Dedicated to Academician S.K. Godunov on the occasion of his 90th birthday

# Method of Difference Potentials for Evolution Equations with Lacunas

S. V. Petropavlovsky<sup>*a*</sup> and S. V. Tsynkov<sup>*b*,\*</sup>

 <sup>a</sup> National Research University Higher School of Economics, Moscow, 101000 Russia
 <sup>b</sup> Department of Mathematics, North Carolina State University, Box 8205, Raleigh, NC 27695, USA \*e-mail: tsynkov@math.ncsu.edu
 Received November 14, 2019; revised November 14, 2019; accepted December 16, 2019

**Abstract**—A boundary method for computing unsteady wave propagation in three-dimensional space is proposed. The described approach is based on the method of difference potentials and the Huygens principle, which makes it possible to update the solution on the scatterer boundary by using a fixed time interval.

**Keywords:** method of difference potentials, Huygens principle, lacunas, wave equation **DOI:** 10.1134/S0965542520040144

# 1. INTRODUCTION

Boundary methods for solving problems of mathematical physics have been long and successfully applied to primarily elliptic problems. The main advantage of the boundary formulation is that the dimension of the problem is reduced by one after passing to equations for unknowns specified only on the boundary of the original domain [1]. A direct generalization of this approach to unsteady problems faces an obvious difficulty, namely, the boundary for an evolution problem represents a spatiotemporal manifold, i.e., the direct product of the spatial domain boundary and the solution time interval. Moreover, with growing time of integration, this boundary expands, so that increasingly more variables and equations have to be stored and solved [2]. In practice, this approach is not applicable even in the case of short integration times.

In this paper, we describe a boundary method for solving certain hyperbolic equations that is free of the indicated shortcoming. We consider equations satisfying the Huygens principle, in other words, equations whose solutions have a finite backward memory in time. The last property is equivalent to the existence of lacunas in solutions of these equations, i.e., domains in space-time where solutions vanish when the source (the right-hand side of the equation) generating this solution becomes zero. Practically important examples of such equations are the three-dimensional wave equation with constant coefficients and Maxwell's equations in a vacuum. Since the dependence of solutions to these equations is bounded in time, we can split the interval of integration into small subintervals and advance over fixed time steps, sequentially updating the solution of some boundary equations. As a result, the advantages of the boundary formulation (dimension reduction in space variables by one) are combined with a solution-updating algorithm designed in the spirit of a usual difference scheme for an evolution equation. Due to the dimension reduction, the resulting algorithm is *computationally more efficient than the conventional solution based on an explicit difference scheme* (this property holds starting at a certain duration of computation).

Another feature of the proposed approach is the methods used for reducing and especially solving the boundary value problem. The traditional approach is based on discretizing integrals taken over the boundary and solving the resulting algebraic system. For domains with complex geometry, the indicated technique may cause considerable computational difficulties. An additional difficulty is associated with the fact that the kernels in the convolutions are singular. Our presentation relies on the method of difference potentials [3], in which the arising convolutions are computed by solving an auxiliary problem in a geometrically simple domain (say, cube) with the help of a suitable difference scheme on a simple rectangular

grid. Due to the last circumstance, the algorithm is easy to implement and provides opportunities to control and improve the numerical accuracy by using high-accuracy schemes and other advantages inherent in the finite-difference approach. Moreover, there is no loss of accuracy associated with the approximation of curvilinear boundaries/boundary conditions on a rectangular grid.

Below, the method is described as applied to an exterior problem for the three-dimensional wave equation. In other words, we solve the problem of wave scattering by an obstacle with a boundary of arbitrary complex geometry; more specifically, we are interested in the reflected field. As applied to scattering problems, an additional advantage of any boundary method, including the one described below, is that the radiation condition at infinity is exactly taken into account. In the case of volume integration methods, radiation conditions at infinity are replaced by specially constructed artificial boundary conditions on the outer boundary of the computational domain (see, e.g., [4]). Additionally, our computations rely on a high (fourth) order accurate difference scheme, which allows us to effectively cope with numerical dispersion.

The general idea of the method in a continuous formulation is presented in Section 2. The main point is a time advancing scheme with small step sizes. A discretization of the algorithm is described in detail in Section 3. The results of test computations are given in Section 4.

## 2. IDEA OF THE METHOD

Consider the following exterior problem for the three-dimensional wave equation with constant coefficients:

$$\Box_{c} u = 0, \quad (\mathbf{x}, t) \in \mathbb{R}^{3} \setminus \Omega \times (0, T], \tag{2.1}$$

$$\mathbf{l}_{\Gamma} u = \phi, \quad (\mathbf{x}, t) \in \partial \Omega \times (0, T], \tag{2.2}$$

$$u_{|_{t=0}} = \partial u / \partial t_{|_{t=0}} = 0, \tag{2.3}$$

where  $\Box_c \equiv \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta$  is the d'Alembert operator and c is the wave propagation speed. The task is to find

the solution  $u(\mathbf{x}, t)$  outside a bounded domain  $\Omega \subset \mathbb{R}^3$  over time  $t \in (0, T]$ . This problem formulation is typical of (unsteady) wave scattering by an obstacle  $\Omega$ , where  $u(\mathbf{x}, t)$  is the reflected field. With this treatment, the zero initial conditions (2.3) mean that the incident radiation reaches the obstacle  $\Omega$  at the time t = 0. The operator  $\mathbf{l}_{\Gamma}$  in (2.2) specifies boundary conditions on the scatterer surface and determines the type of scattering. The simplest examples of boundary conditions on  $\partial\Omega$  are the Dirichlet condition  $\mathbf{l}_{\Gamma} u \equiv u = -u^{\text{inc}}$  or the Neumann condition  $\mathbf{l}_{\Gamma} u \equiv \frac{\partial u}{\partial \mathbf{n}} = -\frac{\partial u^{\text{inc}}}{\partial \mathbf{n}}$  written in terms of the incident radiation  $u^{\text{inc}}$ (here, **n** is the outward normal vector to the boundary  $\Gamma$  of  $\Omega$ ). In the general case, boundary conditions can be much more complicated, including nonlocal ones, but they ensure the well-posedness of problem (2.1)–(2.3).

Consider a somewhat large auxiliary region  $\Omega' \supset \Omega$  such that the difference  $\Omega' \setminus \overline{\Omega}$  (the bar over  $\Omega$  denotes the closure) contains the computational domain. Assume without loss of generality that  $\Omega'$  is a parallelepiped. Let  $G(\mathbf{x}, t)$  be a retarded Green's function (fundamental solution) of Eq. (2.1). To the fourdimensional domain  $\Omega' \setminus \Omega \times (0, t], t \leq T$  (see [5]), we apply the Green formula

$$u(\mathbf{x},t) = \frac{1}{c^{2}} \underbrace{\int_{\Omega' \setminus \overline{\Omega}} \left\{ \frac{\partial u}{\partial t}(\mathbf{y},0) G(\mathbf{x}-\mathbf{y},t) - u(\mathbf{y},0) \frac{\partial G}{\partial t}(\mathbf{x}-\mathbf{y},t) \right\} d\mathbf{y}}_{=0}$$

$$+ \int_{\Gamma_{t}} \left\{ \frac{\partial u}{\partial \mathbf{n}}(\mathbf{y},t') G(\mathbf{x}-\mathbf{y},t-t') - u(\mathbf{y},t') \frac{\partial G}{\partial \mathbf{n}}(\mathbf{x}-\mathbf{y},t-t') \right\} dt' dS_{\mathbf{y}}$$

$$+ \underbrace{\int_{\Gamma_{t}} \left\{ \frac{\partial u}{\partial \mathbf{n}}(\mathbf{y},t') G(\mathbf{x}-\mathbf{y},t-t') - u(\mathbf{y},t') \frac{\partial G}{\partial \mathbf{n}}(\mathbf{x}-\mathbf{y},t-t') \right\} dt' dS_{\mathbf{y}}}_{=0}$$
(2.4)

which expresses the solution  $u(\mathbf{x}, t)$  in this domain in terms of the solution values on the boundary. The given (three-dimensional) boundary consists of pieces corresponding to the initial time,  $\Omega' \setminus \overline{\Omega} \times \{t = 0\}$ ,

and nonzero times,  $\Gamma_t \equiv \partial \Omega \times (0, t]$  and  $\Gamma'_t \equiv \partial \Omega' \times (0, t]$ ; note that  $\Gamma'_t$  corresponds to the boundary of  $\Omega'$  in space-time.

The first term in (2.4) vanishes because of the homogeneous boundary conditions (2.3). The last inte-

gral in (2.4) is taken over the boundary of the auxiliary domain in space-time,  $\Gamma'_t \equiv \partial \Omega' \times (0, t]$ , and also vanishes, provided that the chosen Green's function is the free-space fundamental solution of the three-dimensional wave equation, i.e.,

$$G(\mathbf{x},t) = \frac{1}{4\pi |\mathbf{x}|} \delta(t - |\mathbf{x}|/c).$$
(2.5)

In this case, the boundary values of the solution and its derivative on  $\Gamma'_t$  do not contribute to the solution  $u(\mathbf{x}, t)$  at interior points of  $\Omega'$ , since the spatial boundary  $\partial \Omega'$  is reached only by outgoing waves leaving  $\Omega'$ . Thus, with the indicated choice of the Green's function, the only term remaining in (2.4) is the second term, which allows us to express the value of the solution in the computational domain  $\Omega' \setminus \Omega$  in terms of its values (and values of its normal derivative) on the scatterer boundary  $\Omega$  at all preceding times.

By analogy with formula (2.4), we introduce Calderon's potential with density  $\xi_{\Gamma_t} = (\xi_0, \xi_1)$  defined on  $\Gamma_t$ :

$$\mathbf{P}_{\bar{\Omega}}\xi_{\Gamma_{t}}(\mathbf{x},t) = \int_{\Gamma_{t}} \left\{ \xi_{1}(\mathbf{y},t')G(\mathbf{x}-\mathbf{y},t-t') - \xi_{0}(\mathbf{y},t')\frac{\partial G}{\partial \mathbf{n}}(\mathbf{x}-\mathbf{y},t-t') \right\} dt' dS_{\mathbf{y}},$$
(2.6)

where  $\mathbf{x} \in \tilde{\Omega} = \mathbb{R}^3 \setminus \overline{\Omega}$ . Note that Calderon potential (2.6) satisfies the wave equation on  $\tilde{\Omega}$ , i.e.,  $\Box_c \mathbf{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_c}(\mathbf{x}, t) = 0$  for an arbitrary density  $\boldsymbol{\xi}_{\Gamma_c}$ .

By comparing formulas (2.4) and (2.6), it is easy to see that the functions  $\xi_0$  and  $\xi_1$  can be interpreted as the traces on  $\partial\Omega$  of the solution leaving  $\Omega'$  and its normal derivative. It can be proved (see [3]) that the pair  $\xi_{\Gamma_r} = (\xi_0, \xi_1)$  is the trace of the outgoing solution if and only if  $\xi_{\Gamma_r}$  satisfies the boundary equation with projection (BEP):

$$\mathbf{P}_{\Gamma_t} \boldsymbol{\xi}_{\Gamma_t} = \boldsymbol{\xi}_{\Gamma_t}.$$

where  $\mathbf{P}_{\Gamma_t} \equiv \mathbf{T} \mathbf{r}_{\Gamma_t} \mathbf{P}_{\Omega} \boldsymbol{\xi}_{\Gamma_t}$  and the trace operator is defined as  $\mathbf{T} \mathbf{r}_{\Gamma_t} f(\mathbf{x}, t) = \left( f, \frac{\partial f}{\partial n} \right)_{\Gamma_t}$ . Obviously, there exists an

(infinite) set of solutions to BEP (2.7), since the original equation (2.1) has a set of outgoing solutions. To identify the solution among them that corresponds to the type of scattering determined by boundary condition (2.2), BEP (2.7) has to be solved together with the boundary condition relating the solution and its normal derivative on the scatterer boundary:

$$\mathbf{I}_{\Gamma}\boldsymbol{\xi}_{\Gamma_{\tau}} = \boldsymbol{\phi}. \tag{2.8}$$

It should be emphasized that boundary condition (2.2) can determine one of the density components, namely,  $\xi_0$  (Dirichlet problem with a function specified on the boundary) or  $\xi_1$  (Neumann problem with a given normal derivative) or the relationship between them (Robin problem and more complicated non-local conditions). However, the two density components (function and its normal derivative at the boundary) cannot be specified simultaneously as that would yield an overdetermined problem with no unique solution.

Thus, BEP (2.7), together with boundary condition (2.8), is an equivalent boundary formulation of the original system (2.2) with the unknown  $\xi_{\Gamma_t}$  (possibly, with only one unknown component in the case of Dirichlet or Neumann conditions). The dimension of the problem is reduced by one as compared with the original system. By using the found density  $\xi_{\Gamma_t}$ , the solution  $u(\mathbf{x}, t)$  in the three-dimensional domain

 $\tilde{\Omega} = \mathbb{R}^3 \setminus \Omega$  is recovered by applying formula (2.6).

It should be underlined that the integral in formula (2.6) is taken over a (2 + 1)-dimensional manifold and, in the case of a scatterer  $\Omega$  of complex geometry, it might represent a computationally nontrivial problem. In this context, it is convenient to use another, equivalent representation of the Calderon poten-

tial. Consider a function  $w(\mathbf{x}, t)$  defined on  $\mathbb{R}^3 \setminus \Omega \times (0, t]$  such that  $\mathbf{Tr}_{\Gamma_t} w = \xi_{\Gamma_t}$  and  $w(\mathbf{x}, 0) = \frac{\partial w(\mathbf{x}, 0)}{\partial t} = 0$ . In other words, the only assumption made about  $w(\mathbf{x}, t)$  is that its trace and the trace of its normal deriv-

COMPUTATIONAL MATHEMATICS AND MATHEMATICAL PHYSICS Vol. 60 No. 4 2020

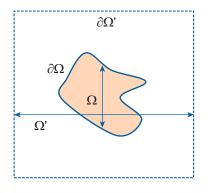


Fig. 1. Scatterer  $\Omega$  and the auxiliary domain  $\Omega'$ .

ative on  $\Gamma_t$  coincide with  $\xi_{\Gamma_t}$  and that the indicated initial conditions are satisfied. In other aspects, this function is arbitrary, specifically, it does not need to be a solution of wave equation (2.1), i.e., in the general case,  $\Box_c w \neq 0$  on  $\mathbb{R}^3 \setminus \Omega \times (0, t]$ . In practice,  $w(\mathbf{x}, t)$  can be constructed as an extension from the boundary  $\Gamma_t$  with the help of Taylor series with the required second and higher order derivatives computed using the original equation (2.1) (see Section 2). By applying the Green formula to the given function on  $\Omega' \setminus \Omega \times (0, t]$  and solving the resulting relation for quantity (2.6) of interest, it is easy to see that the Calderon potential can be represented in the form

$$\mathbf{P}_{\tilde{\Omega}}\boldsymbol{\xi}_{\Gamma}(\mathbf{x},t) = w(\mathbf{x},t) - v(\mathbf{x},t), \quad \mathbf{x} \in \tilde{\Omega},$$
(2.9)

where the function  $v(\mathbf{x}, t) = G * \Box_c w|_{\bar{\Omega}}$  is defined in terms of the convolution of Green's function (2.5) with the quantity  $\Box_c w|_{\bar{\Omega}}$  extended by zero to the scatterer's interior, i.e., to  $\Omega$ . Note that this convolution is taken over the *entire* three-dimensional space  $\mathbb{R}^3$  and the time interval (0, t]. It is convenient to compute this convolution by solving the auxiliary problem (AP)

$$\Box_c v = \Box_c w|_{\tilde{O}}, \tag{2.10}$$

set up formally with homogeneous initial conditions in the unbounded domain  $\mathbb{R}^3$ . In practice, of course, this problem is solved in the bounded domain  $\Omega'$ , but radiation conditions are set on the boundary of  $\Omega'$ . This is equivalent to choosing the required Green's function (2.5). The *transition from computing the Calderon potential in terms of integral* (2.6) *to solving AP* (2.10) *plays a key role in convenience, flexibility, and simplicity of the implementation of the described approach.* 

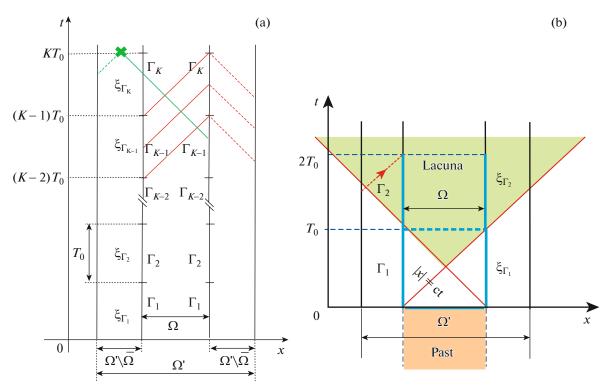
It should be emphasized once again that AP (2.10) is solved in a simple (rectangular) auxiliary domain  $\Omega'$  with no "hole" corresponding to the scatterer  $\Omega$ . The entire information on the geometry of this object (which is possibly complex and does not conform to the Cartesian grid) and on the boundary conditions set on its surface is contained in the function  $w(\mathbf{x}, t)$  and passes into the right-hand side of (2.10) and, next, into formula (2.9). Due to this circumstance, finite-differences on the simplest rectangular grids can be used to compute objects of complex geometry without any loss of accuracy associated with the nonconformity of the object boundaries to the grid.

Now suppose that the task is to find a solution of the problem at a finite time t = T by applying the indicated method. As T grows, the boundary  $\Gamma_T = \partial \Omega \times (0, T]$ , on which the density  $\xi_{\Gamma_T}$  is defined, increases linearly and, even for moderate T, the method becomes hardly applicable because of the need of storing and solving an equation for the quantity  $\xi_{\Gamma_T}$  increasing with time.

To overcome this limitation, the interval (0,T] is partitioned into K subintervals of length  $T_0$ , where  $KT_0 = T$ , and, on each partial boundary in space-time

$$\Gamma_k = \partial \Omega \times ((k-1)T_0, kT_0], \quad k = 1, ..., K, \quad \bigcup_{k=1}^K \Gamma_k = \Gamma_T,$$

in this partition, we introduce corresponding densities  $\xi_{\Gamma_k}$  (see Fig. 2a). At first glance, this formal partition does not resolve the issue of the boundary  $\Gamma_T$  growing with time, since, by virtue of causality, the den-



**Fig. 2.** (a) Partition in time and the characteristic cone of the solution. (b) Lacuna in the solution. The horizontal axis formally represents three-dimensional space.

sity  $\xi_{\Gamma_k}$  on any *k*th partition element has to depend on the densities  $\xi_{\Gamma_s}$ , s = 1, ..., k - 1, on all preceding segments. Seemingly, this prevents us from solving system (2.7), (2.8) for  $\xi_{\Gamma_k}$  separately without using all preceding values  $\xi_{\Gamma_k}$ .

However, it is easy to see that, for the chosen Green's function (2.5), the integral in the Calderon potential (2.6) is taken over the intersection of the light cone with the vertex in  $\Gamma_k$  and the scatterer surface  $\Omega$  at the preceding times (see Fig. 2a, where k = K for illustrative purposes). Considering all points of  $\Gamma_K$  at which we are interested in the density  $\xi_{\Gamma_K}$ , we conclude that this intersection is nonempty at most over the time  $2T_0$  measured back from the last (latest) time of the set  $\Gamma_K$  (i.e., for the case shown in the figure t = T), provided that the partition size satisfies

$$T_0 \ge \frac{1}{c} \operatorname{diam} \Omega. \tag{2.11}$$

In other words, under condition (2.11), the densities  $\xi_{\Gamma_s}$  corresponding to the earlier partition elements  $\Gamma_s$ , s = 1, ..., K - 2, do not influence the density determined on the element  $\Gamma_K$ . In terms of lacunas in the solution of the wave equation in free space, the same situation can be explained as follows: the solution generated by a source (right-hand side) localized in space-time on the boundary of the preceding partition element ( $\Gamma_1$  in Fig. 2b) a fortiori leaves the domain  $\Omega$  during time (2.11). Thus, the back dependence of the solution of Eq. (2.7) is limited to a single partition element. As a result, the density can be updated using the recurrence scheme

$$\mathbf{P}_{\Gamma_k} \boldsymbol{\xi}_{\Gamma_k} + \mathbf{R}_{\Gamma_k} \boldsymbol{\xi}_{\Gamma_{k-1}} = \boldsymbol{\xi}_{\Gamma_k}, \tag{2.12}$$

where

$$\mathbf{R}_{\Gamma_{k}}\xi_{\Gamma_{k-1}}(\mathbf{x},t) = \mathbf{T}\mathbf{r}_{\Gamma_{k}}\int_{\Gamma_{k-1}} \left\{\xi_{1}(\mathbf{y},t')G(\mathbf{x}-\mathbf{y},t-t') - \xi_{0}(\mathbf{y},t')\frac{\partial G}{\partial \mathbf{n}}(\mathbf{x}-\mathbf{y},t-t')\right\}dt'dS_{\mathbf{y}}$$
(2.13)

COMPUTATIONAL MATHEMATICS AND MATHEMATICAL PHYSICS Vol. 60 No. 4 2020

and  $(\mathbf{x}, t) \in \Gamma_k$  in (2.13). Note that integral (2.13) is taken over the preceding partition element  $\Gamma_{k-1}$ , but its value is calculated at a point from the next element  $\Gamma_k$ .

It is convenient to expand the partial densities  $\xi_{\Gamma_k}$  and  $\xi_{\Gamma_{k-1}}$  in series on  $\Gamma_k$  and  $\Gamma_{k-1}$  in terms of some basis functions:

$$\xi_{\Gamma_{k-1}} = \sum_{s} c_{0,s}^{(I)} \psi_{0,s} + c_{1,s}^{(I)} \psi_{1,s}, \quad \xi_{\Gamma_{k}} = \sum_{s} c_{0,s}^{(II)} \psi_{0,s} + c_{1,s}^{(II)} \psi_{1,s}, \quad (2.14)$$

where the two-component basis functions  $\Psi_{0,s} = (\Psi_s, 0)$  and  $\Psi_{1,s} = (0, \Psi_s)$  are used to represent the solution and its normal derivative on the boundary. It is also natural to use the same basis functions for any partition element *k*. For example, in the case of a spherical scatterer  $\Omega$ , the basis functions  $\Psi_s(\mathbf{x}, t)$  can be defined as the direct product of spherical harmonics (in angular variables) and Chebyshev polynomials (in time). Depending on the imposed boundary condition (2.2), some of the coefficients in the expansions can be known; for example, in the case of the Dirichlet condition, the function specified on the boundary uniquely determines  $c_{0,s}^{(I)}$  and  $c_{0,s}^{(II)}$ ; the Neumann condition fixes  $c_{1,s}^{(I)}$  and  $c_{1,s}^{(II)}$ ; and the Robin condition establishes a relation between these sets of coefficients.

Note also that, in view of explicit expression (2.5), the kernel of integrals (2.6) and (2.13) is invariant under time shifts. Therefore, by using the same basis for all partition elements, the action of operators (2.6) and (2.13) on the basis elements on the set  $\Gamma_k$  (the left-hand side of Eq. (2.12)) can be calculated on any two consecutive partition elements of size  $T_0$ , for example,  $\Gamma_1$  and  $\Gamma_2$ , with the results denoted by  $\mathbf{P}_{\Gamma_{T_0}} \Psi_s$  and  $\mathbf{R}_{\Gamma_{T_0}} \Psi_s$ . Then Eq. (2.7) becomes

$$\mathbf{P}_{\Gamma_{T_{0}}}\boldsymbol{\xi}_{\Gamma_{k}} + \mathbf{R}_{\Gamma_{T_{0}}}\boldsymbol{\xi}_{\Gamma_{k-1}} = \boldsymbol{\xi}_{\Gamma_{k}}.$$
(2.15)

It should be emphasized that the actions of these operators are computed using AP (2.10); moreover, the AP for computing  $\mathbf{R}_{\Gamma_{T_0}} \psi_s$  is solved over time  $t \in [0, 2T_0]$ , and AP for  $\mathbf{P}_{\Gamma_{T_0}} \psi_s$ , over  $t \in [T_0, 2T_0]$ . The number of such APs is equal to the number of basis elements in (2.14). After performing this computation, Eq. (2.15) turns into an equation for the expansion coefficients of density on two consecutive partition elements  $\Gamma_k$  and  $\Gamma_{k-1}$ :

$$\sum_{s} c_{0,s}^{(II)} \underbrace{\{\mathbf{P}_{\Gamma_{\tau_{0}}} - \mathbf{I}\}}_{\mathbf{Q}_{\Gamma_{\tau_{0}}}} \Psi_{0,s} + c_{1,s}^{(II)} \underbrace{\{\mathbf{P}_{\Gamma_{\tau_{0}}} - \mathbf{I}\}}_{\mathbf{Q}_{\Gamma_{\tau_{0}}}} \Psi_{1,s} = -\sum_{s} c_{0,s}^{(I)} \mathbf{R}_{\Gamma_{\tau_{0}}} \Psi_{0,s} + c_{1,s}^{(I)} \mathbf{R}_{\Gamma_{\tau_{0}}} \Psi_{1,s},$$
(2.16)

where I denotes the identity operator and  $c_{0,s}^{(I)}$  and  $c_{1,s}^{(I)}$  are known from the preceding step. For choosing the required solution, Eq. (2.16) is supplemented with boundary condition (2.8) written in terms of expansion coefficients:

$$\mathbf{I}_{\Gamma_{K}}\sum_{s}c_{0,s}^{(\mathrm{II})}\boldsymbol{\Psi}_{0,s} + c_{1,s}^{(\mathrm{II})}\boldsymbol{\Psi}_{1,s} = \boldsymbol{\Phi} \equiv \sum_{s}c_{s}^{(\boldsymbol{\Phi})}\boldsymbol{\Psi}_{s}.$$
(2.17)

#### 3. DISCRETIZATION

On the auxiliary domain  $\Omega'$  (parallelepiped), we introduce a rectangular grid with a step size *h* in each space dimension. Once again, it should be stressed that, although the discrete solution of the problem is determined and required only outside the obstacle  $\Omega$ , we discretize the entire domain  $\Omega$  as well. Note also that the obstacle boundary  $\partial\Omega$  may not coincide with lines of the introduced rectangular grid. The solution of the problem is sought at discrete times with step  $\tau$ ; in other words, a grid with the indicated step sizes is introduced on the four-dimensional domain  $\Omega' \times [0, T]$ . Equation (2.2) is discretized using a fourth-order accurate compact difference scheme with a stencil consisting of  $3 \times 3 \times 3 \times 3 = 81$  points:

$$\Delta u^{n+1} - \frac{u^{n+1}}{\theta \tau^2 c^2} = 2 \left( \Delta u^n - \frac{u^n}{\theta \tau^2 c^2} \right) - \left( \Delta u^{n-1} - \frac{u^{n-1}}{\theta \tau^2 c^2} \right) - \frac{1}{\theta} \Delta u^n,$$
(3.1)

with parameter  $\theta = \frac{1}{12}$ . Note that Eq. (3.1) describes only time differencing, which is implicit. At the time level n + 1, Eq. (3.1) is next approximated up to fourth-order accuracy in space on a stencil of  $3 \times 3 \times 3$  points by using the general idea of compact schemes (see [6]).

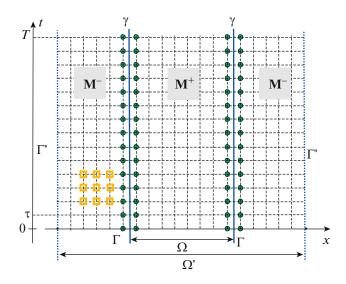


Fig. 3. Grid covering the auxiliary domain  $\Omega'$ . The nodes making up the discrete boundary  $\gamma$  of the scatterer are shown in green. The stencil of the difference scheme is depicted by yellow squares [6].

Let  $\mathbb{N}_m$  denote the grid points belonging to the given 81-point stencil centered at the node m. In what follows, we need several subsets of the spatiotemporal rectangular grid covering  $\Omega' \times [0, T]$ . Specifically, let  $\mathbb{M}^-$  and  $\mathbb{M}^+$  denote the subsets of grid nodes lying in the domains  $\Omega' \setminus \Omega \times [\tau, T - \tau]$  and  $\Omega \times [0, T]$ , respectively. Thus,  $\mathbb{M}^-$  and  $\mathbb{M}^+$  represent the grid nodes lying outside and inside  $\Omega$  at all times  $t \in [0, T]$ . The nodes lying on the boundary  $\partial \Omega$  are included in  $\mathbb{M}^+$ . The center of the stencil  $\mathbb{N}_m$  is inside  $\Omega' \setminus \Omega \times [0, T]$  and  $\Omega \times [0, T]$  if  $m \in \mathbb{M}^-$  and  $m \in \mathbb{M}^+$ , respectively.

Let  $\gamma^+$  denote the subset of nodes satisfying two conditions: these nodes belong to the stencil  $\mathbb{N}_m$  centered at  $m \in \mathbb{M}^-$  and lie inside  $\Omega$ . Similarly,  $\gamma^-$  denotes the subset of nodes belonging to the stencil  $\mathbb{N}_m$  centered at  $m \in \mathbb{M}^+$  and lying outside  $\Omega$ . The union  $\gamma^+ \cup \gamma^- \equiv \gamma$  forms a thin layer of nodes covering the spatiotemporal boundary  $\Gamma$  of  $\Omega$  and replacing  $\Gamma$  in the discrete formulation (see Fig. 3). Additionally, we consider the sets  $\mathbb{N}^+ = \bigcup_{m \in \mathbb{M}^+} \mathbb{N}_m$  and  $\mathbb{N}^- = \bigcup_{m \in \mathbb{M}^-} \mathbb{N}_m$ , which consist of all points of the stencil  $\mathbb{N}_m$  with its center running over all points of  $\mathbb{M}^+$  or  $\mathbb{M}^-$ , respectively. Specifically,  $\mathbb{N}^-$  contains points on the boundary  $\partial \Omega'$ , the first and last time levels  $t = \{0, T\}$  inside  $\Omega' \setminus \Omega$ , and the subset  $\gamma^+$ . The union  $\mathbb{N}^0 = \mathbb{N}^+ \cup \mathbb{N}^-$  is the set of all grid points lying in the stencil  $\mathbb{N}_m$  with  $m \in \mathbb{M}^+ \cup \mathbb{M}^-$ .

All the above-introduced (sub)sets of nodes correspond to a grid covering the entire spatiotemporal domain  $\Omega' \times [0, T]$ , where *T* is a finite moment of time. Obviously, all these constructions can also be defined on any subdomain  $\Omega' \times [0, t]$ , t < T, in which case they are equipped with a subscript *t*. Specifically, the set  $\gamma_t$  is a discrete analogue of the boundary  $\Gamma_t$  from Section 2.

# 3.1. Difference Potentials

We introduce a grid function  $\xi_{\gamma_t}$  defined on the grid boundary  $\gamma_t$ . Additionally, let  $w^{(h)}$  be a grid function defined at points of  $\mathbb{N}_t^0$  such that its trace on  $\gamma_t$  coincides with  $\xi_{\gamma_t}$ :

$$\mathbf{Tr}_{\gamma_t}^{(h)} w^{(h)} = \xi_{\gamma_t}$$

The trace operator  $\mathbf{Tr}_{\gamma_t}^{(h)}$  yields the restriction of the grid function from the set  $\mathbb{N}_t^0$  to the discrete boundary  $\gamma_t \subset \mathbb{N}_t^0$ . Let  $\Box_c^{(h)}$  denote the discrete Laplacian corresponding to the chosen difference scheme. By analogy with formula (2.10), we construct a "right-hand side" extended by zero to grid nodes inside  $\Omega$ :

$$\Box_{c}^{(h)}w^{(h)}\Big|_{\mathbb{M}_{t}^{-}} \equiv \begin{cases} \Box_{c}^{(h)}w^{(h)}, & m \in \mathbb{M}_{t}^{-}, \\ 0, & m \in \mathbb{M}_{t}^{+}. \end{cases}$$

The difference potential with density  $\xi_{\gamma_r}$  is defined as a grid function on  $\mathbb{N}_r^-$  specified according to the rule

$$\mathbf{P}_{\mathbb{N}_{t}^{-}}\boldsymbol{\xi}_{\gamma_{t}} = \boldsymbol{w}^{(h)}\Big|_{\mathbb{N}_{t}^{-}} - \mathbf{G}^{(h)}\Big(\Box_{c}^{(h)}\boldsymbol{w}^{(h)}\Big|_{\mathbb{N}_{t}^{-}}\Big),$$
(3.2)

where  $\mathbf{G}^{(h)}$  is the Green's function (resolvent) for the difference wave equation. The subtrahend  $\mathbf{G}^{(h)}\left(\left[ \prod_{c}^{(h)} w^{(h)} \right]_{\mathbb{M}_{t}^{-}}\right) \equiv v^{(h)}$  on the right-hand side of (3.2) is computed by solving the difference AP

$$\Box_c^{(h)} v^{(h)} = \Box_c^{(h)} w^{(h)} \Big|_{\mathbb{M}_t^-}$$
(3.3)

on the set  $\mathbb{N}^0$  with radiation conditions specified on the outer boundary (cf. (2.10)). Since  $w^{(h)} = \mathbf{G}^{(h)} \square_c^{(h)} w^{(h)}$ , the difference potential (3.2) is the solution of the homogeneous difference wave equation on  $\mathbb{M}_t^-$ :

$$\left. \Box_{c}^{(h)} \mathbf{P}_{\mathbb{N}_{t}^{-}} \boldsymbol{\xi}_{\gamma_{t}} \right|_{\mathbb{M}_{t}^{-}} = 0.$$

The projection of the difference potential onto the set  $\gamma_t$  is defined in terms of its trace on this set:

$$nP_{\gamma_{t}}\xi_{\gamma_{t}} \stackrel{\text{def}}{=} \mathbf{Tr}_{\gamma_{t}}^{(h)}\mathbf{P}_{\mathbb{N}_{t}}\xi_{\gamma_{t}}.$$
(3.4)

By construction, neither difference potential (3.2) nor its projection (3.4) depends on the choice of the auxiliary function  $w^{(h)}$  if  $\mathbf{Tr}_{\gamma_t}^{(h)}w^{(h)} = \xi_{\gamma_t}$ .

It can be shown that the finite-difference BEP

$$\mathbf{P}_{\gamma_t} \boldsymbol{\xi}_{\gamma_t} = \boldsymbol{\xi}_{\gamma_t} \tag{3.5}$$

(cf. (2.7)) holds if and only if  $\xi_{\gamma_t} = \mathbf{Tr}_{\gamma_t}^{(h)} u_{\mathbb{N}_t^-}^{(h)}$ , where  $u_{\mathbb{N}_t^-}^{(h)}$  is a discrete solution of the wave equation  $\Box_c^{(h)} u_{\mathbb{N}_t^-}^{(h)} |_{\mathbb{N}_t^-} = 0$  with zero initial conditions.

As in the continuous formulation, the difference BEP (3.5) set up on the discrete boundary  $\gamma_t$  is equivalent to the difference wave equation  $\left. \Box_c^{(h)} u_{\mathbb{N}_t^-}^{(h)} \right|_{\mathbb{N}_t^-} = 0$  with zero initial conditions on the set  $\mathbb{N}_t^-$ , i.e., out the scatterer  $\Omega$ .

Obviously, there exists a set of solutions  $\xi_{\gamma_t}$  of the difference BEP (3.5), since there exists a set of solutions  $u_{\mathbb{N}_t^-}^{(h)}$  of the difference wave equation for  $\Box_c^{(h)} u_{\mathbb{N}_t^-}^{(h)}$  at exterior (with respect to the scatterer) nodes of  $\mathbb{M}_t^-$ . To choose the required solution, Eq. (3.5) is supplemented with a corresponding condition following from the boundary condition (2.2) on the scatterer. However, conditions (2.2) are set on the analytical boundary  $\Gamma_t$  rather than on its discrete analogue  $\gamma_t$ , where Eq. (3.5) is considered. Accordingly, an additional procedure is needed for transferring boundary data from  $\Gamma_t$  to  $\gamma_t$ .

#### 3.2. Extension of Boundary Data

Suppose that the density  $\xi_{\Gamma_t} = (\xi_0, \xi_1)|_{\Gamma_t}$  on the analytical boundary  $\Gamma_t$  is given. By using a Taylor series with a finite number *P* of terms, we define a function  $v = v(\mathbf{x}, t)$  in the neighborhood of  $\Gamma_t$ :

$$v(\mathbf{x},t) = \sum_{p=0}^{P} \frac{1}{p!} \frac{\partial^{p} v}{\partial \mathbf{n}^{p}} (\mathbf{x}_{0},t) \boldsymbol{\rho}^{p}.$$
(3.6)

The point  $\mathbf{x} \in \mathbb{R}^3$  in formula (3.6) is near the scatterer boundary  $\partial \Omega$ , while the point  $\mathbf{x}_0$  corresponds to the base of the normal to  $\partial \Omega$  pointing to the point  $\mathbf{x}$ . The quantity  $\rho$  is the distance from the point  $\mathbf{x}$  to the surface  $\partial \Omega$  taken with a plus sign for exterior points (with respect to  $\Omega$ ) and with a minus sign for interior points, i.e.,  $\rho = |\mathbf{x} - \mathbf{x}_0|$  if  $\mathbf{x} \notin \Omega$  and  $\rho = -|\mathbf{x} - \mathbf{x}_0|$  if  $\mathbf{x} \in \Omega$ .

The outward normal derivatives on  $\partial\Omega$  in (3.6) are defined as follows:  $v(\mathbf{x}_0, t) = \xi_0(\mathbf{x}_0, t)$  for p = 0 and  $\frac{\partial v}{\partial \mathbf{n}}(\mathbf{x}_0, t) = \xi_1(\mathbf{x}_0, t)$  for p = 1. This choice corresponds to  $\mathbf{Tr}_{\Gamma_t} v = \xi_{\Gamma_t}$ . Higher order derivatives are computed using the wave equation (2.1) considered in a local orthogonal coordinate system with the origin placed at the point  $\mathbf{x}_0$ . This system is chosen so that two of its axes lie in the tangent plane, while the third axis is aligned with the normal  $\mathbf{n}$  (up to its sign). In this case, the three-dimensional Laplacian at the point  $\mathbf{x}_0$  can be written as

$$\Delta v = \frac{\partial^2 v}{\partial \mathbf{n}^2} + \mathbf{L} v,$$

where the operator contains tangential derivatives and, possibly, the derivative with respect to **n** of at most the first order. For example, if  $\partial \Omega$  is a sphere, then, in spherical coordinates, we have

$$\Delta v = \frac{\partial^2 v}{\partial r^2} + \underbrace{\frac{2}{r} \frac{\partial v}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial v}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 v}{\partial \phi^2}}_{\mathbf{L}v}.$$

By using the original equation  $\Box_c v = \frac{1}{c^2} \frac{\partial^2 v}{\partial t^2} - \Delta v = 0$ , the normal derivative of order p = 2 in (3.6) can be represented in the form

$$\frac{\partial^2 v}{\partial \mathbf{n}^2}(\mathbf{x}_0, t) = \frac{1}{c^2} \frac{\partial^2 v}{\partial t^2}(\mathbf{x}_0, t) - \mathbf{L} v(\mathbf{x}_0, t).$$
(3.7)

On the right-hand side of (3.7), the derivatives with respect to **n**, if any, have at most the first order. Substituting the known quantities  $\xi_0$  and  $\xi_1$  into this expression, we find the second normal derivative. To obtain normal derivatives of order p > 2, Eq. (3.7) is differentiated with respect to **n** and, if necessary, the second derivative with respect to **n** appearing on the right-hand side is recursively expressed via Eq. (3.7). A conceptually similar technique is often used in solving evolution equations by a finite-difference method when analytical Cauchy data specified at t = 0 have to be extended to the first time level  $t = \tau$  in order to start the difference scheme. The function  $v(\mathbf{x}, t)$  obtained according to (3.6) is called the extension of the boundary data  $\xi_{\Gamma}$  with the help of the original equation.

If the density  $\xi_{\Gamma_t}$  corresponds to some solution  $u(\mathbf{x}, t)$  of the wave equation, i.e., if  $\xi_0$  and  $\xi_1$  are the traces of this solution and its normal derivative on  $\Gamma_t$ , then the function  $v(\mathbf{x}, t)$  constructed according to (3.6) approximates this solution up to  $\mathbb{O}(|\rho|^{P+1})$  accuracy. Formally, this technique for boundary data transfer can be applied to any pair of functions  $\xi_{\Gamma_t} = (\xi_0, \xi_1)|_{\Gamma_t}$ , which do not need to be consistent or be the traces of some solution and its derivative. In that case, rule (3.6) merely defines a new function. Within the described approach, we are interested in an extension of (3.6) to the nodes of the discrete boundary  $\gamma_t$  lying near the exact boundary  $\Gamma_t$ . This extension is denoted as follows:

$$\boldsymbol{\xi}_{\boldsymbol{\gamma}_t} = \mathbf{E} \mathbf{x} \boldsymbol{\xi}_{\boldsymbol{\Gamma}_t}, \tag{3.8}$$

where **Ex** is the extension operator determined by formulas (3.6), (3.7). In this way, any basis element  $\Psi_{0,s}$ ,  $\Psi_{1,s}$  specified on the exact boundary  $\Gamma_t$  can be extended to  $\gamma_t$ , i.e., we can compute the grid functions **Ex** $\Psi_{0,s}$  and **Ex** $\Psi_{1,s}$ .

### 3.3. Scheme for Updating the Solution in Time

Now the partition of the boundary in time described in Section 2 is applied to the discrete boundary  $\gamma$ . Let  $\mathbf{P}_{\gamma_{T_0}}$  denote the difference analogue of the operator  $\mathbf{P}_{\Gamma_{T_0}}$  defined by formula (3.4). The difference analogue of  $\mathbf{R}_{\Gamma_{T_0}}$  is defined as

$$\mathbf{R}_{\gamma_{T_0}} \boldsymbol{\xi}_{\gamma_{T_0}} \stackrel{\text{def}}{=} \mathbf{Tr}_{\gamma_{(T_0,2T_0)}}^{(h)} \mathbf{P}_{\mathbb{V}_{2T_0}} \boldsymbol{\xi}_{\gamma_{T_0}}, \qquad (3.9)$$

where  $\xi_{\gamma_{\tau_0}}$  is obtained by extending the density from the exact boundary to the set  $\gamma_{T_0}$  according to (3.8). Once again, we emphasize that the argument of  $\mathbf{R}_{\gamma_{\tau_0}}$  (density  $\xi_{\gamma_{\tau_0}}$ ) is defined for times  $0 < t \le T_0$ , while the difference potential is calculated over the time  $0 < t \le 2T_0$  as the solution of AP (3.3), and the trace of this solution is preserved on the "upper" part of two consecutive partition elements of the discrete boundary  $\gamma_{(T_0,2T_0]} = \gamma_{2T_0} \setminus \gamma_{T_0}$ . The scheme for updating coefficients (2.16) in the difference formulation has the form

$$\mathbf{Q}_{\gamma_{\tau_0}}^{(0)} \mathbf{c}_0^{(1)} + \mathbf{Q}_{\gamma_{\tau_0}}^{(1)} \mathbf{c}_1^{(1)} = -\mathbf{R}_{\gamma_{\tau_0}}^{(0)} \mathbf{c}_0^{(1)} - \mathbf{R}_{\gamma_{\tau_0}}^{(1)} \mathbf{c}_1^{(1)}, \qquad (3.10)$$

where the right-hand-side coefficients

$$\mathbf{c}_{0}^{(1)} = [c_{0,1}^{(1)} \dots c_{0,s}^{(1)} \dots c_{0,s}^{(1)}]^{\mathsf{T}}, \quad \mathbf{c}_{1}^{(1)} = [c_{1,1}^{(1)} \dots c_{1,s}^{(1)} \dots c_{1,s}^{(1)}]^{\mathsf{T}}$$

are known from the preceding step and the unknowns are the sets of coefficients (possibly, only one of them in the case of Dirichlet or Neumann conditions)

$$\mathbf{c}_{0}^{(\mathrm{II})} = [\mathbf{c}_{0,1}^{(\mathrm{II})} \dots \mathbf{c}_{0,s}^{(\mathrm{II})} \dots \mathbf{c}_{0,S}^{(\mathrm{II})}]^{\mathrm{T}}, \quad \mathbf{c}_{1}^{(\mathrm{II})} = [\mathbf{c}_{1,1}^{(\mathrm{II})} \dots \mathbf{c}_{1,s}^{(\mathrm{II})} \dots \mathbf{c}_{1,S}^{(\mathrm{II})}]^{\mathrm{T}}.$$

The columns of the matrices in (3.10) correspond to individual elements of the used basis:

$$\mathbf{Q}_{\gamma_{T_{0}}}^{(0)} = [\underbrace{\mathbf{P}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{0,1} - \mathbf{E}\mathbf{x}\psi_{0,1}}_{\text{column $\#1$}} \dots \underbrace{\mathbf{P}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{0,s} - \mathbf{E}\mathbf{x}\psi_{0,s}}_{\text{column $\#s$}} \dots \underbrace{\mathbf{P}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{0,s} - \mathbf{E}\mathbf{x}\psi_{0,s}}_{\text{column $\#s$}}],$$
(3.11)  
$$\mathbf{Q}_{\gamma_{T_{0}}}^{(1)} = [\mathbf{P}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{1,1} - \mathbf{E}\mathbf{x}\psi_{1,1} \dots \mathbf{P}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{1,s} - \mathbf{E}\mathbf{x}\psi_{1,s} \dots \mathbf{P}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{1,s} - \mathbf{E}\mathbf{x}\psi_{1,s}],$$
$$\mathbf{R}_{\gamma_{T_{0}}}^{(0)} = [\underbrace{\mathbf{R}}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{0,1} \dots \underbrace{\mathbf{R}}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{0,s} \dots \underbrace{\mathbf{R}}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{0,s}],$$
$$\mathbf{R}_{\gamma_{T_{0}}}^{(1)} = [\mathbf{R}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{1,1} \dots \mathbf{R}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{1,s} \dots \mathbf{R}_{\gamma_{T_{0}}}\mathbf{E}\mathbf{x}\psi_{1,s}].$$
(3.12)

The size of these matrices is  $|\gamma_{T_0}| \times S$ , where *S* is the dimension of the basis and  $|\gamma_{T_0}|$  is the number of points in the set  $\gamma_{T_0}$ . Note that matrices (3.11) need to be computed only once before solving the problem. This computation requires solving 4*S* auxiliary problems (3.3) over the time  $T_0$  for matrices (3.11) and over  $2T_0$  for matrices (3.12). These problems are solved in a suitable three-dimensional rectangular domain without holes. The grid do not need to conform to the boundary of  $\Omega$ . Chosen according to (2.11), the fixed time  $T_0$  of computing data for AP is usually a tiny fraction of the total computation time:  $T_0 \ll T$ . Note that the basis dimension *S* can be rather large, which requires solving a large number of APs. However, all these APs are completely independent of one another, so these computations can be effectively parallelized.

After matrices (3.11) and (3.12) have been computed, the recurrence relation (3.10) is solved, together with the scatterer boundary condition (2.17), for the unknown coefficients. The solution is sought in the least squares sense by using QR decompositions of the matrices  $\mathbf{Q}_{\gamma\tau_0}^{(0)}$  and  $\mathbf{Q}_{\gamma\tau_0}^{(1)}$ , since the number of rows of matrices (3.11) and (3.12) is, as a rule, considerably greater than the number of their columns and the system for the unknown coefficients is overdetermined. Note that the most computationally expensive part of the solution (QR decompositions) has to be performed only once before starting the computations,

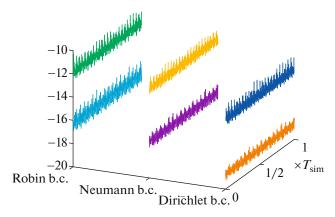


Fig. 4. Binary logarithm of the error in the numerical solution on two sequential grids for three types of boundary conditions. The Robin boundary condition is specified as  $u + \frac{\partial u}{\partial u} = 0$ .

so that the recurrence update of the coefficients in (3.10) is reduced to back substitution in the QR decomposition method.

Note also that, since the matrices do not contain information on a specific boundary condition on the scatterer  $\Omega$ , they are universally suitable for any type of scattering. In other words, to recalculate the problem with another type of boundary condition on  $\partial\Omega$ , it is sufficient to solve recurrence relation (3.10) with boundary condition (2.17) of the new type without relatively expensive recalculation of matrices (3.11), (3.12).

## 4. NUMERICAL EXPERIMENT

The demonstrate the performance of the method described above, we consider the scattering of a plane wave by a sphere of radius  $R_0 = 1$  cm. This classical problem has an analytical solution in the form of a series (see [5]), which will be compared with the numerical solution. As incident radiation, we use the sum of two plane waves with incomparable angular frequencies,  $\omega_1 = 3 \text{ s}^{-1}$  and  $\omega_2 = \omega_1/\sqrt{2}$ , thus obtaining a time-aperiodic solution. At the chosen frequencies, the incident wavelength is a quantity on the order of the scatterer diameter  $2R_0$ . We are interested in the solution within a spherical layer around the scatterer with  $R_0 < r < R_1$ , where  $R_1 = 1.5$  cm.

The auxiliary domain  $\Omega'$  is specified as a cube  $[-R_2, R_2]^3$ ,  $R_2 > R_1$  such that, over the maximum computation time  $2T_0$  used for AP, the waves reflected from the outer boundary  $\partial\Omega'$  do not reach the computational domain  $R_0 < r < R_1$  (see Fig. 2b). It is easy to see that, for this purpose,  $R_2$  has to satisfy the condition  $2R_2 - R_0 - R_1 > 2cT_0$ . With this choice of the size of the auxiliary domain, arbitrary boundary conditions, rather than approximate radiation conditions, can be set on  $\partial\Omega'$  and the solution of AP (3.3) can be obtained over the time interval  $[0, 2T_0]$  for  $R_0 < r < R_1$  as if AP is solved in an unbounded domain. Note that this technique makes it possible to model reflected waves going to infinity exactly without using any approximation process, which is a significant advantage of the described method. This possibility is ensured by the short computation time of AP (at most  $2T_0$ ), which is required for generating matrices (3.11), (3.12).

The domain  $\Omega'$  thus constructed is covered with a rectangular grid, on which the above-mentioned fourth-order difference scheme is used [6]. The convergence of the algorithm can be examined by reducing the mesh size (see Fig. 4). It can be seen that the binary logarithm of the error is decreased by four when the mesh size is halved, which confirms the correct work of the algorithm. Note also that this figure presents the result of a sufficiently long computation: the terminal simulation time  $T_{\text{sim}}$  corresponds to a time interval over which a signal crosses a ball of  $r \leq R_0$  about 6000 times. There is no evidence that the error increases with time.

Note also that the basis  $\Psi_{0,s}$ ,  $\Psi_{1,s}$  is constructed using the direct product of Chebyshev polynomials  $T_n(t)$  (in time) and spherical harmonics  $Y_{lm}(\vartheta, \varphi)$  (for decomposition on the boundary of  $\Omega$ , i.e., on a sphere). As was shown in the experiment, the maximum order n = 10 and l = 12 are more than enough to obtain results with a level of accuracy presented in Fig. 4.

### 5. CONCLUSIONS

An algorithm for computing unsteady wave propagation was proposed that (i) reduces the dimension of the problem by one by transforming it to a boundary formulation, (ii) applies to domains of complex geometry with the use of standard difference schemes on simple rectangular grids without loss of accuracy associated with approximation of boundaries, (iii) exactly takes into account radiation conditions for exterior problems, and (iv) effectively exploits the opportunities of parallel computations.

Let us discuss items (i) and (iv) in more detail. Obviously, the update of the solution on a partition element of length  $T_0$  according to (3.10) takes less time than its advance over the same time with the use of an explicit difference scheme, since the dimension of the problem in the former case is less by one. However, before solving recurrence relation (3.10), we need to calculate the matrices involved in (3.10). This is the most computationally long part of the algorithm, since 4S problems have to be solved over time at most  $2T_0$  at this stage. As a result, for short computation times, a common explicit scheme takes less time than the proposed algorithm. For longer computation times, the time cost of computing the matrices  $\mathbf{Q}_{y_{TD}}^{(0)}$ ,

 $\mathbf{Q}_{\gamma_{\tau_0}}^{(1)}$ ,  $\mathbf{R}_{\gamma_{\tau_0}}^{(0)}$ , and  $\mathbf{R}_{\gamma_{\tau_0}}^{(1)}$  is compensated for by the faster (than in an explicit scheme) advance based on (3.10). Thus, there exists a computation time starting at which the proposed algorithm becomes more efficient than the most obvious, simple, and fast solution based on an explicit difference scheme. Importantly, the matrices  $\mathbf{Q}_{\gamma_{\tau_0}}^{(0)}$ ,  $\mathbf{Q}_{\gamma_{\tau_0}}^{(1)}$ ,  $\mathbf{R}_{\gamma_{\tau_0}}^{(0)}$ , and  $\mathbf{R}_{\gamma_{\tau_0}}^{(1)}$  are computed in parallel, since their columns are independent of one another. The more cores, nodes, etc., are used in the computation, the less time is required and the sooner (with less computation time) the described algorithm becomes more efficient than an explicit scheme. Note also that a detailed study of the described method as applied to interior problems can be found in [7].

A further development of the method is associated with its generalization to Maxwell's equations and objects with a boundary of arbitrary shape with the use of suitable splines.

## FUNDING

This work was supported by the United States Army Research Office (grant no. W911NF-16-1-0115) and by the US–Israel Binational Science Foundation (grant no. 2014048).

#### REFERENCES

- 1. R. E. Kleinman and G. F. Roach, "Boundary integral equations for the three-dimensional Helmholtz equation," SIAM Rev. 16, 214–236 (1974).
- 2. F.-J. Sayas, *Retarded Potentials and Time Domain Boundary Integral Equations: A Road Map* (Springer, Cham, Switzerland, 2016).
- 3. V. S. Ryaben'kii, *Method of Difference Potentials and Its Applications* (Fizmatlit, Moscow, 2002; Springer-Verlag, Berlin, 2002).
- I. L. Sofronov, "About using transparent boundary conditions in aeroacoustics," Mat. Model. 19 (8), 105–112 (2007).
- 5. P. M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw-Hill, New York, 1953).
- 6. F. Smith, S. Tsynkov, and E. Turkel, "Compact high order accurate schemes for the three dimensional wave equation," J. Sci. Comput. **81** (3), 1181–1209 (2019).
- S. Petropavlovsky, S. Tsynkov, and E. Turkel, "A method of boundary equations for unsteady hyperbolic problems in 3D," J. Comp. Phys. 365, 294–323 (2018).

Translated by I. Ruzanova