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NUMERICAL METHODS

Numerical Solution of the Three-Dimensional Dirichlet Problem for Inhomogeneous Media by the Method of Integral Equations

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Abstract—We consider the three-dimensional Dirichlet problem for equations of elliptic type in inhomogeneous media. The problem can be reduced to a system of loaded Fredholm integral equations of the second kind over the volume. We prove the uniqueness of a classical solution of the problem. We suggest a numerical solution algorithm of iterative type. An example of the numerical solution of the problem is considered, and the convergence of the iterative procedure is demonstrated numerically.

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1. INTRODUCTION

The three-dimensional Dirichlet problem in a piecewise homogeneous medium was considered in [1] and solved by the method of boundary integral equations, which permitted one to pose and solve a number of inverse problems of electrocardiography [2]. However, there are cases in which the medium parameters are continuous functions of the space variables (the gradient of the parameters is nonzero). The results in [1] do not directly apply to these cases.

In the present paper, we consider a three-dimensional boundary value problem for an equation of elliptic type in inhomogeneous media. The problem is reduced to a system of loaded Fredholm integral equations of the second kind over the volume. We suggest an iterative numerical solution algorithm for this problem.

2. STATEMENT OF THE PROBLEM. UNIQUENESS THEOREM

Consider the domain

$$\Omega = \Omega_0 \cup \Omega_1 \cup \cdots \cup \Omega_N \subset \mathbb{R}^3$$

(Fig. 1). The boundaries Γ_i of the domains Ω_i $(i = 0, \ldots, N)$ are sufficiently smooth and have no common points. We pose the following problem: find a function $u(x) \in C(\overline{\Omega})$, $u(x) = u_i(x)$, $x \in \Omega_i$, $i = 0, \ldots, N$, where $u_i(x) \in C^2(\Omega_i) \cap C^1(\overline{\Omega}_i)$ and

$$\operatorname{div}\{\sigma_i(x) \operatorname{grad} u_i(x)\} = 0, \qquad x \in \Omega_i, \qquad i = 0, \ldots, N. \tag{1}$$

The parameters σ_i, $i = 0, \ldots, N$, are continuously differentiable functions in Ω_i and are positive and finite. In addition, the Dirichlet boundary condition

$$u(x) = y(x), \qquad x \in \Gamma_0, \tag{2}$$

is satisfied, where $y(x) \in C(\Gamma_0)$ is a given function. The coupling conditions

$$u_0(x) = u_i(x), \qquad x \in \Gamma_i, \qquad i = 1, \ldots, N, \tag{3}$$

$$\sigma_0(x)\frac{\partial u_0(x)}{\partial n} = \sigma_i(x)\frac{\partial u_i(x)}{\partial n}, \qquad x \in \Gamma_i, \qquad i = 1, \ldots, N, \tag{4}$$

are satisfied on the boundaries Γ_i, $i = 1, \ldots, N$.

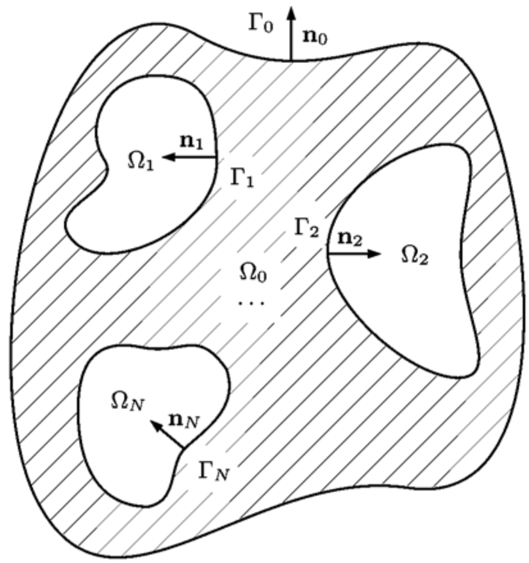

Fig. 1. The domain Ω.

Similar problems were considered, e.g., in [3, pp. 291–390]. Note that condition (4) is treated in the limit sense, and the normals are directed into the domains Ω_i, $i = 1, \ldots, N$. A function $u(x)$, $x \in \overline{\Omega}$, is called a *classical solution* of the problem if it satisfies relations (1)–(4).

Theorem 1. *The classical solution of problem* (1)–(4) *is unique.*

Proof. Suppose that there exist two classical solutions $u^{\{1\}}$ and $u^{\{2\}}$ of the problem and introduce the function $v(x) = u^{\{1\}}(x) - u^{\{2\}}(x) \neq 0$ and the differential operator

$$Lv \equiv \operatorname{div}\{\sigma(x) \operatorname{grad} v(x)\}. \tag{5}$$

We apply the first Green formula [4, p. 57] to the differential operator (5) and to the function v in the multiply connected domain Ω_0,

$$\int_{\Omega_0} v_0 L v_0 \, d\Omega = \int_{\Gamma_0} \sigma_0 v_0 \frac{\partial v_0}{\partial n} \, d\Gamma + \sum_{i=1}^{N} \int_{\Gamma_i} \sigma_0 v_0 \frac{\partial v_0}{\partial n} \, d\Gamma - \int_{\Omega_0} \sigma_0 |\operatorname{grad} v_0|^2 \, d\Omega \tag{6}$$

and

$$\int_{\Omega_i} v_i L v_i \, d\Omega = -\int_{\Gamma_i} \sigma_i v_i \frac{\partial v_i}{\partial n} \, d\Gamma - \int_{\Omega_i} \sigma_i |\operatorname{grad} v_i|^2 \, d\Omega, \qquad i = 1, \ldots, N, \tag{7}$$

in each domain Ω_i. By adding formulas (6) and (7) and by using the relations $Lv_i = 0$, $i = 0, \ldots, N$, and $v_0(x) = 0$, $x \in \Gamma_0$, we obtain

$$\sum_{i=1}^{N} \int_{\Gamma_i} \sigma_0 v_0 \frac{\partial v_0}{\partial n} \, d\Gamma - \sum_{i=1}^{N} \int_{\Gamma_i} \sigma_i v_i \frac{\partial v_i}{\partial n} \, d\Gamma - \sum_{i=0}^{N} \int_{\Omega_i} \sigma_i |\operatorname{grad} v_i|^2 \, d\Omega = 0.$$

In view of condition (4), the last expression acquires the form

$$\sum_{i=0}^{N} \int_{\Omega_i} \sigma_i |\operatorname{grad} v_i|^2 \, d\Omega = 0$$

or

$$\int\limits_{\Omega} \sigma |\operatorname{grad} v|^2 \, d\Omega = 0.$$

Since $\sigma(x) > 0$, we have $\operatorname{grad} v = 0$, or

$$\frac{\partial v(x)}{\partial x_1} = 0, \qquad \frac{\partial v(x)}{\partial x_2} = 0, \qquad \frac{\partial v(x)}{\partial x_3} = 0, \qquad x \in \overline{\Omega},$$

whence we obtain $v(x) = \text{const}$, and it follows from the condition $v(x) = 0$, $x \in \Gamma_0$, that $v(x) = 0$. Therefore, the solution of problem (1)–(4) is unique. The proof of the theorem is complete.

3. SYSTEM OF LOADED INTEGRAL EQUATIONS

Let us construct a system of integral equations of the second kind. Suppose that there exists a solution of the boundary value problem. Without loss of generality, in the derivation of the system of integral equations, we assume that $N = 1$; i.e., there is only one domain Ω_1 inside the domain Ω_0.

By the assumptions of the problem, $\sigma_i \in C^1(\Omega_i)$ and $u_i \in C^2(\Omega)$; therefore, Eq. (1) can be represented in the form

$$\Delta u_i = -\sigma_i^{-1} \operatorname{grad} u_i \operatorname{grad} \sigma_i, \qquad x \in \Omega_i, \qquad i = 0, 1. \tag{8}$$

For the representation (8), in the domain Ω_0, we write out the third Green formula

$$\begin{aligned} u_0(P) = &\int\limits_{\Gamma_0} \left[\frac{\partial u_0(Q)}{\partial n} G(P,Q) - u_0(Q) \frac{\partial G(P,Q)}{\partial n} \right] d\Gamma \\ &+ \int\limits_{\Gamma_1} \left[\frac{\partial u_0(Q)}{\partial n} G(P,Q) - u_0(Q) \frac{\partial G(P,Q)}{\partial n} \right] d\Gamma \\ &+ \int\limits_{\Omega_0} \frac{\operatorname{grad} u_0(Q) \operatorname{grad} \sigma_0(Q)}{\sigma_0(Q)} G(P,Q) \, d\Omega, \qquad P \in \Omega_0, \end{aligned} \tag{9}$$

where P is a fixed point, Q is the integration variable, and $G(P,Q)$ is the fundamental solution of the Laplace equation,

$$G(P,Q) = \frac{1}{4\pi} \frac{1}{|Q - P|}.$$

In what follows, for convenience, in the integral relations, we omit the explicit mention of the variables P and Q in the arguments of the functions; we assume that these relations have the same structure as (9).

We introduce the notation

$$\begin{aligned} &\varrho_i(x) \equiv u_0(x), \qquad \mu_i(x) \equiv \frac{\partial u_0(x)}{\partial n}, \qquad x \in \Gamma_i, \qquad i = 0, 1, \\ &\nu_{i1} \equiv \frac{\partial u_i(x)}{\partial x_1}, \qquad \nu_{i2} \equiv \frac{\partial u_i(x)}{\partial x_2}, \qquad \nu_{i3} \equiv \frac{\partial u_i(x)}{\partial x_3}, \qquad x \in \Omega_i, \qquad i = 0, 1, \\ &\operatorname{grad} u_i \equiv (\nu_{i1}, \nu_{i2}, \nu_{i3}), \qquad x \in \Omega_i, \qquad i = 0, 1. \end{aligned}$$

In (9), we land the point P from the domain Ω_0 onto the surfaces Γ_0 and Γ_1 and obtain

$$\begin{aligned} c_i \varrho_i = &\int\limits_{\Gamma_0} \left[\mu_0 G - \varrho_0 \frac{\partial G}{\partial n} \right] d\Gamma + \int\limits_{\Gamma_1} \left[\mu_1 G - \varrho_1 \frac{\partial G}{\partial n} \right] d\Gamma \\ &+ \int\limits_{\Omega_0} \frac{(\nu_{01}, \nu_{02}, \nu_{03}) \operatorname{grad} \sigma_0}{\sigma_0} G \, d\Omega, \qquad P \in \Gamma_i, \qquad i = 0, 1, \end{aligned} \tag{10}$$

where the coefficients c_0 and c_1 depend only on the geometric properties of the surfaces Γ_0 and Γ_1 and are equal to 1/2 for smooth surfaces.

Let us differentiate relation (9) with respect to x_1, x_2, and x_3,

$$\nu_{0j} = \int\limits_{\Gamma_0} \left[\mu_0 \frac{\partial G}{\partial x_j} - \varrho_0 \frac{\partial^2 G}{\partial x_j \partial n}\right] d\Gamma + \int\limits_{\Gamma_1} \left[\mu_1 \frac{\partial G}{\partial x_j} - \varrho_1 \frac{\partial^2 G}{\partial x_j \partial n}\right] d\Gamma$$
$$+ \int\limits_{\Omega_0} \frac{(\nu_{01}, \nu_{02}, \nu_{03}) \operatorname{grad} \sigma_0}{\sigma_0} \frac{\partial G}{\partial x_j} d\Omega, \qquad P \in \Omega_0, \qquad j = 1, 2, 3. \tag{11}$$

Likewise, by virtue of the coupling conditions (3) and (4) and the inward direction of normals, for the domain Ω_1, we obtain

$$-c_1 \varrho_1 = \int\limits_{\Gamma_1} \left[\frac{\sigma_0}{\sigma_1}\mu_1 G - \varrho_1 \frac{\partial G}{\partial n}\right] d\Gamma + \int\limits_{\Omega_1} \frac{(\nu_{11}, \nu_{12}, \nu_{13}) \operatorname{grad} \sigma_1}{\sigma_1} G \, d\Omega, \quad P \in \Gamma_1, \tag{12}$$

$$-\nu_{1j} = \int\limits_{\Gamma_1} \left[\frac{\sigma_0}{\sigma_1}\mu_1 \frac{\partial G}{\partial x_j} - \varrho_1 \frac{\partial^2 G}{\partial x_j \partial n}\right] d\Gamma$$
$$+ \int\limits_{\Omega_1} \frac{(\nu_{11}, \nu_{12}, \nu_{13}) \operatorname{grad} \sigma_1}{\sigma_1} \frac{\partial G}{\partial x_j} d\Omega, \qquad P \in \Omega_1, \qquad j = 1, 2, 3. \tag{13}$$

By combining Eqs. (10)–(13), we obtain a system of loaded integral equations of the second kind for the unknown functions ϱ_1, μ_i, and ν_{ij}, $i = 0, 1$, $j = 1, 2, 3$.

The theory of such equations is identical to the theory of Fredholm integral equations of the second kind [5, pp. 156–160]. By using the constructed system of integral equations and by following [1], one can prove the existence of a classical solution of the original differential problem.

4. NUMERICAL SOLUTION METHOD

For problem (1)–(4), one can construct an iterative solution algorithm that is based on the method of boundary integral equations and does not require the computation of volume integrals. We illustrate the main idea of that method for the following problem. In the domain $\Omega \subset \mathbb{R}^3$ with sufficiently smooth boundary Γ, find a function $u(x)$, $u \in C^2(\Omega) \cap C^1(\overline{\Omega})$, such that

$$\operatorname{div}\{\sigma(x) \operatorname{grad} u(x)\} = 0, \qquad x \in \Omega, \qquad u(x) = y(x), \qquad x \in \Gamma, \tag{14}$$

where $y(x) \in C(\Gamma_0)$ and $\sigma(x) \in C^1(\overline{\Omega})$ are given functions.

Just as in the derivation of the system of loaded integral equations, we reduce the expression (14) to the form

$$\Delta u = -\sigma^{-1} \operatorname{grad} u \operatorname{grad} \sigma, \qquad x \in \Omega,$$

and construct an iterative process on the kth iteration of which one solves the following boundary value problem for the Poisson equation:

$$\Delta u^{(k)} = b^{(k-1)}, \qquad x \in \Omega, \qquad u^{(k)}(x) = y(x), \qquad x \in \Gamma, \tag{15}$$

where

$$b^{(k-1)} = -\sigma^{-1} \operatorname{grad} u^{(k-1)} \operatorname{grad} \sigma, \qquad k = 1, 2, \dots, \qquad b^{(0)} = 0.$$

Consider an algorithm for solving the Poisson equation at the kth step of the iterative method by the method of boundary integral equations. For notational convenience, we omit the index k in forthcoming expressions.

In the domain Ω, we write out the third Green formula

$$u + \int\limits_{\Gamma} \left[u\frac{\partial G}{\partial n} - \frac{\partial u}{\partial n} G \right] d\Gamma = -\int\limits_{\Omega} \Delta u \, G \, d\Omega, \qquad P \in \Omega.$$

By virtue of condition (15), we have $\Delta u = b$, and the Green formula acquires the form

$$u + \int\limits_{\Gamma} \left[u\frac{\partial G}{\partial n} - \frac{\partial u}{\partial n} G \right] d\Gamma = -\int\limits_{\Omega} b \, G \, d\Omega, \qquad P \in \Omega. \tag{16}$$

We approximately represent [6] the function b in the form of the series

$$b = \sum_{i=1}^{L} \alpha_i \varphi_i \tag{17}$$

in the basis functions φ_i such that each basis function can be represented in the form

$$\varphi_i = \Delta \phi_i, \qquad i = 1, \ldots, L. \tag{18}$$

We substitute the expansions (17) and (18) into (16),

$$u + \int\limits_{\Gamma} \left[u\frac{\partial G}{\partial n} - \frac{\partial u}{\partial n} G \right] d\Gamma = -\sum_{i=1}^{L} \alpha_i \int\limits_{\Omega} \Delta \phi_i \, G \, d\Omega, \qquad P \in \Omega. \tag{19}$$

By using the third Green formula, in the expression (19), we reduce the volume integral to a surface integral,

$$u + \int\limits_{\Gamma} \left[u\frac{\partial G}{\partial n} - \frac{\partial u}{\partial n} G \right] d\Gamma = \sum_{i=1}^{L} \alpha_i \left\{ \phi_i + \int\limits_{\Gamma} \left[\phi_i \frac{\partial G}{\partial n} - \frac{\partial \phi_i}{\partial n} G \right] d\Gamma \right\}, \qquad P \in \Omega. \tag{20}$$

In (20), we land the point P onto the surface Γ and obtain the integral equation

$$cu + \int\limits_{\Gamma} \left[u\frac{\partial G}{\partial n} - \frac{\partial u}{\partial n} G \right] d\Gamma = \sum_{i=1}^{L} \alpha_i \left\{ c\phi_i + \int\limits_{\Gamma} \left[\phi_i \frac{\partial G}{\partial n} - \frac{\partial \phi_i}{\partial n} G \right] d\Gamma \right\}, \qquad P \in \Gamma, \tag{21}$$

from which one can find the normal derivative of the function u on the surface Γ.

To make the next step of the iterative process, one should compute the gradient of the function u. To this end, we differentiate relation (20) with respect to x_1, x_2, and x_3,

$$\begin{aligned} \frac{\partial u}{\partial x_j} &= -\int\limits_{\Gamma} \left[u \frac{\partial^2 G}{\partial x_j \partial n} - \frac{\partial u}{\partial n} \frac{\partial G}{\partial x_j} \right] d\Gamma \\ &+ \sum_{i=1}^{L} \alpha_i \left\{ \frac{\partial \phi_i}{\partial x_j} + \int\limits_{\Gamma} \left[\phi_i \frac{\partial^2 G}{\partial x_j \partial n} - \frac{\partial \phi_i}{\partial n} \frac{\partial G}{\partial x_j} \right] d\Gamma \right\}, \qquad P \in \Omega, \quad j = 1, 2, 3. \end{aligned} \tag{22}$$

In the approximate representation of the function b, for the functions φ, it is convenient to use RBF-functions [6; 7, pp. 36–98]. To this end, it suffices to introduce M points in the domain Ω and N points on the surface Γ arbitrarily. The set of these points forms the RBF-interpolation nodes S_i, $i = 1, \ldots, L$, $L = M + N$, and the interpolation functions φ_i depend on the distance to the node S_i,

$$\varphi_i(Q) = f(|Q - S_i|), \qquad i = 1, \ldots, L.$$

The approximate values of the function b at the nodes S_i are computed by the formula

$$R\boldsymbol{\alpha} = \mathbf{b},$$

whence we obtain

$$\boldsymbol{\alpha} = R^{-1}\mathbf{b}, \tag{23}$$

where $\mathbf{b} = [b(S_1), b(S_2), \ldots, b(S_L)]$, $\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_L]$, and

$$R = \begin{bmatrix} f(0) & f(|S_1 - S_2|) & \ldots & f(|S_1 - S_L|) \\ f(|S_2 - S_1|) & f(0) & \ldots & f(|S_2 - S_L|) \\ \ldots & \ldots & \ldots & \ldots \\ f(|S_L - S_1|) & f(|S_L - S_2|) & \ldots & f(0) \end{bmatrix}.$$

In discrete form, the boundary integral equation (21) can be represented as follows (for details on the discretization, see [1]) :

$$H\mathbf{u} - G\mathbf{q} = \sum_{i=1}^{L} \alpha_i \left(H\phi_i - G\frac{\partial \phi_i}{\partial n} \right),$$

or

$$H\mathbf{u} - G\mathbf{q} = (H\hat{U} - G\hat{Q})\boldsymbol{\alpha}, \tag{24}$$

where $\mathbf{u}$ stands for the discrete values of the function u, $\mathbf{q}$ stands for the discrete values of the normal derivative of u, the matrices H and G are discrete representations of surface integrals with kernels $\partial G/\partial n$ and G, respectively, and the matrices $\hat{U}$ and $\hat{Q}$ consist of values of the functions ϕ_i and $\partial\phi_i/\partial n$, $i = 1, \ldots, L$, at each discretization node on the surface Γ.

By virtue of relation (23), Eq. (24) can be represented in the form

$$H\mathbf{u} - G\mathbf{q} = (H\hat{U} - G\hat{Q})R^{-1}\mathbf{b},$$

whence we find the vector

$$\mathbf{q} = G^{-1}[H\mathbf{u} - (H\hat{U} - G\hat{Q})R^{-1}\mathbf{b}]. \tag{25}$$

By substituting these discrete values of the function u on the surface Γ into the expression (25), we find the desired values of the normal derivative $\mathbf{q}$.

Likewise, from (22), we obtain expressions for the computation of discrete values of the gradient of the function u :

$$\mathbf{q}_j = -T_j\mathbf{u} + S_j\mathbf{q} + (\hat{\mathbf{q}}_j + T_j\hat{U} - S_j\hat{Q})R^{-1}\mathbf{b}, \qquad j = 1, 2, 3,$$

where $\mathbf{q}_1$, $\mathbf{q}_2$, and $\mathbf{q}_3$ are discrete values of the partial derivatives of the function u with respect to x_1, x_2, and x_3, $\hat{\mathbf{q}}_1$, $\hat{\mathbf{q}}_2$, and $\hat{\mathbf{q}}_3$ are discrete values of the partial derivatives of the functions ϕ_i with respect to x_1, x_2, and x_3, and the matrices T_j and S_j are discrete representations of the surface integrals with kernels $\partial^2 G/(\partial x_j \partial n)$ and $\partial G/\partial x_j$, respectively.

To illustrate the suggested method, we analyze the results of numerical solution of the following problem. In the domain $\Omega \subset \mathbb{R}^3$, find a function $u(x)$, $u \in C^2(\Omega) \cap C^1(\overline{\Omega})$, such that

$$\operatorname{div}\left\{ \frac{1}{\varepsilon + r(x)^2} \operatorname{grad} u(x) \right\} = 0, \qquad x \in \Omega,$$
$$u(x) = x_1, \qquad x \in \Gamma,$$

where $x = (x_1, x_2, x_3)$, $r(x) = \sqrt{x_1^2 + x_2^2 + x_3^2}$, and $\varepsilon = 10^{-5}$.

The design domain is an ellipse with center the point $O(0.0, 0.0, 0.0)$ and semiaxes $a_0 = 1.0$ and $a_1 = 0.5$. The surface was approximately represented by a polygon grid consisting of plane triangles.

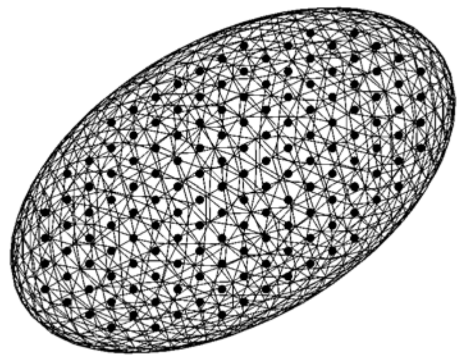

Fig. 2. Geometric structure of the design domain.

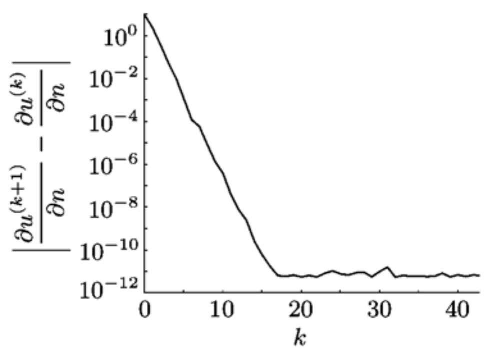

Fig. 3. Convergence of the algorithm in the logarithmic scale.

The number of boundary elements was $N_{\text{bound}} = 1920$, and the number of boundary nodes was $N = 962$. The RBF-interpolation nodes on the surface Γ coincided with the boundary nodes, the RBF-interpolation nodes in the domain Ω were chosen at the nodes of a uniform volume grid, and the number of such nodes was $M = 288$ (see Fig. 2). For the interpolation RBF-functions, we chose the functions

$$\phi = \frac{r^3}{12} + \frac{r^2}{6}, \qquad \nabla\phi = \frac{r}{4}\mathbf{r} + \frac{1}{3}\mathbf{r}, \qquad \varphi = \Delta\phi = r + 1.$$

The normal derivative $\partial u/\partial n$ of the function u on the surface Γ was found by the above-suggested method, after which the values of the function u at interior points of the domain Ω were computed. Next, the same problem was independently solved by the finite-element method with the use of the SfePy software package [8], and values of the function u at the same internal points of the domain Ω were computed. The values thus obtained were compared, and the relative error of the solution

$$\varepsilon_{\mathbf{u}} = \frac{\|\mathbf{u}_{fem} - \mathbf{u}_{bem}\|}{\|\mathbf{u}_{fem}\|}$$

was computed, which was equal to $\varepsilon_u = 3.68 \times 10^{-3}$, where $\mathbf{u}_{bem}$ is the solution found by the above-suggested algorithm and $\mathbf{u}_{fem}$ is the solution found by the finite-element method.

Figure 3 presents the graph of the convergence of the iterative process in the logarithmic scale; the x-axis represents the iteration number, and the y-axis represents the norm of the difference of solutions at the $(k+1)$st and kth steps. Figure 4 presents the values of the gradient of the function u at interior nodes of the domain Ω at the 1st and 20th iterations.

Therefore, the above-suggested algorithm of iterative type permits one to solve the Dirichlet problem in inhomogeneous media by the method of boundary integral equations.

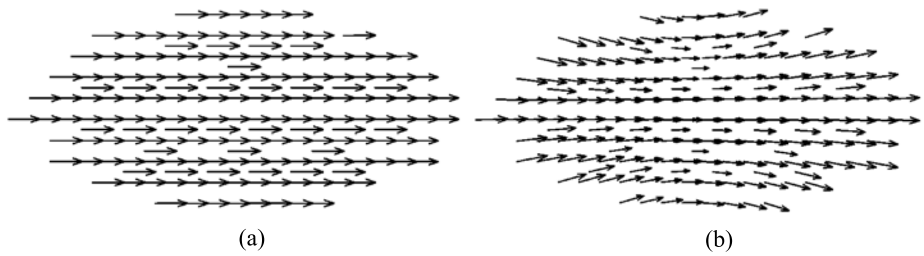

Fig. 4. The gradient of the function at interior points; (*a*) the 1st iteration; (*b*) the 20th iteration.

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