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ON THE METHOD OF FUNDAMENTAL SOLUTIONS AND SOME ASPECTS OF ITS APPLICATION

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Abstract. The paper describes a general scheme of the application of the Method of Fundamental Solutions (MFS) for boundary value problems and the particular features of the application of this method. It is emphasized that to obtain accurate results when applying the method, one should take into account the physical meaning of fundamental solutions, an adequate choice of an auxiliary surface and therefore of a structure of the location of auxiliary points (simulation sources) on this surface. This is illustrated by the results of numerical experiments in which the dynamics of the solution accuracy of boundary value problems is given depending on a choice of an auxiliary surface and the number of simulation sources.

To outline the main idea of the solution of boundary value problems of mathematical physics by means of the MFS, let us consider a general stationary problem for the homogeneous equation

$$Lu(x) = 0\,, \quad x \in D\,, \tag{1}$$

$$lu(x)|_S \equiv lu(y) = g(y)\,, \quad y \in S \tag{2}$$

where D in the general case is a multiply connected domain in the Euclidian space $R^n (n = 2, 3)$ bounded by the surface S, L is a linear vector differential operator of the elliptic type, l is some operator defined on S; $u(x)$ and $g(y)$ are elements of some vector functional spaces $R_1(D)$ and $R_2(S)$,

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respectively. It is assumed that $g(y) \in L_2(S)$, where $L_2(S)$ is the space of square integrable functions on S.

The method of fundamental solutions (functions) is a particular case of the general method of solution of boundary value problems by expansion in nonorthogonal functions which can be described as follows:

Let $\{\psi_k(x)\}_{k=1}^{\infty}$ be a system of vector functions ψ_k which satisfies the following conditions:

1. Each function $\psi_k(x)$ satisfies the equation $L\psi_k(x) = 0$ in D.

2. A new function $l\psi_k(y)$, where l is the operator of the boundary condition (2), is defined for each function $\psi_k(x)$ on S.

3. The system of functions $\{l\psi_k(y)\}_{k=1}^{\infty}$ is linearly independent and complete in the space $L_2(S)$ of square integrable vector functions on S.

After finding the coefficients $a_k^{(N)}$ of the best (in the sense of $L_2(S)$) expansion of $g(y)$ in the first N functions of the system $\{l\psi_k(y)\}_{k=1}^{\infty}$,

$$g(y) \approx \sum_{k=1}^{N} a_k^{(N)} l\psi_k(y)\,,$$

an approximate solution of problem (1),(2) is

$$u^{(N)}(x) = \sum_{k=1}^{N} a_k^{(N)} \psi_k(x)\,,$$

which tends to an exact solution $u(x)$ for $N \to \infty$, provided that problem (1),(2) is correctly posed.

In [1-4] it is proved that a system of fundamental solutions of equation (1) constructed in usual manner satisfies the above-listed conditions. Mathematically the function $\psi(x, y)$ is called a fundamental solution of the operator L if $L\psi(x, y) = \delta(x - y)$, where $\delta(x - y)$ is the Dirac function $(x, y \in R^n)$.

As shown in [1-4], in the role of a system of vector functions $\{\psi_k(x)\}_{k=1}^{\infty}$ one can take a system of fundamental solutions of the operator L, $\{\psi(x, z_k)\}_{k=1}^{\infty}$, where $\{z_k\}_{k=1}^{\infty}$ is a countable set of points lying densely everywhere on the auxiliary closed surface S_1 (i. e. an arbitrarily small area of S_1 contains at least one point of the set $\{z_k\}_{k=1}^{\infty}$) which contains the domain $\overline{D} = D + S$ and $\min \rho(S, S_1) > O$, where ρ is the distance between S and S_1; if D is multiply connected, i. e. S consists of separate closed surfaces, then S_1 consists of the same number of closed surfaces.

As is known (see [1-4]), in the case of spaces R^3 (R^2) it is sufficient for S_1 to be the Liapunov surface (curve).

Remark 1. It is proved in [1-4] that if L is the Laplace operator in the plane case and S is a piecewise-smooth curve, then under the above-listed conditions,$\{\frac{1}{2\pi} \ln |x - z_k|\}_{k=1}^{\infty}$, the system of fundamental solutions of the operator L is lineraly independent and complete not only in the space $L_2(S)$, but also in the space $C(S)$ of continuous functions.

The principal restrictions of the FSM are as follows:

(a) the necessity to know the fundamental solutions of that differential operator for which the boundary value problem is posed;

(b) the absence of a general rule of the choice of S_1 and locations of auxiliary points z_k on S_1 in the case of solving the concrete problems;

(c) the method can be used only for homogeneous equations (it is obvious that the method will work for that inhomogeneous equations which might be reduced to the homogeneous equations).

The advantages of the MFS include:

1. The method can be used to solve both internal and external boundary value problems.

2. Since an approximate solution of problem (1),(2) is represented by the sum of concrete fundamental (elementary) functions which are continuous and continuously differentiable an arbitrary number of times in $\overline{D}$, the MFS enables one to compute easily both the value of an approximate solution of problem (1),(2) and its derivative of any order in the domain $\overline{D}$.

3. The method makes it possible to obtain an *a posteriori* of error estimate, since the only reason for which an error may arise is a somewhat inexact satisfaction of the boundary conditions (the principal homogeneous equation is satisfied exactly).

4. The method enables one to solve boundary value problems which, strictly speaking, are not completely well-defined; such problems frequently arise in geophysics (they should not be confused with classical incorrect boundary value problems), for example, when the geophysical fields are known and one has to determine the sources of these fields (see [5], [6]).

5. From the computation standpoint, the most important feature of the MFS as compared with the variational methods is that the approximation in that case is carried out on the surface S and not in the domain D, which thus saves computation time.

As for an approximate solution of problem (1),(2), it has the form

$$u^{(N)}(x) = \sum_{k=1}^{N} a_k^{(N)} \psi(x, z_k)\,, \tag{3}$$

assuming that the points z_k $(k = 1\,,\ 2\,, \cdots\,,\ N)$ are "uniformly" arranged on the auxiliary surface S_1; $a_k^{(N)}$ are the coefficients of the expansion of $g(y)$ in a series in terms of the first N functions of the system $\{l\psi(y, z_k)\}_{k=1}^{\infty}$ $(y \in S)$.

If the coefficients $a_k^{(N)}$ of expansion of the boundary function $g(y)$ in fundamental solutions are determined using the least squares method or the collocation method [3], to determine the coefficients $a_k^{(N)}$ we obtain a system of linear algebraic equations of the form

$$\sum_{k=1}^{N} a_k^{(N)} (l\psi_k\,,\ l\psi_j) = (g\,,\ l\psi_j)\,, \quad (j = 1\,,\, 2\,, \cdots\,,\, N)\,, \tag{4}$$

where $\psi_k(y) = \psi(y\,,\, z_k)$ and $(l\psi_k\,, l\psi_j) = \int\limits_S l\psi_k(y) l\psi_j(y) d_y S$ or

$$\sum_{k=1}^{N} a_k^{(N)} \psi(y_j\,, z_k) = g(y_j) \tag{5}$$

and the collocation points y_j $(j = 1\,, 2\,, \cdots, N)$ are "uniformly" distributed on S.

It is proved [3] that for the determinants $|A|$ and $|A'|$ of systems (4) and (5), respectively, the asymptotic relations

$$0 < |A| \le O(N^{-N})\,, \quad |A'| \le O(C_0^{N/2}) \quad (N \to \infty)\,, \tag{6}$$

hold, where C_0 is the constant not depending on N, $|A|$ is the Gram's determinant (Gramian) for the system $\{\psi_k(y)\} = \{\psi(y\,, z_k)\}$ $(k = 1\,, 2\,, \cdots, N)$, and $|A| \neq 0$ because the system of functions $\{\psi(y\,, z_k)\}_{k=1}^{\infty}$ is linearly independent of S, but it is not excluded that $|A'|$ may happen to be equal to zero (which, in practice, occurs very seldom, see [3], [8]). In that case, for the numerical implementation one should pass to system (4) or change the location structure of auxiliary (collocation) points. However numerical experiments have shown that, with the same N and the "uniform" location of collocation nodes on S, the matrix of system (5) is much better conditioned than the matrix A of system (4). Moreover, in the case of using the collocation method, to find the coefficients $a_k^{(N)}$ from system (5) we have a gain in computation time as compared with the solution of system (4).

Note that, in solving boundary value problems by the MFS, to obtain sufficient accuracy it is of principal importance to have an adequately chosen system $\{l\psi(y\,, z_k)\}_{k=1}^{N}$ (i. e. points z_k), since an increase of the number N does not lead, as a rule, to the desired results both because of the size of the corresponding Gram's determinant and because of the finiteness of digits of a computer used to solve the problem. Hence the functions of this system must be chosen so that already the first several dozen (hundred) functions provide the desired accuracy. However, in solving boundary value problems, an adequate choice of the system $\{\psi(y\,, z_k)\}_{k=1}^{N}$ (or points z_k) demands a deep understanding of the real problem which is reduced to the boundary value problem, as well as knowledge of the physical meaning of fundamental solutions.

Actually, since the fundamental solutions depend on the physical characteristics of the medium for which the problem is posed (e. g. the fundamental solutions depend on elastic constants in the case of boundary value problems of elasticity theory) and the simulation sources are placed outside the domain D, therefore while solving the boundary problems by MFS the space R^n $(D \in R^n)$ is filled (independently of us) by the same matter, as the medium D, and the simulation sources located at the points z_k $(k = 1\,, 2\,, \cdots, N)$ are used to construct the simulation model which

corresponds to the real physical model. An approximate solution of problem (1), (2) is actually the superposition of information (waves and fields) coming from the points z_k into which the sources get included simultaneously (in the statics case) and instantly. Moreover, when solving particular problems (for example, in geophysics), the FSM enables us to construct the desired solution on the basis of physical arguments and express it in terms of well-defined potentials.

For example, if L is the Laplace operator in the plane case and a solution is to be found in form (3), then $z_k (k = 1, 2, \ldots, N)$ are the points of location of simulation charges of intensity $2\pi a_k^{(N)}$. The fundamental solution $\frac{1}{2\pi} \ln |x - z_k|$ of the Laplace operator is an electric potential at the point x generated by the unit charge located at the point z_k (as known, $\Delta \ln |x - z_k| = 2\pi\delta(x - z_k)$).

Remark 2. It is easy to show that in the plane case if the simply connected domain $\overline{D}$ is contained within the unit circle whose center x_0 lies within D and we take the circumference $|x| = 1$ in the role of the auxiliary contour S_1, then for the Laplace operator we have $u^{(N)}(x) \to u(x)$, $x \in \overline{D}$, provided that $u(x_0) = 0$.

Note that if problem (1),(2) is the dynamic (nonstationary) one, then, taking into account the characteristics of wave propagation in the space R^n and the fact that the boundary of D depends on the geometry of S, then we have to determine not only the values of z_k, $a_k^{(N)}$ but also the time moments t_k $(k = 1, 2, \cdots, N)$ of inclusion of sources at the points z_k.

Therefore one should not expect accurate results when boundary value problems are solved by the MFS without taking into account the physical meaning and, accordingly, without having an adequate choice of the auxiliary surface S_1 and the structure of location of simulation sources z_k $(k = 1, 2, \cdots, N)$ on the surface S_1.

Remark 3. Many years of experience in the solution of boundary value problems by the MFS show that the highest accuracy in the sense of the approximation of $g(y)$ is obtained when the surface (curve) S_1 is similar to S. In that case the surface (contour) S_1 is the boundary of the figure D_1 similar to the figure D with the same orientation so that D and D_1 have the same gravity center. As for the choice of values $\rho(S, S_1)$ (ρ is the distance between the curves (surfaces) S and S_1) and N, they can be chosen during the numerical realization of the algorithm, taking into account *a posteriori* estimates of the accuracy of the results.

As known, the basic problems of the theory of approximate methods are considered by the successive steps as follows: 1) constructing an algorithm; 2) establishing the convergence; 3) estimation of error. It is shown in [1-4] that for the MFS the first two problems have been solved. As for an estimate of the difference $\varepsilon^{(N)}(y) = \|g(y) - lu^{(N)}(y)\|$, $\forall y \in S$, i. e., an error (depending on N) of the approximate solution of the boundary value

problem by the MFS, such an estimate is absent in the Kupradze-Aleksidze's method. As known, the real *a priori* estimate (i. e. the error depending on N) can be obtained only for a limited number of problems. Hence *a posteriori* estimates become no less important the more so that such an estimate can be obtained by computer techniques and it can be used to change automatically the further computation scheme.

For a small error $\varepsilon^{(N)}(y)\,(\forall y \in S)$ we can state that the error $[u(x) - u^{(N)}(x)]$ will also be sufficiently small for any point $x \in D$. This fact immediately follows from the assumption that problem (1), (2) is correctly posed or from theorems of the maximum principle type in the theory of harmonic functions. When the difference $\|g(y) - lu^{(N)}(y)\|$ exceeds the admissible values, we should analyse causes leading to high values of the error $\varepsilon^{(N)}(y)$. In our analysis we used the following reasoning: for large $\varepsilon^{(N)}(y)$ either the functions $l\psi(y, z_k)\,(k = 1, 2, \cdots, N)$ are not quite suitable for the expansion of $g(y)$ or the expansion coefficients are derived with a high error.

As for *a priori* estimates of the solution of boundary value problems by the MFS, we should mention the interesting articles [7-10], concerning mathematical study of MFS (the charge simulation method), where it is shown that if in problem (1), (2) L is two-dimensional Laplace operator, l-unit operator, D is a simply connected domain bounded by the analytic Jordan curve S and $g(y)$ is an analytic boundary function on S, then there exists a structure of the location of auxiliary points z_k and collocation points y_k $(k = 1\,, 2\,, \cdots, N)$ and constants $c > 0$, N_0, $0 < \tau < 1$, such that

$$\sup_{x \in \overline{D}} |u(x) - u^{(N)}(x)| \leq c\tau^N$$

for all $N \geq N_0$.

This result has a more theoretical value, than practical because to determine the location of the points y_k and z_k $(k = 1\,, 2\,, \cdots, N)$ we must have a function that conformally maps the unit circle G with boundary γ on the domain D (or the neighburhood of the circumference γ on the neighburhood of the contour S). However an exact or approximate construction of this function for a given simply connected domain (the exception is a rather limited family of domains) is a highly difficult mathematical problem.

Examples of the Application of the MFS to Obtain Approximate Solutions of Boundary Value Problems for the Plane Case

Numerous experiments on the solution of boundary value problems by means of the MFS confirm that the method is fully competitive for solving problems of mathematical physics and prove that the method is characterized by a high accuracy under an adequate choice of simulation sources.

We give some tables to illustrate, on the basis of experiments, the dynamics of the solution accuracy of boundary value problems depending on

a choice of the auxiliary contour S_1 and N. It is assumed that the auxiliary points z_k and the collocation points y_k $(k = 1\,, 2\,, \cdots\,, N)$ are located on the contours S_1 and S, respectively. Thus all examples deal with the same Dirichlet boundary value problem for the Laplace operator

$$\Delta u(x) = 0\,, \quad x \in D \tag{7}$$

$$u(y) = -\ln|y|\,, \quad y \in S \tag{8}$$

where $x = (x^1\,, x^2)$, $y = (y^1\,, y^2)$.

In all the examples considered below, the coefficients $a_k^{(N)}$ of an approximate solution

$$u^{(N)}(x) = \sum_{k=1}^{N} a_k^{(N)} \ln|x - z_k|$$

were determined from system (5) using the collocation method.

In the tables N is the number of collocation points, i. e. the number of "uniformly" located points on the contours S and S_1, $\varepsilon_{\max}$ is an *a posterioiri* estimate of the solution error of problem (7),(8),

$$\varepsilon_{\max} = |g(y_j) - u^{(N)}(y_j)|\,,$$

where $g(y_j) = -\ln|y_j|$, the points y_j $(j = 1\,, 2\,, \cdots\,, M)$ are located "uniformly" on the boundary S and $M \gg N$. In numerical experiments $M = 50000$ and computations were performed with double accuracy. For the sake of brevity some values are written with exponent E, i. e. E is used as radix 10.

Example 1. It is assumed that the domain D consists of the interior of the ellipse $S : y^1 = a\,\mathrm{cost},\ y^2 = b\,\mathrm{sint}$ $(0 \le t \le 2\pi)$ and the auxiliary contour is the ellipse $S_1 : z^1 = (a+\delta)\,\mathrm{cost}\,,\ z^2 = (b+\delta)\,\mathrm{sint}$ $(0 \le t \le 2\pi\,,\ \delta > 0)$.

In numerical experiments the collocation points y_j $(j = 1\,, 2\,, \cdots\,, N)$ and auxiliary points z_k $(k = 1\,, 2\,, \cdots\,, N)$ were located uniformly along the parameter t on the ellipses S and S_1 $(t_j = \frac{2\pi}{N}(j-1)\quad j = 1\,, 2\,, \cdots\,, N)$, respectively. Similarly, for an *a posteriori* estimate of the solution error of problem (7), (8) we used the points y_k $(k = 1\,, 2\,, \cdots\,, M)$ uniformly laying along the parameter t on S, i. e. $t_k = \frac{2\pi}{M}(k-1)$ $(k = 1\,2,, \cdots\,, M)$.

In Ttable 1 we present the results of numerical experiments for various values of $a\,, b\,, \delta$ and N.

Table 1

$a=5\,;\quad b=2$				
δ	N=100 $\varepsilon_{\max}$	N=200 $\varepsilon_{\max}$	N=300 $\varepsilon_{\max}$	N=400 $\varepsilon_{\max}$
0.5	$0.1E-04$	$0.1E-08$	$0.6E-13$	$0.13E-13$
1.0	$0.7E-07$	$0.1E-13$	$0.7E-14$	$0.12E-13$
1.5	$0.5E-07$	$0.4E-12$	$0.8E-14$	$0.19E-12$
2.0	$0.1E-07$	$0.5E-14$	$0.7E-14$	$0.17E-12$
$a=5\,;\quad b=1$				
0.1	$0.2E-01$	$0.17E-02$	$0.16E-03$	$0.1E-04$
0.2	$0.4E-02$	$0.56E-02$	$0.6E-06$	$0.1E-07$
0.3	$0.9E-03$	$0.76E-05$	$0.4E-08$	$0.9E-11$
0.4	$0.1E-01$	$0.14E-04$	$0.3E-10$	$0.1E-13$

In Table 2 is given the results of numerical experiments for narrow ellipses.

Table 2

a	b	δ	N	$\varepsilon_{\max}$
10	1	1	600	$0.1E-12$
20	1	1	600	$0.3E-08$
40	1	1	600	$0.2E-06$

Example 2. The domain D is a rectangle with center at the origin, whose sides are parallel to the coordinate axes and equal to 4 and 1. If a rectangle with center at the origin and sides 5 and 2 (parallel to axes) is taken as auxilary, then we obtain the results given in Table 3.

Table 3

N	$\varepsilon_{\max}$	N	$\varepsilon_{\max}$	N	$\varepsilon_{\max}$
50	$0.14E-05$	100	$0.5E-07$	200	$0.8E-11$

Example 3. It is assumed that the domain D consists of the interior of the astroid $S:\ \ y^1=2\,cos^3t$, $y^2=2\,sin^3t\ \ (0\le t\le 2\pi)$, and the auxiliary contour is the astroid S_1: $z^1=2\delta\,cos^3t,\quad z^2=2\delta\,sin^3t$.

In numerical experiments, like in Example 1, the collocation points, auxiliary points and points for an *a posteriori* estimate were located uniformly along the perimeter t on the curves S and S_1, respectively. In Table 4 we present the results for various values of δ and N.

Table 4

δ	N=200 $\varepsilon_{\max}$	N=400 $\varepsilon_{\max}$	N=600 $\varepsilon_{\max}$
1.1	$0.4E-03$	$0.2E-06$	$0.4E-09$
1.2	$0.3E-05$	$0.2E-09$	$0.4E-13$
1.5	$0.2E-06$	$0.4E-09$	$0.5E-10$
2.0	$0.1E-04$	$0.8E-06$	$0.2E-06$

In the Aleksidze's monograph [3] it is shown that: 1) for fixed number of N points there exist optimal auxiliary contour S_1 (or optimal location of z_k points)in the sense of accuracy of approximated solution; 2) if auxiliary contour S_1 is moving from basic boundary S then the conditionality of the matrix is deteriorated and on the contrary, by moving S_1 to the S , improving. (In this case for achieving the necessary accuracy it is enough to increase N).

The experience of using the method fundamental solutions shows that for fixed N there existed a class of auxiliary contours S_j (j=1,2, ... ,L) which obey to the mentioned conditions (see remark 3) and give the necessary accuracy for the solution of the problem. If $\varepsilon_{\max}^{(j)}$ is an accuracy for the S_j (j=1,2, ... ,L) auxiliary contour we say that S_k from this class is an optimal (for fixed N) if $\varepsilon_{\max}^{(k)} = \min \varepsilon_{\max}^{(j)}$.

Experience shows that theoretically existed optimal auxiliary contour has a neighborhood where all contours which satisfy the conditions stated in Remark 3 give satisfactory accuracy. Thus it is good hint to look for optimal one among those contours.

The Table 1 shows that for the ellipse (a=5,b=2) optimal auxiliary contour is ellipse with $1 \leq \delta \leq 2$.

In the example 2 optimal contour (by the experimental sense) is rectangle with sides 5 and 2. In Table 4 optimal auxiliary contour will be chosen from contours for which $1.2 \leq \delta \leq 1.5$.

Concluding comments

Finally it must be mentioned that simplicity and high speed of convergance of the MFS makes it popular among reserchers.

By means of modern computer techniques MFS might be successfully used for solving problems of mathematical physics and theory of conformal mapping.

At last, after some modification of MFS it might be used for approximate solution of Dirichlet plane external boundary value problem for the Laplace equation.

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