Computer Approach to an Analytically Numerical Method of the Solution of Boundary Value Problems in Mechanics

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A development of an analytically-numerical method of the solution of boundary value problems of applied mechanics is considered. The symbolic programming is applied to enable full computer approach to the Rvachev R-function method in domains of arbitrary shape, that may be concave and multiconnected. The method is realized in two steps. In the first step so called general structure of the solution is automatically derived in the analytical form. Numerous and laborous analytical operations, especially differentiation of complicated elementary functions are necessary then. In the original version of the method they had to be manually performed by the user.

The general solution strictly satisfies all prescribed boundary conditions and moreover contains some free functions. In the second step, which is of numerical character, these free functions are approximately determined by means of any known discrete procedure in order to satisfy the considered differential equation or to minimize the given functional.

A study set of subroutines written in the FORTRAN STANDARD code was worked out, to realize various required symbolic operations. They were associated with the Chebychev approximation and the least square approach to enable solution of wide class of boundary value problems. A numerical test is presented.

1. Introduction

An analitically - numerical method of solution of boundary-value problems of applied mechanics is presented. The symbolic programming was used to obtain fully automatic computer approach to the R-function method [6,7], applied in one or multi-connected domains of an arbitrary shape. The method is realized in two steps. In the first step so called structure of the solution is derived in the analytical form. It is a mapping $B = B(\Phi)$ of a set of functions defined in the considered domain into another set, also defined in Ω, but strictly satisfying prescribed boundary conditions and moreover containing some free functions Φ. In the second step, having obtained the above mentioned formulas, one may use various discrete methods [1] for the numerical determination of these functions in order to satisfy the considered equation or to minimize the given functional.

To build the solution structure $B(\Phi)$ in the R-function method the functions $\omega : R^n \longrightarrow R$ satisfying:

$$\begin{aligned} &\omega(x) > 0 \quad \text{if} \quad x \in \Omega , \\ &\omega(x) = 0 \quad \text{if} \quad x \in \partial\Omega , \\ &\omega(x) < 0 \quad \text{if} \quad x \notin \bar{\Omega} \end{aligned} \tag{1}$$

and $\varphi : R^n \longrightarrow R$ satisfying all prescribed boundary conditions $l_i \varphi_i(x) = \varphi_i(x)$ at $x \in \partial\Omega_i$, $i = 1,2,\ldots k$, are used. The form of the ω and φ functions depends on the shape of the domain Ω. In the case of complicated domains they are derived using set theory operations applied to the equations of simple subdomains.

The following R-functions are the most frequently used to derive the ω function:

$$x \wedge_* y = \left(x + y - \sqrt{x^2 + y^2}\right)\left(x^2 + y^2\right)^{\frac{m}{2}} , \tag{2}$$

$$x \vee_* y = \left(x + y + \sqrt{x^2 + y^2}\right)\left(x^2 + y^2\right)^{\frac{m}{2}} . \tag{3}$$

They correspond to 'or' and 'and' operations respectively. Using these R-functions one may obtain the arbitrarily smooth ω and φ functions for domains of any shape and to derive structures of solution for the wide class of boundary value problems of mathematical physics. Since R-functions are elementary ones this task may be programmed on computers. In the present paper the first version of such program is given to derive the structure of the solution in the analytical form. Algorithms and corresponding symbolic programs were prepared to realize automatic generation of a source code of a subroutine calculating:

- the function ω in an arbitrary point of R^n;
- partial derivatives $\frac{\partial^{i+j}\omega}{\partial x^i \partial y^j}$ of an arbitrary order.

Using these subroutines and a discretized method a study computer program was prepared to solve selected boundary problems in mechanics.

2. R-functions and generation of the domain of an arbitrary shape

R-functions [6,7] are real functions of many variables. The sign of each R-function is uniquely defined by the sign of its arguments. R-function are related to the functions of k-valued logics. For our purposes, however, functions of two and three-valued logics are sufficient.

Let us denote by B_3 the set $\{0,1,2\}$ and introduce the following operations:

$$X \vee Y = \max\{X,Y\}, \quad X,Y \in B_3 ,$$
$$X \wedge Y = \min\{X,Y\}, \quad X,Y \in B_3 ,$$

that respectively denote alternative and conjunction. Moreover let us define the mapping $F : B_3^k \longrightarrow B_3$ called the function of three- valued logics, and

$$S_3(x) = \operatorname{sgn} x + 1, \quad x \in R .$$

Using these denotations we may write the following definition:

R-function associated with a function F of three-valued logics is the mapping $f: R^k \longrightarrow R$, such that for each $x = (x_1,..,x_k) \in R^k$ holds

$$S_3[f(x_1,..,x_k)] = F[S_3(x_1),...S_3(x_k)] .$$

The relation between R-function and equations $\omega_i = 0$ of subdomains $\Omega_i \subset R^n$, $i = 1,...,k$ in n- dimensional Euclidean space is explained by the following theorem:

let

$$\omega_i : R^n \longrightarrow R, \quad i = 1,...,k,$$
$$\Omega_i = \{ x \in R^n : \omega_i(x) > 0 \} , \quad i = 1,..., k,$$

are open sets while

$\omega_i(x) = 0$ if $x \in \partial\Omega_i$, $\omega_i(x) < 0$ if $x \notin \bar{\Omega}_i$;

$F : B_3^k \longrightarrow B_3$ is an arbitrary function of three- valued logics,

$\Omega = \{ x \in R^n : F(S_3(\omega_1(x)),..., S_3(\omega_k(x)) = 2 \}$, and

f is an R-function associated with F, then the function

$$\omega(x) = f(\omega_1(x),... \omega_k(x)) \text{ at } x \in R^n$$

fulfils the relations (1).

The function (2) eg is associated with conjunction, whence

$$S_3(x \wedge_* y) = S_3(x) \wedge S_3(y),$$

while the function (3) corresponds to alternative, whence

$$S_3(x \vee_* y) = S_3(x) \vee S_3(y) .$$

From the theorem above mentioned one may conclude how to get the function $\omega : R^n \longrightarrow R$ where

$$\operatorname{sgn} \omega(x) = \begin{cases} +1 & \text{if } x \in \Omega , \\ 0 & \text{if } x \in \partial\Omega , \\ -1 & \text{if } x \notin \bar{\Omega} . \end{cases}$$

The domain Ω is obtained using the theory of set operations applied to known simple subdomains Ω_i, i = 1,...,k, defined by the given equations $\omega_i = 0$, where functions ω_i satisfy conditions (1). The required function ω is the R-function associated with a function of logics F corresponding to the theory of set operations used to build the domain Ω. The arguments of that function are functions $\omega_1,\ldots,\omega_k$. It is worth to mention, that since the composition of R-functions corresponds to a composition of associated functions of logics, in order to obtain the required function ω it is sufficient to use the R-functions related to alternative and conjunction only [6,7].

Similar basis are needed to form the function φ strictly satisfying all prescribed boundary conditions. For boundary value problem every type, in a local $Lu = g$ or a global $\int_\Omega Lu\, d\Omega = \min$ formulation, the theory of R-function supply us with the proper structure of solution $B(\omega, \varphi, \Phi)$.

3. Computer approach

3.1 The computer approach is realized in two steps. In the first one the structure of the solution $B(\omega, \varphi, \Phi)$ in the analytical form is automatically derived. This comes to the generation of subroutines calculating the functions ω and φ, their derivatives and LB. Symbolic programming [2-5] was applied ie automatic generation of series of chars, which in our case correspond to FORTRAN expression. They are brought later on to the form of required subroutines. Such approach allows user to avoid very laborous and time consuming operations, necessary for the manual derivation of all formulas appearing in the first step of the R-functions method and required so far in the original version of the method.

General idea of calculation procedure is presented in the Fig.1

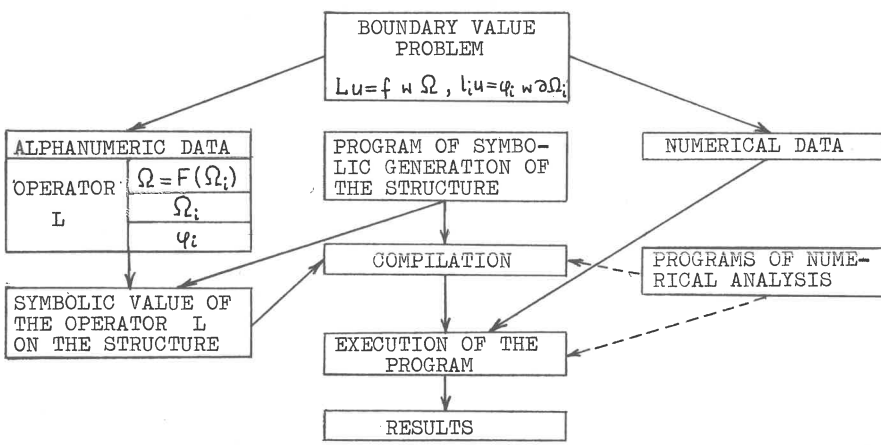

Fig.1

3.2. Symbolic operations

Subsequent step of the symbolic programming applied are shown in the flow chart (Fig.2)

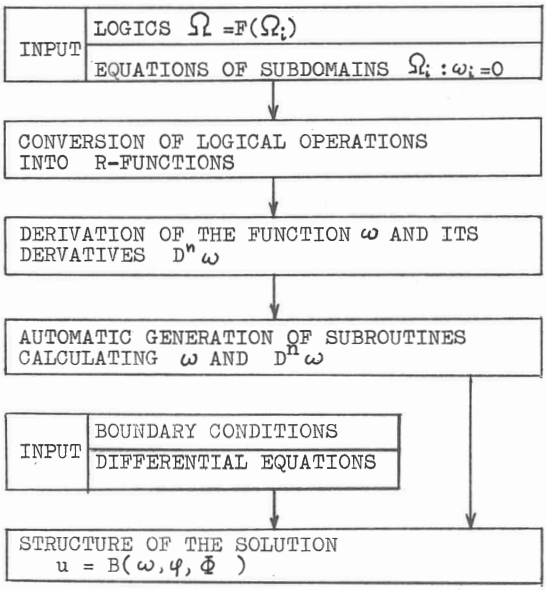

Fig.2

Alphanumeric data, are introduced according to the rules presented in the Table 1. R-function assumed are described by the formulas

Table 1

Symbol	Operations				Arguments			
	set theory		R-function		set theory		R-function	
math.	$\cap$	$\cup$	$\wedge_*$	$\vee_*$	Ω	Ω_i	ω	ω_i
FORTRAN	*	+	AIL	SUM	F	F(I)	F	F(I)

(2) and (3) were assumed as basic ones. The data are transformed later on into the form of functions. Let us explain such transformation on the following example. Let the domain be

$$\Omega = \Omega_1 \cap (\Omega_2 \cup \Omega_3) \cup \Omega_4 \cup \Omega_5 \ .$$

The input data in this case are:

F(1) * (F(2) + F(3)) + F(4) + F(5) ,

and finally we get

SUM(AIL(F(1), SUM(F(2), F(3) , SUM(4), F(5))) .

This expression is transformed into simple expressions using formulas (2) and (3). Later on all neccessary derivatives are generated, provided the functions F(I) are replaced by corresponding initial data. Finally the required subroutines of FUNCTION type are formed.

3.3. Numerical solution

Let the structure of the solution $u = B(\omega, \varphi, \Phi)$ of the boundary value problem

$$Lu = f \quad \text{in} \quad \Omega ,$$
$$l_i u = \varphi_i , \quad i = 1,\ldots,k \quad \text{in} \quad \partial\Omega_i$$

is found. The following relations hold then:

$$l_i B(\Phi) = \varphi_i , \quad \forall\, \Phi \in \mathcal{M} ,$$

where $\mathcal{M}$ is a space of the functions defined on the Ω . If $v_1,\ldots,v_N \in \mathcal{M}$ form the base of this space and $\lambda_1,\ldots,\lambda_N \in R$ are coefficients, one may write

$$\Phi = \sum_{i=1}^{N} \lambda_i v_i \ .$$

Using any known discrete method one may find λ_i .

3.4 Numerical test

As a simple tests the torsion of the prismatic bars of the square cross-section and three quarter of circle one were considered:

$$\Delta u = -2 \quad \text{in} \quad \Omega , \quad u = 0 \quad \text{in} \quad \partial\Omega$$

the structure of the solution is $u = \omega\Phi$ then [6] . An aproximation by three Chebychev polynomials

$$v_{ij} = T_i(x)\, T_j(y) , \quad i = 1,2,3$$

combined with the least-square approach was applied. Numerical results referred to the central point of the square are presented in the table 2.

Table 2

Number of integration points in Ω	Value u in the central point
20 x 20 = 400	0,154594
25 x 25 = 625	0,146572
30 x 30 = 900	0,142635
35 x 35 = 1225	0,140023
38 x 38 = 1444	0,140167

4. Final remarks

A full computer approach to the analitically numerical R-function method of solution of boundary-value problems is presented. All analytical formulas are generated by symbolic programming. When compared with the FF and FD methods the following advantage, of the method considered may be mentioned:

- significant decrease of the total number of degrees of freedom is possible
- boundary conditions are satisfied exactly,
- real, curvilinear shape of the boundary is assumed.

On the other hand some disadvantages may be observed:

- complicated form of the solution,
- complicated algebraic expressions have to be derived and calculated,
- $\frac{0}{0}$ type expressions of a definite value may appear at the intersection of boundaries given by two different equations.

Though the present paper is a preliminary study, the results obtained so far encourage to further investigations like:

- combination of the method with various numerical approach-es like FEM, FDM, Ritz, Galerkin etc,
- analysis of the generation procedure of the structure of solution in order to secure results of required smoothness,
- investigation of effectiveness of the method,
- various improvements of the computer program,
- application to a wide class of boundary value problems in applied mechanics.

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