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NORMAL VARIABLES TRANSFORMATION METHOD APPLIED TO FREE BOUNDARY VALUE PROBLEMS*

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We extend the application of group analysis approach to determining the numerical solution of free boundary value problems.

If the differential problem is invariant under a translation group of transformations we will formulate a non-iterative method of solution. This is done by introducing the concept of normal variables. Application of the method to two problems in the class characterized produces correct numerical results. Moreover, introducing a parameter into the differential problem and requiring invariance under an extended stretching group we give an iterative method applicable to any free boundary value problem.

As further result of the knowledge of the group properties we point out that these methods are self-validating.

Finally we suggest application of numerical transformation methods to boundary value problems.

KEY WORDS: Free boundary value problem, non-iterative and iterative numerical methods, similarity properties.

C.R. CATEGORY: G.1.7

1. INTRODUCTION

The purpose of this paper is to investigate further application of group properties to the numerical solution of free boundary value problems. Generally only iterative methods of solution are known to be applicable to these problems, see for instance [3, 5, 14, 16].

Recently, for some classes of problems, we proposed, in [8], a non-iterative transformation method, based upon invariance properties. Indeed, that non-iterative method is limited because we have to require invariance of the differential equation under stretching or spiral group of transformations. Nevertheless, an interesting application of that method to a non-linear hyperbolic problem has been given in [9].

For completeness we restate the method in point in Section 3.

In Section 4, by introducing the concept of normal variables, we try to extend to every problem invariant at least with respect to a one-parameter group of transformations that non-iterative method. Here we have to say that a very

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sensitive question is to obtain "consistent boundary conditions" (see Section 3 for a formal definition) after application of normal variables.

In section 5 we deal with the application of normal variables to the class of problems invariant under a translation group of transformations.

The theory given in Sections 3 and 5 is applied to the model problems of Section 2 and the related numerical results are listed in Section 6.

In Section 7, following the original idea already formulated in [8], we extend our method to every free boundary value problem. This is done by introducing in the differential problem a parameter and requiring invariance under an extended stretching group. In this way we get an iterative method of solution. A first application of this iterative method was given in [8].

Moreover we remark that in any case our methods are self-validating. In fact the same value of the free boundary must be found with different guesses of it [6]. Therefore the last numerical integration has to give a "good" approximation of the assigned initial value [7].

In the next section we state a general free boundary value problem and we give some examples.

2. FREE BOUNDARY PROBLEMS

We consider free boundary value problems

$$\frac{d^2u}{dx^2}=f\left(x,u,\frac{du}{dx}\right) \qquad x\in(a,s) \tag{2.1a}$$

$$u(a)=\alpha; \quad u(s)=\beta; \quad \frac{du}{dx}(s)=\gamma. \tag{2.1b}$$

The conditions $u(s)=\beta$ and $(du/dx)(s)=\gamma$ define the free boundary s.

The solution of this problem is given by a pair (s,u), $s\in(a,\infty)$ and $u\in C^2(a,s)$ that solve (2.1).

Next we give two examples of problems like (2.1).

A Linear Oxygen Absorption Model [5, 8]

We consider a simple one-dimensional steady-state model for the diffusion and absorption of oxygen in cellular tissue. At the cell wall, that 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

$$\frac{d^2u}{dx^2}=q(x)u+p(x); \qquad x\in(0,s) \tag{2.2a}$$

$$u(0)=1; \quad u(s)=\frac{du}{dx}(s)=0. \tag{2.2b}$$

In (2.2) $u(x)$ is the concentration of oxygen in the tissue, $q(x)$ that we assume to be non-negative will be 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.

For existence and uniqueness of problem (2.2) we refer to [5].

A Nonlinear Dynamical Problem [14]

We suppose a non-linear force equal to $-u\exp(-u)$ acts upon a unit mass, here u is the mass position on the axis of motion. We assume that initially the mass is located at the origin $u=0$. We want to know the initial velocity and the duration of motion s such that for a given point $u=u_0$, $u_0>0$, the velocity of the mass is exactly zero.

Applying Newton's second law of motion we can find the following free boundary value problem

$$\frac{d^2u}{dx^2}=-u\exp(-u) \qquad x\in(0,s) \tag{2.3a}$$

$$u(0)=0; \quad u(s)=u_0; \quad \frac{du}{dx}(s)=0. \tag{2.3b}$$

A similar problem was already considered in [12]. The non-linear force acting on the mass was equal to $-1-u-(du/dx)^2$.

We do not know any result about existence and uniqueness of solution for these problems, see [12] and [14].

3. STRETCHING GROUP AND NON-ITERATIVE TRANSFORMATION METHOD

In this section we consider invariance under the stretching group of transformations, that in finite form can be written as

$$x^*=\lambda^\delta x; \quad u^*=\lambda u. \tag{3.1}$$

We suppose δ different from zero, so that the class of invariant problems is characterized by

$$f=u^{1-2\delta}F\left(xu^{-\delta},\frac{du}{dx}u^{\delta-1}\right). \tag{3.2}$$

Definition We will call (2.1b) consistent boundary conditions in the particular case where $a=0$, $\alpha\neq 0$ and $u(s)=\beta$, $(du/dx)(s)=\gamma$ are invariant with respect to (3.1).

In the case of consistent boundary conditions a non-iterative numerical method was developed in [8]. Let us restate the non-iterative method in point. In order to find the value of s by the first numerical integration we guess a value of $s^*\neq 0$.

Then we integrate inwards in $[0, s^*]$ to evaluate numerically $u^*(0)$. Usually $u^*(0)$ will be different from α. However, from (3.1) we have $s^* = \lambda^\delta s$ and $u^*(0) = \lambda\alpha$ then we get

$$s = s^*(\alpha/u^*(0))^\delta. \tag{3.3}$$

We remark that the same value of s must be found by different values of the guess s^* [6]. Moreover within a second numerical integration we can validate the numerical solution. In fact we accept our results if we get a "good" approximation of the boundary value α [7].

4. GROUP INVARIANCE AND NORMAL VARIABLES

First we focus our attention only on the differential equation; the crucial point of transformation of boundary conditions will be considered later. We assume that the differential equation (2.1a) will be at least invariant with respect to the one-parameter group of transformations [2, 10]

$$x^* = x + \mu X(x, u); \quad u^* = u + \mu U(x, u) \tag{4.1}$$

where μ is the group parameter while X and U are the so-called generators.

The infinitesimal generator D of (4.1) is given by

$$D = X(x, u)\frac{\partial}{\partial x} + U(x, u)\frac{\partial}{\partial u}. \tag{4.2}$$

Now we introduce a particular variable transformation $t = t(x, u)$ and $z = z(x, u)$. Then we can write (4.2) as

$$D = \left(X\frac{\partial t}{\partial x} + U\frac{\partial t}{\partial u}\right)\frac{\partial}{\partial t} + \left(X\frac{\partial z}{\partial x} + U\frac{\partial z}{\partial u}\right)\frac{\partial}{\partial z}. \tag{4.3}$$

We will call t and z "normal variables" if they transform as

$$t^* = t(1 + \mu\tau); \quad z^* = z(1 + \mu). \tag{4.4}$$

We note that (4.4) is the infinitesimal form of a stretching group. In the case of normal variables taking into account (4.3) and (4.4) we get

$$\begin{aligned} X\frac{\partial t}{\partial x} + U\frac{\partial t}{\partial u} &= \tau t \\ X\frac{\partial z}{\partial x} + U\frac{\partial z}{\partial u} &= z. \end{aligned} \tag{4.5}$$

The general solution of (4.5) can be found by integrating

In (2.2) $u(x)$ is the concentration of oxygen in the tissue, $q(x)$ that we assume to be non-negative will be 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.

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$$\frac{dx}{X(x,u)} = \frac{du}{U(x,u)} = \frac{dt}{\tau t} = \frac{dz}{z}. \tag{4.6}$$

Integration of the first equation gives us the so-called group invariant $\omega = \omega(x, u)$ whereupon we have

$$\begin{aligned} t &= t_0(\omega) \exp\left(\tau \int \frac{dx}{X(x, u(x, \omega))}\right) \\ z &= z_0(\omega) \exp\left(\int \frac{dx}{X(x, u(x, \omega))}\right) \end{aligned} \tag{4.7}$$

where $t_0(\omega)$ and $z_0(\omega)$ are arbitrary functions of the invariant.

The introduction of normal variables allows us to apply (in all cases for which the transformed boundary conditions are consistent) the proposed non-iterative transformation method.

Let us show that the request to obtain consistent boundary conditions is not a trivial one.

To this end we discuss application of normal variables to the special case of $\delta = 0$ in (3.1) and (3.2). We introduce the normal variables as follows

$$t = xu^{\tau}; \quad z = u. \tag{4.8}$$

After (4.8) the boundary conditions (2.1b) will become:

$$z(a\alpha^{\tau}) = \alpha; \quad z(s\beta^{\tau}) = \beta; \quad \frac{dz}{dt}(s\beta^{\tau}) = \frac{\gamma}{\beta^{\tau} + \tau\beta^{\tau-1}s\gamma}. \tag{4.9}$$

Then in any case we must require $a = 0$ and $\alpha \neq 0$. Moreover the choice $\tau = 1$ leaves the value of γ arbitrary. While for $\tau \neq 1$ we have to require $\gamma = 0$. However for every value of τ it is impossible to find a value of β in order the condition $z(s\beta^{\tau}) = \beta$ be invariant.

5. TRANSLATION GROUP OF TRANSFORMATIONS

In this section we use the normal variables to investigate a class of problems characterized by invariance under a translation group. Then we suppose the differential equation (2.1a) to be invariant with respect to the translation group

$$x^* = x + \mu; \quad u^* = u. \tag{5.1}$$

It is worthwhile to remark that, if we identify x as temporal variable, all problems in classical mechanics have to be invariant under the group (5.1). The class of problems invariant under (5.1) is easily found to be characterized by

$$f=\Sigma\left(u,\frac{du}{dx}\right) \tag{5.2}$$

where Σ is an arbitrary function of its arguments.

Here we pay also attention to the boundary conditions (2.1b). In fact we cannot directly apply the non-iterative transformation method of Sections 3 and 4. That is because, once the normal variables have been introduced, the first boundary condition $u(a)=\alpha$ will transform to $z(\exp a)=\alpha\exp a$. Since $\exp a\neq 0$ we do not obtain consistent boundary conditions.

In order to overcome this difficulty we set

$$v(x)=\frac{u(x)-\alpha}{\beta-\alpha};\quad \beta-\alpha\neq 0 \tag{5.3}$$

and we make a hodograph transformation

$$y=v;\quad w=x. \tag{5.4}$$

After (5.3) and (5.4) we have also that

$$\frac{du}{dx}=(\beta-\alpha)\frac{1}{dw/dy};\quad \frac{d^2u}{dx^2}=-(\beta-\alpha)\frac{d^2w/dy^2}{(dw/dy)^3} \tag{5.5}$$

and the boundary conditions

$$w(0)=a;\quad w(1)=s;\quad \frac{dw}{dy}(1)=\frac{\beta-\alpha}{\gamma}. \tag{5.6}$$

The introduction of the normal variables leads to set $\tau=1$ in (4.7). So that we have

$$t=y\exp w;\quad z=\exp w \tag{5.7}$$

whereupon

$$\begin{aligned}\frac{dw}{dy}&=\frac{z(dz/dt)}{z-t(dz/dt)}\\ \frac{d^2w}{dy^2}&=\frac{z^3(dz/dt)^2-tz^2(dz/dt)^3+z^4(d^2z/dt^2)}{(z-t(dz/dt))^3}.\end{aligned} \tag{5.8}$$

Then we can find the transformed free boundary problem that has consistent boundary conditions

Table 1 Numerical results of (2.2) through the solution of (6.2). The exact value of s is 1.31696. We used indifferently $S^*=0.5$ or $S^*=1.0$

$s=\ln(S)$	$u(0)=z(0)$	$\frac{du}{dx}(0)=-\frac{1}{(dz/dx)(0)}$
1.31696	1.00000	−1.73205

$$z(0)=\exp a; \quad z(S)=S$$
$$\frac{dz}{dt}(S)=\frac{\beta-\alpha}{\gamma+\beta-\alpha}; \quad S=\exp s. \tag{5.9}$$

It is evident that we have to require

$$\gamma \neq \alpha-\beta. \tag{5.10}$$

6. NUMERICAL RESULTS

Here we report some numerical results for the model problems listed in Section 2. First we consider the problem (2.2) with $q(x)=p(x)=1$, see [5].

The exact solution of this problem is

$$u(x)=\cosh(x-s)-1 \tag{6.1}$$

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

In [8] the same problem was solved with the iterative method of the next section. Since this particular differential equation is invariant with respect to the translation group (5.1) we will use now the non-iterative transformation method outlined in Sections 3 and 5.

By making use of (5.3)–(5.9) we find the transformed free boundary value problem given by

$$\frac{d^2z}{dt^2}=\frac{1}{z}\left(2\frac{dz}{dt}-1\right)\left(\frac{dz}{dt}\right)^2$$
$$z(0)=1; \quad z(S)=S; \quad \frac{dz}{dt}(S)=1; \quad S=\exp s. \tag{6.2}$$

Table 1 reports numerical results obtained from different value of S^* and application of the procedure of Section 3.

As a second and more interesting example we consider the free boundary value problem (2.3). Using the same procedure as in the previous example we get the transformed free boundary value problem

Table 2 Numerical results of (2.3) through the solution of (6.3). Here we used $S^*=0.5$

u_0	$s=\ln(S)$	$u(0)=z(0)-1$	$\frac{du}{dx}(0)=\frac{u_0}{(dz/dt)(0)}$
0.1	1.63889	0.00001	0.09673
0.5	1.94107	0.0	0.42473
1.0	2.39606	0.00001	0.72693
3.0	5.52586	−0.0001	1.26544

Table 3 Numerical results obtained directly from the integration of (2.3) with the values of s given in Table 2

u_0	s	$u(0)$	$\frac{du}{dx}(0)$
0.1	1.63889	0.0	0.09674
0.5	1.94107	−0.00001	0.42475
1.0	2.39606	−0.00003	0.72697
3.0	5.52586	−0.00084	1.26557

$$\frac{d^2z}{dt^2}=\frac{t}{z^2}\left(\exp\left(-u_0\frac{t}{z}\right)+1\right)\left(\frac{dz}{dt}\right)^3-\frac{1}{z}\left(\frac{dz}{dt}\right)^2$$
$$z(0)=1;\quad z(S)=S;\quad \frac{dz}{dt}(S)=1;\quad S=\exp s. \tag{6.3}$$

The numerical solution of (6.3) with the method outlined in Section 3 produces the results for the original problem listed in Table 2. Table 3 reports a direct validation of the values of s listed in Table 2. Here we integrate numerically (2.3) as an initial value problem inwards in $[0,s]$.

7. A GENERAL ITERATIVE TRANSFORMATION METHOD

We try here to generalize the transformation method of Section 3. A first attempt in this sense was successfully made in [8]. Let us extend that idea.

We do not require now the differential equation (2.1a) to be invariant with respect to any transformation group. Moreover we do not need to have consistent boundary conditions too.

We suppose $\alpha\neq 0$, otherwise we can introduce a new dependent variable as $u(x)+1$. Then we set a new independent variable

$$\xi=x-a \tag{7.1}$$

in order to transform the boundary conditions (2.1b) into

$$u(0)=\alpha; \quad u(m)=\beta; \quad \frac{du}{d\xi}(m)=\gamma \tag{7.2}$$

where $m=s-a$ is the transformed free boundary. Next we consider the free boundary problem

$$\begin{gathered} \frac{d^2u}{d\xi^2}=f\left(\xi, u, \frac{du}{d\xi}, h\right) \\ u(0)=\alpha; \quad u(m)=\beta h^{1/\sigma}; \quad \frac{du}{d\xi}(m)=\gamma h^{(1-\delta)/\sigma}. \end{gathered} \tag{7.3}$$

In other words, we introduce in the original problem a parameter h. Then we require invariance of the differential equation in (7.3) under an extended stretching group

$$\begin{aligned} \xi^* &= \lambda^\delta \xi \\ u^* &= \lambda u \\ h^* &= \lambda^\sigma h. \end{aligned} \tag{7.4}$$

This means that problems with different values of h are transformed under (7.4) one into another [4].

Then we guess two values m^*, h^* and we integrate inwards in $[0, m^*]$ to find $u^*(0)$. Applying group properties we get

$$\begin{aligned} m &= m^*(\alpha/u^*(0))^\delta \\ h &= h^*(\alpha/u^*(0))^\sigma. \end{aligned} \tag{7.5}$$

In order to find the right value of m we have to require that $h=1$. Once the value of m^* has been fixed, as occurs, we have

$$h=H(h^*). \tag{7.6}$$

Then we have to find a solution of the equation

$$\Gamma(h^*)=H(h^*)-1=0 \tag{7.7}$$

where, of course, the functional form of $H(h^*)$ is not known. This can be done iteratively starting from two pairs $h_0^*, \Gamma(h_0^*)$ and $h_1^*, \Gamma(h_1^*)$, and applying a root finder like the bisection or the secant method [15].

8. CONCLUDING REMARKS

We have seen that the introduction of normal variables seems to be a direct way to extend the application of group properties to determining numerical solutions of differential problems invariant under groups different from stretching or spiral one.

However it is also clear that the necessity of obtaining consistent boundary conditions was a fundamental one.

In the case of a translation group we pointed out that a simple hodograph transformation gives us the key in order to obtain consistent boundary conditions. We quoted also two examples of physical interest that can be solved by the normal variables transformation method. Since the two transformed free boundary value problems (6.2) and (6.3) were nonlinear we used the IVPAG integer, in the IMSL MATH/LIBRARY, with step size and error control [11]. Moreover as the second example was nonlinear and very difficult to solve we chose to validate the numerical results directly. This despite the fact that, as we noticed, our transformation method is self-validating.

As far as the group analysis theory is concerned, we would like to point out that it is possible to find systematically all invariant transformation group of a given second order differential equation [2].

However, it is possible to find some second order equation that does not admit any invariant group of transformations [10].

So, we think that from a theoretical point of view it is very important the extension, given in Section 7, of our method to any free boundary value problem. For an application of this extended method we refer to [8]. In this way the method becomes an iterative method of solution.

If we consider two-point boundary value problems we can formulate invariant transformation methods in some different ways [1, 7 and 13]. The outlined numerical transformation methods could be applied to boundary value problems as well.

So if, according to Na [14], we ask if it is possible to apply transformation methods to any differential problem invariant under transformation group different from the stretching or spiral one the normal variable method of this paper is only a partial answer to this question.

However, the general iterative transformation method proposed in Section 7 goes behind this purpose. In principle the method seems to be correct. In any case we need to gain more experience in the practical application to problems of interest. Further application of that iterative method is in progress.

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