International Journal of Computer Mathematics
Vol. 80, No. 12, December 2003, pp. 1549–1560

A FREE BOUNDARY APPROACH AND KELLER'S BOX SCHEME FOR BVPs ON INFINITE INTERVALS

RICCARDO FAZIO*

Department of Mathematics, University of Messina, Salita Sperone 31, 98166 Messina, Italy

(Revised 10 February 2003; In final form 25 July 2003)

A free boundary approach for the numerical solution of boundary value problems (BVPs) governed by a third-order differential equation and defined on infinite intervals was proposed recently [SIAM J. Numer. Anal., 33 (1996), pp. 1473–1483]. In that approach, the free boundary (that can be considered as the truncated boundary) is unknown and has to be found as part of the solution. This eliminates the uncertainty related to the choice of the truncated boundary in the classical treatment of BVPs defined on infinite intervals. In this article, we investigate some open questions related to the free boundary approach. We recall the extension of that approach to problems governed by a system of first-order differential equations, and for the solution of the related free boundary problem we consider now the reliable Keller's box difference scheme. Moreover, by solving a challenging test problem of interest in foundation engineering, we verify that the proposed approach is applicable to problems where none of the solution components is a monotone function.

Keywords: Nonlinear boundary-value problems; Infinite intervals; Free boundary formulation; Finite difference methods

AMS Subject Classification: 65L10; 65L12; 34B15

C.R. Categories: G.1.7

1 INTRODUCTION

Boundary value problems (BVPs) on infinite intervals arise in several branches of science. A classical numerical treatment of these problems is to replace the original problem by the one defined on a finite interval, say $[a, x_\infty]$ where x_∞ is a truncated boundary (see, for instance, Collatz [9, pp. 150–151] or Fox [21, p. 92]). Often the original problem is solved by comparing the numerical results obtained for several values of x_∞. In particular, the value of x_∞ is varied until the computed results stabilize, at least, to a prefixed number of significant digits. For instance, in the case of the von Karman swirling flows, the opportunity to use values of x_∞ up to 200 was reported by Lentini and Keller [28] in order to investigate a fourth branch of the flow.

A theory for defining asymptotic boundary conditions to be imposed at the truncated boundary has been developed by de Hoog and Weiss [24], Lentini and Keller [27] and Markowich [31]. See also the related work by Markowich [32], Markowich and Ringhofer [33], Schmeiser [40]

* E-mail: rfazio@dipmat.unime.it

ISSN 0020-7160 print; ISSN 1029-0265 online
DOI: 10.1080/00207160310001614990

and Mattheij [34]. In the last decade, the asymptotic boundary conditions have been applied successfully to the numerical approximation of the so-called 'connecting orbits' problems of dynamical systems (see Refs. [4–6, 8, 10–12, 22, 23, 38, 39, 37]; more on this topic in the last section). Those problems are of interest, not only in connection with dynamical systems, but also in the study of traveling wave solutions of partial differential equations of parabolic (and, in time, hyperbolic) type as shown by Beyn [5], Friedman and Doedel [22], Bai *et al.* [3], and Liu *et al.* [30]. However, a truncated boundary allowing for a satisfactory accuracy of the numerical solution has to be determined by trial, and that seems to be the weakest point of the classical approach. Hence, a priori definition of the truncated boundary was indicated by Lentini and Keller [27] as an important area of research.

A different approach was proposed recently by this author in Ref. [17], where a free boundary formulation was introduced and the unknown free boundary was identified with a truncated boundary. In this approach, the free boundary is unknown and has to be found as part of the solution, which is a possible way to eliminate the uncertainty related to the choice of the truncated boundary. Moreover, the free boundary approach overcomes the need for a priori definition of the truncated boundary. The new approach has been applied to the Blasius problem [15], the Falkner–Skan equation with relevant boundary conditions [16], and a model describing the flow of an incompressible fluid over a slender parabola of revolution [17] (see also the recent survey in Ref. [19]).

The paper is structured as follows. In Section 2, we recall the extension of the approach proposed in Ref. [17] and worked out in Ref. [19] to a more general class of two-point BVPs. The main result is given by convergence of the solution of the free boundary problem to the solution of the original problem as a parameter, introduced within the formulation, goes to zero (see Theorem 1). In Section 3, we verify the applicability of a classical finite difference method within the mentioned approach (in substitution of the initial value methods, defined within group invariance theory, used in Refs. [15–17]). In that section, we consider the box difference scheme for the numerical solution of the obtained free BVPs and we recall the main properties of that scheme as shown by Keller [25]. In Sections 4 and 5, we introduce and solve a challenging test problem in foundation engineering [27]. Interest for that problem is motivated by the reason that all the problems solved earlier via the proposed approach are governed by a third-order differential equation where the second-order derivative of the solution is a positive monotone function that goes to zero at infinity. The main aim of this study is to verify the applicability of our approach when, for the problem under consideration, a similar property does not hold. The considered test problem is of particular concern here because none of the solution components is monotone on the interval of interest (see the bottom frame of Fig. 1 in Sec. 5). Moreover, by introducing a different free boundary formulation it is verified that the proposed approach can be also applied when the sign of the introduced parameter is unknown (see Tab. IV in Sec. 5). As far as the numerical solution of the free BVPs are concerned, we use a constant step-size implementation of the box difference scheme, in contrast to the application made in Ref. [15–17] of IMSL routines [26]. This results in lack of software control over the achieved accuracy; therefore, we choose to validate the obtained numerical results via a mesh refinement and Richardson's extrapolation. Meaningful results are reported for illustrative purposes in Section 5.

Section 6 deals with conclusions supported by evidences of the present work and indicate a possible way to extend the proposed approach to BVPs defined on the whole real line. Provided we are able to define an additional boundary condition, the free boundary approach is easily extended to the most general class of two-point BVPs defined on an infinite interval; the box difference scheme, if suitably applied within the proposed approach, provides accurate numerical results; the validity of the free boundary approach does not depend on the monotonicity of the solution of the original BVP.

2 THE FREE BOUNDARY APPROACH

Let us consider the class of BVPs defined on an infinite interval

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}), \quad x \in [a, \infty],$$
$$\mathbf{g}(\mathbf{y}(a), \mathbf{y}(\infty)) = \mathbf{0}, \tag{2.1}$$

where $\mathbf{y}(x)$ is an n-dimensional vector with $y_\ell(x)$ for $\ell = 1, \ldots, n$ as components, $\mathbf{f}$: $[a, \infty) \times \mathbb{R}^n \to \mathbb{R}^n$, a is a finite value (but see the last section for $a = -\infty$) and $\mathbf{g}$: $\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$. Note that the BVP (2.1) may admit several or even an infinite number of solutions (as an example consider the von Karman swirling flows investigated numerically by Lentini and Keller [28]). In applications, we require some regular behavior of the solution at infinity; consequently, one or more additional boundary conditions are available [see, Ref. 1, p. 486]. Additional boundary conditions also may be defined by applying physical considerations (see, for instance, the BVP defined in Sec. 4).We assume that at least one additional boundary condition is available

$$h(\mathbf{y}(a), \mathbf{y}(\infty)) = 0, \tag{2.2}$$

where h: $\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$. In that case, a free boundary formulation for Eq. (2.1) can be introduced as follows:

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}), \quad x \in [a, x_\varepsilon],$$
$$\mathbf{g}(\mathbf{y}(a; \varepsilon), \mathbf{y}(x_\varepsilon; \varepsilon)) = \mathbf{0},$$
$$h(\mathbf{y}(a; \varepsilon), \mathbf{y}(x_\varepsilon; \varepsilon)) = \varepsilon, \tag{2.3}$$

where $0 < |\varepsilon| \ll 1$, the solution of Eq. (2.3) depends on ε, that is $\mathbf{y}(x; \varepsilon)$. We would like $\mathbf{y}(x; \varepsilon)$ to be an approximation to $\mathbf{y}(x)$ on $[a, x_\varepsilon]$, and x_ε is unknown. Note that a solution of Eq. (2.3) is given by an ordered pair $(\mathbf{y}(x; \varepsilon), x_\varepsilon)$ and also that for $\varepsilon = 0$, Eq. (2.3) reduces to Eqs. (2.1) and (2.2); hence, if we set $\varepsilon = 0$, then $(\mathbf{y}(x), \infty)$ is a solution of Eq. (2.3).

The conditions for the uniform convergence of $\mathbf{y}(x; \varepsilon)$ to $\mathbf{y}(x)$ are given in the following theorem.

THEOREM 1 *Let us assume that each solution* $\mathbf{y}(x)$ *of Eq.* (2.1) *and* $\mathbf{y}(x; \varepsilon)$ *of Eq.* (2.3) *at least on a neighborhood of* $\varepsilon = 0$ *are 'isolated'* (*this implies that they are locally unique*). *Furthermore, we assume that* x_ε *is a differentiable function of* ε *on a neighborhood* I_0 *of* $\varepsilon = 0$ *and that the limit of* $dx_\varepsilon/d\varepsilon$ *as* ε *goes to zero exists. If all the components of* $\mathbf{y}(x; \varepsilon)$ *and of* $(d\mathbf{y}/d\varepsilon)(x; \varepsilon)$ *are continuous functions on the domain* $[a, x_\varepsilon] \times I_0$, *then the solution of Eq.* (2.3) *converges uniformly to the solution of Eq.* (2.1), *as* ε *tends to zero.*

Main idea of the Proof As a consequence of our hypotheses $M_i = \|\partial y_i(x; \varepsilon)/\partial\varepsilon\|_\infty$ is bounded for $i = 1, 2, \ldots, n$, and from the mean value theorem it follows that

$$\|y_i(x; \varepsilon) - y_i(x)\|_\infty \le M_i|\varepsilon| \text{ on } [a, x_\varepsilon], \qquad \text{for } i = 1, 2, \ldots, n,$$

where each M_i is independent from ε. Hence as $\varepsilon \to 0$ we get the uniform convergence result. ■

We have ignored technical details related to the limiting process $\varepsilon \to 0$. For the omitted details, see Lemma 1 and the proof of Theorem 1 in Ref. [17].

Let us note that there is no guarantee of convergence as ε goes to zero when $\|\partial y_i(x;\varepsilon)/\partial\varepsilon\|_\infty$ is not bounded for some $i = 1, 2, \ldots, n$. On the other hand, we can verify numerically that if $0 < \varepsilon_1 < \varepsilon_2$ or $\varepsilon_2 < \varepsilon_1 < 0$, then $x_{\varepsilon_2} < x_{\varepsilon_1}$. For results concerning the continuous dependence and differentiability of the solution of BVPs with respect to the boundary data, see Refs. [7, 13, 14].

The error related to our approach is first order in $|\varepsilon|$. For comparison, we have to notice that: (1) the error obtained within the truncated boundary approach for the Blasius problem is proportional to x_∞ as shown by Rubel [36]; (2) at least for connecting orbit problems, the best error estimate obtained within the asymptotic boundary approach is exponential small in x_∞, see Ref. [37].

Let us rewrite the free BVP (2.3) in standard form (see, Ref. [2]). To this end, we define $y_{n+1} = x_\varepsilon$ and the new independent variable

$$z = \frac{(x-a)}{(y_{n+1}-a)}; \tag{2.4}$$

so that, from Eq. (2.3) we get the following BVP:

$$\begin{gathered}\frac{\mathrm{d}\mathbf{Y}}{dz} = \mathbf{F}(z, \mathbf{Y}), \quad z \in [0, 1], \\ \mathbf{G}\left(\mathbf{Y}(0), \mathbf{Y}(1)\right) = \mathbf{0},\end{gathered} \tag{2.5}$$

where we have defined

$$\begin{aligned}\mathbf{Y}(z) &\equiv (\mathbf{y}(z), y_{n+1})^T, \\ \mathbf{F}(z, \mathbf{Y}) &\equiv ((y_{n+1}-a)\mathbf{f}((y_{n+1}-a)z + a, \mathbf{y}), 0)^T, \\ \mathbf{G}(\mathbf{Y}(0), \mathbf{Y}(1)) &\equiv (\mathbf{g}(\mathbf{y}(0), \mathbf{y}(1)), h(\mathbf{y}(0), \mathbf{y}(1)) - \varepsilon)^T.\end{aligned} \tag{2.6}$$

To simplify the notation, in Eqs. (2.5) and (2.6) and in the following, we omit the dependence of $\mathbf{y}$ and $\mathbf{Y}$ on ε.

It is an open question to verify if to each isolated solution of Eq. (2.1) will correspond, in general, an isolated solution of Eq. (2.3) or Eqs. (2.5) and (2.6). The author experiences that multiple solutions of free BVPs can arise for ordinary differential equations (ODEs) admitting periodic solutions (as reported in Ref. [18]). However, when an ODE admits periodic solutions it is inappropriate to set for it a boundary condition at infinity. As an example, let us consider the simplest ODE admitting periodic solutions given by $\mathrm{d}^2y/\mathrm{d}x^2 = -k^2y$, with $k = \text{const}$, which admits the general solution $y(x) = c_1\cos(kx + c_2)$; so that, we cannot define $y(\infty)$. Moreover, to investigate the existence and uniqueness of solution of free boundary problems we can apply a numerical test developed in Ref. [18]. Finally, let us remark here that, given a particular problem, Eqs. (2.5) and (2.6) are a BVP written in standard form and therefore it is possible to study the variational problem for Eqs. (2.5) and (2.6) to verify if their solutions are isolated (see, Refs. [1, 25, pp. 89–91]).

3 KELLER'S BOX SCHEME AND ITS PROPERTIES

Let us introduce a mesh of points $z_0 = 0$, $z_j = \sum_{i=1}^{j}\Delta z_i$ for $j = 1, 2, \ldots, J$ of nonuniform spacing Δz_i for $i = 1, 2, \ldots, J$ with $\Delta z = \max_j\{\Delta z_j\}$ and naturally $\sum_{i=1}^{J}\Delta z_i = 1$. We denote by the $(n+1)$-dimensional vector $\mathbf{V}_j$ the numerical approximation to the solution $\mathbf{Y}(z_j)$ of

Eq. (2.5) at the points of the mesh, that is for $j = 0, 1, \ldots, J$. Keller's box scheme for Eq. (2.5) can be written as follows:

$$\mathbf{V}_j - \mathbf{V}_{j-1} - \Delta z_j \mathbf{F}\left(z_{j-1/2}, \frac{\mathbf{V}_j + \mathbf{V}_{j-1}}{2}\right) = \mathbf{0}, \quad \text{for } j = 1, 2, \ldots, J$$
$$\mathbf{G}(\mathbf{V}_0, \mathbf{V}_J) = \mathbf{0}, \tag{3.1}$$

where $z_{j-1/2} = (z_j + z_{j-1})/2$. It is evident that Eq. (3.1) is a nonlinear system with respect to the unknown $(n+1)(J+1)$-dimensional vector $\mathbf{V} = (\mathbf{V}_0, \mathbf{V}_1, \ldots, \mathbf{V}_J)^T$. Following Keller, we apply the classical Newton's method along with a suitable termination criterion for the solution of Eq. (3.1) (see Sec. 5).

Let us recall now the main properties of the box scheme proved by Keller in the main theorem of Ref. [25]. Under the assumption that $\mathbf{Y}(z)$ and $\mathbf{F}(z, \mathbf{Y})$ are sufficiently smooth, each isolated solution of Eq. (2.5) is approximated by a difference solution of Eq. (3.1), which can be computed by Newton's method, provided a sufficiently fine mesh and an accurate initial guess are used for the Newton's method. As far as the accuracy question is concerned, the truncation error has an asymptotic expansion in powers of $(\Delta z)^2$; so that, Richardson's extrapolation can be employed to get two orders of magnitude improvement for application (see, for details, the discussion related to Tab. III in Sec. 5). Moreover, for separated boundary conditions, the Jacobian matrix has a special block tridiagonal form that can be solved by very efficient block-elimination procedures without destroying its zero structure.

4 A TEST PROBLEM

Here we consider a problem that was already used by Lentini and Keller [27] to test the asymptotic boundary conditions approach. That problem is of special interest here because none of the solution components is a monotone function (see the bottom frame of Fig. 1 in Sec. 5). Let $u(x)$ be the deflection of a semi-infinite pile embedded in soft soil at a distance x below the surface of the soil. The governing differential equation for the movement of the pile, in dimensionless form, is given by:

$$\frac{d^4u}{dx^4} = -P_1(1 - \exp^{-P_2 u}), \quad 0 < x < \infty,$$

where P_1 and P_2 are positive material constants. At the origin, a zero moment and a positive shear are assumed

$$\frac{d^2u}{dx^2}(0) = 0, \quad \frac{d^3u}{dx^3}(0) = P_3.$$

Moreover, from physical considerations it follows that $u(x)$ and all its derivatives go to zero at infinity; so that, the asymptotic boundary conditions

$$u(\infty) = 0, \quad \frac{du}{dx}(\infty) = 0$$

can be imposed. This problem is of interest in foundation engineering; for instance, in the design of drilling rigs above the ocean floor.

The governing differential equation can be rewritten as a first-order system by setting

$$y_i(x) = \frac{\mathrm{d}^{i-1}u}{\mathrm{d}x^{i-1}}(x), \qquad \text{for } i = 1, 2, 3, 4.$$

As far as the boundary condition (2.2) is concerned, several options can be taken into consideration. Since $y_3(\infty) = 0$ and $y_4(\infty) = 0$, to take into account both conditions, we can consider

$$h(\mathbf{y}(0), \mathbf{y}(\infty)) = |y_3(\infty)| + |y_4(\infty)|$$

and in this way the free boundary problem specializes to (note that $y_5 \equiv x_\varepsilon$):

$$\begin{aligned}
\frac{\mathrm{d}y_1}{\mathrm{d}z} &= y_5 y_2, \\
\frac{\mathrm{d}y_2}{\mathrm{d}z} &= y_5 y_3, \\
\frac{\mathrm{d}y_3}{\mathrm{d}z} &= y_5 y_4, \\
\frac{\mathrm{d}y_4}{\mathrm{d}z} &= -y_5 P_1 (1 - \exp^{-P_2 y_1}), \\
\frac{\mathrm{d}y_5}{\mathrm{d}z} &= 0,
\end{aligned} \tag{4.1}$$

$$\begin{gathered}
y_3(0) = 0, \quad y_4(0) = P_3, \\
y_1(1) = 0, \quad y_2(1) = 0, \quad |y_3(1)| + |y_4(1)| = \varepsilon;
\end{gathered} \tag{4.2}$$

that is,

$$\begin{aligned}
\mathbf{Y} &= (y_1, y_2, y_3, y_4, y_5)^T \\
\mathbf{F}(z, \mathbf{Y}) &= (y_5 y_2, y_5 y_3, y_5 y_4, -y_5 P_1 (1 - \exp^{-P_2 y_1}), 0)^T \\
\mathbf{G}(\mathbf{Y}(0), \mathbf{Y}(1)) &= (y_3(0), y_4(0) - P_3, y_1(1), y_2(1), |y_3(1)| + |y_4(1)| - \varepsilon)^T
\end{aligned}$$

in Eq. (2.5).

A second free boundary formulation for the considered test problem can be obtained by setting for the definition of Eq. (2.2) the following condition

$$h(\mathbf{y}(0), \mathbf{y}(\infty)) = y_4(\infty);$$

that is,

$$\begin{aligned}
\mathbf{Y} &= (y_1, y_2, y_3, y_4, y_5)^T \\
\mathbf{F}(z, \mathbf{Y}) &= (y_5 y_2, y_5 y_3, y_5 y_4, -y_5 P_1 (1 - \exp^{-P_2 y_1}), 0)^T \\
\mathbf{G}(\mathbf{Y}(0), \mathbf{Y}(1)) &= (y_3(0), y_4(0) - P_3, y_1(1), y_2(1), y_4(1) - \varepsilon)^T
\end{aligned}$$

in Eq. (2.5). The main difference between the two free boundary formulations is that while we know a priori that ε is a positive parameter in the former, we do not have any information on the sign of ε in the latter.

Representative numerical results, both for the first and the second free boundary formulation, are reported for comparison in Section 5.

5 NUMERICAL RESULTS

In this section, we report some of the numerical results obtained for the test problem introduced in the previous section. For comparative purposes, we used the same parameter values employed by Lentini and Keller [27]:

$$P_1 = 1, \quad P_2 = \frac{1}{2} \quad \text{and} \quad P_3 = \frac{1}{2}.$$

Moreover, we choose to consider the values of the missing initial conditions $y_1(0)$ and $y_2(0)$ as representative results. A direct way to proceed is to fix a fine grid and to perform a convergence test for decreasing values of ε, note that we should set $\varepsilon \ll 1$ (see Tab. I). Here and in the following, the exponential indicates a single precision arithmetic. We used constant step-sizes due to application of Richardson's extrapolation.

Figure 1 displays the numerical results related to different values of ε obtained by setting $J = 2000$. As it is easily seen, none of the solution components is monotone on the interval of interest.

To verify the numerical accuracy, we applied a mesh refinement obtained by fixing a value of $M > 0$ and setting $J = 2^k M$ for $k = 0, 1, 2, \ldots$. For the results reported in Table II, we fixed $M = 125$ and $J = 2^k M$ for $k = 0, 1, 2, \ldots, 7$.

For Newton's method, we used a simple termination criterion

$$\frac{1}{(n+1)(J+1)} \sum_{\ell=1}^{n+1} \sum_{j=0}^{J} |\Delta V_{j\ell}| \leq \text{TOL},$$

where $\Delta V_{j\ell}$, for $j = 0, 1, \ldots, J$ and $\ell = 1, 2, \ldots, n+1$, is the difference between two successive iterate components and TOL is a fixed tolerance. The results listed in Tables I and II were computed by setting $\text{TOL} = 1 \times 10^{-6}$.

A different validation is reported in Table III. The listed values were obtained by the extrapolation formula

$$T_k^r = \frac{4^r T_k^{r-1} - T_{k-1}^{r-1}}{4^r - 1}, \quad \text{for } k, r = 0, 1, 2, \ldots,$$

where T_k^0 is a result of interest, say $y_1(0)$ or $y_2(0)$, computed by a mesh of $2^k M + 1$ points and r is the extrapolation index. Note that from the extrapolation formula we get $T_k^r = T_k^{r-1}$ when $T_k^{r-1} = T_{k-1}^{r-1}$; so that, there is no need to extend Table III with further rows.

The key point for the numerical solution of the difference system is that Newton's method converges only locally. Therefore, some preliminary numerical experiments may be helpful

TABLE I Numerical Results for the BVP (4.1) and (4.2), Here $J = 1000$.

ε	*it*	$y_1(0)$	$y_2(0)$	$y_3(1)$	$y_4(1)$	$y_5(0) = y_5(1)$
1×10^{-1}	9	1.41566	−0.805665	-5.9×10^{-2}	-4.1×10^{-2}	6.46
1×10^{-2}	11	1.42148	−0.808104	-4.4×10^{-3}	5.6×10^{-3}	8.84
1×10^{-3}	13	1.42154	−0.808146	8.9×10^{-4}	1.1×10^{-4}	13.13
1×10^{-4}	28	1.42154	−0.808144	-7.0×10^{-5}	-3.0×10^{-5}	17.75

Note: The 'it' column indicates the number of iterations.

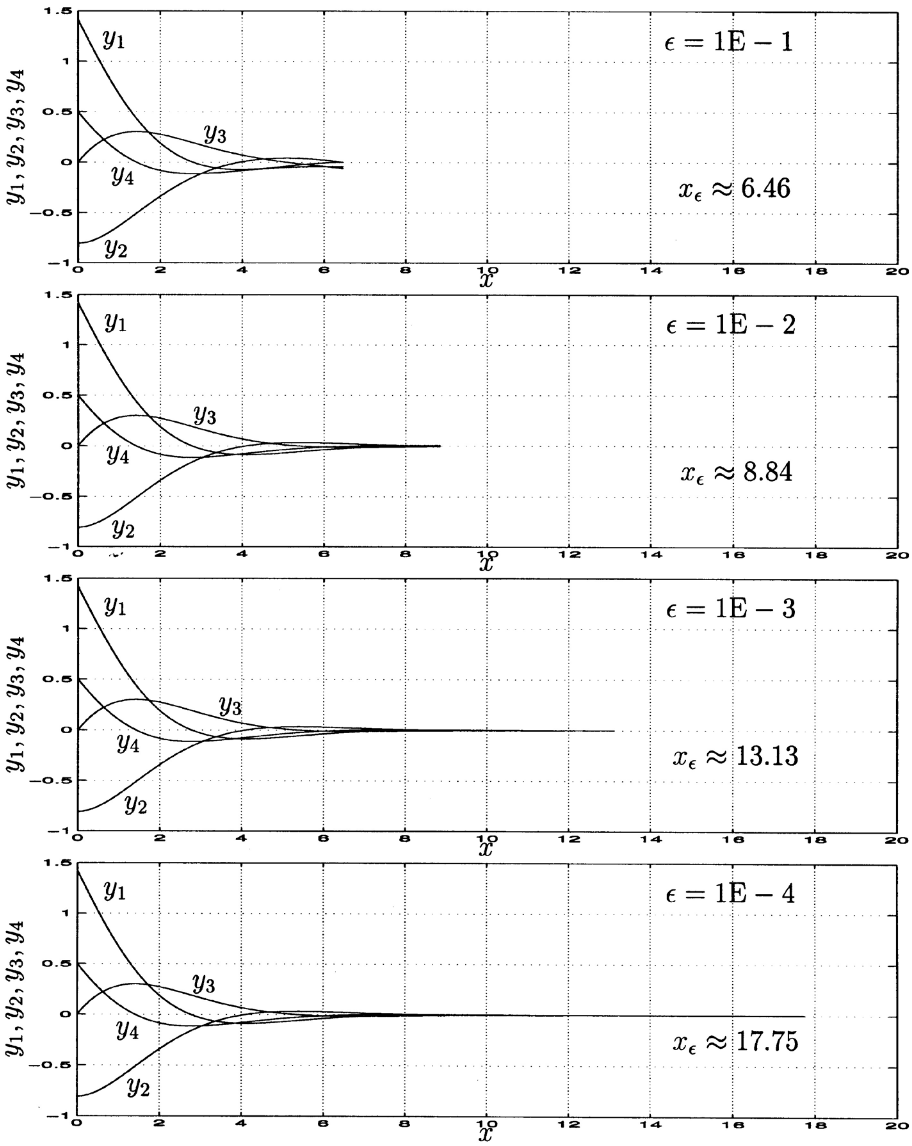

FIGURE 1 The numerical solution of the pile problem by the free boundary approach.

and are worth consideration. However, for the results reported in Tables I and II, our initial guess to start the iterations was always as follows:

$$\begin{aligned}
y_1(z) &= 10(1-z),\\
y_2(z) &= 10(1-z),\\
y_3(z) &= \varepsilon,\\
y_4(z) &= P_3(1-z)+\varepsilon,\\
y_5(z) &= 10.
\end{aligned}$$

TABLE II Numerical Results Computed via a Mesh Refinement. Here $\varepsilon = 1 \times 10^{-4}$.

J	*Iterations*	$y_1(0)$	$y_2(0)$
125	22	1.421166	−0.807913
250	24	1.421450	−0.808089
500	24	1.421521	−0.808133
1000	22	1.421539	−0.808144
2000	22	1.421543	−0.808147
4000	22	1.421544	−0.808148
8000	22	1.421545	−0.808148
16 000	22	1.421545	−0.808148

Note: When $J = 2000$ we get $y_3(1) = -7 \times 10^{-5}$, $y_4(1) = -3 \times 10^{-5}$ and $y_5(0) = y_5(1) = 17.747988$.

A remark is due about this initial guess: $y_1(z)$ is several times over-estimated, $y_2(z)$ has the wrong sign, etc., and last but not least the starting value of $y_5(z)$ could be related to the value of ε because $y_5(z)$ should be a decreasing function of ε. We have verified with further computations that the number of iterations is reduced by a more accurate initial guess. Moreover, a drastic reduction in the number of iterations was observed by adopting a continuation philosophy; that is, by considering the numerical results for a value of ε as the initial guess for Newton's method with the next value of ε. This is the main advantage of finite difference against initial value methods because for the former we can consider ε as the continuation parameter. By implementing this continuation idea the numerical results listed in Table I were found again with the following sequence of iterations: 9, 6, 8, 9.

In the following, we report the results related to the second free boundary formulation of the previous section. In this case, the sign of ε is not defined a priori; so that, we have to consider ε going to zero, separately, from the right and from the left. The numerical results listed in Table IV were obtained with the following initial guess:

$$
\begin{aligned}
y_1(z) &= 10(1 - z),\\
y_2(z) &= 10(1 - z),\\
y_3(z) &= 0,\\
y_4(z) &= P_3(1 - z),\\
y_5(z) &= 50.
\end{aligned}
$$

Note that the lack of convergence in the case corresponding to $\varepsilon = -1 \times 10^{-5}$ and $J = 25$ indicates that the initial guess is not sufficiently accurate. We have verified that by setting $y_5(z) = 25$, in the initial guess reported above, the applied termination criterion is verified within 19 iterations. We remark that for the missing initial conditions the same results are obtained when ε goes to zero from the right and from the left. Moreover, these results are

TABLE III Extrapolation of Some of the Results Listed in Table II with $M = 125$ and the Indicated Values of k.

k	$y_1(0)^0_k$	$y_2(0)^0_k$	$y_1(0)^1_k$	$y_2(0)^1_k$
0	1.421166	−0.807913		
1	1.421450	−0.808089	1.421545	−0.808148
2	1.421521	−0.808133	1.421545	−0.808148

TABLE IV Numerical Results for Different Mesh-Spacings. Here TOL $= 5 \times 10^{-6}$.

ε	J	*it*	$y_5(0) = y_5(1)$	$y_3(1)$	$y_1(0)$	$y_2(0)$
1×10^{-5}	25	25	21.4	1.4×10^{-5}	1.40823	−0.79991
1×10^{-5}	50	21	21.0	5.0×10^{-6}	1.41825	−0.80611
1×10^{-5}	100	23	19.2	-1.2×10^{-5}	1.42085	−0.80772
1×10^{-5}	200	21	19.3	-1.0×10^{-5}	1.42137	−0.80804
1×10^{-5}	400	21	19.3	-6.0×10^{-6}	1.42150	−0.80812
1×10^{-5}	800	21	19.3	-1.0×10^{-5}	1.42153	−0.80814
1×10^{-5}	1600	21	19.3	-1.0×10^{-5}	1.42154	−0.80815
1×10^{-5}	3200	21	19.3	-1.0×10^{-5}	1.42154	−0.80815
-1×10^{-5}	25	NC				
-1×10^{-5}	50	19	18.1	-5.2×10^{-5}	1.41983	−0.80662
-1×10^{-5}	100	18	18.2	-4.7×10^{-5}	1.42092	−0.80776
-1×10^{-5}	200	18	18.2	-4.6×10^{-5}	1.42139	−0.80805
-1×10^{-5}	400	18	18.2	-4.6×10^{-5}	1.42151	−0.80812
-1×10^{-5}	800	18	18.2	-4.6×10^{-5}	1.42154	−0.80814
-1×10^{-5}	1600	18	18.2	-4.6×10^{-5}	1.42154	−0.80815
-1×10^{-5}	3200	18	18.2	-4.6×10^{-5}	1.42154	−0.80815

Note: NC is an abbreviation for no convergence; '*it*' = number of iterations.

in good agreement with those obtained in Tables I–III. All computations were performed in FORTRAN on a SUN Ultra 5 workstation.

6 FINAL REMARKS AND CONCLUSIONS

The classical numerical treatment of BVPs defined on infinite intervals is based on the introduction of a truncated boundary x_∞ where suitable boundary conditions are imposed. To define the boundary conditions to be imposed at the truncated boundary an asymptotic analysis was developed by de Hoog and Weiss [24], Lentini and Keller [27], and Markowich [31]. As far as the test problem of Section 4 is concerned, the related asymptotic boundary conditions are given by:

$$y_2(x_\infty) + 2^{-1/2} Q^{-1} y_3(x_\infty) + 2^{-1/2} Q^{-3} P_1 [1 - \exp^{-P_2 y_1(x_\infty)}] = 0,$$
$$2^{-1/2} Q^{-1} y_3(x_\infty) - Q^{-2} y_4(x_\infty) - 2^{-1/2} Q^{-3} P_1 [1 - \exp^{-P_2 y_1(x_\infty)}] = 0,$$

where $Q = (1/2)^{1/4}$, as reported by Lentini and Keller [27]. Note that the free boundary approach is as simple as the truncated boundary one in contrast to the asymptotic boundary approach (in this context see also the opinion expressed by Ockendon [35]).

Following the idea introduced in Ref. [17], we propose to formulate BVPs on infinite intervals as free BVPs. Let us remark that the two limiting processes, namely $\Delta x \to 0$ and $\varepsilon \to 0$, are independent, but from a numerical viewpoint the order in which they are performed does matter. In fact, to solve effectively a BVP defined on an infinite interval by the free boundary approach we have to find out first of all a suitable value of ε that will assure an acceptable error according to the proof of Theorem 1. After that we can consider a mesh refinement or a Richardson's extrapolation in order to improve the accuracy of the numerical solution. Let us stress that by a mesh refinement or a Richardson's extrapolation we may hope to get an accurate solution of the free BVP for a fixed value of ε; to obtain an accurate approximation of the original problem on $[a, x_\varepsilon]$ we must identify first an appropriate value of ε. In this context, the numerical results in Table I are essential for the correct application of the free boundary approach. Moreover, the above discussion explains the way we used $J = 1000$ in Table I and $J = 2000$ with $\varepsilon = 1 \times 10^{-4}$ in Table II.

As far as the missing initial conditions for the test problem are concerned, a comparison of the obtained values of $y_1(0)$ and $y_2(0)$ can be made, respectively, with the values 1.4215 and -0.80814 reported by Lentini and Keller [27]. They used the mentioned asymptotic boundary conditions and employed PASVAR, a routine based upon the trapezoidal difference scheme with automatic mesh refinement and deferred corrections as described by Lentini and Pereyra [29]. The code is rather sophisticated because it adjusts automatically the mesh and the order of accuracy.

In conclusion, the free boundary approach is easily extended to the most general class of two-point BVPs defined on an infinite interval. The present work indicates that the validity of our approach does not depend on the monotonicity of the solution of the BVP. As we have shown in Refs. [15–17] and herein, accurate numerical results within the proposed approach are obtained either by initial value or finite difference methods.

Let us discuss, at the end of this work, a possible way to extend the free boundary approach to the numerical solutions of problems defined on the whole real line (for instance, the connecting orbits problems mentioned in Sec. 1). For these problems, all boundary conditions are imposed at plus or minus infinity, so that we set $a = -\infty$ in Eqs. (2.1) and (2.2). A free boundary formulation can be defined by substituting the boundary condition (2.2) with

$$h(\mathbf{y}(-x_\varepsilon), \mathbf{y}(x_\varepsilon)) = \varepsilon.$$

Moreover, the resulting free BVP can be rewritten in standard form by setting again $y_{n+1} = x_\varepsilon$ and introducing the independent variable transformation

$$z = \frac{x + y_{n+1}}{2y_{n+1}}$$

instead of Eq. (2.4). The above transformation maps $[-x_\varepsilon, x_\varepsilon]$ to $[0, 1]$.

An application of the free boundary approach to a homoclinic orbit problem can be found in Ref. [20].

Acknowledgement

The research of this work was partially supported by the Italian “MURST”.

References

[1] U. M. Ascher, R. M. M. Mattheij, and R. D. Russell, *Numerical Solution of Boundary Value Problems for Ordinary Differential Equations*, Prentice Hall, Englewood Cliffs, New Jersey (1988).

[2] U. Ascher and R. D. Russell, Reformulation of boundary value problems into ‘standard’ form, *SIAM Rev.*, 23 (1981) 238–254.

[3] F. Bai, A. Spence, and A. M. Stuart, The numerical computation of heteroclinic connections in systems of gradient partial differential equations, *SIAM J. Appl. Math.*, 53 (1993) 743–769.

[4] W.-J. Beyn, Global bifurcation and their numerical computation, In: D. Rossed, B. D. Dier, and A. Spence (Eds.), *Bifurcation: Numerical Techniques and Applications*, Kluwer, Dordrecht (1990), pp. 169–181.

[5] W.-J. Beyn, The numerical computation of connecting orbits in dynamical systems, *IMA J. Numer. Anal.*, 9 (1990) 379–405.

[6] W.-J. Beyn, Numerical methods for dynamical systems, In: W. Light (Ed.), *Advances in Numerical Analysis*, Clarendon Press, Oxford (1991–1992), pp. 175–236.

[7] R. Brantley and J. Henderson, Some analogues of a theorem of Peano for boundary value problems, *Tamkang J. Math.*, 22 (1991) 83–98.

[8] A. R. Champneys and Yu. A. Kuznetsov, Numerical detection and continuation of codimension-two homoclinic bifurcations, *Int. J. Bifurcation and Chaos*, 4 (1994) 785–822.

[9] L. Collatz, *The Numerical Treatment of Differential Equations*, 3rd ed., Springer-Verlag, Berlin (1960).

[10] E. J. Doedel, AUTO: A program for the automatic bifurcation analysis of autonomous systems, *Congr. Numer.*, 30 (1981) 265–284.

[11] E. J. Doedel and J. P. Kernevez, AUTO: software for continuation and bifurcation problems in ordinary differential equations, *Technical Report*, Applied Mathematics, California Institute of Technology, Pasadena, CA (1986).

[12] E. J. Doedel and M. J. Friedman, Numerical computation of heteroclinic orbits, *J. Comp. Appl. Math.*, 26 (1989) 155–170.

[13] J. A. Ehme, Differentiation of solutions of boundary value problems with respect to nonlinear boundary conditions, *J. Differential Equations*, 101 (1993) 139–147.

[14] J. A. Ehme and D. N. Brewley, Continuous data dependence for a class of nonlinear boundary value problems, *Commun. Appl. Nonlinear Anal.*, 3 (1996) 59–65.

[15] R. Fazio, The Blasius problem formulated as a free boundary value problem, *Acta Mech.*, 95 (1992) 1–7.

[16] R. Fazio, The Falkner–Skan equation: Numerical solutions within group invariance theory, *Calcolo*, 31 (1994) 115–124.

[17] R. Fazio, A novel approach to the numerical solution of boundary value problems on infinite intervals, *SIAM J. Numer. Anal.*, 33 (1996) 1473–1483.

[18] R. Fazio, A numerical test for the existence and uniqueness of solution of free boundary problems, *Appl. Anal.*, 66 (1997) 89–100.

[19] R. Fazio, A similarity approach to the numerical solution of free boundary problems, *SIAM Rev.*, 40 (1998) 616–635.

[20] R. Fazio, A survey on free boundary identification of the truncated boundary in numerical BVPs on infinite intervals, *J. Comp. Appl. Math.*, 140 (2002) 331–344.

[21] L. Fox, *Numerical Solution of Two-Point Boundary Value Problems in Ordinary Differential Equations*, Clarendon Press, Oxford (1957).

[22] M. J. Friedman and E. J. Doedel, Numerical computation and continuation of invariant manifolds connecting fixed points, *SIAM J. Numer. Anal.*, 28 (1991) 789–808.

[23] M. J. Friedman and E. J. Doedel, Computational methods for global analysis of homoclinic and heteroclinic orbits: a case study, *J. Dynamics Diff. Eqns.*, 5 (1993) 59–87.

[24] F. R. de Hoog and R. Weiss, An approximation theory for boundary value problems on infinite intervals, *Computing*, 24 (1980) 227–239.

[25] H. B. Keller, Accurate difference methods for nonlinear two-point boundary value problems, *SIAM J. Numer. Anal.*, 11 (1974) 305–320.

[26] *Math/Library User's Manual, Fortran Subroutines for Mathematical Applications*, Version 1.1, 1989.

[27] M. Lentini and H. B. Keller, Boundary value problems on semi-infinite intervals and their numerical solutions, *SIAM J. Numer. Anal.*, 17 (1980) 577–604.

[28] M. Lentini and H. B. Keller, The von Karman swirling flows, *SIAM J. Appl. Math.*, 38 (1980) 52–64.

[29] M. Lentini and V. Pereyra, An adaptive finite difference solver for two-point boundary value problems with mild boundary layers, *SIAM J. Numer. Anal.*, 14 (1977) 91–111.

[30] L. Liu, G. Moore and R. D. Russell, Computation and continuation of homoclinic and heteroclinic orbits with arclength parameterization, *SIAM J. Sci Comp.*, 18 (1997) 69–93.

[31] P. A. Markowich, A theory for the approximation of solution of boundary value problems on infinite intervals, *SIAM J. Math. Anal.*, 13 (1982) 484–513.

[32] P. A. Markowich, Analysis of boundary value problems on infinite intervals, *SIAM J. Math. Anal.*, 14 (1983) 11–37.

[33] P. A. Markowich and C. A. Ringhofer, Collocation methods for boundary value problems on "long" intervals, *Math. Comp.*, 40 (1983) 123–150.

[34] R. M. M. Mattheij, On the computation of BVP on infinite intervals, *Math. Comp.*, 48 (1987) 522–549.

[35] J. R. Ockendon, *Math. Rev.*, 84c:34021.

[36] L. A. Rubel, An estimation of the error due to the truncated boundary in the numerical solution of the Blasius problem, *Quart. Appl. Math.*, 13 (1955) 203–206.

[37] B. Sandstede, Convergence estimates for the numerical approximation of homoclinic solutions, *IMA J. Numer. Anal.*, 17 (1997) 437–462.

[38] S. Schecter, Numerical computation of saddle-node homoclinic bifurcation points, *SIAM J. Numer. Anal.*, 30 (1993) 1155–1178.

[39] S. Schecter, Rate of convergence of numerical approximations to homoclinic bifurcation points, *IMA J. Numer. Anal.*, 15 (1995) 23–60.

[40] C. Schmeiser, Approximate solution of boundary value problems on infinite intervals by collocation methods, *Math. Comp.*, 46 (1986) 479–490.