1.43
1/160	$1.39 \cdot 10^{-4}$	1.52	$4.05 \cdot 10^{-4}$	1.45
1/320	$4.86 \cdot 10^{-5}$	1.52	$1.46 \cdot 10^{-4}$	1.47

Table 3. Example (26): Maximum of errors at the mesh points and experimental order of convergence (EOC).

is known that the convergence order of these two methods is $1+\alpha$ and $2-\alpha$ if the solution is smooth (see [3,8]). Since in this example, this is not the case we can observe a decreasing of the convergence order when the FBDM is used (the theoretical one, for $\alpha = 1/2$, will be 1.5 for both).

From the results listed in Tables 1 and 2 we observe that the errors and estimates of convergence order are similar for the two choices of collocation parameters. In both cases the maximum of the error at the collocation points is obtained at a collocation point that is not a grid point, (compare E_h and ε_h in Tables 1 and 2). On the other hand, for both cases the error at the mesh points converges to zero with order $p \sim 1.5$.

Using the nonpolynomial collocation method (NPCM) applied to the example (26) we are able to solve the initial value problem

$$\begin{aligned} &D_*^{1/2} y(t) = -\frac{1}{4}t^{3/2} + \frac{3\sqrt{\pi}}{4}t + \frac{1}{4}y = f(t,y), \quad t \in (0,b], \\ &y(0) \sim y_0, \end{aligned} \tag{27}$$

with y_0 given by the proposed algorithm with stepsize h, and obtain the approximate solution of (26) on the interval $[0,b]$ $(b>a)$.

In Table 4 we list the values of $y(0)$ and the absolute errors at $t=1$ obtained with the NPCM on the space $V_{h,1}^{1/2}$.

In Figure 1 we present the absolute errors, on the interval $[0,1]$, for several choices of the stepsize h, and the results for both choices of the collocation parameters are extremely similar.

Remark 6. It is important to remark that when we used the NPCM on the space $V_{h,2}^{1/2}$ to solve (26), we obtained the exact solution, as expected, once the solution belongs to $V_2^{1/2}$.

As a second example we consider a multi-term boundary value problem

$$\begin{aligned} &D^2 y(t) + D^{0.5} y(t) + y(t) = t^3 + 6t + \frac{3.2t^{2.5}}{\Gamma(0.5)}, \quad t>0, \\ &y(0.1) = 0.001, \quad y'(0.1) = 0.03, \end{aligned} \tag{28}$$

whose analytical solution is known and given by $y(t) = t^3$.

	Collocation parameters			
	Radau points		Gauss points	
h	$y(0)$	Absolute error at $t=1$	$y(0)$	Absolute error at $t=1$
$1/20$	$7.750273504 \cdot 10^{-4}$	$2.14 \cdot 10^{-5}$	$3.759557731 \cdot 10^{-4}$	$1.75 \cdot 10^{-4}$
$1/40$	$2.775894907 \cdot 10^{-4}$	$6.05 \cdot 10^{-6}$	$9.473442333 \cdot 10^{-5}$	$4.44 \cdot 10^{-5}$
$1/80$	$9.917472973 \cdot 10^{-5}$	$1.64 \cdot 10^{-6}$	$2.382480307 \cdot 10^{-5}$	$1.12 \cdot 10^{-5}$
$1/160$	$3.534384896 \cdot 10^{-5}$	$3.52 \cdot 10^{-6}$	$5.982525181 \cdot 10^{-6}$	$2.82 \cdot 10^{-6}$
$1/320$	$1.256956138 \cdot 10^{-5}$	$8.78 \cdot 10^{-7}$	$1.500418875 \cdot 10^{-6}$	$7.09 \cdot 10^{-7}$

Table 4. Example (27) with $b = 1$: Comparison with the exact solution at the point $t = 1$ and corresponding values of y_0 of the initial value problem (27).

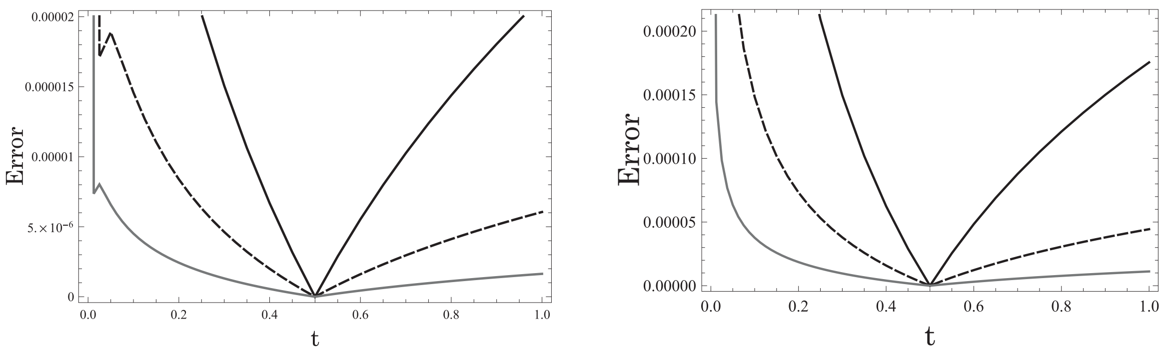

Figure 1. Example (26): Absolute errors using the NPCM on the space $V_{h,1}^{1/2}$, with Radau points (left) and Gauss points (right) as collocation parameters, with $h = 1/20$ (black line), $h = 1/40$ (dashed line) and $h = 1/80$ (gray line).

First, we convert this problem into the equivalent linear system of equations

$$\begin{cases} D^{0.5}y_1(t) = y_2(t), \\ D^{0.5}y_2(t) = y_3(t), \\ D^{0.5}y_3(t) = y_4(t), \\ D^{0.5}y_4(t) = -y_1(t) - y_2(t) + t^3 + 6t + \dfrac{3.2t^{2.5}}{\Gamma(0.5)}, \end{cases} \tag{29}$$

together with the conditions

$$y_1(0.1) = 0.001, \quad y_2(0.1) = y_{2a}, \quad y_3(0.1) = 0.03, \quad y_4(0.1) = y_{4a},$$

where y_{2a} and y_{4a} are unknown constants.

From [15, Theorem 1] the solution of (28) is unique which implies that $y_1(0), y_2(0), y_3(0)$ and $y_4(0)$ exist, are unique and moreover, taking [6, Lemma 2.1] into account, we must have $y_2(0) = y_4(0) = 0$ (the derivative of noninteger order, at $t = 0$, must be zero).

Therefore, given the initial value problem (29) equipped with the conditions

$$y_1(0) = y_{10}, \quad y_2(0) = 0, \quad y_3(0) = y_{30}, \quad y_4(0) = 0,$$

we can determine its approximate solution, say $(\widetilde{y}_1, \widetilde{y}_2, \widetilde{y}_3, \widetilde{y}_4)$, using any standard numerical initial solver. After that, we adjust the unknowns y_{10}, y_{30}, y_{2a} and y_{4a} in order to satisfy the

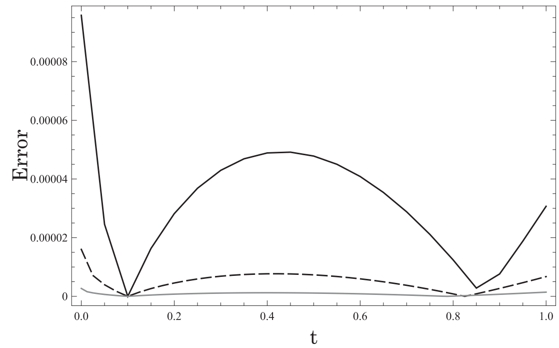

Figure 2. Example (28): Absolute errors using the NPCM on the space $V_1^{1/2}$, with Radau points as collocation parameters, with $h = 1/20$ (black line), $h = 1/40$ (dashed line) and $h = 1/80$ (gray line).

following linear system of equations:

$$\begin{aligned}
&\widetilde{y}_1(0.1) - 0.001 = 0,\\
&\widetilde{y}_2(0.1) - y_{2a} = 0,\\
&\widetilde{y}_3(0.1) - 0.03 = 0,\\
&\widetilde{y}_4(0.1) - y_{4a} = 0.
\end{aligned}$$

In our numerical experiments we have used the nonpolynomial collocation method, described in Section 2, on the space $V_{1,h}^{1/2}$, to solve the initial value problems. For that we must rewrite the system of fractional equations (29) as a system of integral equations and apply the nonpolynomial collocation method to the system of integral equations. In our numerical experiments we used the Radau points as collocation parameters.

In Figure 2 we present the absolute error, on the interval $[0, 1]$, for a sequence of stepsizes. In Table 5 we can see that the maximum of the errors at the collocation and mesh points converges to zero with the same order $p \sim 2.6$.

The results presented in Table 6 are computed using the NPCM on the space $V_{1,h}^{1/2}$, the Adams method (AM) and the fractional backward difference method (FBDM) to solve the initial value problems. We have compared the results obtained at $t = 1$ and for example (28) the method proposed in this work seems converge to zero with a higher order than the other two methods. However, we can also see that the computational cost of the method is considerably higher, by looking at the relative CPU times.

Finally, we consider a nonlinear example:

$$\begin{aligned}
D_*^\alpha y(t) &= \frac{40320}{\Gamma(9-\alpha)} t^{8-\alpha} - 3\frac{\Gamma(5+\alpha/2)}{\Gamma(5-\alpha/2)} t^{4-\alpha/2} + \frac{9}{4}\Gamma(\alpha+1)\\
&\quad + \left(\frac{3}{2}t^{\alpha/2} - t^4\right)^3 - (y(t))^{3/2}, \quad t \in (0, 1],\\
y(1) &= 1.
\end{aligned} \tag{30}$$

The exact solution of this boundary value problem is $y(t) = t^8 - 3t^{4+\alpha/2} + \frac{9}{4}t^\alpha$, meaning that the solution $y(t)$ can be written as $y(t) = u(t) + v(t)$ with $u(t) = \frac{9}{4}t^\alpha \in V_m^\alpha$ and $v(t) = t^8 - 3t^{4+\alpha/2} \in C^m([0, 1])$, $m = 1, 2$.

In Tables 7 and 8 we list the results obtained by the application of the NPCM to solve the initial value problems corresponding to the terminal value problem (30) (several values of α are considered) on the space $V_{1,h}^\alpha$ and $V_{2,h}^\alpha$, respectively.

h	ε_h	EOC	E_h	EOC
1/10	$1.391 \cdot 10^{-3}$	—	$5.690 \cdot 10^{-4}$	—
1/20	$2.248 \cdot 10^{-4}$	2.63	$9.579 \cdot 10^{-5}$	2.57
1/40	$3.691 \cdot 10^{-5}$	2.61	$1.601 \cdot 10^{-5}$	2.58
1/80	$6.140 \cdot 10^{-6}$	2.59	$2.690 \cdot 10^{-6}$	2.57

Table 5. Example (28): Maximum of the errors at the collocation and mesh points and estimates of the convergence order (EOC) using the NPCM on the space $V_{1,h}^{\alpha}$ to solve the initial value problems.

	NPCM			AM			FBDM		
h	$\lvert\widetilde{y}_1(1)-y(1)\rvert$	EOC	CPU	$\lvert\widetilde{y}_1(1)-y(1)\rvert$	EOC	CPU	$\lvert\widetilde{y}_1(1)-y(1)\rvert$	EOC	CPU
1/10	$1.413 \cdot 10^{-4}$	—	1.311	$8.717 \cdot 10^{-2}$	—	0	$7.204 \cdot 10^{-2}$	—	0.016
1/20	$3.069 \cdot 10^{-5}$	2.20	5.429	$3.096 \cdot 10^{-2}$	1.49	0.031	$2.674 \cdot 10^{-2}$	1.43	0.047
1/40	$6.724 \cdot 10^{-6}$	2.19	21.964	$1.109 \cdot 10^{-2}$	1.48	0.171	$9.709 \cdot 10^{-3}$	1.46	0.109
1/80	$1.427 \cdot 10^{-6}$	2.24	88.999	$3.965 \cdot 10^{-3}$	1.48	5.927	$3.487 \cdot 10^{-3}$	1.48	0.343

Table 6. Example (28): Absolute error at $t = 1$, estimates of the convergence order (EOC) and the CPU running-time (CPU) in seconds.

	$\alpha = 1/4$		$\alpha = 1/3$		$\alpha = 1/2$		$\alpha = 2/3$	
Colloc.	0.25, 0.5, 0.75, 1		0.3, 0.6, 1		0.5, 1		0.5, 1	
h	ε_h	EOC	ε_h	EOC	ε_h	EOC	ε_h	EOC
1/10	$1.67{\cdot}10^{-2}$	—	$3.23{\cdot}10^{-3}$	—	$1.18{\cdot}10^{-3}$	—	$5.21{\cdot}10^{-3}$	—
1/20	$9.69{\cdot}10^{-4}$	4.10	$2.69{\cdot}10^{-4}$	3.58	$8.50{\cdot}10^{-4}$	—	$2.21{\cdot}10^{-3}$	1.24
1/40	$5.63{\cdot}10^{-5}$	4.10	$2.67{\cdot}10^{-5}$	3.33	$3.83{\cdot}10^{-4}$	1.15	$7.26{\cdot}10^{-4}$	1.61
1/80	$3.27{\cdot}10^{-6}$	4.11	$3.03{\cdot}10^{-6}$	3.14	$1.32{\cdot}10^{-4}$	1.54	$2.13{\cdot}10^{-4}$	1.77
1/160	$1.89{\cdot}10^{-7}$	4.11	$3.71{\cdot}10^{-7}$	3.03	$4.00{\cdot}10^{-5}$	1.72	$5.87{\cdot}10^{-5}$	1.85

Table 7. Example (30) for several values of α: Maximum of the errors at the collocation points and estimates of the the convergence order (EOC) using the NPCM on the space $V_{1,h}^{\alpha}$ to solve the initial value problems.

	$\alpha = 1/3$		$\alpha = 1/2$		$\alpha = 2/3$		$\alpha = 9/10$	
Colloc.	$0.165 \cdot i$ $(i = 1, \dots, 5)$, 1		$0.25 \cdot i$ $(i = 1, \dots, 4)$		0.2, 0.4, 0.6, 0.8		0.2, 0.4, 0.6, 0.8	
h	ε_h	EOC	ε_h	EOC	ε_h	EOC	ε_h	EOC
1/10	$9.89{\cdot}10^{-3}$	—	$1.10{\cdot}10^{-3}$	—	$8.17{\cdot}10^{-4}$	—	$2.11 \cdot 10^{-4}$	—
1/20	$5.55{\cdot}10^{-4}$	4.15	$6.02{\cdot}10^{-5}$	4.06	$4.06{\cdot}10^{-5}$	4.33	$9.58 \cdot 10^{-6}$	4.46
1/40	$3.11{\cdot}10^{-5}$	4.16	$3.29{\cdot}10^{-6}$	4.19	$2.01{\cdot}10^{-6}$	4.34	$4.36 \cdot 10^{-7}$	4.46
1/80	$1.74{\cdot}10^{-6}$	4.16	$1.80{\cdot}10^{-7}$	4.19	$9.98{\cdot}10^{-8}$	4.33	$1.98 \cdot 10^{-8}$	4.46
1/160	$9.73{\cdot}10^{-8}$	4.16	$9.86{\cdot}10^{-9}$	4.19	$4.95{\cdot}10^{-9}$	4.33	$9.06{\cdot}10^{-10}$	4.45

Table 8. Example (30) for several values of α- Maximum of the errors at the collocation points and estimates of the the convergence order (EOC) using the NPCM on the space $V_{2,h}^{\alpha}$ to solve the initial value problems.

The numerical results presented in Tables 7 and 8 indicate a much better rate of convergence than would have been expected for this method, and this merits detailed consideration in a sequel to this work.

5. Conclusions

Here we proposed a standard shooting algorithm to approximate the solution of fractional terminal value problems. The main advantage of this method is that in order to obtain an optimal order of convergence it is not necessary to impose restrictive smoothness conditions on the solution. We have presented some numerical results illustrating the performance of the numerical scheme even in the case where the solution is nonsmooth. For future work, and in order to avoid the computational effort caused by the nonlocal nature of the fractional differential operator, we intend to adapt the numerical method already developed for solving initial value problems to solve terminal value problems without using shooting. This, in principle, will be possible if we discretise equation (3) directly.

Acknowledgments

The work was supported by an International Research Excellence Award funded through the Santander Universities scheme. The authors are pleased to thank the referees and Editor for their valuable advice which has led to several improvements in the paper.

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