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BVPs on infinite intervals: A test problem, a nonstandard finite difference scheme and a posteriori error estimator

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As far as the numerical solution of boundary value problems defined on an infinite interval is concerned, in this paper, we present a test problem for which the exact solution is known. Then we study an a posteriori estimator for the global error of a nonstandard finite difference scheme previously introduced by the authors. In particular, we show how Richardson extrapolation can be used to improve the numerical solution using the order of accuracy and numerical solutions from 2 nested quasi-uniform grids. We observe that if the grids are sufficiently fine, the Richardson error estimate gives an upper bound of the global error.

KEYWORDS
boundary value problems, global error estimator, nonstandard finite difference, order of accuracy, quasi-uniform grid

1 | INTRODUCTION

The main aim of this paper is to show how Richardson extrapolation can be used to define an error estimator for a nonstandard finite difference scheme applied to boundary value problems (BVPs) defined on the infinite interval. We construct at first a quasi-uniform map from a reference finite domain, and we build on the original domain a nonstandard finite difference scheme. As far as the novelty of this approach is concerned, we solve a given BVP on a semi-infinite interval by introducing a stencil that is constructed in a way to avoid the singularity at infinity, see Fazio and Jannelli[1] for more details.

Without loss of generality, we consider the class of BVPs

$$\begin{aligned} &\frac{d\mathbf{u}}{dx} = \mathbf{f}\,(x, \mathbf{u})\,, \qquad x \in [0, \infty), \\ &\mathbf{g}\,(\mathbf{u}(0), \mathbf{u}(\infty)) = \mathbf{0}, \end{aligned} \tag{1}$$

where $\mathbf{u}(x)$ is a d-dimensional vector with components ${}^{\ell}u(x)$ for $\ell = 1, \ldots, d$, $\mathbf{f} : [0, \infty) \times \mathrm{R}^d \to \mathrm{R}^d$, and $\mathbf{g} : \mathrm{R}^d \times \mathrm{R}^d \to \mathrm{R}^d$. Here, and in the following, we use Lambert notation for the vector components.[[2], pp1-5] Existence and uniqueness results, as well as results concerning the solution asymptotic behavior, for classes of problems belonging to Equation 1 have been reported in the literature, see for instance Granas et al,[3] Countryman and Kannan,[4] and Agarwal et al.[5-7]

Numerical methods for problems belonging to Equation 1 can be classified according to the numerical treatment of the boundary conditions imposed at infinity. The oldest and simplest treatment is to replace infinity with a suitable finite value, the so-called truncated boundary. However, this simple approach has revealed some drawbacks that suggest not to apply it. This is especially true if we have to face a given problem without any clue on its solution behavior. Several other treatments have been proposed in the literature to overcome the shortcomings of the truncated boundary approach. In this research area, they are worth of consideration: the formulation of the so-called asymptotic boundary conditions by de Hoog and Weiss,[8] Lentini and Keller,[9] and Markowich[10,11]; the reformulation of the given problem in a bounded domain as studied first by de Hoog and Weiss and more recently by Kitzhofer et al[12]; the free boundary formulation proposed by Fazio[13] where the unknown free boundary can be identified with a truncated boundary; the treatment on the original domain via pseudo-spectral collocation methods, see the book by Boyd[14] or the review by Shen and Wang[15] for more details on this topic; and, finally, a nonstandard finite difference scheme on a quasi-uniform grid defined on the original domain by Fazio and Jannelli.[1]

When solving a mathematical problem by numerical methods, one of the main concerns is related to the evaluation of the global error. For instance, Skeel[16] reported 13 strategies to approximate the numerical error. Here, we want to show how within Richardson extrapolation theory an error estimate can be derived. For any component U of the numerical solution, the global error e can be defined by

$$e = u - U, \tag{2}$$

where u is the exact analytical solution component. Usually, we have several different error sources: discretization, round-off, iteration, and programming errors. Discretization errors are due to our replacement of a continuous problem with a discrete one: The related error decreases by reducing the discretization parameters, enlarging the value of N, the number of grid points in our case. Round-off errors arise from the utilization of floating-point arithmetic to implement the algorithms available to solve the discrete problem. This kind of error usually decreases by using higher precision arithmetic, double or, when available, quadruple precision. Iteration errors are due to stopping an iteration algorithm that is converging but only as the number of iterations becomes large. Of course, we can reduce this kind of error by requiring more restrictive termination criteria for our iterations, in the present case, the iterations of Newton's method. Programming errors are behind the scope of this work, but they can be eliminated or at least reduced by adopting what is called structured programming. When the numerical error is caused prevalently by the discretization error and in the case of smooth enough solutions, the discretization error can be decomposed into a sum of negative powers of N

$$u = U_N + C_0\left(\frac{1}{N}\right)^{p_0} + C_1\left(\frac{1}{N}\right)^{p_1} + C_2\left(\frac{1}{N}\right)^{p_2} + \cdots , \tag{3}$$

where C_0, C_1, C_2, $\ldots$ are coefficients that depend of u and its derivatives, but are independent on N, and $p_0, p_1, p_2, \ldots$ are the true orders of the error. The value of each p_k, for $k = 0, 1, 2, \cdots$, is usually a positive integer with $p_0 < p_1 < p_2 < \cdots$. All together, the p_k's constitute an arithmetic progression of ratio $p_1 - p_0$, see Joyce.[17] The value of p_0 is called the asymptotic order or the order of accuracy of the method or of the numerical solution U.

2 | THE NUMERICAL SCHEME

To solve a problem in the class 1 on the original domain, we discuss first quasi-uniform grids maps from a reference finite domain. We introduce on the original domain a nonstandard finite difference scheme, developed by Fazio and Jannelli in previous study,[1] that allows us to impose the given boundary conditions exactly. As far as the novelty of our approach is concerned, we solve a given BVP on a semi-infinite interval by introducing a stencil that is constructed in such a way as to avoid the singularity at infinity.

2.1 | Quasi-uniform grids

Let us consider the smooth strict monotone quasi-uniform maps $x = x(\xi)$, the so-called grid generating functions, see Boyd[[14], pp325-326] or Canuto et al,[[18], p96]

$$x = -c \cdot \ln(1 - \xi), \tag{4}$$

and

$$x = c\frac{\xi}{1 - \xi}, \tag{5}$$

where $\xi \in [0, 1]$, $x \in [0, \infty]$, and $c > 0$ is a control parameter. So that a family of uniform grids $\xi_n = n/N$ defined on the interval $[0, 1]$ generates one parameter family of quasi-uniform grids $x_n = x(\xi_n)$ on the interval $[0, \infty]$. The 2 maps 4 and 5 are referred as logarithmic and algebraic map, respectively. As far as the authors' knowledge is concerned, van de Vooren and Dijkstra[19] were the first to use this kind of maps. We note that more than half of the intervals are in the domain with length

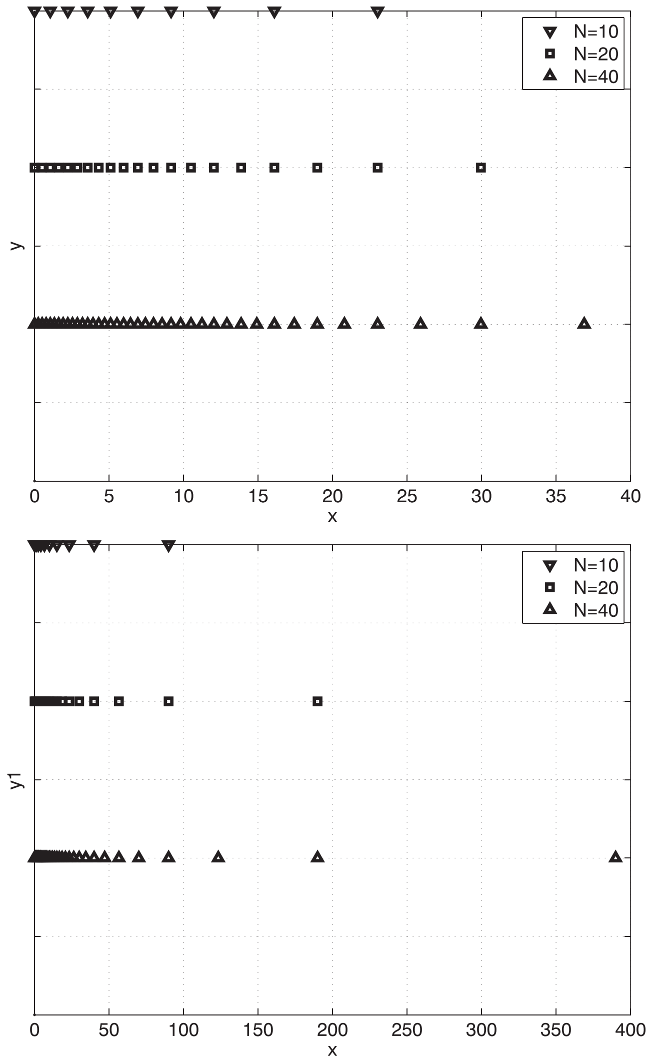

FIGURE 1 Quasi-uniform grids: top frame for Equation 4 and bottom frame for Equation 5. We note that, in both cases, the last mesh point is $x_N = \infty$

approximately equal to c and $x_{N-1} = c \ln N$ for Equation 4, while $x_{N-1} \approx cN$ for Equation 5. For both maps, the equivalent mesh in x is nonuniform with the most rapid variation occurring with $c \ll x$. The logarithmic map 4 gives slightly better resolution near $x = 0$ than the algebraic map 5, while the algebraic map gives much better resolution than the logarithmic map as $x \to \infty$. In fact, for all ξ, but $\xi = 0$, see Figure 1, it is easily verified that

$$-c \cdot \ln(1 - \xi) < c\frac{\xi}{1 - \xi}.$$

The problem under consideration can be discretized by introducing a uniform grid ξ_n of $N + 1$ nodes in $[0, 1]$ with $\xi_0 = 0$ and $\xi_{n+1} = \xi_n + h$ with $h = 1/N$, so that x_n is a quasi-uniform grid in $[0, \infty]$. The last interval in Equations 4 and 5, namely, $[x_{N-1}, x_N]$, is infinite but the point $x_{N-1/2}$ is finite, because the noninteger nodes are defined by

$$x_{n+\alpha} = x\left(\xi = \frac{n + \alpha}{N}\right),$$

with $n \in \{0, 1, \ldots, N - 1\}$ and $0 < \alpha < 1$. These maps allow us to describe the infinite domain by a finite number of intervals. The last node of such grid is placed at infinity, so the right boundary conditions are taken into account correctly. Figure 1 shows the 2 quasi-uniform grids $x = x_n$, $n = 0, 1, \ldots, N$ defined by Equations 4 and 5 with $c = 10$ and N equal to 10, 20, and 40, respectively, from top to bottom.

To derive the finite difference formulae, for the sake of simplicity, we consider a generic scalar variable $u(x)$. We can approximate the values of this scalar variable at mid-points of the grid by

$$u_{n+1/2} \approx \frac{x_{n+3/4} - x_{n+1/2}}{x_{n+3/4} - x_{n+1/4}} u_n + \frac{x_{n+1/2} - x_{n+1/4}}{x_{n+3/4} - x_{n+1/4}} u_{n+1}. \tag{6}$$

As far as the first derivative is concerned, we can apply the following approximation

$$\left.\frac{du}{dx}\right|_{n+1/2} \approx \frac{u_{n+1} - u_n}{2\left(x_{n+3/4} - x_{n+1/4}\right)}. \tag{7}$$

These formulae use the value $u_N = u(\infty)$, but not $x_N = \infty$. For a system of differential equations, Equations 6 and 7 can be applied component-wise.

2.2 | A nonstandard finite difference scheme

A nonstandard finite difference scheme on a quasi-uniform grid for the class of BVPs (Equation 1) can be defined by using the approximations given by Equations 6 and 7 above. A finite difference scheme for Equation 1 can be written as follows:

$$\begin{aligned}
&\mathbf{U}_{n+1} - \mathbf{U}_n - a_{n+1/2}\mathbf{f}\left(x_{n+1/2}, b_{n+1/2}\mathbf{U}_{n+1} + c_{n+1/2}\mathbf{U}_n\right) = \mathbf{0}, \\
&\text{for} \quad n = 0, 1, \ldots, N-1 \\
&\mathbf{g}\left(\mathbf{U}_0, \mathbf{U}_N\right) = \mathbf{0},
\end{aligned} \tag{8}$$

where

$$\begin{aligned}
a_{n+1/2} &= 2\left(x_{n+3/4} - x_{n+1/4}\right), \\
b_{n+1/2} &= \frac{x_{n+1/2} - x_{n+1/4}}{x_{n+3/4} - x_{n+1/4}}, \\
c_{n+1/2} &= \frac{x_{n+3/4} - x_{n+1/2}}{x_{n+3/4} - x_{n+1/4}},
\end{aligned} \tag{9}$$

for $n = 0, 1, \ldots, N-1$. The finite difference formulation 8 has order of accuracy $O(N^{-2})$. It is evident that Equation 8 is a nonlinear system of $d(N+1)$ equations in the $d(N+1)$ unknowns $\mathbf{U} = (\mathbf{U}_0, \mathbf{U}_1, \ldots, \mathbf{U}_N)^T$. For the solution of Equation 8, we can apply the classical Newton's method along with the simple termination criterion

$$\frac{1}{d(N+1)} \sum_{\ell=1}^{d} \sum_{n=0}^{N} |\Delta^{\ell} U_n| \leq \text{TOL}, \tag{10}$$

where $\Delta^{\ell} U_n$, for $n = 0, 1, \ldots, N$, $\ell = 1, 2, \ldots, d$, is the difference between 2 successive iterate components and TOL is a fixed tolerance.

3 | RICHARDSON EXTRAPOLATION AND ERROR ESTIMATE

The utilization of a quasi-uniform grid allows us to improve our numerical results. The algorithm is based on the Richardson extrapolation, introduced by Richardson in 2 studies,[20,21] and it applies to many finite difference methods: for numerical differentiation or integration, or for solving systems of ordinary or partial differential equations, see for instance, Sidi.[22] To apply Richardson extrapolation, we perform several calculations on embedded uniform or quasi-uniform grids with total number of nodes N_g for $g = 0, 1, \ldots, G$. For the numerical results reported in the next section, for instance, we have used 5, 10, 20, 40, 80, 160, 320, 640, 1280, 2560, or 5120 grid points. We can identify these grids with the index $g = 0$, the coarsest one, 1, 2, and so on towards the finest grid denoted by $g = G$. Between 2 adjacent grids, all nodes of the coarser one are identical to the even nodes of finer grid due to uniformity. To find a more accurate approximation, we can apply k Richardson extrapolations on the used grids

$$U_{g+1,k+1} = U_{g+1,k} + \frac{U_{g+1,k} - U_{g,k}}{2^{p_k} - 1}, \tag{11}$$

where $g \in \{0, 1, 2, \dots, G-1\}$, $k \in \{0, 1, 2, \dots, G-1\}$, the value $2 = N_{g+1}/N_g$ appearing in the denominator is the grid refinement ratio, and p_k is the true order of the discretization error. We note that each value of $U_{g+1,k+1}$ requires the computation of 2 solution U in 2 embedded grids, namely, $g+1$ and g at the extrapolation level k. For any g, the level $k = 0$ represents the numerical solution of U without any extrapolation, which is obtained as described in Section 2.2. In this case, Richardson extrapolation uses 2 solutions on embedded refined grids to define a more accurate solution that is reliable only when the grids are sufficiently fine. The case $k = 1$ is the classical single Richardson extrapolation, which is usually used to estimate the discretization error or to improve the solution accuracy. If we have computed the numerical solution on $G+1$ nested grids then we can apply Equation 11G times performing G Richardson extrapolations.

The theoretical orders of accuracy p_k of the numerical solution U with k extrapolations verify the relation

$$p_k = p_0 + k(p_1 - p_0), \tag{12}$$

where this equation is valid for $k \in \{0, 1, 2, \dots, G-1\}$. In any case, the values of p_k can be obtained a priori by using appropriate Taylor series or a posteriori as explained below.

To show how Richardson extrapolation can also be used to get an error estimate for the computed numerical solution, we use the notation introduced above. Taking into account Equation 11, we can conclude that the error estimate by Richardson extrapolation is given by

$$E_{g+1,k} = \frac{U_{g+1,k} - U_{g,k}}{2^{p_k} - 1}, \tag{13}$$

for $g \in \{0, 1, 2, \dots, G-1\}$, $k \in \{0, 1, 2, \dots, G-1\}$. Here, p_k is the true order of the discretization error. Hence, these values give estimations of the global error without knowledge of the exact solution. Of course, p_k can be found by

$$p_k \approx \frac{\log(|U_{g,k} - u|) - \log(|U_{g+1,k} - u|)}{\log(2)}, \tag{14}$$

where u is again the exact solution (or, if the exact solution is unknown, a reference solution computed with a suitable large value of N) evaluated at the same grid points of the numerical solution. We note that $E_{g+1,k}$ is the error estimate for the more accurate numerical solution $U_{g+1,k}$ but only on the grid points of N_g.

4 | AN APPLICATION: A BVP IN COLLOIDS THEORY

In this section, we consider a test problem with known exact solution for our error estimator. All numerical results reported in this paper were performed on an ASUS personal computer with i7 quad-core Intel processor and 16 GB of RAM memory running the Windows 8.1 operating system. The nonstandard finite difference scheme described above has been implemented in FORTRAN. The results listed in this section were computed by setting

$$\text{TOL} = 1E - 12. \tag{15}$$

The following test problem arises in the theory of colloids, see Alexander and Johnson[23]

$$\begin{aligned} &\frac{d^2u}{dx^2} - 2\sinh(u) = 0 \qquad x \in [0, \infty), \\ &u(0) = u_0, \qquad u(\infty) = 0, \end{aligned} \tag{16}$$

where $u_0 > 0$. The exact solution of the BVP 16, namely,

$$u(x) = 2\ \ln\left(\frac{(e^{u_0/2}+1)\,e^{-\sqrt{2}\,x} + (e^{u_0/2}-1)}{(e^{u_0/2}+1)\,e^{-\sqrt{2}\,x} - (e^{u_0/2}-1)}\right), \tag{17}$$

has been found by Countryman and Kannan,[4,24] and the missing initial condition is given by

$$\frac{du}{dx}(0) = -2\,\sqrt{\cosh(u_0) - 1}. \tag{18}$$

We rewrite the governing differential equation as a first-order system and indicate the exact solution by $\mathbf{u} = ({}^1u, {}^2u)^T$ and the numerical solution by $\mathbf{U} = ({}^1U, {}^2U)^T$. To fix a specific problem, as a first case, we consider $u_0 = 1$. As mentioned before, we apply 5, 10, 20, 40, 80, 160, 320, 640, 1280, 2560, or 5120 grid points, so that $G = 10$, and we adopt a continuation approach for the choice of the first iterate. This means that the accepted solution for $N = 5$ is used as first iterate for $N = 10$, where the new grid values are approximated by linear interpolations, and so on. The first iterate for the grid with $N = 5$, where the field variable was taken with a constant value 1 and its derivative was taken with a constant value −1, is shown on the top

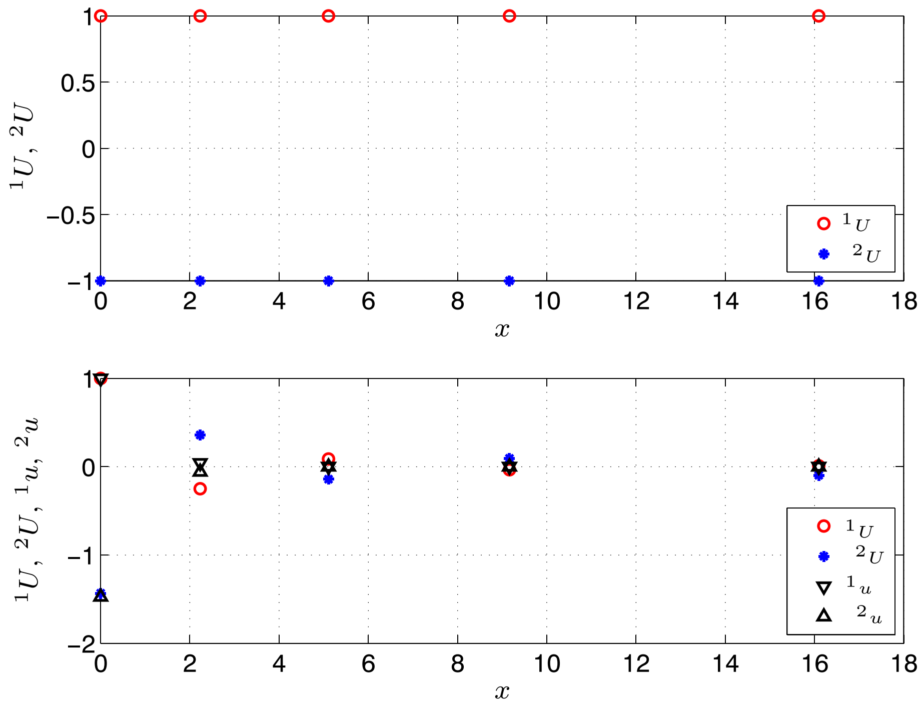

FIGURE 2 Sample iterates for problem 16 with $u_0 = 1$ [Colour figure can be viewed at wileyonlinelibrary.com]

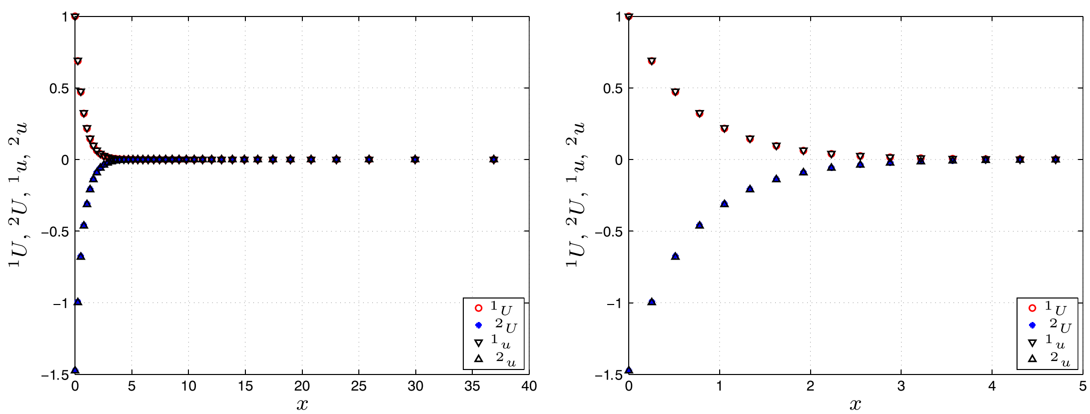

FIGURE 3 Final iterate and exact solution for problem 16 with $u_0 = 1$ and $N = 40$. On the left, solutions on the quasi-uniform grid, and on the right, zoom of the transient behavior in $[0, 5]$ [Colour figure can be viewed at wileyonlinelibrary.com]

frame of Figure 2. The bottom frame of the same figure shows the accepted numerical solution. Our relaxation algorithm takes 7 iterations to verify the termination criterion 10 with TOL given by Equation 15. Once the continuation approach has been initialized, the iteration routine needs 3 or 4 iterations to get a numerical solution that verifies the stopping criterion. For the sake of completeness in Figure 3, we display the numerical solution for $N = 40$ along with the exact solution.

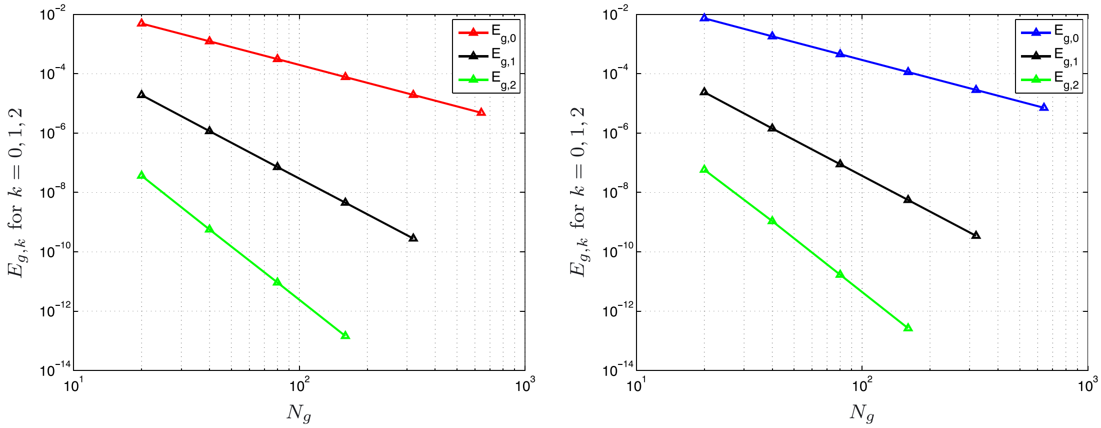

FIGURE 4 Problem 16 with $u_0 = 1$, global errors for the field variable on the left and its first derivative on the right [Colour figure can be viewed at wileyonlinelibrary.com]

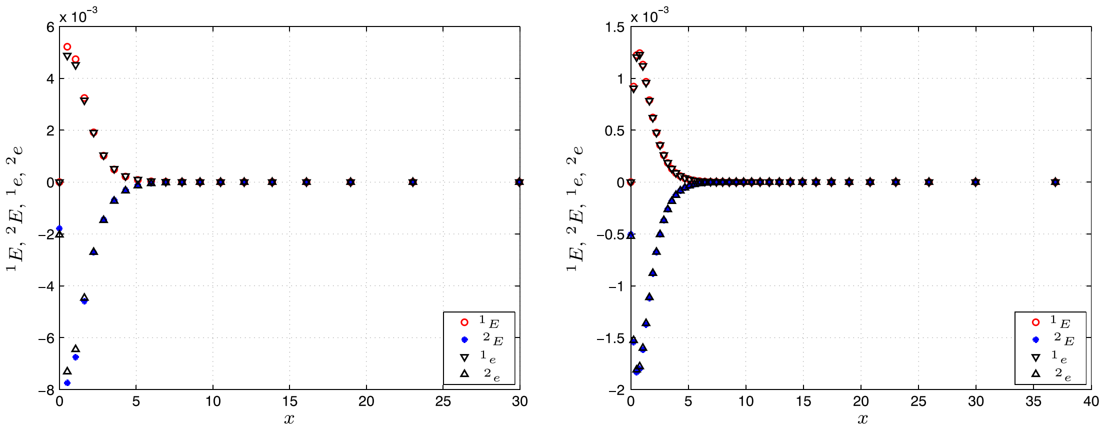

FIGURE 5 Global and a posteriori error estimates for the field variable and its first derivative for Equation 16 with $u_0 = 1$. Left: $N = 20, 40$, right: $N = 40, 80$. Here, ^1e and ^2e are the global errors defined by Equation 2, whereas ^1E and ^2E are the error estimates provided by Equation 13 [Colour figure can be viewed at wileyonlinelibrary.com]

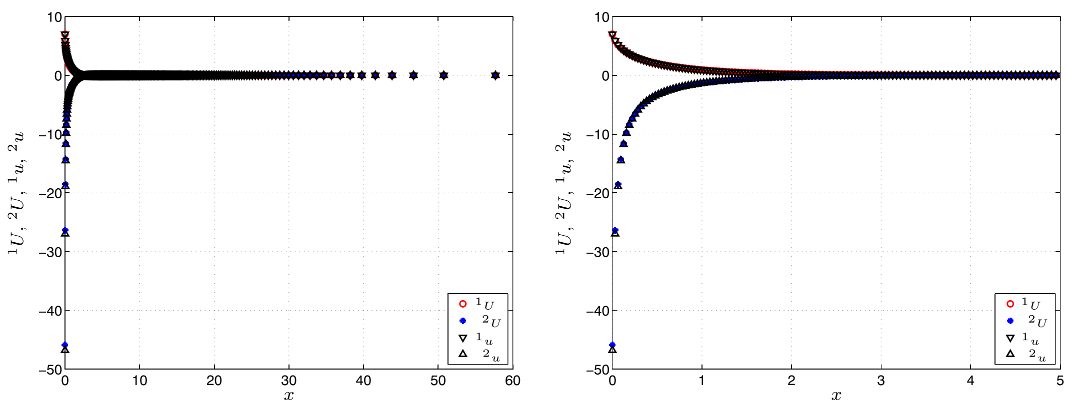

FIGURE 6 Final iterate and exact solution for problem 16 with $u_0 = 7$ and $N = 320$. On the left, solutions on the quasi-uniform grid, and on the right, zoom of the transient behavior in $[0, 5]$ [Colour figure can be viewed at wileyonlinelibrary.com]

Figure 4 shows in a log-log scale the computed empirical errors. We can compute the orders of accuracy p_0, p_1, and p_2 according to the formula 14. As it is easily seen from Figure 4, we obtained $p_0 \approx 2$, $p_1 \approx 4$, and $p_2 \approx 6$ for both the field variable and its first derivative. As far as the a posteriori error estimator is concerned in Figure 5, we report the computation related to 2 sample cases: namely, the estimate obtained by using $N = 20, 40$ and $N = 40, 80$. We note that the global error, for both the solution components, is of order 10^{-3} and decreases as we refine the grid. It is easily seen that the estimator defined by Equation 13 provides upper bounds for the global error.

A more challenging test case is given by setting $u_0 = 7$. The (inaccurate) accepted numerical solution for the grid with $N = 320$ is shown on Figure 6. Indeed, the chosen grid is unable to resolve the transient behavior at $x = 0$ of the first derivative of the solution. In Table 1, we list the computed as well as the extrapolated values obtained for the missing initial condition 18.

TABLE 1 Richardson extrapolation for $\frac{du}{dx}(0)={}^2U_0$

N_g	${}^2U_{g,0}$	${}^2U_{g,1}$	${}^2U_{g,2}$
160	−43.835177171609345		
320	−45.864298511341850	−46.540672291252690	
640	−46.537797149336093	−46.762296695334179	−46.777071655606278
1280	−46.725033491934731	−46.787445606134277	−46.789122200187620
2560	−46.773360098843838	−46.789468967813541	−46.789603858592159
5120	−46.785544794016836	−46.789606359074504	−46.789615518491907

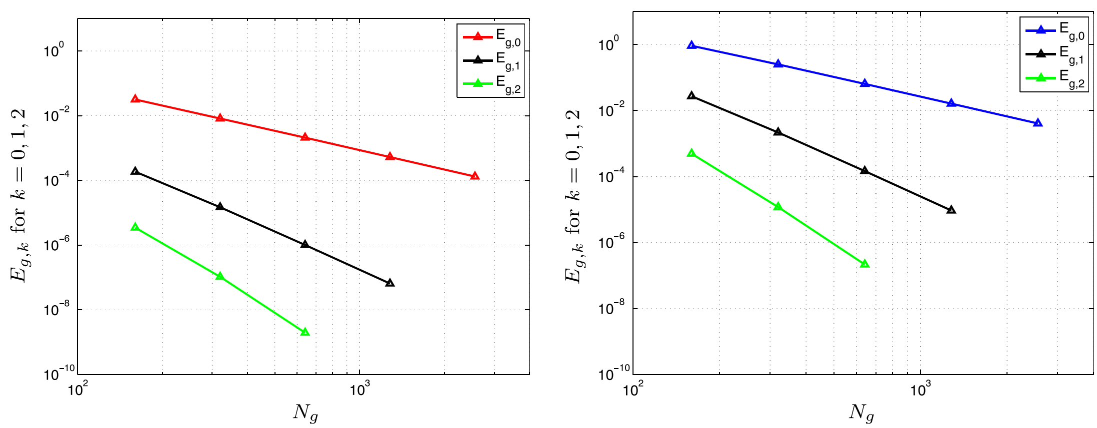

FIGURE 7 Problem 16 with $u_0 = 7$, global errors for the field variable on the left and its first derivative on the right [Colour figure can be viewed at wileyonlinelibrary.com]

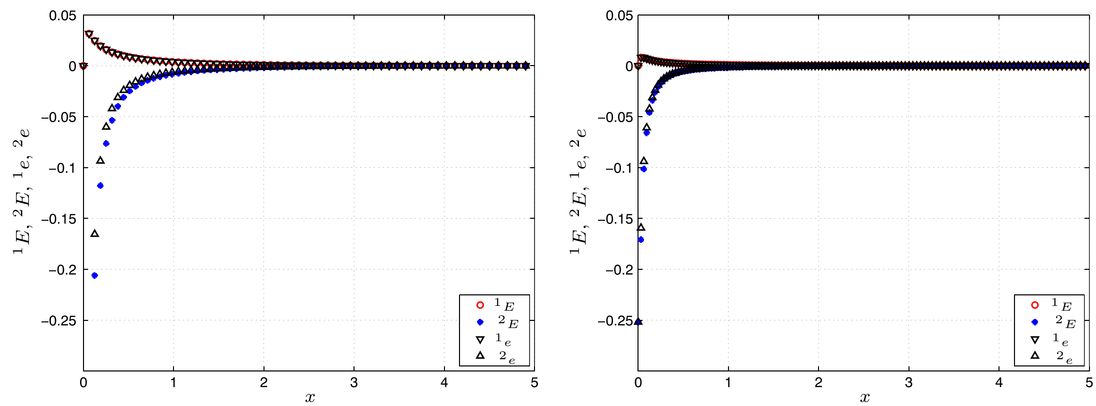

FIGURE 8 Zoom in the domain related to the initial transient behavior for the global errors and a posteriori error estimates for the field variable and its first derivative for Equation 16 with $u_0 = 7$. Left: $N = 160, 320$, right: $N = 320, 640$. Here, ${}^1e$ and ${}^2e$ are the global errors by Equation 2, whereas ${}^1E$ and ${}^2E$ are the error estimates provided by Equation 13 [Colour figure can be viewed at wileyonlinelibrary.com]

For the sake of brevity, in this table, we do not report the less accurate values obtained with the coarser grids. These results can be compared with the exact value, $\frac{du}{dx}(0) \approx -46.789615734913319$, obtained by Equation 18.

Figure 7 shows in a log-log scale the computed errors. From Figure 7, it is clear that the computed orders, using Equation 14, are slightly different from the theoretical ones, namely, $p_0 \approx 1.99$, $p_1 \approx 3.96$, and $p_2 \approx 5.77$.

As far as the a posteriori error estimator is concerned in Figure 8, we report the computation related to 2 sample cases: namely, the estimate obtained by using $N = 160, 320$ and $N = 320, 640$. Once again, the global error, for both the solution components, decreases as we refine the grid and the estimator defined by Equation 13 provides upper bounds for the global error.

5 | CONCLUSIONS

In this paper, we have defined an a posteriori estimator for the global error of a nonstandard finite difference scheme applied to BVPs defined on an infinite interval. A test problem was examined for which the exact solution is known. We tested our error estimator for 2 sample cases: a simpler one with smooth solution and a more challenging one presenting an initial fast transient behavior for one of the solution components. For this second test case, we showed how Richardson extrapolation can be used to improve the numerical solution using the order of accuracy and numerical solutions from 2 nested quasi-uniform grids.

In our previous paper,[1] instead of Equation 6, we derived the finite difference formula

$$u_{n+1/2} \approx \frac{x_{n+1} - x_{n+1/2}}{x_{n+1} - x_n} u_n + \frac{x_{n+1/2} - x_n}{x_{n+1} - x_n} u_{n+1}. \tag{19}$$

However, by setting $n = N - 1$ and $x_N = \infty$, this formula 19 reduces to $u_{N-1/2} = u_{N-1}$ that does not involve the boundary value u_N. Therefore, the boundary condition cannot be used. In Fazio and Jannelli,[1] this was the reason that forced us the use of a modification of this formula at $n = N-1$, see Fazio and Jannelli[1] for details. The novel approach proposed by the new formula 6 in this paper completely overcomes this drawback.

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