

SIMILARITY AND NUMERICAL ANALYSIS FOR FREE BOUNDARY VALUE PROBLEMS*

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We consider the similarity properties of nonlinear ordinary free boundary value problems, i.e.,

$$\begin{aligned}u'' &= f(x, u, u') \quad x \in (0, s) \quad s > 0 \\ u(0) &= \alpha; \quad u(s) = u'(s) = 0; \quad \alpha \neq 0.\end{aligned}$$

By making use of group properties we show that for the two classes of problems

$$\begin{aligned}f &= u^{1-2\delta} F(x/u^\delta, u'/u^{1-\delta}) \\ f &= e^{-2\delta u} \Phi(xe^{-\delta u}, u'e^{\delta u}),\end{aligned}$$

it is possible to define a method that allows us to find the location of the free boundary s through the first numerical integration and the numerical solution by means of a second integration.

Moreover, by requiring invariance of some parameter, we give an important extension of the method to solve a problem that does not belong to the two classes in point.

Finally we remark that the method is self-validating.

KEY WORDS: Free boundary value problem, similarity properties.

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1. INTRODUCTION

In recent years the group analysis approach has proved to be a useful tool either for finding out exact solutions or for developing numerical procedures to mathematical models of relevant interest. Most of the literature about utilization of group properties in applicative problems make use of some computations.

In connection with partial differential equations we can quote the works of [2]–[6], [8]–[10] and [17].

This paper is concerned with ordinary differential equation problems. Within such a context, the first application was given by Toepfer [18] without direct consideration of group properties. In his attempt to solve Blasius's equation in boundary layer theory, by using a series expansion method he discovered a transformation which converts the boundary value problem into an initial value

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problem. It was in the paper of Klamkin [12] and later of Na [14] that this transformation was regarded as a consequence of the invariance of the governing model under the action of the stretching group. Some important extensions of the method were given in [14] where boundary value problems on finite and infinite domains and invariance under a different group of transformations, namely the spiral group, were considered. A further extension to eigenvalue problems was made by Ames and Adams [1].

For a general review before 1979, we refer to [15].

Recently in [11] a different way to apply the group properties was stated and we characterized the classes of problems for which the method is applicable. Moreover in [10] we give an extension of the method to elliptic problems in more than one dimension.

In the present paper we consider the application of group properties to free boundary value problems. Our aim is to find the exact free boundary location within the first numerical integration.

We also point out the classes of problems for which it is possible to define this method of solution. We remark that the procedure is self-validating. In fact we have to find the same value of the free boundary, with different values of the "initial guess" (see [9] for a first application of this method of approach). Moreover if we perform a second numerical integration we have to get a good approximation of the given initial boundary value. The same idea was used in [11] to validate the numerical solutions.

In Section 3 we list the numerical results related to a physical model for the diffusion and absorption of oxygen in cellular tissue.

2. SIMILARITY PROPERTIES OF SECOND ORDER EQUATIONS

We consider free boundary value problems

$$u'' = f(x, u, u') \quad x \in (0, s) \quad (2.1a)$$

$$u(0) = \alpha; \quad u(s) = u'(s) = 0; \quad \alpha \neq 0, \quad (2.1b)$$

where a prime indicates derivative with respect to x .

The conditions $u(s) = u'(s) = 0$ define the free boundary s .

We assume the problem (2.1) to be well posed, then we look for a pair (s, u) , $s \in (0, \infty)$ and $u \in C^2(0, s)$ that solve (2.1).

First we consider the stretching group of transformations

$$u^* = \lambda u; \quad x^* = \lambda^\delta x, \quad (2.2)$$

where λ is an arbitrary parameter different from zero, while δ is an arbitrary constant.

Requiring invariance of (2.1a) under (2.2) we characterize the class of problems [11]

$$f = u^{1-2\delta} F(x/u^\delta, u'/u^{1-\delta}). \quad (2.3)$$

In order to find the value of s with the first numerical integration we guess a value of $s^* \neq 0$. Then we integrate inwards in $[s^*, 0]$ to evaluate numerically $u^*(0)$. Generally $u^*(0)$ will be different from α .

However, from (2.2) we have

$$s = s^*(\alpha/u^*(0))^\delta. \quad (2.4)$$

Considering the spiral group of transformations

$$u^* = u + \mu; \quad x^* = \lambda^\delta x; \quad \lambda = e^\mu \quad (2.5)$$

we characterize the class of problems [11]

$$f = e^{-2\delta u} \Phi(xe^{-\delta u}, u'e^{\delta u}). \quad (2.6)$$

If we guess a value $s^* \neq 0$ and evaluate numerically $u^*(0)$ we can find the value of s by

$$s = s^* e^{-\delta(u^*(0) - \alpha)}. \quad (2.7)$$

We remark here that the same value of s has to be found with different values of s^* [9]. Moreover performing a second numerical integration we can validate the numerical solution. In fact we can accept our results if we get a good approximation of the boundary value α [11].

At this point of the analysis we have to say the drawback that the differential problem has to be in the classes (2.3) or (2.6) can be overcome. This is done by introducing in the differential problem some parameters and requiring that they transform themselves in (2.2) or (2.5), (see [15]).

An explicit example will be given in the next section.

3. A PHYSICAL EXAMPLE

We consider a simple one-dimensional steady-state model for the diffusion and absorption of oxygen in cellular tissue. At the cell wall, which we take to be $x=0$, oxygen enters into the cell, where it diffuses and is absorbed. The phenomenon is governed by the following free boundary problem

$$u'' = q(x)u + p(x); \quad x \in (0, s) \quad (3.1a)$$

$$u(0) = 1; \quad u(s) = u'(s) = 0, \quad (3.1b)$$

where $u(x)$ is the concentration of oxygen in the tissue, $q(x)$ is assumed to be nonnegative and different from zero in the hypothesis that absorption depends on concentration and $p(x) > 0$ represents the rate at which oxygen is absorbed by the tissue.

Table 1 The exact value of s is 1.4427. The asterisk indicates a guessed value

s^*	s	$U(0)$	$U'(0)$
0.5	1.44278	0.99919	-1.15542
1	1.44274	0.99917	-1.15537

Remark: Step size of $-1E+03$.

For existence and uniqueness we refer to [7].
The differential problem is in the class (2.3) if

$$q(x) = hx^{-2}; \quad h \geq 0; \quad p(x) = kx^{(1-2\delta)/\delta}; \quad k > 0. \quad (3.2)$$

In a similar way, the differential problem is in the class (2.6) if

$$q(x) = 0; \quad p(x) = kx^{-2}; \quad k > 0. \quad (3.3)$$

As a first example, we consider the simple problem

$$u'' = x^{1/2} \quad (3.4)$$

with boundary conditions (3.1b). This is in the class (3.2) with $h=0, k=1$ and $\delta=5/2$. The exact solution of (3.4), (3.1b) is given by

$$u(x) = (4/15)(x^{5/2} - s^{5/2}) - (2/3)s^{3/2}(x - s), \quad (3.5)$$

where $s = (5/2)^{(2/5)}$.

Table 1 reports on some results from different choices of the initial guess.
The second example

$$u'' = u + 1 \quad (3.6)$$

with boundary conditions (3.1b) is not in the class (3.2) or (3.3). So in order to apply our method we require the parameter h in (3.2) to change itself using the transformations (2.2), i.e.

$$h^* = \lambda^{-\theta - 2\delta} h. \quad (3.7)$$

This means that problems with different values of h are transformed one into another [15]. In so doing we can deal with the class of problems $q(x) = hx^\theta, h > 0$.

Then in order to apply the method we guess $s^* \neq 0$ and $h^* \neq 0$ and integrate inwards in $[s^*, 0]$ to find $u^*(0)$. After that we have s given by (2.4) and h from

$$h = (u^*(0)/\alpha)^{\theta + 2\delta} h^*. \quad (3.8)$$

Our problem becomes

Table 2 The exact value of s is 1.31696. The asterisk indicates a guessed value

s^*	s	h^*	h	$U(0)$	$U'(0)$
0.5	1.31729	6.94115	1.00002	0.99986	-1.73195
1	1.31712	1.73485	1.00002	0.99986	-1.73195

$$u'' = hu + 1 \quad (3.9)$$

with boundary conditions (3.1b). Here we have $h \neq 0$, $k=1$, $\delta=1/2$ and $\theta=0$. Suppose $h=H(h^*)$ with $H \in C^r$ for a suitable r . We have to find a zero of the equation

$$\Gamma(h^*) = H(h^*) - 1 = 0. \quad (3.10)$$

If we assume that $r \geq 2$ and $H'(h) \neq 0$, we can use Newton's method in this case, since we do not know explicitly the functional form of H , we have to use a finite difference formula in order to approximate H' . Otherwise we can apply the bisection method in order to approximate the value of h . Given two values h_{i-2} and h_{i-1} such that

$$\Gamma(h_{i-2})\Gamma(h_{i-1}) < 0 \quad (3.11)$$

we define the sequence

$$h_i = (h_{i-1} + h_{i-2})/2; \quad i = 2, 3, \dots \quad (3.12)$$

and h_{i-1} as h_{i-1} or h_{i-2} so that (3.11) is verified.

We stop the iteration when $|h_i - 1|$ is less than a given tolerance. Thus we get an iterative method of solution.

The exact solution to the problem (3.6),(3.1b) is

$$u(x) = (1/2)(e^{x-s} + e^{s-x} - 2), \quad (3.13)$$

where $s = \ln(2 + 3^{1/2}) \sim 1.31696$.

When we apply the outlined procedure we find the values listed in Table 2.

4. CONCLUDING REMARKS

The method given in Section 2 seems to be efficient. If we deal with a problem that belongs to the classes characterized here we will have a non-iterative method of solution.

Although the two model problems solved in the previous section are of physical interest they are linear and very simple. We considered these problems because in

this way we can easily show the features of the method. Certainly, we expect more important and interesting applications of the established method.

By introducing the transformation of some parameter we give also an important extension of the method to a model problem that is not in the classes characterized. But in this way the method becomes an iterative method of solution. So we have to ask whether it is possible to extend the method to any free boundary problem invariant under some infinitesimal group of transformations. The answer to this question seems to be negative. In fact this is an open question for boundary value problems from the paper of Na [14].

The simple numerical integrations were obtained with the classical Runge-Kutta method of fourth-order and step size of $-1E01$. In a more difficult problem we can use extrapolation or multistep methods [13] or eventually a polyalgorithm integrator [16].

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ADDENDUM et ERRATA

Corrections to: Similarity and numerical analysis for free boundary value problems, by R. Fazio and D. J. Evans, *Intern. J. Computer Math.* **31**, pp. 215–220, 1990.

The non-iterative numerical method introduced can be applied with more general free boundary conditions. As far as a stretching group is involved we can consider

$$u(s) = \beta s^{1/\delta}; \quad \frac{du}{dx}(s) = \gamma s^{(1-\delta)/\delta} \quad (1)$$

where β and γ are arbitrary constants. In the work we considered for (1), the simple case $\beta = \gamma = 0$. Beyond this, the case (1) where $\beta = \delta = 1$ is also possible, (see R. Fazio, Normal variables transformation method applied to free boundary value problems, *Intern. J. Computer Math.*, **37**, pp. 189–199, 1990).

The free boundary conditions invariant with respect to the spiral group are

$$u(s) = \beta + \frac{1}{\delta} \ln(s); \quad \frac{du}{dx}(s) = \frac{\gamma}{s} \quad (2)$$

where, again β and γ are arbitrary constants. This result shows that now the condition $u(s) = 0$ is not consistent with the non-iterative numerical method. Therefore the non-iterative method cannot be applied when the transformation group is the spiral one and the free boundary conditions are homogeneous.

The correct value of δ in the first numerical example was 2/5. Finally, in all numerical integrations we used a constant step size of $-1E-03$, where the symbol E indicates simple precision arithmetic.