Volume Singular Integral Equation Method for Solving Problems of Diffraction of Electromagnetic Waves by a Dielectric Inhomogeneous Body in a Rectangular Waveguide

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***Abstract*—The problem of diffraction of an external electromagnetic field by a locally inhomogeneous body placed in a rectangular waveguide with perfectly conducting walls is considered. The formulated problem is reduced to a volume singular integral equation. The problem is solved with the use of the numerical collocation method. Volume singular integral equation method is applied to analyze the problem for structures of a complex geometric shape. Since the problem is highly computer-intensive, it is solved with the use of parallel algorithms realized on a supercomputer.**

Index Terms - Maxwell equations, volume singular integral equation, Galerkin method, numerical results.

I. Introduction

The study of problems of diffraction of electromagnetic waves in waveguides leads to the solution of three-dimensional vector problems to the complete electrodynamic formulation.

At present, solution of such problems is one of the topical tasks in electromagnetics. The solution that is based on mathematical methods and guarantees the accuracy suitable for practice at the electrodynamic level of rigor necessitates a very large amount of computation, which cannot be implemented even on the state of the art supercomputers. Solution of inverse electrodynamic problems for a complex system of surfaces and bodies in the resonance frequency region is the most urgent task. This problem arises when the parameters of nanocomposite materials and nanostructures are to be determined.

Solving the aforementioned problems with the help of expensive applied software packages using traditional finite difference techniques or finite element methods does not always lead to sufficiently accurate results.

Since exact solutions of diffraction problems can be obtained for a limited set of bodies with a regular geometry, it is important for many applications to develop various approximate numerical methods valid for bodies of arbitrary shapes. Thus, it is necessary to develop new methods for solving this kind of problems.

One of the promising methods is the method of volume singular integral equations (VSIE), by means of which the boundary problem is reduced to solving a VSIE [1], [2], [3], [4]. Generally, the obtained integral equation can be solved only by numerical methods but, since the dimensionality of the problem is reduced due to the reduction of the problem to a surface integral, numerical calculation is significantly simplified. Solving such problems with an accuracy appropriate for practice requires a considerable amount of computational effort.

At present, a rapid progress in the computer technology facilitates wide application of computer simulation methods for solving such problems for screens of canonical shapes.

In this work, the development of a software based on subhierarchical method is proposed and implemented. The method presented in this paper makes it possible to solve the problems for inhomogeneous bodies of complex geometric shapes using the results of the solution of the problem for bodies of basic shapes.

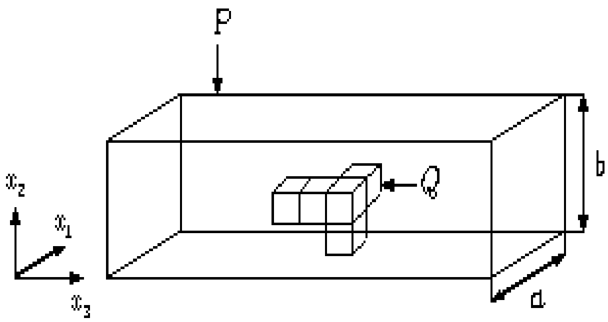
II. FORMULATION OF THE PROBLEM

Consider the following diffraction problem. In Cartesian coordinates, let $P = \{x : 0 < x_1 < a, 0 < x_2 < b, -\infty < x_3 < +\infty\}$ be a waveguide with perfectly conducting surface ∂P (Fig. 1). The waveguide contains volume body Q ($Q \subset P$ being a region) characterized by constant permeability μ_0 and positive 3×3 tensor permittivity function $\hat{\varepsilon}(x)$. The components of $\hat{\varepsilon}(x)$ are bounded functions in region $\bar{Q}$, inverse tensor $\hat{\varepsilon} \in L_\infty(Q)$ exists in Q, and its components are also bounded in Q .

Fig 1. The body Q in the waiveguide P.

The region ∂Q is assumed to have a piecewise smooth boundary Q . We assume, in addition, that the body Q does not touch the waveguide walls, i.e. $\partial Q \cap \partial P = \emptyset$. Beyond $P \backslash \bar{Q}$, the medium is isotropic, homogeneous, and characterized by constants $\varepsilon_0 (> 0),\ \mu_0 (> 0)$.

It is necessary to determine the electromagnetic field's $E, H \in L_{2,loc}(P)$ (and, hence, $E,\ H \in L_2(Q)$) excited in



the waveguide by an external field with, the time dependence $\exp(-i\omega t)$, where ω is the circular frequency.

In region $P \subset R^3$, the standard differential operators $grad,\ div$ and $curl$ are understood in the sense of generalized functions.

We seek weak (generalized) solutions to the system of Maxwell equations

$$\begin{array}{l} curlH = -i\omega\hat{\varepsilon}E \\ curlE = i\omega\mu_0 H,\ x \in P. \end{array} \quad (1)$$

These solutions must satisfy the conditions at infinity: fields E and H for $|x_3| > C$ and rather large $C > 0$ are represented as

$$\left(\begin{array}{c} E \\ H \end{array}\right) = \left(\begin{array}{c} E^0 \\ H^0 \end{array}\right) +$$

$$+\sum_p R_p^{\pm} exp(i\gamma_p^1 |x_3|) \left(\begin{array}{c} \lambda_p^{(1)} \Pi_p \vec{e_3} - i\gamma_p^1 \nabla_2 \Pi_p \\ -i\omega\varepsilon_0 (\nabla_2 \Pi_p) \times \vec{e_3} \end{array}\right)$$

$$+\sum_p Q_p^{\pm} exp(i\gamma_p^2 |x_3|) \left(\begin{array}{c} i\omega\mu_0 (\nabla_2 \psi_p) \times \vec{e_3} \\ \lambda_p^{(2)} \psi_p \vec{e_3} - i\gamma_p^{(2)} \nabla_2 \psi_p \end{array}\right) \quad (2)$$

("+" and "–" correspond to $+\infty$ and $-\infty$, respectively), where $\vec{e}_{1,2,3}$are units vectors in the Cartesian coordinate frame, $\gamma_p^{(j)} = \sqrt{k_0^2 - \lambda_p^{(j)}}$, $Im\gamma_p^{(j)} > 0$ or $Im\gamma_p^{(j)} = 0$, $k_0\gamma_p^{(j)} \geq 0$ and $Im\gamma_p^{(j)} = 0$, $k_0\gamma_p^{(j)} \geq 0$ sets of eigenvalues and eigenfunctions (orthonormal in $L_2(\Pi)$) of 2D Laplace operator $-\Delta$ in the rectangle $\Pi := \{(x_1, x_2) : 0 < x_1 < a, 0 < x_2 < b\}$ with the Dirichlet and Neumann conditions, respectively; $k_0^2 = \varepsilon_0\mu_0\omega^2$.

The coefficients $R_p^{(\pm)}$ and $Q_p^{(\pm)}$ appearing in the right hand side of (2) are estimated to have the behavior

$$R_p^{(\pm)}, Q_p^{(\pm)} = O(p^m), p \to \infty \quad (3)$$

for certain $m \in N$.

E^0 and H^0, appearing in (2) are known incident fields, and they are the solutions of the boundary value problem in the absence of an inhomogeneous body Q.

From a physical viewpoint, conditions expressed in (2) that the scattered field is the superposition of normal waves emanating from the body. Conditions (3) provide for the exponential convergence of series (2) and the possibility of their term-wise differentiation with respect to x_j performed an arbitrary number of times.

The field E must satisfy the boundary condition on the waveguide's walls

$$E_\tau|_{\partial P} = 0. \quad (4)$$

Relationships (1)–(4) for the field E yield the integrodifferential equation [4]

$$E(x) = E^0(x) + k_0^2 \int_Q \hat{G}_E(r) \left(\frac{\widehat{\varepsilon}(y)}{\varepsilon_0} - \hat{I}\right) E(y)\, dy +$$

$$graddiv \int_Q \hat{G}_E(r) \left(\frac{\widehat{\varepsilon}(y)}{\varepsilon_0} - \hat{I}\right) E(y)\, dy,\ \ x \in Q \quad (5)$$

where $\hat{I}$ is the unit tensor.

The components of the diagonal Green's tensor $\hat{G}_E = diag\left(G_E^1, G_E^2, G_E^3\right)$ have the following form [4], [6], [7], [8]:

$$G_E^1 = \frac{2}{ab} \sum_{n=0}^{\infty} \sum_{m=1}^{\infty} \frac{\exp(-\gamma_{nm}|x_3 - y_3|)}{\gamma_{nm}(1 + \delta_{0n})} \times$$
$$\cos\frac{\pi n}{a} x_1 \sin\frac{\pi m}{b} x_2 \cos\frac{\pi n}{a} y_1 \sin\frac{\pi m}{b} y_2,$$

$$G_E^2 = \frac{2}{ab} \sum_{n=1}^{\infty} \sum_{m=0}^{\infty} \frac{\exp(-\gamma_{nm}|x_3 - y_3|)}{\gamma_{nm}(1 + \delta_{0m})} \times$$
$$\sin\frac{\pi n}{a} x_1 \cos\frac{\pi m}{b} x_2 \sin\frac{\pi n}{a} y_1 \cos\frac{\pi m}{b} y_2,$$

$$G_E^3 = \frac{2}{ab} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\exp(-\gamma_{nm}|x_3 - y_3|)}{\gamma_{nm}} \times$$
$$\sin\frac{\pi n}{a} x_1 \sin\frac{\pi m}{b} x_2 \sin\frac{\pi n}{a} y_1 \sin\frac{\pi m}{b} y_2.$$

In these expressions, $\gamma_{nm} = \sqrt{\left(\frac{\pi n}{a}\right)^2 + \left(\frac{\pi m}{b}\right)^2 - k_0^2}$ the branch of the square root is chosen such that $Im\gamma_{nm} \geq 0$.

Equation (5) can be solved by means of various numerical methods. In this study, we apply the collocation method, because the use of the Galerkin method leads to more cumbersome formulas and calculations.

III. THE COLLOCATION METHOD

For the equation $A\phi = f, (\phi, f \in X)$, with linear bounded operator $A : X \to X$ in Hilbert space X, we consider the collocation method that is formulated as follows. Approximate solution $\phi_n \in X_n$ is determined from the equation $P_n A\phi_n = P_n f$. Here, $\phi_n \in X_n$ (X_n is an n-dimensional subspace of space X), and $P_n : X \to X_n$ is result of the projection of X onto a finite dimensional subspace, by using the operator defined below.

Let us split the region Q into elementary subdomains $Q_i$with piecewise smooth boundaries ∂Q_i so that the conditions $Q_i \cap Q_j = \emptyset$ are fulfilled when $i \neq j$ and$\overline{Q} = \underset{i}{\cup}\overline{Q_i}$. In each subdomain Q_i , we choose the collocation point (node) x^i. Consider the basis functions $v_i = \begin{cases} 1, x \in Q_i \\ 0, x \notin Q_i \end{cases}$. Let subspaces be linear hulls of basis functions: $X_n = \text{span}\{v_l,\ \ldots,\ v_n\}$.

We require that the chosen basis functions satisfy the approximation condition

$$\forall x \in X \ \lim_{n\to\infty} \inf_{\bar{x}\in X_n} \|x - \bar{x}\| = 0.$$

Let us define operator $P_n : X \to X_n$ as follows: $(P_n\phi)(x) = \phi(x^i),\ x \in Q_i$

Note that, in this situation, the values of functions $(P_n\phi)(x)$ for $x \in \partial Q_i$ are not defined, but this is not important, because $X = L_2$ in our case.

The equation $P_nA\phi_n = P_nf$ is equivalent to the following:

$$(A\phi_n)(x^j) = f(x^j),\quad j = 1,\ \ldots,\ n.$$

Let us represent the approximate solution as a linear combination of basis functions: $\phi_n = \sum\limits_{k=1}^{n} c_k v_k$

The substitution of this representation into the scheme of the collocation method yields the system of linear algebraic equations for unknown coefficients c_k:

$$\sum_{k=1}^{n} c_k(Av_k)(x^j) = f(x^j),\ j = 1,\ \ldots,\ n.$$

Now, let us construct a scheme for solving the integral equation by means of the collocation method.

We formulate the method for integrodifferential equation (5). Assume that the tensor $\left(\frac{\hat{\varepsilon}(x)}{\varepsilon_0} - \hat{I}\right)$ is invertible in $\bar{Q}$, $\left(\frac{\hat{\varepsilon}(x)}{\varepsilon_0} - \hat{I}\right)^{-1} \in L_\infty(Q)$.

Let us introduce the notation

$$\hat{\xi} = \left(\frac{\hat{\varepsilon}(x)}{\varepsilon_0} - \hat{I}\right)^{-1},\ J = \left(\frac{\hat{\varepsilon}(x)}{\varepsilon_0} - \hat{I}\right)E \quad ,$$

and pass to the next equation

$$AJ \equiv \hat{\xi}(x)\vec{J}(x) - k_0^2 \int\limits_Q \hat{G}_E(x,y)J(y)dy -$$

$$graddiv \int\limits_Q \hat{G}_E(x,y)J(y)dy = J^0(x) \quad , \quad x \in Q. \qquad (6)$$

Equation (6) can be represented as a system of three scalar equations:

$$\sum_{i=1}^{3} \xi_{li}J^i(x) - k_0^2 \int\limits_Q \hat{G}_E(x,y)J^l(y)dy -$$

$$\frac{\partial}{\partial x_l} div_x \int\limits_Q \hat{G}_E(x,y)J(y)dy = E^{0l}(x),\ l = 1,2,3. \qquad (7)$$

We define the components of the approximate solution $J_n = (J_n^1, J_n^2, J_n^3)$ as follows:

$$J_n^1 = \sum_{k=1}^{n} a_k f_k^1(x),\ J_n^2 = \sum_{k=1}^{n} b_k f_k^2(x),\ J_n^3 = \sum_{k=1}^{n} c_k f_k^3(x),$$

where f_k^i are the basis step functions.

Below, we construct functions f_k^1. Assume that Q is a parallelepiped:

$$Q = \{x : a_1 < x_1 < a_2,\ b_1 < x_2 < b_2,\ c_1 < x_3 < c_2\}.$$

Let us split Q into elementary parallelepipeds:

$$\Pi_{klm} = \{x : x_{1,k} < x_1 < x_{1,k+1}, x_{2,l} < x_l < x_{2,l+1},$$
$$x_{3,m} < x_3 < x_{3,m+1}\}$$
$$x_{1,k} = a_1 + \frac{a_2 - a_1}{n}k,\ x_{2,l} = b_1 + \frac{b_2 - b_1}{n}l,$$
$$x_{3,m} = c_1 + \frac{c_2 - c_1}{n}m,$$

where $k, l, m = 0, ..., n-1$.

We obtain the following formulas for f_{klm}^i, $i = 1,2,3$:

$$f_{klm}^i = \begin{cases} 1,\ x \in \bar{\Pi}_{klm} \\ 0,\ x \notin \bar{\Pi}_{klm} \end{cases}.$$

The constructed set of basis functions satisfies the necessary approximation condition in $L_2^3 = L_2 \times L_2 \times L_2$.

In order to construct matrix elements, we integrate the components of the Green's tensor over the parallelepiped $P_{i_1i_2i_3} = \{(x_1, x_2, x_3) : i_1 \le \frac{x_1}{h_1} \le i_1 + 1, i_2 \le \frac{x_2}{h_2} \le i_2 + 1, i_3 \le \frac{x_3}{h_3} \le i_3 + 1\}$ and denote these components G_I^1, G_I^2, G_I^3. Then, we obtain

$$G_I^1 = \frac{8}{\pi^2}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{f_{nm}^0(x_3)}{\gamma_{nm}^2 nm}\cos(nX_1)\sin(mX_2)\sin\left(\frac{nH_1}{2}\right)$$
$$\times\cos(nH_1(i_1+0.5))\sin(mH_2(i_2+0.5))\sin\left(\frac{mH_2}{2}\right) +$$
$$\frac{2H_2}{\pi^2}\sum_{m=1}^{\infty}\frac{f_{0m}^0(x_3)}{\gamma_{0m}^2 n}\sin(mX_2)\sin(mH_2(i_2+0.5))\sin\left(\frac{mH_2}{2}\right)$$

$$G_I^2 = \frac{8}{\pi^2}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{f_{nm}^0(x_3)}{\gamma_{nm}^2 nm}\sin(nX_1)\cos(mX_2)\sin\left(\frac{nH_1}{2}\right)$$
$$\times\sin(nH_1(i_1+0.5))\cos(mH_2(i_2+0.5))\sin\left(\frac{mH_2}{2}\right) +$$
$$\frac{2H_1}{\pi^2}\sum_{n=1}^{\infty}\frac{f_{n0}^0(x_3)}{\gamma_{n0}^2 m}\sin(nX_1)\sin(nH_1(i_1+0.5))\sin\left(\frac{nH_1}{2}\right)$$

$$G_I^3 = \frac{8}{\pi^2}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{f_{nm}^0(x_3)}{\gamma_{nm}^2 nm}\sin(nX_1)\sin(mX_2)\sin\left(\frac{nH_1}{2}\right)$$
$$\times\sin(nH_1(i_1+0.5))\sin(mH_2(i_2+0.5))\sin\left(\frac{mH_2}{2}\right)$$

Here,

$$X_1 = \frac{\pi x_1}{a}, X_2 = \frac{\pi x_2}{b}, Y_1 = \frac{\pi y_1}{a},$$
$$Y_2 = \frac{\pi y_2}{b}, H_1 = \frac{\pi h_1}{a}, H_2 = \frac{\pi h_2}{b},$$

$$x_1 = j_1 h_1,\ \ x_2 = j_2 h_2,\ y_1 = i_1 h_1,\ y_2 = i_2 h_2,$$

$$\gamma_{nm} = \sqrt{\left(\frac{\pi n}{a}\right)^2 + \left(\frac{\pi m}{b}\right)^2 - k_0^2},$$

$$f_{nm}^0(x_3) = \begin{cases} exp(-(x_3 - (i_3+1)h_3)\gamma_{nm}) \\ -exp(-(x_3 - i_3 h_3)\gamma_{nm}), \\ x_3 > (i_3+1)h_3 \\ \\ exp(-(i_3 h_3 - x_3)\gamma_{nm}) \\ -exp(-((i_3+1)h_3 - x_3)\gamma_{nm}), \\ x_3 < i_3 h_3 \\ \\ 2 - exp(-(x_3 - i_3 h_3)\gamma_{nm}) \\ -exp(-((i_3+1)h_3 - x_3)\gamma_{nm}), \\ i_3 h_3 < x_3 < (i_3+1)h_3 \end{cases}$$

The values of the integrated components of the Green's tensor at a collocation point are obtained by summating slowly convergent series and their second order derivatives. The computation of slowly convergent series is accelerated by separating the singularity.

It is convenient to represent the extended matrix obtained according to the collocation method in a block form:

$$\left(\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & B_1 \\ A_{21} & A_{22} & A_{23} & B_2 \\ A_{31} & A_{32} & A_{33} & B_3 \end{array}\right)$$

Elements A_{kl} and B_k are determined from the relationships

$$A_{kl}^{ij} = \xi_{kl} f_i^l(x_j) - \delta_{kl} k_0^2 \int\limits_Q G^k(x_j, y) f_i^l(y) dy$$

$$-\frac{\partial}{\partial x_k} \int\limits_Q \frac{\partial}{\partial x_l} G^l(x_j, y) f_i^l(y) dy, \qquad (8)$$

$$B_k^i = E_0^k(x_i) \qquad (9)$$

where the coordinates of the collocation points are

$$x_i = (x_{i1}, x_{i2}, x_{i3}),\ \ x_{i1} = (i_1 + 0.5) h_1,$$

$$x_{i2} = (i_2 + 0.5) h_2,\ \ x_{i3} = (i_3 + 0.5) h_3,$$

$$k, l = 1, 2, 3; i_1, i_2, i_3,\ \ j_1, j_2, j_3 = 0, \ldots, n-1.$$

Thus, we have obtained the necessary formulas for calculating the matrix coefficients of the collocation method applied to solve the volume singular integral equation in the problem of determination of the permittivity of a material.

IV. THE SUBHIERARCHIAL ALGORITHM

Let $Q = \{x : a_1 < x_1 < a_2, b_1 < x_2 < b_2, c_1 < x_3 < c_2\}$ be a filled waveguide section ($a_1 = 0,\ a_2 = a,\ b_1 = 0,\ b_2 = b,\ c_1 = 0,\ c_2 = c$). The algorithm of calculation of the electromagnetic field inside a filled waveguide section has been described in the foregoing. Let us consider the algorithm of calculation of the electromagnetic field in a rectangular waveguide for a body of a complex geometric shape. We use the matrix obtained according to the collocation method for a filled section. The problem of diffraction by a body of a complex shape can be solved when the body entirely fits into the considered waveguide section and consists of grid elements [5], [9], [10], [11], [12].

The subhierarchical method makes it possible to compose a matrix for determination of the electromagnetic fields inside a body of a complex shape with the use of the matrix calculated for the complete waveguide section. In the constructed structure, we introduce a new numeration of elementary parallelepipeds belonging to the structure of a complex shape and form a new grid. This grid will be employed for calculating the field on the body of a complex shape.

We solve the system of linear algebraic equations for the matrix composed with the use of the new grid and find the values of the field inside the structure of a complex shape. The speed of construction of the new matrix depends on the dimensions of the structure and the dimensions of the grid. The considered method makes it possible to avoid bulky calculation of matrix elements. This method is especially efficient for calculation of a series of problems for bodies of various shapes. Because of the computationally intensive nature of the formulated problem, the matrix for the case of a filled section has been calculated at the computational cluster of the Research Computing Center of the Moscow State University.

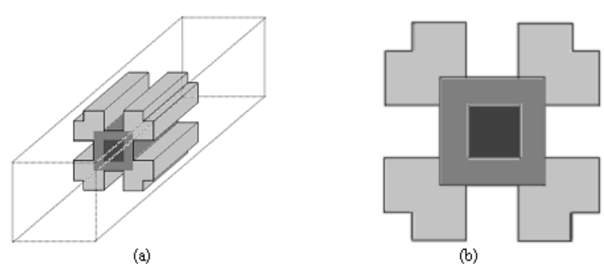


Fig 2. The body shape of Q

Let us present the calculated electric current on a structure of a complex shape (Fig. 2).. The results have been obtained with the use of a $8 \times 8 \times 8$ grid. The incident wave propagates along the $0z$axis. The right hand side of the matrix equation is $E^0 = A \sin\left(\frac{\pi x_1}{a}\right) e^{-i\gamma_1 x_3}$.

The shape of the body is displayed in Fig. 2a, and its material the parameter are shown in Fig. 2b. The absolute values of the second component of the electric field in the first, third, sixth and eighth layers are shown in Figs. 3a–3d, respectively. Thus, a subhierarchical method has been proposed for solving the problem of diffraction by a dielectric body that has an arbitrary shape and is located in a waveguide.

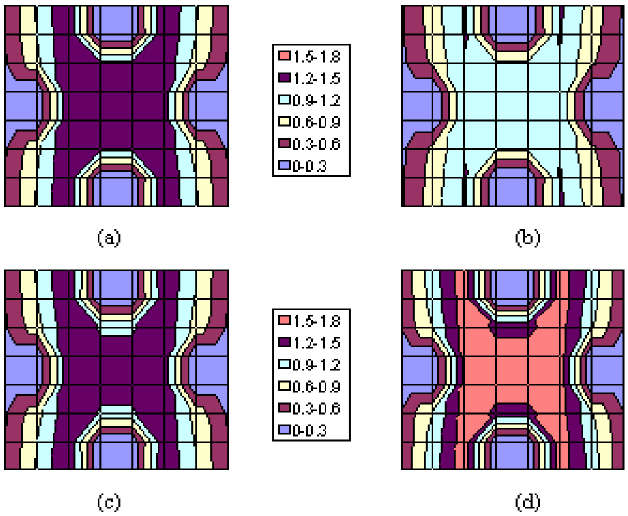


Fig 3. The modulus of solution of integral equation on the body Q

The method has been implemented on a supercomputer calculation, and the are memory required to store the matrix is 38 MB for 8x8x8 grid. Program execution time is three minutes using 512 processors. We have compared these results with an analytic solution to the diffraction problem for (full) homogeneous diaphragm in the waveguide. The relative error estimation is approximately $1 - 2\%$ for the magnitude of the electric field.

V. CONCLUSION

The advantages of the method presented in the paper are as follows: i) The integral equation is solved only on the bounded body in spite of the fact that the original boundary value problem is formulated in the infinite domain; ii) Orders of the matrices in the problem are much less than orders of similar matrices in the finite difference method or the finite elements method; iii) Since coefficients of the matrices can be calculated independently, it provides us an opportunity to use parallel algorithms to determine the unknown coefficients; hence these coefficients can efficiently computed by using supercomputers, as has been done in this work.

This method can be generalized to handle similar problems involving waveguides with circular cross-sections. We further believe that this approach can be implemented in (commercial) software packages to solve a variety of diffraction problems, involving inhomoge-neous objects of the arbitrary shape.

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