Algorithms for numerical solution of integral equations of three-dimensional scalar diffraction problem

A A Kashirin, S I Smagin
Computing Center, Far Eastern Branch, Russian Academy of Sciences; 65 Kim Yu Chena St., Khabarovsk, 680000, Russian Federation
E-mail: elomer@mail.ru, smagin@ccfebras.ru

Abstract. The three-dimensional diffraction problem of stationary acoustic waves on a homogeneous inclusion is considered. It is reduced to the weakly singular boundary Fredholm integral equations of the first kind with one unknown function, each of which is conditionally equivalent to the original problem. By using the original method of averaging the integral operators kernels, these equations are approximated by systems of linear algebraic equations. The resulting systems are solved numerically by the generalized minimal residual method (GMRES). Then the solution of the initial problem is calculated. To find the solution on the spectrum of integral operators, where the condition of equivalence of integral equations to the original problem is violated, the interpolation solution method is proposed. It does not require knowledge of the spectrum and allows us to find the approximated solutions with high accuracy. The proposed algorithms have been implemented in the computing cluster of Computing Center FEB RAS. The results of the calculations that allow us to assess the possibilities of this approach are presented.

1. Introduction
Three-dimensional diffraction problems are found in various fields of science and technology. Their analytical solutions can be found only in exceptional cases. Therefore, the diffraction problems are mainly solved numerically.

In this work, the initial problem is reduced to weakly singular boundary integral Fredholm equations of the first kind with one unknown function. Each of these equations is conditionally equivalent to the diffraction problem. Using the special method of averaging the integral operators kernels with weak singularities, these equations are approximated by systems of linear algebraic equations. The resulting systems are solved numerically by means of the generalized minimal residual method (GMRES). Then approximate solutions of the original problem are calculated [1], [2].

Integral operators of these equations have a spectrum. It is a countable set of positive wave numbers. For each of these numbers the condition of integral equations equivalence to the initial problem is violated. Herein the method of solution interpolation is proposed. It does not require knowledge of the spectrum and allows us to find a solution of the diffraction problem for all positive wave numbers [3].
This research was supported in through computational resources provided by the Shared Facility Center Data Center of FEB RAS (Khabarovsk) [4]. The results of numerical experiments are presented. They allow us to assess the potential of this approach.

2. The initial problem and its equivalent integral equations
Let us formulate the initial problem.

Problem 1. In bounded domain $\Omega_i$ of three-dimensional Euclidean space $R^3$ and in unbounded domain $\Omega_e = R^3 \setminus \bar{\Omega}_i$ separated by a closed surface $\Gamma \in C^{r+\beta}$, $r + \beta > 1$, find complex-valued functions $u_i(e) \in H^1(\Omega_i(e), \Delta)$, satisfying integral identities

$$\int_{\Omega_i(e)} \nabla u_i(e) \nabla u_i^*(e) dx - k_i^2 u_i(e) u_i^*(e) dx = 0 \quad \forall u_i(e) \in H_0^1(\Omega_i(e)), \quad (1)$$

matching conditions at the interface of media from $\Omega_i$ and $\Omega_e$

$$\langle u_i^- - u_i^+, \mu \rangle_{\Gamma} = \langle f_0, \mu \rangle_{\Gamma} \quad \forall \mu \in H^{-1/2}(\Gamma), \quad (2)$$

$$\langle \eta, p_i N^- u_i - p_e N^+ u_e \rangle_{\Gamma} = \langle \eta, p_e f_1 \rangle_{\Gamma} \quad \forall \eta \in H^{1/2}(\Gamma),$$

as well as the radiation condition at infinity for $u_e$

$$\partial u_e / \partial |x| - i k_e u_e = o \left( |x|^{-1} \right), \quad |x| \to \infty, \quad (3)$$

if functions $f_0 \in H^{1/2}(\Gamma)$ and $f_1 \in H^{-1/2}(\Gamma)$ are set on the boundary $\Gamma$.

Here $v^*$ is a complex conjugate function to $v$, $(\cdot, \cdot)_{\Gamma}$ is duality ratio on $H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)$, generalizing the scalar product in $H^0(\Gamma)$, $u^\pm \equiv \gamma^\pm u$, $\gamma^- : H^1(\Omega_i) \to H^{1/2}(\Gamma)$, $\gamma^+ : H^1(\Omega_e) \to H^{1/2}(\Gamma)$ are trace operators, $N^\pm : H^1(\Omega_i, \Delta) \to H^{-1/2}(\Gamma)$, $N^+ : H^1(\Omega_e, \Delta) \to H^{-1/2}(\Gamma)$ are operators of normal derivatives [5], $f_0 = u_0^\pm$, $f_1 = N^+ u_0$,

$$k_i^2 = \omega \left( \omega + i \gamma_i(e) \right) / c_i^2, \quad \text{Im}(k_i(e)) \geq 0, \quad p_i(e) = c_i^2 \gamma_i(e) k_i^2 - 1$$

$\omega$ is a circular oscillation frequency, $c_i(e) > 0$, $\rho_i(e) > 0$, $\gamma_i(e) \geq 0$. Definitions of the functional spaces used hereafter are available in [5].

Let us introduce the following notations:

$$\left( A_i(e) q \right)(x) \equiv \left\langle G_i(e)(x, \cdot), q \right\rangle_{\Gamma}, \quad \left( B_i(e) q \right)(x) \equiv \left\langle N_{g} G_i(e)(x, \cdot), q \right\rangle_{\Gamma}, \quad (4)$$

$$\left( B_i^* q \right)(x) \equiv \left\langle N_{g} G_i(e)(x, \cdot), q \right\rangle_{\Gamma}, \quad G_i(e)(x, y) = \exp \left( i k_i(e) |x-y| \right) / (4\pi |x-y|).$$

We will search for the solution of problem 1 in the form of potentials

$$u_e(x) = \left( A_e q \right)(x), \quad x \in \Omega_e, \quad (5)$$

$$u_i(x) = (p_{ei} A_i \left( N^+ u_e + f_1 \right) - B_i^* (u_e^+ + f_0)) (x), \quad x \in \Omega_i,$$

where $q \in H^{-1/2}(\Gamma)$ is an unknown density, $f_0 \in H^{1/2}(\Gamma)$, $f_1 \in H^{-1/2}(\Gamma)$, $p_{ei} = p_e / p_i$.

The kernels of the integral operators here are the fundamental solutions of the Helmholtz equations and their normal derivatives. Therefore, they satisfy the identities (1) and the radiation condition at infinity (3). Furthermore, the fulfillment of the first matching conditions (2) for them automatically means the fulfillment of the second. By substituting potentials (5)
into the first condition, we obtain a weakly singular Fredholm integral equation of the first kind to find unknown density $q$:

$$\langle Cq, \mu \rangle_{\Gamma} = \langle f_2, \mu \rangle_{\Gamma} \quad \forall \mu \in H^{-1/2}(\Gamma),$$

(6)

where

$$C = (0.5 + B^*_i) A_e + p_{ei} A_i (0.5 - B_e), \quad f_2 = -(0.5 + B^*_i) f_0 + p_{ei} A_i f_1.$$

Problem 1 allows for another equivalent formulation in the form of an integral Fredholm equation of the first kind with a weak singularity in the kernel. We will seek its solution in the form of

$$u_i(x) = (A_i q)(x), \quad x \in \Omega_i,$$

(7)

$$u_e(x) = (A_e \left( f_1 - p_{ie} N - u_i \right) - B^*_e \left( f_0 - u_i \right)) \quad x \in \Omega_e,$$

where $q \in H^{-1/2}(\Gamma)$ is an unknown density, $f_0 \in H^{1/2}(\Gamma)$, $f_1 \in H^{-1/2}(\Gamma)$, $p_{ie} = p_i/p_e$.

In this case, problem 1 is reduced to equation

$$\langle Dq, \mu \rangle_{\Gamma} = \langle f_0, \mu \rangle_{\Gamma} \quad \forall \mu \in H^{-1/2}(\Gamma),$$

(8)

$$D = (0.5 - B^*_e) A_i + p_{ie} A_e (0.5 + B_i).$$

Theorem 1. Let $f_0 \in H^{1/2}(\Gamma)$, $f_1 \in H^{-1/2}(\Gamma)$, $\gamma_e > 0$ or $\omega$ is not the eigenfrequency of the following problem

$$\Delta u + k^2 u = 0, \quad x \in \Omega_i, \quad u^− = 0.$$  

(9)

Then equations (6) and (8) are correctly solvable in the class of densities $q \in H^{-1/2}(\Gamma)$ and formulas (5) and (7) give the solution of problem 1.

3. Numerical method

Let us construct surface cover $\Gamma$ by system $\{\Gamma_m\}_{m=1}^M$ of the neighborhoods of node points $x'_m \in \Gamma$ lying inside the spheres of radii $h_m$, with the centers in $x'_m$, and denote its subordinate unity partition as $\{\varphi_m\}$. We shall use functions

$$\varphi_m(x) = \varphi_m(x) \left( \sum_{k=1}^M \varphi_k(x) \right)^{-1}, \quad \varphi'_m(x) = \left\{ \begin{array}{cl} (1 - r_m^2/h_m^2)^{\beta}, & r_m < h_m, \\ 0, & r_m \geq h_m, \end{array} \right.$$  

where $x \in \Gamma$, $r_m = |x - x'_m|$, $\varphi_m \in C^1(\Gamma)$ if $\Gamma \in C^{r+\beta}$, $r + \beta > 1$.

The approximate solutions of equations (6) and (8) will be sought on the grid $\{x_m\}$,

$$x_m = \frac{1}{\varphi_m} \int_{\Gamma} x \varphi_m d\Gamma, \quad \varphi_m = \int_{\Gamma} \varphi_m d\Gamma,$$

whose nodes are the centers of gravity of functions $\varphi_m$. We assume that for all $m = 1, 2, \ldots, M$ inequalities

$$0 < h' \leq |x_m - x_n|, \quad m \neq n, \quad n = 1, 2, \ldots, M,$$

$$h' \leq \sigma_m \leq h_m \leq h, \quad h/h' \leq q_0 < \infty,$$

are satisfied where $h$, $h'$ are positive numbers depending on $M$, $q_0$ does not depend on it, $\sigma_m^2 = 0.5\varphi_m$.  

3
Integral operators from (4) on $\Gamma$ are approximated by expressions [2]

$$\langle A_{i(e)}q, \varphi_m \rangle_{\Gamma} \approx \sum_{n=1}^{M} A_{i(e)}^{mn} q_n, \quad m = 1, 2, \ldots, M, \quad (10)$$

$$A_{i(e)}^{mn} = A_{mn} \left( k_{i(e)} \right), \quad A_{mn} \left( k \right) = \frac{\bar{\varphi}_m \varphi_n}{8\pi r_{mn}} \exp \left( \frac{\mu^2}{2} - \frac{\gamma^2}{2} \right) \left( w \left( z_{mn}^- \right) - w \left( z_{mn}^+ \right) \right), \quad n \neq m,$$

$$\mu_{mn} \left( k \right) = \frac{r_{mn}^2}{4\pi} \exp \left( \mu_{mn}^{2} \right) \left( ikw \left( \mu_{mn} \right) + \frac{\sqrt{2\pi}}{\varphi_m} \left( \frac{\varphi_m}{\mu} + 2\mu - \frac{k^2 \sigma_m^2}{3} \right) \right),$$

$$\sigma_{mn}^2 = \sigma_m^2 + \sigma_n^2, \quad \mu_{mn} = 0.5k\sigma_{mn}, \quad z_{mn}^\pm = \mu_{mn} \pm i\gamma_{mn}, \quad \gamma_{mn} = r_{mn}/\sigma_{mn}, \quad i^2 = -1,$$

$$w \left( z \right) = -\frac{2i}{\sqrt{\pi}} \exp \left( -z^2 \right) \int_{z}^{\infty} \exp \left( t^2 \right) dt,$$

$$\langle aq + B_{i(e)}q, \varphi_m \rangle_{\Gamma} \approx \sum_{n=1}^{M} B_{i(e)}^{mn} q_n, \quad m = 1, 2, \ldots, M, \quad a = \pm 0.5, \quad (11)$$

$$\langle aq + B_{i(e)}^*q, \varphi_m \rangle_{\Gamma} \approx \sum_{n=1}^{M} B_{i(e)}^{mn} q_n, \quad m = 1, 2, \ldots, M, \quad (12)$$

$$B_{i(e)}^{mn} = \frac{n_{mn}}{4\pi r_{mn}^2} \exp \left( ik_{i(e)}r_{mn} \right) \left( ik_{i(e)}r_{mn} - 1 \right) \varphi_m \varphi_n, \quad n \neq m,$$

$$B_{i(e)}^{mn} = (-|a| + a + G_{sm}) \varphi_m, \quad \eta_{mn} = \sum_{l=1}^{3} n_{ml} \frac{x_{ml} - x_{mn}}{r_{mn}}, \quad G_{sm} = -\sum_{n \neq m}^{M} \frac{\eta_{mn} \varphi_n}{4\pi r_{mn}^2}.$$

$n_{ml}$ are components of the unit vector of the external normal to surface $\Gamma$ at the point $x_m$.

Operators on the left-hand sides of equations (6) and (8) are approximated by compositions of operators (10)–(12):

$$\langle Cq, \varphi_m \rangle_{\Gamma} \approx \sum_{n=1}^{M} C_{i(e)}^{mn} q_n, \quad \langle Dq, \varphi_m \rangle_{\Gamma} \approx -\sum_{n=1}^{M} C_{i(e)}^{mn} q_n, \quad m = 1, 2, \ldots, M, \quad (13)$$

$$C_{i(e)}^{mn} = B_{i(e)}^{mn} A_e^{mn} - p_{ei} A_{i(e)}^{mn} B_e^{mn},$$

whereas those on the right-hand sides of equations (6) – (8) – by formulas

$$\langle f_2, \varphi_m \rangle_{\Gamma} \approx \sum_{n=1}^{M} \left( p_{ei} A_{i(e)}^{mn} f_{1n} - B_{i(e)}^{mn} f_{0m} \right), \quad \langle f_0, \varphi_m \rangle_{\Gamma} = \varphi_m f_{0m}, \quad (14)$$

$$f_{lm} = \langle f_l, \varphi_m / \varphi_m \rangle_{\Gamma}, \quad l = 0, 1, \quad m = 1, 2, \ldots, M.$$

By solving the corresponding systems of linear equations, we find the approximate values of the densities of integral equations at the points of discretization. After that, the diffraction problem solution can be easily and accurately calculated with the help of integral representations both in the near and far zones.
3.1. Problem solution on the spectrum

For the numerical solution of integral equations on the spectrum, we are going to use the following scheme. Let $k_e > 0$ denotes some eigenvalue of the problem (9), and $q(k_e)$ is a particular solution of the inhomogeneous equation (6) or (8) depending on it. We choose a number $\delta > 0$. Then the interpolation formula

$$q(k_e) = 4q(k_e + i\delta) - q(k_e - \delta + i\delta) - q(k_e + \delta + i\delta) - q(k_e + 2i\delta) + O(\delta^4)$$

(15)

is valid for the particular solution of the integral equation. Here all densities in the right part are solutions of correctly solvable integral equations. The substitution of the density in formulas (5) or (7) gives an approximate solution of the original problem.

4. Results of numerical experiments

The program for numerical solution of diffraction problems is written in Fortran 90, which is a console application designed to work on multiprocessor computing systems. Intel Fortran is used as a compiler, complimented by Intel Math Kernel Library (Intel MKL). OpenMP standard is implemented for this compiler.

The correctness and accuracy of the numerical method have been verified by means of numerical solution of test problems with known exact solutions. As such internal and external boundary value Dirichlet and Neumann problems for the Helmholtz equation in areas bounded by a unit sphere and a three-axis ellipsoid, as well as the problem of plane wave diffraction on a unit ball were used. The convergence of approximate solutions to exact solutions of the same problems on thickening grids was also checked. In all the cases considered, there was a good agreement of decisions [2].

Example 1. The diffraction problem of a plane acoustic wave on a unit ball with a center at the origin and three different sets of parameters of the medium and inclusion is considered.

The complex amplitude of the initial pressure wave field has the form

$$u_0(x) = \exp(ik_e x_3),$$

media parameters: I) $k_i = 12.5, \rho_i = 4, k_e = 7.725251836937, \rho_e = 3$; II) $k_i = 7, \rho_i = 2, k_e = 16.923621852138, \rho_e = 5$; III) $k_i = 21, \rho_i = 7, k_e = 13.6980231532492, \rho_e = 4.5$.

The eigenvalues of the problem (9) are chosen as $k_e$.

The main aim has been to demonstrate the potential of the solution interpolation method. In this regard, the problem from example 1 was solved twice with and without interpolation of the solution (formula (15), $\delta = 0.01$). It was formulated in the form of equation (8). The number of discretization points $M$ varied from 500 to 128,000. The exact solution of the diffraction problem is given in [2].

Figures 1 and 2 show the values of relative solution errors of the diffraction problem from example 1 calculated in the norm of grid functions spaces $H_0^1(\Omega_i)$ (fig. 1 – without interpolation of the solution, fig. 2 – with interpolation of the solution). The solid line denotes the errors of functions $u_i$, the dotted line denotes the errors of functions $u_e$. The results of calculations relating to the first, second and third set of parameters are marked on the charts by triangles, circles and squares, respectively. It is seen that the solution interpolation method can be effectively used to find approximate solutions of diffraction problems on the spectrum of the problem (9). For sufficiently large $M$ the order of solution error is not lower than $h^2 \sim M^{-1}$.

The results of other numerical experiments are given in [2], [3].

5. Conclusions

The work presents the numerical method for the diffraction problem of acoustic waves on three-dimensional homogeneous inclusions. This problem formulated in the form of boundary integral Fredholm equations of the first kind with one unknown function. Based on the results of computational experiments, it can be concluded that the proposed numerical method has a
Figure 1. Diffraction problem solution errors from example 1 found without solution interpolation.

Figure 2. Diffraction problem solution errors from example 1 found with solution interpolation.

sufficiently high accuracy. With a large number of discretization points $M$ it is a second-order method with respect to the "step" $h$ given the surface grid. The method allows for calculations in a wide range of wave numbers and can be used to solve other problems of mathematical physics formulated in the form of weakly singular boundary or volume Fredholm integral equations. Further development of the proposed approach to the numerical solution of diffraction problems may be connected with a decrease in its computational complexity, for example, by using fast methods of matrix-vector multiplication [6].

Acknowledgments
This work was supported by the Russian Foundation for Basic Research (project 17-01-00682) and Basic Research Program of the Far Eastern Branch of the Russian Academy of Sciences (project 18-5-100).

References
[1] Kashirin A A and Smagin S I 2014 Numerical solution of integral equations for a scalar diffraction problem *Doklady Mathematics* **90** 549-552
[2] Kashirin A A and Smagin S I 2018 Numerical solution of integral equations for the three-dimensional scalar diffraction problems Comput. Technologies **23** 20-36 (In Russ.)
[3] Kashirin A A and Smagin S I 2018 Numerical solution of integral equations on the spectrum for acoustic waves diffraction *Informatika i Sistemy Upravleniya* **58** 141-149 (In Russ.)
[4] Sorokin A A, Makogonov S V and Korolev S P 2017 The information infrastructure for collective scientific work in the Far East of Russia *Scientific and Technical Information Processing* **44** 302-304
[5] McLean W 2000 *Strongly Elliptic Systems and Boundary Integral Equations* (Cambridge: Cambridge University Press)
[6] Kashirin A A, Smagin S I and Taltykina M Yu 2016 Mosaic-skeleton method as applied to the numerical solution of three-dimensional Dirichlet problems for the Helmholtz equation in integral form *Comput. Math. and Math. Phys.* **56** 612-625