METHODS OF ARTIFICIAL INTELLIGENCE IN SOLVING BOUNDARY VALUE PROBLEMS
[Artificial intelligence and boundary problems]

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Abstract: The given article traces the development of methods of solving boundary-value problems and presents a comparative analysis of these methods from the perspective of reliability of the solutions. An attempt to develop the fictitious canonic regions method using the technology of genetic algorithms is made.

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1. Introduction

Boundary-value problems of mathematical physics were addressed in the end of the XVIII – beginning of the XIX centuries in the fundamental works by J.L. d'Alembert and J.B.J. Fourier. For more than two centuries they have been one of the most important trends in mathematical modeling applied to engineering calculations. Let us first trace the development of methods of boundary-value problem solving and outline the difficulties and obstacles, which the authors of these methods confronted with.

In general view we will present the statement of linear boundary value problem in the following way. It's required to find the function $U(\mathbf{x})$, satisfying within some domain $D \subset R^3$ the partial differential equation

$$L\,U(\mathbf{x}) = L^*(\mathbf{x}), \quad \mathbf{x} \in D \tag{1}$$

and on the surface S of D satisfying the boundary conditions

$$B\,U(\mathbf{x}) = B^*(\mathbf{x}), \quad \mathbf{x} \in S \tag{2}$$

where L and B are linear differential operators with constant coefficients; $L^*(\mathbf{x})$ and $B^*(\mathbf{x})$ are given functions of position $\mathbf{x}$.

According to Fourier method of separation of variables, solution of boundary value problem (1)-(2) is constructed in the form of infinite sum

$$U(\boldsymbol{x}) = \sum_{n=1}^{\infty} c_n U_n(\boldsymbol{x}) \tag{3}$$

where c_n are constant coefficients, and $U_n(\boldsymbol{x})$ are functions of coordinates $\mathbf{x}$.

The sum (3) is an analytical expression, which identically satisfies the differential equation (1) and the boundary condition (2). Therefore, it is said that it is the exact analytical solution of the boundary value problem (1)-(2).

In XIX-XX centuries by means of Fourier method a number of exact analytical solutions of boundary value problems were successfully found for the simplest domains: circle, sphere, cylinder, parallelepiped, infinite slab, etc., called canonic domains. For more complicated computational domains, which occur in engineering practice, the use of Fourier method faced serious difficulties. So, mathematicians simplified the task. Instead of finding exact analytical solutions they began limiting themselves to finding approximate analytical solutions of boundary value problems. These approximate solutions differ from exact solutions by some small error value $\varepsilon(\boldsymbol{x})$. Three groups of approximate analytical methods appeared.

1. Ritz type methods.

Solution of the boundary value problem (1)-(2) is constructed in the form of finite sum

$$U(\boldsymbol{x}) = \sum_{n=1}^{N} c_n U_n(\boldsymbol{x}) \tag{4}$$

such that it approximately satisfies the differential equation (1) and identically satisfies the boundary conditions (2).

2. Trefftz type methods.

Solution of the boundary value problem (1)-(2) is constructed in the form of finite sum (4) such that it, as opposed to Ritz method, identically satisfies the differential equation (1) and approximately satisfies the boundary conditions (2).

3. Reissner type methods.

Solution of the boundary value problem (1)-(2) is constructed in the form of finite sum (4) such that it approximately satisfies the differential equations (1) and the boundary conditions (2).

In such simplified statement boundary value problems for non-canonic domains had been solved up to the middle of the XX century. Notably that with the development of approximate analytical methods, error estimation methods of approximate solutions also developed, that was extremely important for applying found solutions in engineering practice.

The emergence of high-speed computers in the middle of the XX century gave new opportunities and opened up new prospects for using approximate analytical methods. However it turned out that they were less effective in comparison to an alternative approach, which happened to be more adapted to the use of computer machinery. It turned out that if we split the solution domain of a boundary value problem into a set of small sub-domains, and for every sub-domain we introduce conjectures, reducing physical characteristics of the continuum, the process of differential equation integration can be traced to a set of simple arithmetic operations – additions, subtractions, multiplications, divisions. Thus it became possible to solve boundary-value problems of mathematical physics by means of computers with «brute force approach», finding solution not by way of analytic formulae, but as arrays of numbers. Numerical methods of the boundary value problems solution replaced classical analytical methods. It so happened because numerical methods proved out to be more easily formalized and programmed. Soon one more advantage of numerical methods over analytical

methods was found: computer programs, implementing numerical methods, and developed for solving one boundary value problem, without any sufficient alterations were suitable for solving other problems, belonging to the same class. As for algorithms, based on analytical methods, they were not so all-purpose.

Above-mentioned circumstances resulted in that on the modern market of software, designed to solve boundary value problems, there are a great number of all-purpose software packages, based on numerical methods, such as ANSYS, COSMOS, LS-DYNA, NASTRAN, PATRAN, FEMLAB, APM WINMACHINE, BEASY, and virtually there are not any software packages, implementing analytical methods.

Thus, by the beginning of the XXI century the development of methods of boundary value problem solving resulted in the situation when the vast majority of engineering problems are solved by means of all-purpose software packages based on numerical methods. These packages let engineers find numerical solutions of boundary value problems of almost any complexity. But another serious problem emerged: generally it is not possible to estimate accuracy of such numerical solutions for complicated engineering problems. In the book by L.N. Yasnitskiy and T.V. Danilevich "Modern problems of science" [1] this paradoxical situation is called "modern crisis of applied mathematics; crisis, which, judging by catastrophic growth of technogenic accidents and disasters, threatens to escalate into crisis of modern civilization".

The thing is that solutions received by numerical methods represent arrays of numbers, errors of which can be estimated only by the way they behave with the growth of element number the domain divided. It is usually supposed that results can be trusted if they stop changing with the mesh refinement. But theoretical inconsistency of this opinion was shown long ago. Firstly, the theorems, according to which the approximate computational solutions converge to the exact ones, are proven under such conditions, which are rarely fulfilled in engineering practice. Secondly, with the refinement of the finite element meshes, the condition number of resolving linear equation system always increases. So in case of solving two-dimensional boundary value problems for second order differential equations and application of uniform mesh with linear shape functions this dependence is used:

$$\alpha = Ch^{-2} \tag{5}$$

where α – spectral condition number of the system of linear equations, h – maximum size of finite element, C – is a constant that depends on the specificity of the problem. According to this formula when h decreases, α increases. It means that the system of linear equations becomes ill-conditioned: slight changes of the matrix coefficients lead to significant changes in system solution. It means that errors connected with matrix coefficient rounding in computer calculations, or errors introduced into these coefficients during the process of its formation affect the result of system solution. And it means that when $h \to 0$ approximate finite element solutions do not converge to the desired solution of boundary value problem, as it is schematically shown in figure 1.

It follows from this analysis that the results received with numerical methods should be treated carefully. Exactly the problem of error estimation is the most serious drawback of numerical methods, and it makes the search for the new methods and approaches more actual.

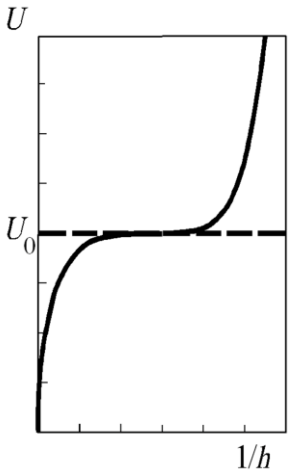


Figure 1. Typical dependency of the numerical solution of the boundary value problem from the maximum size of finite element h. U_0 -exact problem solution.

2. Errors of approximate analytical methods

Let's try to compare analytical methods from the point of view of their reliability.

We will start with Trefftz Method. According to what has been said, the solution received with this method identically satisfies differential equations (1) and approximately satisfies boundary conditions (2).

It means that instead of solving boundary value problem (1)-(2), this method leads to the exact solution of another boundary value problem with changed boundary conditions:

$$L\,U(\mathbf{x}) = L^{*}(\mathbf{x}), \quad \mathbf{x} \in D \tag{6}$$

$$B\,U(\mathbf{x}) = B^{**}(\mathbf{x}), \quad \mathbf{x} \in S \tag{7}$$

The difference between the given condition $B^{*}(\mathbf{x})$ and changed boundary condition $B^{**}(\mathbf{x})$ in each specific case can be easily found. It is always possible to substitute the solution received with Trefftz method into the left part of the equation (2) and after making calculations of this part on the boundary of solution domain, when ($\mathbf{x} \in S$), to recreate the statement of the changed boundary value problem, which was exactly solved with Trefftz method. And finally it is always possible to evaluate the replacement of boundary value problem (substitution of the given boundary value problem (1)-(2) for the changed boundary value problem (6)-(7)) from the engineering point of view. And if this substitution is possible from the engineering point of view the solution errors received with Trefftz method should not be discussed at all.

If for example we needed to calculate the temperature in some object, on the surface of which the given temperature is 500°C. Using Trefftz method we will find the function $U(\mathbf{x})$ which identically satisfies boundary value problem differential equations and on the surface off the object boundary conditions are hold approximately. For example when calculating the

value of the function $U(\mathbf{x})$ on S, we see that instead of 500 °C the function $U(\mathbf{x})$ changes its value within 499°C to 501°C. So the difference between the given boundary condition of the temperature $B^*(\mathbf{x})$ and the boundary condition of the changed boundary value problem do not exceed 1°C. And if these temperature perturbations on the surface of the object are acceptable from the engineering point of view, we can change the statement of the problem, replacing $B^*(\mathbf{x})$ with $B^{**}(\mathbf{x})$ and state that the problem is solved without errors at all.

So this method allows to receive exact analytical solutions of the boundary value problems but not the given ones but those which differ with their boundary conditions with a slight value and this difference in every specific case can be easily evaluated.

Now let's appeal to Ritz Method. Reasoning the same way, we see that applying this method leads to the exact analytical solution of the following boundary value problem:

$$L\,U(\mathbf{x}) = L^{**}(\mathbf{x}), \quad \mathbf{x} \in D \tag{8}$$

$$B\,U(\mathbf{x}) = B^{*}(\mathbf{x}), \quad \mathbf{x} \in S \tag{9}$$

This problem statement differs from the given boundary value problem with the different form of differential equation. But as opposed to the previous case, here the possibility of substituting the given problem (1)-(2) with the changed one (8)-(9), is not so evident from the engineering point of view. The same conclusion can be made in case of using Reissner method.

So among the whole taken analytical methods, Trefftz method is the most reliable one for solving boundary value problems.

3. Trefftz method and its development

Let's study the history and the problems of applying Trefftz method more properly.

This method was presented by German mathematician and mechanic Trefftz in 1926. In his speech on The Second International Congress on Technical Mechanics in Zurich he presented his analytical method of solving boundary value problems, the essence of which is enclosed here.

Let us find function $U(\mathbf{x})$ satisfying Laplace's equation within some domain $D \subset R^3$

$$\Delta U(\mathbf{x}) = 0, \quad \mathbf{x} \in D \tag{10}$$

and on the boundary S of domain D satisfying boundary conditions

$$U(\mathbf{x}) = B^{*}(\mathbf{x}), \quad \mathbf{x} \in S \tag{11}$$

According to Trefftz method solution of the boundary value problem is searched as the following sum

$$U(\mathbf{x}) = \sum_{n=1}^{N} c_n U_n(\mathbf{x}), \quad \mathbf{x} \in D \tag{12}$$

Where $U_n(\mathbf{x})$ are basis functions of coordinates that are chosen in such a way that each of them identically satisfies differential equation (10), and c_n are constant coefficients determined by the minimization of functional

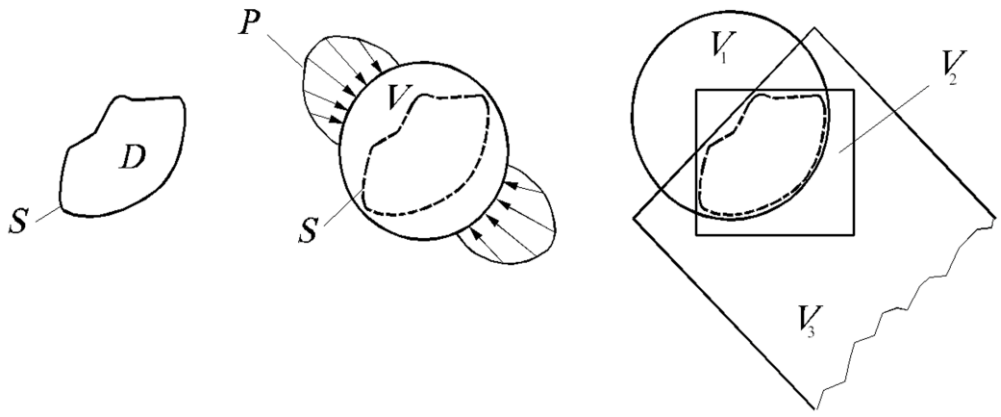
$$J(U) = \int_D (gradU(\mathbf{x}))^2 dD \tag{13}$$

that is equal to the boundary conditions (11).

As each item of the sum identically satisfies the differential equation, the whole sum has this characteristic. Thereby the solution of the boundary value problem $U(\mathbf{x})$ identically satisfies the differential equation and after the minimization of functional (13) it approximately satisfies the boundary conditions (11). As it was mentioned above, this magnificent feature of Trefftz method makes it different from other approximate methods and it is a serious advantage of the method, which is especially significant in modern conditions, where the quality and reliability of computational results are of great importance.

The approach suggested by E. Trefftz in 1926 at those times was the cause of the series of scientific works dedicated to the issues of its development and application. Among them we should mention fundamental works by E. Reissner, L. Leibenzon, S. Mihlin, M. Birman, G. Grinberg, L. Collatz. However, in spite of the unique features and attention of mathematicians, Trefftz method had been remaining useless for a wide practical application for a long period of time. The point is that the problem of selection of basis functions $U_n(\mathbf{x})$ that satisfy the differential equation of the boundary value problem and that provide the convergence of the method remained unsolved. Only in rare cases by means of increase of the basis functions number N it was possible to decrease difference between $B^*(\mathbf{x})$ and $B^{**}(\mathbf{x})$ to the acceptable values and thereby justify the possibility of substitution of the given boundary value problem (1) – (2) by the altered boundary value problem (6) – (7). As a result the success of application of Trefftz method completely depended on experience and intuition of the mathematician and sometimes even on luck.

Geometrical interpretation that was developed in 1973 [3] made it possible to examine the problems of convergence and correctness and to set up the technique of basis functions choice, that ensure the success of the use of Trefftz method. The essence of geometrical interpretation can be illustrated by an example. Let us assume that the stress-strain state of elastic body D that is depicted in fig.2 (a) is needed to be calculated. Displacement or (and) stress boundary conditions on surface S of body D are assigned.



a b c

Figure 2. Given body D (a) is mentally immersed in canonic region V (b) or in the crossing section of several canonic regions: $V_1 \cap V_2 \cap V_3$ (*c*)

Alongside with D some fictitious canonic region V is introduced, within which the contours of a given body are mentally (on fig.2, b – in dotted line) distinguished. By virtue of the fact that the region *V* is canonic, then the solution of differential equation (for example, equations of the theory of elasticity) may be set up for this area by means of Fourier method. The above mentioned solution takes the form

$$U(\mathbf{x}) = \sum_{n=1}^{N} c_n U_n(\mathbf{x}), \qquad N \to \infty, \qquad \mathbf{x} \in V \tag{14}$$

where $U_n(\mathbf{x})$ are functions of coordinates, which by reason of a specific character of Fourier method, identically satisfy differential equation, and c_n - are constant coefficients, determined by the boundary conditions on the surface of region V.

This solution is general in the sense that by selecting values of coefficient c_n some partial solutions may be pointed out from the general solution. These partial solutions can satisfy sufficiently arbitrary boundary conditions on the surface of body V. If we now produce such loading P on this surface that on the boundary of body D there will be displacements or (and) stresses, that satisfy given boundary conditions on surface S, then the solution for *V*, that fits loading P will be at the same time the solution of the original problem for body D. The latter is just by virtue of the fact that partial solution pointed out from (14) satisfies within body D elasticity equations and on its surface it satisfies given boundary conditions.

From the mathematical point of view the objective of the loading of fictitious body V is implemented by selecting coefficients in sum (14) that provide the fulfillment of given conditions on S. If we take a finite number N of row summands (14), the problem may be solved approximately by minimizing the functional of boundary conditions. The latter may be formulated with the help of Trefftz method (13) by using energy representation or by

means of least squares method etc.

The above mentioned geometrical interpretation to Trefftz mathematical apparatus made it possible to understand physically and account for the reasons of many unsuccessful attempts of its use. For example if body D on fig.2 had internal holes filled with high pressure gas then the formation of such boundary conditions on D by means of matching of loading P of fictitious body V would be hardly possible. By intuition we can guess that V should be a multiply connected region, but we will discuss it later. Now it should be pointed out that geometrical interpretation that for the first time was brought out by L.N. Yasnitskiy in his scientific work [3], made it possible in this work to give a definition and the first proof of the convergence theorem, to suggest a choice-technique of basis functions and also to suggest and give a proof of error estimation method for solutions of boundary value problems, i.e. to lay theoretical basis for mathematical apparatus, which later was named a fictitious canonic region method (FCRM) [4].

Now let us turn our attention to this method in more detail. The essence of choice criterion of fictitious canonic region consists in requirement of *extendability* of the original problem solution within region V. Under the term "extendability" we understand the possibility of extension of the original problem solution (as a function satisfying differential equations of the problem) beyond the boundaries of computational domain D to the whole space, which is occupied by bigger domain V. Moreover V is implied as a minimal domain that contains body *D* and belongs to the set of regions, for which the series expansion (14) is valid.

As a separate canonic region V (fig.2, b), and an intersection of several canonic regions can be chosen $V = V_1 \cap V_2 \cap ... \cap V_K$ (fig.2, c). In this case instead of (14) the sum of K decompositions is used, referring accordingly to $V_1, V_2, ..., V_K$.

The criterion of choice of the fictitious canonic regions is based on that, when meeting the condition of extendability of the original problem solution within V this solution is the sum of basis functions for V. So the expansion (14) (or the sum of K expansions in case of superposition of fictitious regions (fig.2, c)) for limited N is a segment of the series and for it appropriate convergence theorems are applicable. If there is no extendability, so there is no such series. The sum of the right part of the formula (14) can be considered only as a linear combination of functions $U_n(\mathbf{x})$ approximating in D the original problem solution. But for this approximation the problem of finding coefficients c_n is not correct by Hadamard. In this case, it is proved by S.J. Guzman [5] that when increasing N some of coefficients c_n grow unlimitedly. It means that during the practical calculation on computers it is impossible to get the solution of the problem with error, that is lesser than some positive number ε_0, dependent on original boundary value problem and computer memory.

The failure of extendability can happen because of some singularities, points where the original problem solution becomes infinite or discontinuous, has discontinuous derivatives etc. As a rule, in real boundary value problems singular points of solutions are located out of domain D (fig.3) or on its boundary. So, the task of choice of the fictitious canonic region is:

1. To predict possible places of singular points.

2. To locate the fictitious canonic region in that way when singular points of the original problem solution will be out of the region V (or on its boundary).

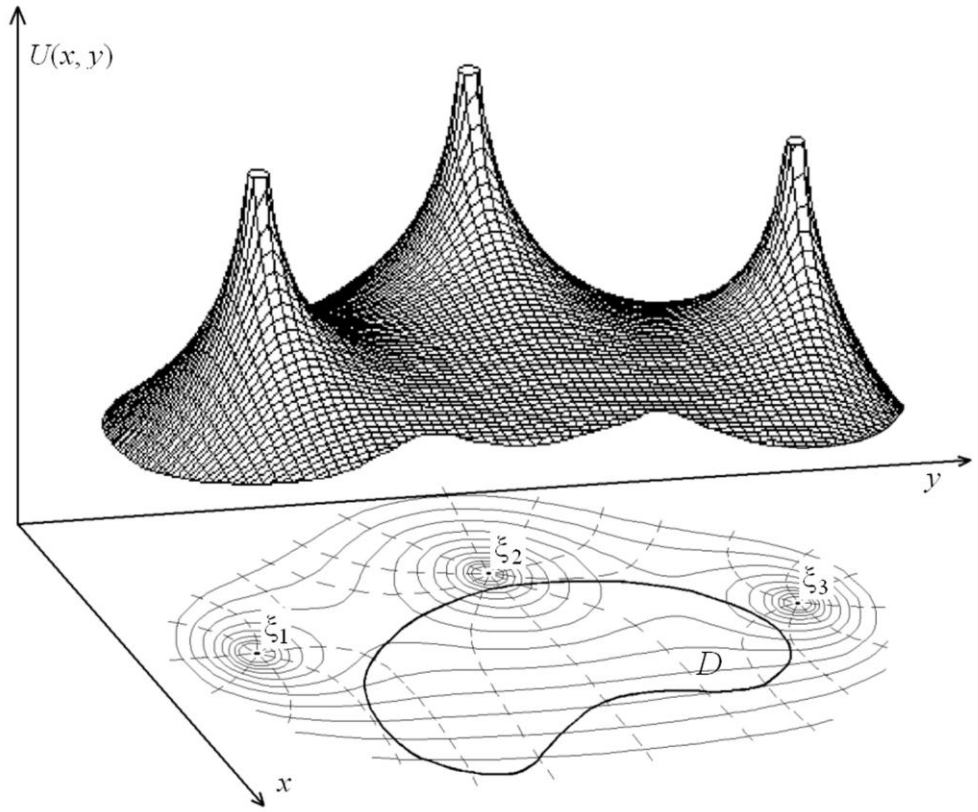
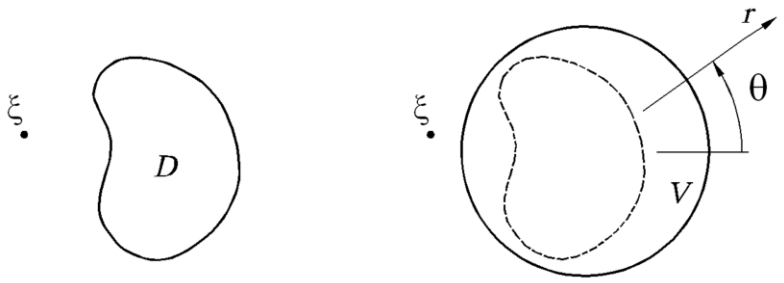


Figure 3. The exact solution of a boundary-value problem, which exists within domain D and beyond its limits. Singular points $\xi_1, \xi_2, ..., \xi_n$ (where the function $U(x.y)$ becomes infinite) located out of domain D.

Let us show the method of choice of fictitious canonic region in following problems.

Problem 1. Laplace equation for plane domain D on fig. 4 needs to be solved, so it is known that the problem solution has a singular point ξ, located near D.



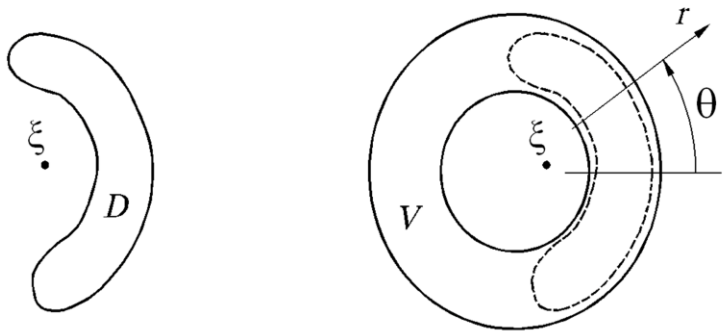
a b

Figure 4. Given domain D (a) is placed into the circle V (b). ξ – a singular point of the problem solution.

As fictitious region V in this case a circle can be used as an example, for which the solution of Laplace equation found by Fourier method of separation of variables [6] is the following:

$$U = \sum_{n=0}^{N} r^n (a_n \cos n\theta + b_n \sin n\theta), \quad N \to \infty \tag{15}$$

where r, θ - polar coordinates, a_n and b_n - constant coefficients. According to the criterion of extendability the circle should be placed in such a way, that it contains domain D and does not contain the singular point ξ. The example of such an arrangement is shown in figure 4, b.

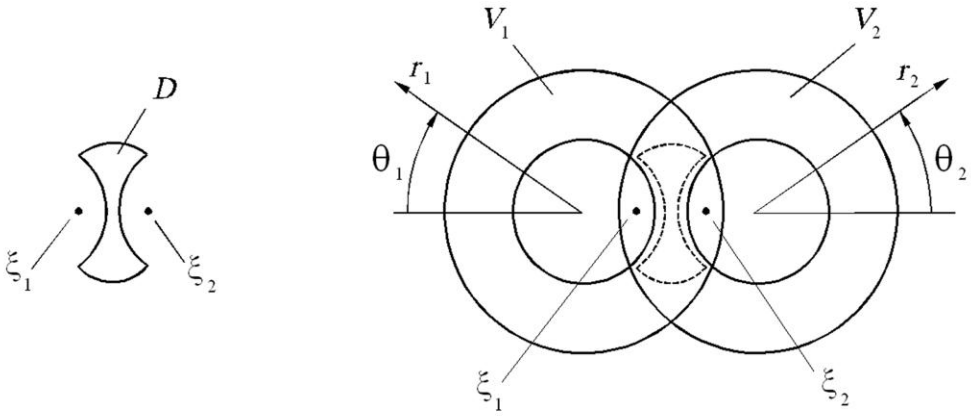


a b

Figure 5. Given domain D (a) is immerged into circular domain V (b)

Problem 2. In figure 5, *a* it is an example, when it is impossible to choose a circle satisfying the criterion of extendability. So as V in fig. 5, b a circular region is offered, for which (under [6]) the solution of Laplace equation is the following:

$$U = \sum_{n=-N}^{N} r^n (a_n \cos n\theta + b_n \sin n\theta) + c_0 \ln r, \quad N \to \infty \tag{16}$$



a b

Figure 6. Given domain D (a) is immerged into region of intersection of two fictitious rings V_1 and V_2 (b)

Problem 3. In figure 6, *a* a more complicated case is shown, when near domain D there are two singular points ξ_1 and ξ_2. In this case, neither circle nor ring fit for it, so here the method of superposition of fictitious canonic regions [7] is recommended: D is immerged into the intersection of two ring regions $V = V_1 \cap V_2$. The expansion for *V* is the sum of two series:

$$U = U_1 + U_2 \tag{17}$$

The first

$$U_1 = \sum_{n=-N}^{N} r_1^{\,n} (a_{n1} \cos n\theta_1 + b_{n1} \sin n\theta_1) + c_1 \ln r_1, \quad N \to \infty \tag{18}$$

belongs to region V_1, and the second –

$$U_2 = \sum_{n=-N}^{N} r_2^{\,n} (a_{n2} \cos n\theta_2 + b_{n2} \sin n\theta_2) + c_2 \ln r_2, \quad N \to \infty \tag{19}$$

belongs to region V_2.

As follows from the fig. 6, *b*, singular points ξ_1 and ξ_2 turn out beyond the limits of the intersection of fictitious rings and so the original problem solution is extendable into $V = V_1 \cap V_2$.

In all examples fictitious canonic regions are chosen and placed in that way, that the condition of the main theorem of FCR method (extendability theorem) is fulfilled – that provides the convergence of the method, and so the successful solution of a boundary – value problem. Seemingly, the theoretical basics of FCR method can be considered to be formed. But, the following problems remain to be unsolved:

1. Singular points of the original problem solution can be defined by the view of this function after that, when it is constructed, that is after that when the solution of the boundary value problem is found. But before the problem is solved, this function is unknown. So in practice of FCR method application the prediction of singular point locations of the original problem solution is performed intuitively.

2. Usually there is a great number of variants and location of FCR, providing the fulfillment of extendability condition. For instance, in fig. 7 there is another variant of FCR choice for the solution of problem 3 – initial domain D is immerged into the intersection of three fictitious canonic regions $V = V_1 \cap V_2 \cap V_3$: two fictitious circular hollows in infinite space V_1 and V_2, for which the general solution of Laplace equation has the following form:

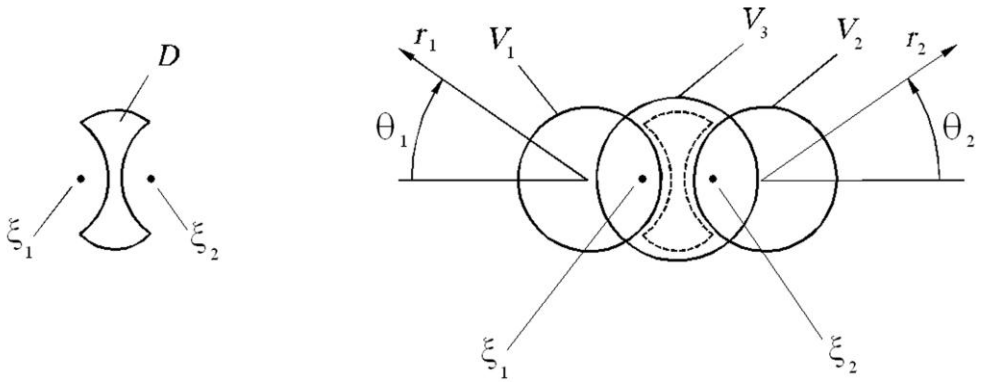
$$U_1 = \sum_{n=-N}^{0} r_1^{\,n} (a_{n1} \cos n\theta_1 + b_{n1} \sin n\theta_1) + c_1 \ln r_1, \qquad N \to \infty \tag{20}$$

$$U_2 = \sum_{n=-N}^{0} r_2^{\,n} (a_{n2} \cos n\theta_2 + b_{n2} \sin n\theta_2) + c_2 \ln r_2, \quad N \to \infty \tag{21}$$

and a circle V_3 for which the general solution of Laplace equation has the following form:

$$U_3 = \sum_{n=0}^{N} r_3^{\,n} (a_{n3} \cos n\theta_3 + b_{n3} \sin n\theta_3) + c_3 \ln r_3. \qquad N \to \infty \tag{22}$$

What variant of FCR choice and location (fig. 6 or fig. 7) is the best - is an unsolved problem.



a b

Figure 7. The domain D (a) is immerged into the intersection of two fictitious circular hollows V_1 and V_2, and circle V_3 (b)

4. Gradient method of optimizing the location of the fictitious canonic regions

S.L. Gladkiy attempted in his work [8] to create an algorithm for solving the problem of FCR location in means of an optimization problem. The essence of the algorithm is as follows.

Let the boundary value problem be solved for the domain D. Somehow (for example, on the basis of intuitive considerations of mathematician, who is solving the boundary problem), let fictitious regions and their initial location be selected. It's necessary to change the positions of the fictitious canonic regions in order to ensure the best quality solution.

The square error of the boundary conditions is taken as the quality criteria of the optimization problem:

$$\varepsilon = \int_S \left(B^*(\mathbf{x}) - B^{**}(\mathbf{x})\right)^2 dS \tag{23}$$

Let the initial location of a FCR be defined by the position of its center C_0 (fig. 8). All the points at the distance of dL are taken into consideration. The value of dL is an input parameter of the algorithm and is set by users in fractions of the characteristic size L of the domain D. Further, with the help of the golden section method the direction of movement (angle) of the FCR center is determined, providing the decrease in value of the selected quality criteria. The center of FCR is placed in the point C_1 and the new value of quality criteria is calculated. If it is smaller than in the previous position, the center of FCR remains at the point C_1, and further some similar actions are performed. If the value of the quality criteria increases, then the value of dL will decrease. The degree of decrease in the parameter dL is also considered to be as an input parameter of the algorithm. After several iterations for one FCR, it moves to the point C_n. Further we consider other FCR for which similar iterative algorithm is implemented, and the initial value of dL is restored every time.

The process of the sequential movement of the FCR centers is done as long as the value of the quality criteria will decrease by the predefined times or the total number of iterations will not exceed the maximum allowable value.

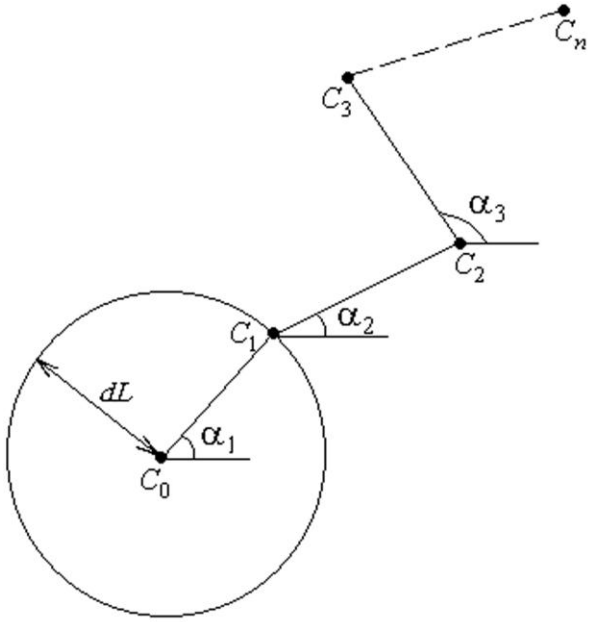


Figure 8. Scheme of sequential FCR movements.

According to computational experiments, the use of the optimization algorithm in some cases allows to find good solutions of boundary value problems. However, this algorithm has significant drawbacks:

1. The result of applying the algorithm depends on the initial approximation: the selected by a mathematician type of fictitious canonic regions (circle, ring, hollow, layer, etc.), their count and the number of summands N, retained in the general solutions (14), relating to fictitious canonic regions.

2. Functional (23) has not one, but a lot of extremes, and therefore the application of the described optimization algorithm, which is originally gradient, allows, as a rule, to find not global, but some of the many local extreme points.

In this regard, we have attempted to create a genetic algorithm for solving this optimization problem, which is deprived of these shortcomings.

5. Genetic algorithm for fictitious canonic regions selection and positioning

Genetic algorithms are one of the newest sections of the artificial intelligence [9]. They originate from the evolutionary theory of Darwin, and they are based on the use of the mechanisms of natural selection and genetic inheritance to solve optimization problems. Optimization problem is formulated in such a way that its solution could be represented as a vector (chromosome), whose components are the parameters ("genes") that characterize this

decision. Randomly it generates a certain amount of initial vectors (initial population). They are evaluated using criteria of solution quality (fitness function), resulting in each vector is assigned a specific value, which determines the probability of survival of the organism represented by this chromosome vector. Then, using these values of fitness function, "natural selection" is done - "individuals" who have sufficiently high value of fitness function have a chance to survive. Then some genetic operations are produced on "surviving" individuals - "cross" and "mutation", resulting in a "new generation". Specimens of the new generation are also evaluated using the fitness function, then the selection is made again, some genetic operations are applied etc. This is a model of an "evolutionary process", which runs for several life cycles: each generation replaces the previous one up to that point when the criterion of algorithmic stop is fulfilled. The criteria might be: global or local minimum found; the number of generations for evolution exceeded; the computational time expired.

We can distinguish the following stages of the genetic algorithm:

- Creation of the initial population.
- Determination of fitness function for individuals in a population.
- Start the cycle of evolution:
- Selecting individuals from the current population (selection).
- Crossover and mutation.
- Calculation of fitness function for all individuals.
- Formation of a new generation.
- The end of the evolution cycle.

In drawing up the genetic algorithm of FCR positions optimization we will consider the functional (23) as a function of fitness because it is an integral characteristic of the solution error.

Let us introduce the notion of *individual* and present it in the form of the following structure:

Table 1. Representation of individual's structure

Field name	*K*	FCR type	*x*	*y*	*N*	…	FCR type	*x*	*y*	*N*
Data type	Int	Int	Real	Real	Int	…	Int	Real	Real	Int

Where:

K is the number of FCR, encoded by the number of type Integer.

FCR type is one of the possible FCR kinds (circle {0}, ring {1}, hollow {3}, infinite slab {4} etc.), encoded by the number of type Integer.

X is the coordinate of FCR centre on horizontal axis, has the data type Real.

Y is the coordinate of FCR centre on vertical axis, has the data type Real.

N is the number of summands that are held in the general solution (14), encoded by the number of type Integer.

Thus, the notion of *individual* in this case means one of the variants of FCR, which chromosome genes are as follows: number of FCR, their type, coordinates that determine the FCR spatial position, and also the number of summands held in general solutions related to FCR. The aim of genetic algorithm is to find an individual for which the fitness function (functional) has the least value – a global minimum.

Two types of genetic algorithm were tested. They are called *continuous and discrete* variants. In a continuous variant the FCR centre point falls in any point of computational domain of a boundary value problem. Thus, the global minimum will be found on an infinite set of FCR positions, constrained only by a possibility of presenting the real number in a computer. In a discrete variant before the algorithm starts, a grid is formed in a computational domain. Then every FCR in every individual must have its center in the grid node. So, the global minimum will be found already on the finite set of FCR positions.

Admittedly incorrect individuals must not be used in a genetic algorithm; these are organisms that contradict the physical sense of the problem. An FCR of the type "hollow", which centre point is inside the computational domain, may serve as an example, though it is evident that the centre point of an FCR of the type "hollow" must be outside the computational domain of a boundary value problem. The test of an individual correctness is realized in the genetic algorithm.

The first population of individual organisms is generated in a random manner. The number of individuals in a population is determined according to the input parameters of genetic algorithm. The number of FCR, their type and coordinates and also the number of summands for every FCR are also generated as random values.

According to the chosen type of algorithm (continuous or discrete) the centre points of every FCR are chosen in the problem solution domain. If the continuous variant is chosen, then FCR centre points fall in any point of computational domain and uniform distribution is used for coordinates x and y. If the discrete variant is used, then the FCR centre points fall in the grid nodes and the probabilities of falling in all nodes are the same.

After generation every individual takes a test on correctness. If the organism is incorrect for the problem, then the regeneration of an individual organism is performed.

After the computation of fitness function value by formula (23) every individual from the population undergoes sorting by the value. An individual with the best fitness function value takes the first leading position; it is not subjected to mutation and necessarily passes selection in the next generation in order to get better (or the same) value for the leading individual at the next algorithm iteration.

Two variants of selection of individuals for crossover are implemented.

In the first variant every individual is crossed with one of the remaining individuals, chosen in a random manner. So, in this variant every individual takes place in the crossover at least once.

The second variant is called "roulette" algorithm. A probability value for crossing is formed for every individual. The better the fitness function value is the more is the probability value for crossover.

According to probability values M random pairs are formed. They produces M descendents. In the general case individuals-descendents in the "roulette" algorithm have a smaller fitness function value than in the first variant of selection of individuals for crossover.

After fulfilling the crossover process a test of a generated individual on correctness takes place. If an individual is incorrect for the given problem, the crossover process is performed again.

Five variants of crossover operator are implemented.

Simple method. The integer number *K* is chosen in the interval from 1 to *M*, where *M* is the number of FCR in an individual. Then the first *K* fictitious regions from the first individual are chosen to be individuals-descendents, the rest FCRs are selected from the second individual.

Flat method. FCRs taking correlative positions in individuals are crossed. The centre point of a new FCR is chosen in a random manner from the interval that is made by FCR-parent centre points. The type of a new FCR is chosen in a random manner from the types that FCR-parents have.

Mixed method. FCRs taking correlative positions in individuals are crossed. The centre point of a new FCR is chosen in a random manner from the interval that is made by FCR-parent centre points. This interval is increased by means of a coefficient that is the parameter of crossover method. The type of a new FCR is chosen in a random manner from the type that FCR-parents possessed.

Discrete method. The integer number *K* is chosen in a random manner from the interval from 1 to *M*, where *M* is the number of FCRs in an individual. Then *K* FCRs from the first individual in the random manner is included into the individual-descendent, the rest FCRs are chosen from the second individual.

Fuzzy method. FCRs taking correlative positions in individuals are crossed. The probability of FCR-descendent centre point to fall closer to the FCR-parent centre point is increased.

After fulfilling the crossover stage the mutation stage takes place. Every individual may mutate with a certain degree of probability that is the input parameter of a genetic algorithm. During mutation only one gene can be changed in an individual. FCR that will be subjected to mutation is selected in a random manner. The type of selected FCR may be changed only to one of the remaining types, or one of centre point coordinates may be changed. The change of a coordinate takes place near the initial coordinate.

After fulfilling the mutation stage the test of a generated individual on correctness takes place. If an individual is incorrect for the given problem, the mutation process is fulfilled again.

Then a selection phase comes. This phase provides a test that indicates the existence of replicated individuals. If such replicated individual exists, it will be replaced by a new random individual. When there is no replicated individual remained in the population, values of fitness function will be calculated for each individual left. Individuals in the population are sorted according to their values of fitness function and in the next generation we may see a half of these individuals that have better values of fitness function.

6. Genetic and gradient methods in comparison

Problem 1. Find the temperature distribution in the biconnected domain (figure 9), where the temperature on the outer circuit is 100^{O}C and on the internal – 3320^{O}C

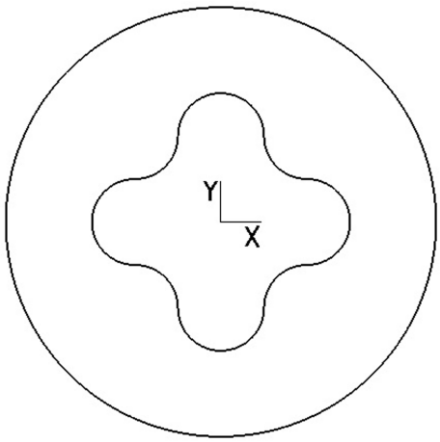


Figure 9. Biconnected domain, presenting a cross section of a solid-fuel rocket engine.

Optimization with the gradient method. To solve a boundary value problem, using FCR and the gradient method, it is necessary to set the initial number, the type and the position of fictitious canonic regions and the number of held summands in general solutions for the chosen FCRs. An experience of such problems solution shows that it is rational to use only 1 FCR of "a ring" type, for which a general solution of Laplace equation has the form (16) and 8 FCRs of a circular hollow in infinite space type, for which it has the form (20) or (21). Initially all FCRs were placed in the origin of the coordinate system.

To solve an optimization problem with the gradient method, the maximum number of algorithm iterations was set to 1000. As a result of first 20 iterations, the error $\varepsilon = 0{,}20\%$ was achieved, and then its value didn't reduce during all iterative process.

Figure 10 presents an optimal position of FCRs, obtained with the gradient method.

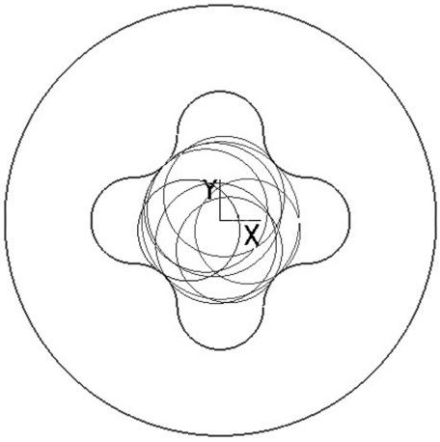


Figure 10. A scheme of the optimal positions of FCRs, obtained with the gradient method.

Optimization with the genetic algorithm. To solve this problem a genetic algorithm with the following input parameters was launched:

- The number of individuals in a population – 100;
- Initial number of FCRs in an individual – 9;
- Initial number of held summands – 20;
- The probability of a mutation – 5%;
- The maximum number of generations – 100.

After the replacement of 10 generations an error of the boundary value problem reduced to $\varepsilon = 0{,}20\%$, the value, achieved by gradient method. Then the genetic method continued its work and as a result of 100 generation replacement the error $\varepsilon = 0{,}007\%$ was achieved and this error is 28 times less than the error of the gradient method.

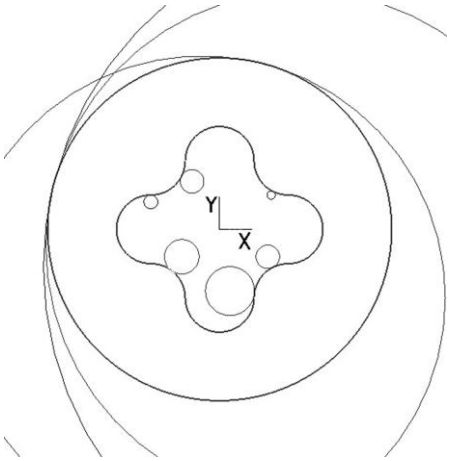


Figure 11. A scheme of the optimal positions of FCRs, obtained with the genetic algorithm.

Boundary value solution in a form of temperature isolines, obtained with the FCR method and the gradient algorithm, is given in the figure 12.

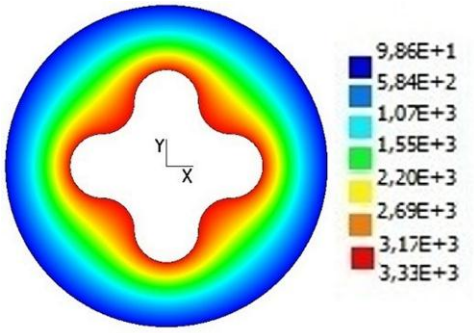


Figure 12. A solution of the boundary value problem 1 – temperature isolines in a cross section of a solid-fuel rocket engine.

Problem 2. Find a solution of a boundary value problem of the theory of elasticity in the biconnected domain, depicted in the figure 9. The rigid constraint is set on the outer boundary and on the internal boundary a uniform pressure distribution is set - 152 MPa (1500 atm).

As well as in the preceding case, in the solution of this problem gradient and genetic algorithms of functional minimization of boundary conditions were used. General solution of the theory of elasticity equations in the cylindrical coordinate system (r,θ,z) were used (plane-strain deformed state is supposed) [8]

$$u_r = \frac{d_0}{r} - 2(1-2\nu)\, f_0\, r + \sum_{m=2}^{\infty} \cos m\theta \left\{ d_m^1\, m\, r^{m-1} - f_m^2\, (m+2-4\nu)\, r^{-m+1} \right\} -$$

$$- \sum_{m=1}^{\infty} \cos m\theta \left\{ d_m^2\, m\, r^{-m-1} - f_m^1 \left(m-2+4\nu\right) r^{m+1} \right\}$$

$$u_\theta = -\sum_{m=2}^{\infty} \sin m\theta \left\{ d_m^1\, m\, r^{m-1} + f_m^2\, (m-4+4\nu)\, r^{-m+1} \right\} -$$

$$- \sum_{m=1}^{\infty} \sin m\theta \left\{ d_m^2\, m\, r^{-m-1} + f_m^1\, (m+4-4\nu)\, r^{m+1} \right\}$$

$$u_z = -c_0\, 2\, (1-2\nu)\, z \qquad (24)$$

Three types of FCRs can be distinguished from this solution: “a ring” type includes all basis functions, “a circle” type – only nonsingular functions, and “circular hollow in the infinite space” type – only singular basis.

The gradient method allowed us to obtain an exact analytical solution of the boundary value problem which differs from the original boundary conditions by the value $\varepsilon = 1{,}75\%$, and the genetic algorithm allowed to reduce the error to the value $\varepsilon = 0{,}67\%$. The final solution of the boundary value problem in the form of von Mises stress intensity distribution is presented in fig. 13. Here the dangerous stress concentration is seen (red isolines at the inner surface of the computational domain), which could have been one of the possible reasons of the crash of the American spaceship «Challenger» in 1986.

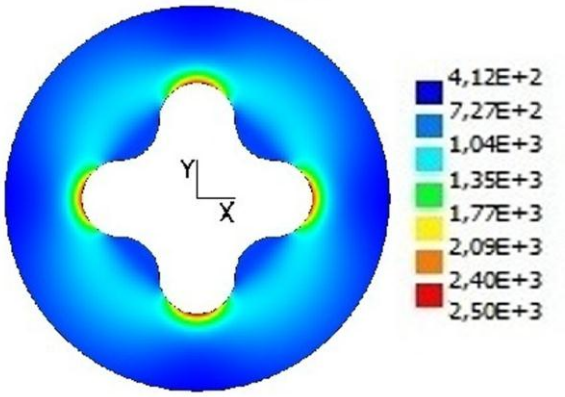


Figure 13. The solution of boundary value problem 2 – von Mises stress intensity distribution in cross section of the solid-fuel rocket engine.

Problem 3. It is necessary to obtain the solution of a boundary value problem of the steady heat conduction in a three-dimensional cylindrical solid with a hole in the side surface which is shown at fig. 14. At the solid's surface the conditions of the third type are set: the temperature of the environment at the outer and side surfaces equals 0, at the inner surface and at the surface of hole it equals 1. The coefficient of heat emission at the whole surface equals 1 (all values are given in dimensionless form).

Figure 14. Cylindrical solid with a hole in the side surface.

For application of the FCR method to the solution of three-dimensional steady problems of heat conduction we need general solutions of Laplace equation for various spatial canonic regions – sphere, cylinder etc. Let us use general solutions given in [6], obtained by Fourier method of separation of variables. According to [6] the general solution of Laplace equation in spherical coordinate system (r,φ,θ) can be presented in the following way:

$$T(r,\varphi,\theta)=c_0+c_1\,t_1(r)+\sum_{n=1}^{\infty}\sum_{m=1}^{n}\sum_{i=1}^{4}c_{nmi}\,t_{nmi}(r,\varphi,\theta)+\sum_{n=1}^{\infty}\sum_{i=5}^{6}c_{n0i}\,t_{n0i}(r,\theta)$$

$$t_1(r) = \frac{1}{r},$$

$$t_{nm1}(r,\varphi,\theta) = r^n \sin(m\varphi)\, P_n^m(\cos(\theta))$$

$$t_{nm2}(r,\varphi,\theta) = r^n \cos(m\varphi)\, P_n^m(\cos(\theta))$$

$$t_{nm3}(r,\varphi,\theta) = \frac{\sin(m\varphi)\, P_n^m(\cos(\theta))}{r^{n+1}}$$

$$t_{nm4}(r,\varphi,\theta) = \frac{\cos(m\varphi)\, P_n^m(\cos(\theta))}{r^{n+1}}$$

$$t_{n05}(r,\theta) = r^n\, P_n(\cos(\theta))$$

$$t_{n06}(r,\theta) = \frac{P_n(\cos(\theta))}{r^{n+1}} \qquad (25)$$

where P_n – Legendre polynomials, P_n^m – associated Legendre functions.

The given solution is the general solution for a hollow sphere, i.e. by the choice of coefficients of the given solution it is possible to satisfy rather arbitrary boundary conditions at the surface of a hollow sphere with any outer and inner radius. If we leave in the given solution only nonsingular basis functions, we will obtain the general solution for a solid ball, if we leave only singular – the general solution for a spherical hollow in the infinite space.

Further, according to [6] the general solution of Laplace equation in cylindrical coordinate system (r,φ,z) can be presented in the following way:

$$T(r,\varphi,z) = c_0 + c_1\, t_1(r) + c_2\, t_2(z) + \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\sum_{i=1}^{16} c_{nmi}\, t_{nmi}(r,\varphi,z) +$$

$$+ \sum_{n=1}^{\infty}\sum_{i=17}^{24} c_{n0i}\, t_{n0i}(r,z) + \sum_{m=1}^{\infty}\sum_{i=25}^{28} c_{0mi}\, t_{0mi}(r,\varphi) + \sum_{m=1}^{\infty}\sum_{i=29}^{32} c_{0mi}\, t_{0mi}(r,\varphi,z)$$

$$t_1(r) = \ln(r)$$

$$t_2(z) = z$$

$$t_{nm1}(r,\varphi,z) = I_m(\mu r)\sin(m\varphi)\sin(\mu z)$$

$$t_{nm2}(r,\varphi,z) = I_m(\mu r)\sin(m\varphi)\cos(\mu z)$$

$$t_{nm3}(r,\varphi,z) = I_m(\mu r)\cos(m\varphi)\sin(\mu z)$$

$$t_{nm4}(r,\varphi,z) = I_m(\mu r)\cos(m\varphi)\cos(\mu z)$$

$$t_{nm5}(r,\varphi,z) = K_m(\mu r)\sin(m\varphi)\sin(\mu z)$$

$$t_{nm6}(r,\varphi,z) = K_m(\mu r)\sin(m\varphi)\cos(\mu z)$$

$$t_{nm7}(r,\varphi,z) = K_m(\mu r)\cos(m\varphi)\sin(\mu z)$$

$$t_{nm8}(r,\varphi,z) = K_m(\mu r)\cos(m\varphi)\cos(\mu z)$$

$$t_{nm9}(r,\varphi,z) = J_m(\mu r)\sin(m\varphi)\sinh(\mu z)$$

$$t_{nm10}(r,\varphi,z) = J_m(\mu r)\sin(m\varphi)\cosh(\mu z)$$

$$t_{nm11}(r,\varphi,z) = J_m(\mu r)\cos(m\varphi)\sinh(\mu z)$$

$$t_{nm12}(r,\varphi,z) = J_m(\mu r)\cos(m\varphi)\cosh(\mu z)$$

$$t_{nm13}(r,\varphi,z) = Y_m(\mu r)\sin(m\varphi)\sinh(\mu z)$$

$$t_{nm14}(r,\varphi,z) = Y_m(\mu r)\sin(m\varphi)\cosh(\mu z)$$

$$t_{nm15}(r,\varphi,z) = Y_m(\mu r)\cos(m\varphi)\sinh(\mu z)$$

$$t_{nm16}(r,\varphi,z) = Y_m(\mu r)\cos(m\varphi)\cosh(\mu z)$$

$$t_{n017}(r,z) = I_0(\mu r)\sin(\mu z)$$

$$t_{n018}(r,z) = I_0(\mu r)\cos(\mu z)$$

$$t_{n019}(r,z) = K_0(\mu r)\sin(\mu z)$$

$$t_{n020}(r,z) = K_0(\mu r)\cos(\mu z)$$

$$t_{n021}(r,z) = J_0(\mu r)\sinh(\mu z)$$

$$t_{n022}(r,z) = J_0(\mu r)\cosh(\mu z)$$

$$t_{n023}(r,z) = Y_0(\mu r)\sinh(\mu z)$$

$$t_{n024}(r,z) = Y_0(\mu r)\cosh(\mu z)$$

$$t_{0m25}(r,\varphi) = r^m \sin(m\varphi)$$

$$t_{0m26}(r,\varphi) = r^m \cos(m\varphi)$$

$$t_{0m27}(r,\varphi) = r^{-m} \sin(m\varphi)$$

$$t_{0m28}(r,\varphi) = r^{-m} \cos(m\varphi)$$

$$t_{0m29}(r,\varphi,z) = r^m \sin(m\varphi)\, z$$
$$t_{0m30}(r,\varphi,z) = r^m \cos(m\varphi)\, z$$
$$t_{0m31}(r,\varphi,z) = r^{-m} \sin(m\varphi)\, z$$
$$t_{0m32}(r,\varphi,z) = r^{-m} \cos(m\varphi)\, z \qquad (26)$$

where $\mu = \frac{\pi n}{L}$, L – the period of temperature distribution by axis z, I_m, K_m, J_m, Y_m – Bessel functions.

The given solution is the general solution for a hollow cylinder. If we leave in the given solution only nonsingular basis values we will obtain the general solution for a solid cylinder, if we leave only singular values – the solution for a cylindrical hole in the infinite space. The solutions containing trigonometric functions of coordinate z correspond to the solution for a long cylinder, hyperbolic functions – to the solution for a short cylinder.

According to the FCR method, the given cylindrical solid should be immerged into the intersection of some FCRs, in the given example it was immerged into «hollow spheres» and «spherical hollows in the infinite space», for which general solutions of Laplace equation were determined in (25). In the result of genetic algorithm's work the optimal location of FCRs was found: the given solid appeared to be immerged into intersection region of one «hollow sphere» V_1 and four «spherical hollows in the infinite space» V_2, V_3, V_4, V_5, as it is shown at fig. 15.

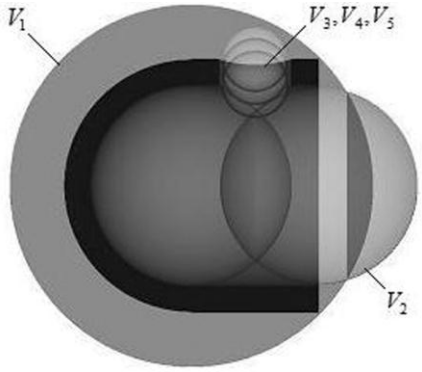


Figure 15. Scheme of the solid immersion into the intersection of FCRs - "hollow sphere" V_1 and "spherical hollows in the infinite space" V_2, V_3, V_4, V_5 (cross section in the middle of the hollow).

The results of the problem solution are presented in figure 16 and figure 17. Maximum error of boundary conditions by heat flow is less than 1%.

It is worth mentioning that in engineering analyses such an error may be considered as a consequence of real boundary conditions' idealization since all the boundary conditions are assigned with some permissible accuracy. That is, this solution is exact for some adjusted boundary conditions which differ insignificantly (less than 1%) from the initial ones.

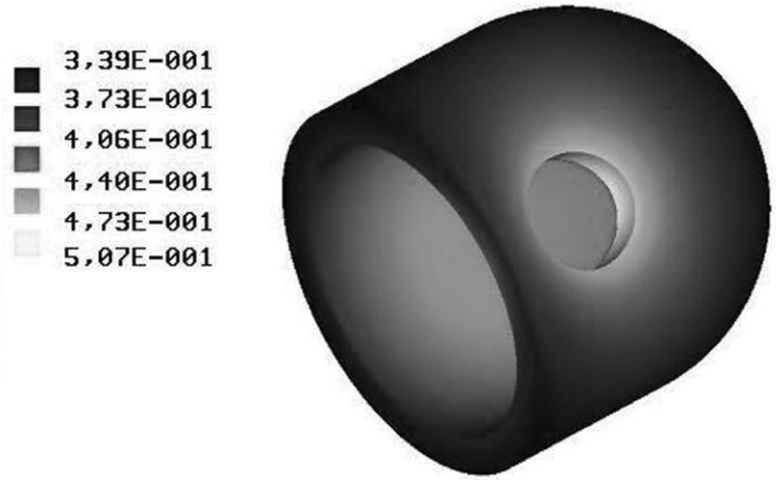


Figure 16. Temperature distribution.

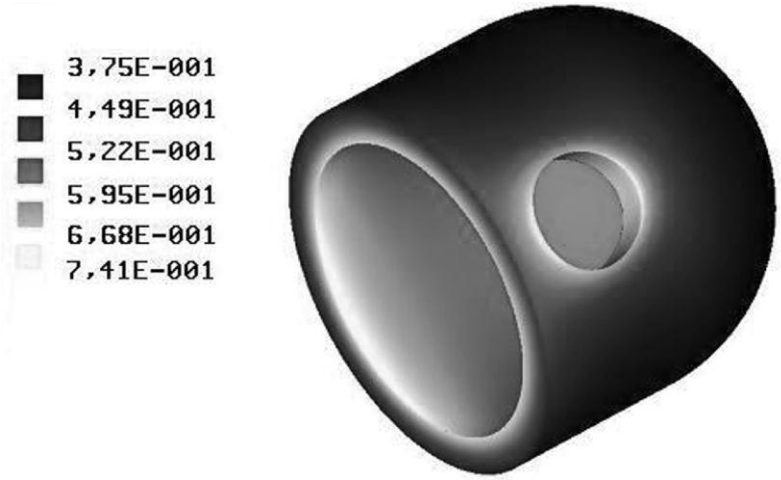


Figure 17. Heat flow distribution.

7. Conclusions

Analytical methods of boundary value problems solution (which lead to solutions in the form of analytical expressions, satisfying differential equations and boundary conditions) are more reliable than numerical methods (which lead to solutions in the form of arrays of numbers). On the other hand, analytical methods are more complicated in implementation than

numerical ones. According to this article, an effective tool for analytical methods implementation is artificial intelligence methods, particularly genetic algorithm technology.

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