A Method of Boundary Equations for Unsteady Hyperbolic Problems in 3D

S. Petropavlovsky, S. Tsynkov and E. Turkel

Abstract We propose an efficient algorithm based on boundary operator equations for the numerical simulation of time-dependent waves in 3D. The algorithm employs the method of difference potentials combined with the (strong) Huygens' principle (lacunae of the solution). It can handle nonconforming boundaries on regular structured grids with no loss of accuracy and offers sublinear computational complexity.

1 Introduction

We present a boundary method for computing the scattering of unsteady waves about general three-dimensional shapes. Boundary methods are common for elliptic and time-harmonic problems, but their generalization to the time-dependent case is far less straightforward. A major limitation is the ever-expanding backward dependence of the solution on time. It manifests itself via the boundary convolutions that go all the way back from the current to the initial moment of time, which makes the computation too costly. The key contribution of the current work is a boundary time-marching algorithm that requires only a narrow time window, which slides over the (2+1)-dimensional boundary of a (3+1)-dimensional space–time computational domain. The reduced dimension of the proposed boundary formulation compared to that of a volumetric integration results in a sublinear complexity of the algorithm.

Truncation of the backward temporal dependence of the solution is an implication of the (strong) Huygens' principle. It is a rare occurrence, but it holds for several

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PDE models important for applications: the wave (d'Alembert) equation, acoustics equations (linearized Euler's), Maxwell's equations in vacuum, and elasticity equations. The Huygens principle as a vehicle for truncating the convolutions is time has been exploited in some numerical methods based on retarded potential boundary integral equations [1]. Our implementation is fundamentally different in that it relies on the lacunae in the solutions and does not require the sophisticated numerical quadratures over the intersection of the light cone with the space–time boundary.

The boundary operators for the sliding window time-marching algorithm are computed by finite differences, including high order, on Cartesian grids. No sophisticated grid generation is required (which is typical, e.g., for finite elements). In doing so, the method of difference potentials (MDP) by Ryaben'kii [2] guarantees no deterioration of accuracy even for nonconforming boundaries.

We demonstrate the performance of our algorithm by solving both interior and exterior initial boundary value problems (IBVPs) for the 3D wave equation.

2 Description of the Method

Consider an exterior IBVP for the homogeneous 3D wave equation:

$$\Box_c u = 0, \quad \text{on} \quad \mathbb{R}^3 \backslash \Omega \times [0, T], \tag{1a}$$

$$\boldsymbol{l}_\Gamma u = \phi, \quad \text{on} \quad \partial\Omega \times [0, T], \tag{1b}$$

$$u|_{t=0} = \partial u/\partial t|_{t=0} = 0, \tag{1c}$$

where $\Box_c \equiv \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta$ is the d'Alembert operator and c is the propagation speed which is assumed constant. The solution u is to be calculated outside a bounded domain $\Omega \subset \mathbb{R}^3$ until the final time T. System (1) describes scattering about the shape Ω, and the unknown quantity u represents the scattered field. The homogeneous initial condition (1c) implies that the incident wave u^{inc} has just reached Ω by the initial time $t = 0$. The operator $\boldsymbol{l}_\Gamma$ in (1b) determines the type of scattering. The simplest examples of the boundary conditions (BCs) on $\Gamma \equiv \partial\Omega$ are the Dirichlet $\boldsymbol{l}_\Gamma u \equiv u = -u^{\text{inc}}$ and Neumann $\boldsymbol{l}_\Gamma u \equiv \frac{\partial u}{\partial \boldsymbol{n}} = -\frac{\partial u^{\text{inc}}}{\partial \boldsymbol{n}}$ conditions written in terms of the incident field. Our approach does not impose any limitations on the type of the initial or boundary conditions except that the entire problem (1) must be well-posed.

Next, consider a larger auxiliary domain $\Omega' \supset \Omega$ and denote by $G(\boldsymbol{x}, t)$ the fundamental solution of the 3D d'Alembert operator of (1a). We will be interested in obtaining the scattered field u on the complimentary domain $\Omega' \backslash \bar{\Omega}$ (the horizontal bar stands for the closure of Ω). Let us apply the Green's formula to the four-dimensional bounded domain $\Omega' \backslash \Omega \times (0, t]$, $t \leq T$ (see, e.g., [3, Eq. (7.3.5)]):

$$u(\boldsymbol{x},t)=\frac{1}{c^2}\int\limits_{\Omega'\setminus\bar{\Omega}}\left\{\frac{\partial u}{\partial t}(\boldsymbol{y},0)G(\boldsymbol{x}-\boldsymbol{y},t)-u(\boldsymbol{y},0)\frac{\partial G}{\partial t}(\boldsymbol{x}-\boldsymbol{y},t)\right\}d\boldsymbol{y}$$
$$+\int\limits_{\Gamma_t}\left\{\frac{\partial u}{\partial \boldsymbol{n}}(\boldsymbol{y},t')G(\boldsymbol{x}-\boldsymbol{y},t-t')-u(\boldsymbol{y},t')\frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x}-\boldsymbol{y},t-t')\right\}dt'dS_{\boldsymbol{y}}$$
$$+\int\limits_{\Gamma'_t}\left\{\frac{\partial u}{\partial \boldsymbol{n}}(\boldsymbol{y},t')G(\boldsymbol{x}-\boldsymbol{y},t-t')-u(\boldsymbol{y},t')\frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x}-\boldsymbol{y},t-t')\right\}dt'dS_{\boldsymbol{y}}. \tag{2}$$

The first integral in (2) is zero because of (1c). The last integral in (2) is taken over the artificial boundary $\Gamma'_t\equiv\partial\Omega'\times(0,t]$ and is also equal to zero. Given that $G(\boldsymbol{x},t)=\frac{1}{4\pi|\boldsymbol{x}|}\delta(t-|\boldsymbol{x}|/c)$ is the Green's function of the 3D wave equation in free space, this implies that all the waves at the outer boundary Γ'_t are outgoing, and there are no waves coming through the boundary Γ'_t back to the domain Ω'. As a result, only the second integral on the right-hand side of (2) remains, where the integration is performed over $\Gamma_t\equiv\partial\Omega\times(0,t]$. Thus, formula (2) allows us to express the solution u inside the computational domain $\Omega'\setminus\bar{\Omega}$ at a given time t only through the boundary values on the surface of the scatterer $\partial\Omega$ at the previous moments of time.

By analogy with (2), we introduce the Calderon potential with vector density $\boldsymbol{\xi}_{\Gamma_t}=(\xi_0,\xi_1)$ defined on Γ_t:

$$\boldsymbol{P}_{\tilde{\Omega}}\boldsymbol{\xi}_{\Gamma_t}(\boldsymbol{x},t)=\int\limits_{\Gamma_t}\left\{\xi_1(\boldsymbol{y},t')G(\boldsymbol{x}-\boldsymbol{y},t-t')-\xi_0(\boldsymbol{y},t')\frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x}-\boldsymbol{y},t-t')\right\}dt'dS_{\boldsymbol{y}}, \tag{3}$$

where $\boldsymbol{x}\in\tilde{\Omega}=\mathbb{R}^3\setminus\bar{\Omega}$. Comparison of (2) and (3) suggests that ξ_0 and ξ_1 can be interpreted as the trace of an outgoing solution to the wave equation (1a) and its normal derivative on $\partial\Omega$, respectively. It turns out that this is the case if and only if the boundary equation with projection (BEP) holds (see [2]):

$$\boldsymbol{P}_{\Gamma_t}\boldsymbol{\xi}_{\Gamma_t}=\boldsymbol{\xi}_{\Gamma_t}, \tag{4}$$

where $\boldsymbol{P}_{\Gamma_t}\equiv\boldsymbol{Tr}_{\Gamma_t}\boldsymbol{P}_{\tilde{\Omega}}\boldsymbol{\xi}_{\Gamma_t}$ is the Calderon projection and for any function w defined on $\tilde{\Omega}$, $\boldsymbol{Tr}_{\Gamma_t}w(\boldsymbol{x},t)\stackrel{\text{def}}{=}\left(w,\frac{\partial w}{\partial \boldsymbol{n}}\right)\Big|_{\Gamma_t}$. To obtain a unique outgoing solution, Eq. (4) should be considered along with the BC (1b) reformulated in terms of $\boldsymbol{\xi}_{\Gamma_t}=(\xi_0,\xi_1)$:

$$\boldsymbol{l}_{\Gamma_t}\boldsymbol{\xi}_{\Gamma_t}=\phi. \tag{5}$$

Thus, Eqs. (4) and (5) form a problem equivalent to the IBVP (1) but set only on the lateral boundary $\partial\Omega$ rather than on the entire 3D domain $\mathbb{R}^3\setminus\Omega$. Once the density $\boldsymbol{\xi}_{\Gamma_t}$ is found from (4), (5), the solution u on $\mathbb{R}^3\setminus\Omega$ is given by formula (3).

The surface integral in (3) may be difficult to compute, especially for a complicated geometry of the scatterer. Therefore, we redefine the Calderon poten-

tial. Take an arbitrary function $w(\boldsymbol{x}, t)$ compactly supported in space and such that $\boldsymbol{Tr}_{\Gamma_t} w = \boldsymbol{\xi}_{\Gamma_t}$. Then, $\boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_t}(\boldsymbol{x}, t) = v(\boldsymbol{x}, t)$, where $v(\boldsymbol{x}, t)$ is a solution to the Cauchy problem: $\Box_c v = \begin{cases} \Box_c w, & \boldsymbol{x} \in \Omega, \\ 0, & \boldsymbol{x} \notin \Omega, \end{cases}$, $v\big|_{t=0} = \begin{cases} w\big|_{t=0}, & \boldsymbol{x} \in \Omega, \\ 0, & \boldsymbol{x} \notin \Omega, \end{cases}$, $\frac{\partial v}{\partial t}\big|_{t=0} = \begin{cases} \frac{\partial w}{\partial t}\big|_{t=0}, & \boldsymbol{x} \in \Omega, \\ 0, & \boldsymbol{x} \notin \Omega. \end{cases}$ This Cauchy problem is referred to as the auxiliary problem (AP).

While formulated for all $\boldsymbol{x} \in \mathbb{R}^3$ and $t \geqslant 0$, in practice it will need to be solved only over a finite short interval of time, which, in turn, requires only a bounded auxiliary domain Ω'.

For a given $\boldsymbol{\xi}_{\Gamma_t} = (\xi_0, \xi_1)$, the function $w(\boldsymbol{x}, t)$ in the vicinity of Γ_t can be built by Taylor's formula: $w(\boldsymbol{x}, t) = \sum_{p=0}^{P} \frac{1}{l!} \frac{\partial^p w}{\partial \boldsymbol{n}^p}(\boldsymbol{x}_0, t) \rho^p$, $\boldsymbol{x}_0 \in \partial\Omega$, where $w(\boldsymbol{x}_0, t) = \xi_0(\boldsymbol{x}_0, t)$, $\frac{\partial w}{\partial \boldsymbol{n}}(\boldsymbol{x}_0, t) = \xi_1(\boldsymbol{x}_0, t)$, and higher order derivatives are obtained by differentiating the d'Alembert equation (1a). The density $\boldsymbol{\xi}_{\Gamma_t}$ is represented as an expansion with respect to a basis on Γ_t: $\xi_0 = \sum_{i=1}^{N} c_{0,i} \psi_i(\boldsymbol{x}, t)$, $\xi_1 = \sum_{i=1}^{N} c_{1,i} \psi_i(\boldsymbol{x}, t)$ so that Eqs. (4), (5) can be reformulated and solved for the coefficients $c_{0,i}, c_{1,i}$. The details of the discretization by means of the MDP can be found in [4].

However, as the time elapses, the boundary Γ_t extends, which makes Eqs. (4), (5) increasingly costly to solve. To overcome this fundamental difficulty, we partition the boundary Γ_T (where T is the final time) into K equal parts: $\Gamma_T = \Gamma_1 \cup \Gamma_2 \cup \ldots \cup \Gamma_K$, where $\Gamma_k = \partial\Omega \times ((k-1)T_0, kT_0]$. Then, we recast system (4), (5) (for $t = T$) in such a way that the corresponding partial densities can be determined consecutively.

From the BEP (4), we derive the following equation for the partial density $\boldsymbol{\xi}_{\Gamma_K}$:

$$\boldsymbol{P}_{\Gamma_{T_0}} \boldsymbol{\xi}_{\Gamma_K} + \sum_{k=1}^{K-1} \boldsymbol{Tr}_{\Gamma_K} \boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_k} = \boldsymbol{\xi}_{\Gamma_K}. \tag{6}$$

It is supplemented by the boundary condition derived from (5):

$$\boldsymbol{l}_{\Gamma_K} \boldsymbol{\xi}_{\Gamma_K} = \phi. \tag{7}$$

Assuming that all $\boldsymbol{\xi}_{\Gamma_k}$ for $k = 1, 2, \ldots, K-1$ are known, Eqs. (6), (7) allow us to determine $\boldsymbol{\xi}_{\Gamma_K}$. As T and K are arbitrary, we can continue consecutive updates $K \mapsto K+1$. This is a time-marching algorithm along the boundary. Still, it inherits full backward dependence on time: $\boldsymbol{\xi}_{\Gamma_K} = \boldsymbol{\xi}_{\Gamma_K}(\boldsymbol{\xi}_{\Gamma_{K-1}}, \ldots, \boldsymbol{\xi}_{\Gamma_1})$.

Let us, however, choose $T_0 \geqslant \frac{1}{c}\operatorname{diam}\Omega$. As $\boldsymbol{P}_{\tilde{\Omega}}$ is convolution with G, there will be no contribution from any of $\boldsymbol{\xi}_{\Gamma_k}$, $k = K-2, \ldots, 1$. Therefore, from (6) we have

$$\boldsymbol{P}_{\Gamma_{T_0}} \boldsymbol{\xi}_{\Gamma_K} + \boldsymbol{Tr}_{\Gamma_K} \boldsymbol{P}_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_{K-1}} = \boldsymbol{\xi}_{\Gamma_K}. \tag{8}$$

Thus, $\boldsymbol{\xi}_{\Gamma_K}$ depends only on the immediately preceding $\boldsymbol{\xi}_{\Gamma_{K-1}}$. Combining (8) with (7), we have a sliding window time marching with respect to K performed along a (2+1)-dimensional boundary Γ_t. The limited backward dependence on time in (8), (7) is an implication of the Huygens' principle. Indeed, the Calderon operators take

advantage of the lacuna of G or, equivalently, of the lacuna in the solution of the AP driven by a source compactly supported on Ω and operating over a finite time T_0.

Expanding the densities $\boldsymbol{\xi}_{\Gamma_K}$ and $\boldsymbol{\xi}_{\Gamma_{K-1}}$ with respect to the basis $\{\psi_i\}$, we recast (8):

$$\boldsymbol{Q}^{(0)}\boldsymbol{c}_0^{(K)} + \boldsymbol{Q}^{(1)}\boldsymbol{c}_1^{(K)} = -\boldsymbol{R}^{(0)}\boldsymbol{c}_0^{(K-1)} - \boldsymbol{R}^{(1)}\boldsymbol{c}_1^{(K-1)}, \tag{9}$$

where $\boldsymbol{c}_0^{(K)} = \{c_{0,i}^{(K)}\}$, $\boldsymbol{c}_1^{(K)} = \{c_{1,i}^{(K)}\}$ are the unknown coefficients and $\boldsymbol{c}_0^{(K-1)}$, $\boldsymbol{c}_1^{(K-1)}$ are considered known. Equation (9) is to be solved together with the boundary condition (7) reformulated using the same basis $\{\psi_i\}$.

The columns of the matrices $\boldsymbol{Q}^{(0,1)}$ and $\boldsymbol{R}^{(0,1)}$ in (9) correspond to individual basis functions ψ_i on Γ_{T_0}. Namely, each vector function $(\psi_i, 0)$ or $(0, \psi_i)$ is extended by Taylor's formula, and the resulting w is used to generate the source term for the AP. Then, the AP is solved on the time interval $2T_0$ and the solution on the special discrete sets of grid nodes near Γ_{T_0} yields the aforementioned columns. Solving multiple APs is the costliest part of the algorithm, because the number of basis functions ψ_i may be substantial. Yet different APs can be very efficiently solved in parallel, because different basis functions ψ_i are completely independent. As the AP is solved on a short time interval (we assume $T_0 \ll T$), we approximate it numerically on a bounded computational domain $\Omega' \supset \Omega$ chosen sufficiently large so that no wave reflected back from the outer boundary $\partial\Omega'$ can reach the physical boundary $\partial\Omega$ before $t = 2T_0$. This approach eliminates the need for artificial boundary conditions on $\partial\Omega'$ and is equivalent to a perfect reflectionless treatment of the outgoing waves.

It is important that Eq. (9) does not depend on the boundary condition (7). The two need to be combined to obtain a unique solution. Therefore, changing the boundary condition is numerically inexpensive, and the proposed methodology appears very well suited for solving multiple similar problems. Moreover, applying the proposed methodology to interior problems requires only insignificant changes.

3 Numerical Demonstrations

For our numerical simulations (of both interior and exterior problems), we choose a unit sphere as the computational domain Ω. The auxiliary domain is a larger cube: $\Omega' \supset \Omega$. It is discretized using a uniform Cartesian mesh, and the boundary $\partial\Omega$ is nonconforming. The wave equation (1a) is approximated using two schemes—the standard explicit second-order accurate central difference scheme and a compact implicit fourth-order accurate scheme [5] that uses a full $3 \times 3 \times 3 \times 3$ stencil.

First, we solve the interior problem with second-order accuracy. The test solution is a plane wave ($\lambda = \operatorname{diam}\Omega$), and we reconstruct it numerically for the boundary condition (1b) of a Dirichlet, Neumann, or Robin type. Table 1 shows the design rate of grid convergence. There is no deterioration of accuracy even though the boundary is nonconforming, and no indication of any difficulties related to cut cells [6].

Table 1 Time-averaged ℓ_∞ error on three successively refined grids (by a factor of 2) and the respective convergence rates for the interior problem

	Grid 1	Grid 2	Rate	Grid 3	Rate
Dirichlet BC	8.03×10^{-5}	2.64×10^{-5}	1.74	6.87×10^{-6}	1.96
Robin BC	2.89×10^{-4}	7.50×10^{-5}	1.96	1.87×10^{-5}	1.99
Neumann BC (∇)	4.86×10^{-4}	1.29×10^{-4}	1.94	3.48×10^{-5}	1.92

Table 2 Average values of the ℓ_∞ error over $0 \leqslant t \leqslant T_{\text{sim}}$ on three successive grids and the respective convergence rates for the exterior scattering problem solved using second-order scheme

Grid	Dirichlet		Neumann		Robin	
	Average error	Rate	Average error	Rate	Average error	Rate
1x	6.55×10^{-3}	–	1.84×10^{-2}	–	2.02×10^{-2}	–
2x	1.52×10^{-3}	4.27	4.84×10^{-3}	3.81	5.74×10^{-3}	3.52
4x	2.91×10^{-4}	5.25	9.69×10^{-4}	4.99	1.41×10^{-3}	4.06

Table 3 Average values of the ℓ_∞ error over $0 \leqslant t \leqslant T_{\text{sim}}$ on two successive grids and the respective convergence rates for the exterior scattering problem solved using fourth-order scheme

Grid	Dirichlet		Neumann		Robin	
	Average error	Rate	Average error	Rate	Average error	Rate
2x	6.52×10^{-5}	–	2.09×10^{-4}	–	2.86×10^{-4}	–
4x	2.44×10^{-6}	26	8.60×10^{-6}	24	1.31×10^{-5}	21

Table 4 CPU time needed to advance the solution to the scattering problem over the time T_0

Grid	Volumetric method+PML		MDP+lacunae	
	CPU time, sec	Scaling, times	CPU time, sec	Scaling, times
1x	1.26	–	0.0474	–
2x	19.8	15.7	0.421	8.87
4x	322	16.3	3.56	8.46

The exterior problem that we solve is that of the scattering of an impinging plane wave about a unit sphere. The exact solution for the scattered field is known in the form of an expansion in spherical harmonics and Hankel functions [3, Vol. 2, Chap. 11, p. 1483]. Tables 2 and 3 present the results of computations with second- and fourth-order accuracy, respectively. The design rates of grid convergence are achieved for all three types of the boundary conditions. Again, the boundary $\partial\Omega$ is nonconforming.

Table 4 compares the CPU time needed to compute the solution by a traditional volumetric scheme terminated with a PML against that for the proposed boundary approach. One can see that in the volumetric case the time scales as 2^4, whereas for the proposed method it scales as 2^3. This is a demonstration of sublinear complexity.

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