Contents lists available at ScienceDirect

Journal of Computational Physics

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3D time-dependent scattering about complex shapes using high order difference potentials \ddagger

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ARTICLE INFO

Article history: Received 18 July 2022 Received in revised form 14 September 2022 Accepted 14 September 2022 Available online 19 September 2022

Keywords: Unsteady acoustic waves CAD surface with patched parameterization High order splines (NURBS) Calderon's boundary equations High-order compact schemes on Cartesian grids Huygens' principle

ABSTRACT

We compute the scattering of unsteady acoustic waves about complex three-dimensional bodies with high order accuracy. The geometry of a scattering body is defined with the help of CAD. Its surface is represented as a collection of non-overlapping patches, each parameterized independently by means of high order splines (NURBS). As a specific example, we consider a submarine-like scatterer constructed using five different patches. The acoustic wave equation on the region exterior to the scatterer is solved by first reducing it to a system of Calderon's boundary operator equations. The latter are obtained using the method of difference potentials coupled with a compact fourth order accurate finite difference scheme. When solving the boundary operator equations, we employ Huygens' principle. It allows us to work on a sliding time window of non-increasing duration rather than keep the entire temporal history of the solution at the boundary. The proposed methodology demonstrates grid-independent computational complexity at the boundary and sub-linear complexity with respect to the grid dimension. It efficiently handles complex non-conforming geometries on Cartesian grids with no penalty for either accuracy or stability due to the cut cells. Its performance does not deteriorate over arbitrarily long simulation times. The exact treatment of artificial outer boundaries is inherently built in. Finally, multiple similar problems can be solved efficiently at a low individual cost per problem. This is important when, for example, the boundary condition on the surface changes but the scattering body stays the same.

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1. Introduction

An acoustic scattering problem is an exterior initial boundary value problem (IBVP) for the wave equation (with a constant propagation speed *c*):

$$\Box_{c} u \equiv \frac{1}{c^{2}} \frac{\partial^{2} u}{\partial t^{2}} - \Delta u = 0, \quad (\boldsymbol{x}, t) \in \mathbb{R}^{3} \setminus \Omega \times [0, T],$$

Work supported by the U.S-Israel Binational Science Foundation (BSF) under grant # 2020128. Corresponding author.

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https://doi.org/10.1016/j.jcp.2022.111632 0021-9991/© 2022 Elsevier Inc. All rights reserved.





(1a)

$$\begin{aligned} l_{\Gamma} u &= \phi, \quad (x,t) \in \Gamma \equiv \partial \Omega \times [0,T], \end{aligned} \tag{1b} \\ u|_{t=0} &= \frac{\partial u}{\partial t} = 0, \quad x \in \mathbb{R}^3 \backslash \Omega. \end{aligned}$$

$$u|_{t=0} = \left. \frac{\partial u}{\partial t} \right|_{t=0} = 0, \quad x \in \mathbb{R}^3 \setminus \Omega,$$

where *u* is the scattered field (perturbation of the acoustic pressure), $\Omega \subset \mathbb{R}^3$ is a bounded scattering body, and *T* is the final time which is arbitrary. The governing d'Alembert equation in (1a) is homogeneous because there are no sources for the scattered field in the exterior region $\tilde{\Omega} \equiv \mathbb{R}^3 \setminus \Omega$ and the solution is driven by a given incident field u^{inc} via the boundary condition (1b) on the scattering surface $\partial\Omega$. In particular, if l_{Γ} is the identity, then (1b) becomes a Dirichlet boundary condition $u|_{\Gamma} = -u^{\text{inc}}|_{\Gamma}$, which corresponds to sound-soft scattering. If $l_{\Gamma} = \frac{\partial}{\partial n}$ (normal derivative), then (1b) becomes a Neumann boundary condition $\frac{\partial u}{\partial n}|_{\Gamma} = -\frac{\partial u^{\text{inc}}}{\partial n}|_{\Gamma}$, which corresponds to sound-hard scattering. Other boundary conditions (1b), for example, impedance (Robin) boundary condition $l_{\Gamma} = \alpha + \sigma \frac{\partial}{\partial n}$, can be considered as well. In addition, we assume that the simulation starts when the incident field reaches the scatterer Ω . Hence, the initial conditions (1c) are homogeneous. Moreover, the scattered field u is assumed outgoing in the sense of [1]. This means that u(x,t) = 0 for all $t \ge 0$ and $|\mathbf{x}| \ge \rho + ct$, where $\rho > 0$ is sufficiently large so that $\Omega \subset \{\mathbf{x}' \in \mathbb{R}^3 | |\mathbf{x}'| \le \rho\}$.

The IBVP (1), as well as other similar problems, can be solved by a variety of numerical methods, including finite difference time domain method (FDTD) [2], time domain finite elements (TD FEM) [3] and discontinuous Galerkin methods (DG) [4], various techniques that combine frequency domain solutions [5–8], and boundary methods, specifically those based on retarded potential boundary integral equations (RPBIEs) [9–16]. The volumetric methods (FDTD and TD FEM) benefit from high order accuracy as it reduces the numerical pollution [17,18]. These methods also require special treatment of artificial outer boundaries [19]. Boundary methods solve the IBVP only on the surface Γ thus reducing the dimension by one. They automatically account for the radiation of waves in the far field. The boundary formulation on Γ typically depends on the type of the boundary conditions, e.g., Dirichlet and Neumann conditions require different representation of the solution at the boundary.

In [20–26], we have developed a class of high order accurate numerical methods for solving the exterior IBVPs of type (1) and the corresponding interior problems. Our methods are based on Calderon's operators and the method of difference potentials (MDP) [27]. They combine the advantages of boundary methods and FDTD. The approach of [20-26] employs the MDP along with compact high order accurate finite difference schemes on regular structured grids. In doing so, the MDP maintains high order accuracy in the case of general non-conforming boundaries. The MDP reduces the IBVP (1) to an equivalent boundary formulation independent of the boundary condition (1b). This enables efficient solution of multiple similar problems, e.g., for various incident waveforms and the same scattering shape, because it is the boundary condition (1b) that characterizes the incident radiation and the type of scattering.

Moreover, the methodology of [20-26] relies on the (strong) Huygens' principle and lacunae of the solution, i.e., voids behind aft fronts of the waves [28-37]. When solving the IBVP (1), lacunae allow one to limit the backward dependence of the MDP algorithm on time and thus compute the Calderon's operators only over a finite non-increasing time interval. The latter depends on the size of the scatterer and speed of propagation, but does not depend on the bandwidth of the signal. As a result, lacunae-based time marching obviates the need for any special treatment of artificial outer boundaries, such as artificial boundary conditions (ABC) or perfectly matched layers (PML) [19]. It also yields a grid-independent complexity of boundary integration and sub-linear complexity of computing the solution in the volume.

A very important feature of any algorithm for the numerical simulation of waves' scattering is its capacity to handle complex geometries. This capacity involves two components: maintaining the accuracy of a discrete approximation of the governing equations (and boundary conditions) on the domain of a complex shape and representation of the domain itself.

Finite differences are very efficient on simple domains discretized by regular grids. They may not perform as well for non-conforming geometries unless supplemented by additional techniques such as [38–40]. The MDP [27] guarantees that the accuracy of a finite difference scheme will remain unaffected by geometry. Finite elements are more flexible than finite differences from the standpoint of geometry but require a mesh generation about complex shapes. For both FD and FEM, the definition of the shape Ω itself is of key importance as it should obviously precede any grid generation or discrete approximation.

Unlike the volumetric methods (FD and FEM), boundary methods do not approximate the original PDEs on $\tilde{\Omega} = \mathbb{R}^3 \setminus \Omega$. They approximate the boundary integral equations on the surface $\partial \Omega$ (more precisely, on $\Gamma = \partial \Omega \times [0, T]$). Therefore, the accuracy considerations for these methods apply to the approximation of the corresponding integrals rather than PDEs. Yet similar to the volumetric methods, the representation of the geometry of Ω and parameterization of the surface $\partial \Omega$ are central for the boundary methods, because they precede the derivation of the boundary integral equations.

In practical scenarios, the geometric shapes are often represented by means of computer-aided design (CAD). For the integration of CAD and FEM, a special approach has been developed known as isogeometric analysis [41,42]. A method of boundary integral equations for CAD-defined shapes has been proposed in [43]. This method relies on a parameterization of the scattering surface via a set of non-overlapping patches, with local coordinates associated with every patch.

To solve the IBVP (1) by means of the MDP, one also needs a parameterization of the scattering surface $\partial \Omega$. In [20,24], we have computed unsteady scattering about spheres and spheroids. The scattering surfaces were represented using spherical and spheroidal coordinates, respectively. It is important that, for the simple shapes Ω such as spheres and spheroids, one can use one coordinate transformation to parameterize the entire surface $\partial \Omega$.



Fig. 1. 3D time-dependent scattering of a Gaussian modulated chirp about a torus.

A parametric representation of a 2D surface in a 3D space is defined as

$$x = x(\sigma, \varphi), \quad y = y(\sigma, \varphi), \quad z = z(\sigma, \varphi), \tag{2}$$

where the parametric coordinates $(\sigma, \varphi) \in \mathbb{R}^2$ and $(x, y, z) \in \mathbb{R}^3$. An example that goes beyond the spheres and spheroids is given by the toroidal coordinates:

$$x = \frac{a \sinh \alpha \cos \varphi}{\cosh \alpha - \cos \sigma}, \quad y = \frac{a \sinh \alpha \sin \varphi}{\cosh \alpha - \cos \sigma}, \quad z = \frac{a \sin \sigma}{\cosh \alpha - \cos \sigma}, \quad (3)$$
$$0 \le \alpha < \infty, \quad -\pi < \sigma \le \pi, \quad -\pi < \varphi \le \pi,$$

where for any fixed value of $\alpha = \text{const} > 0$, equations (3) yield a parametric representation of a toroidal surface in \mathbb{R}^3 in the form (2).

Using the methodology of [20] that employs the MDP and lacunae, we have computed several scattering solutions about a torus; one example is presented in Fig. 1. The entire toroidal surface was represented by parametric coordinates (2), (3) for a fixed α .

There are, however, only a small number of coordinate systems that yield a parametric representation of the entire surface $\partial\Omega$ in the form of (2), see [44, Volume 1]. The corresponding shapes Ω are fairly simple. For more realistic shapes, one has to use patched parametric coordinates, where equations (2) do not extend to the entire surface. Instead, the surface is partitioned into a collection of patches, and each patch has its own representation in the form of (2).

In the current work, we define the scattering body Ω by means of CAD, develop a parametric representation of its surface $\partial \Omega$ using a system of non-overlapping patches, and incorporate this development into the wave equation solver based on the MDP and lacunae [20]. The parameterization of the patches involves high order splines (NURBS). To compute the discrete counterparts of Calderon's boundary operators, we approximate the wave equation on a uniform Cartesian grid with the help of a fourth order accurate in space and time compact scheme [22]. The operators act on the trace of the solution and its normal derivative at the boundary. The trace on every patch is represented as a finite Fourier and/or Chebyshev expansion. The coefficients of this expansion eventually become the unknowns for reconstruction in the sense of least squares. The Huygens' principle enables marching the solution in time along the space-time boundary Γ in increments of a fixed duration. It also guarantees the reflectionless properties of the artificial outer boundary. Neither stability of the time marching nor accuracy of the solution are affected by the geometry that does not conform to the Cartesian discretization grid. Stability is maintained over arbitrarily long integration times. Furthermore, once the Calderon's operators have been computed, the complexity of the time marching along Γ is independent of the grid dimension. The solution in the volume (i.e., on $\hat{\Omega}$) does not need to be computed until the terminal time T (more generally, does not need to be computed except at some predetermined moments of time), and the complexity of this computation is substantially lower than that of the conventional volumetric time marching. Finally, for a given shape Ω , the operators need to be computed only once and then any incident signal and any type of scattering can be accommodated. This facilitates efficient solution of multiple similar problems.

In Section 2, we provide a brief account of the method of difference potentials and its implementation as combined with Huygens' principle for solving the unsteady hyperbolic problems. A detailed description of the MDP+lacunae algorithm can be found in [20,21,24]. In Section 3, we discuss the parametric representation of a 2D surface in a 3D space using splines. In Section 4, we build an equation-based extension operator that maps the Dirichlet and Neumann data at the boundary onto nearby grid nodes. In Section 5, we describe the numerical setting and present the results. Section 6 provides the conclusions.

2. Method of difference potentials and lacunae

2.1. Operators

The fundamental solution $G(x, t) = \frac{c}{2\pi} \theta(t) \delta(c^2 t^2 - |x|^2)$ of the 3D d'Alembert operator \Box_c satisfies $\Box_c G = \delta(x, t)$. The Calderon's potential for the exterior problem (1) is

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$$\boldsymbol{P}_{\tilde{\Omega}}\boldsymbol{\xi}_{\Gamma_{t}}(\boldsymbol{x},t) = \int_{\Gamma_{t}} \left\{ \xi_{1}(\boldsymbol{y},t') \boldsymbol{G}(\boldsymbol{x}-\boldsymbol{y},t-t') - \xi_{0}(\boldsymbol{y},t') \frac{\partial \boldsymbol{G}}{\partial \boldsymbol{n}}(\boldsymbol{x}-\boldsymbol{y},t-t') \right\} dt' dS_{\boldsymbol{y}}, \tag{4}$$

where $\Gamma_t \equiv \partial \Omega \times [0, t]$. The potential (4) is a scalar function on $\tilde{\Omega}$ that satisfies (1a). Its density $\boldsymbol{\xi}_{\Gamma_t} = (\boldsymbol{\xi}_0, \boldsymbol{\xi}_1)$ is a vector function on the space-time boundary Γ_t . For an arbitrary $w = w(\boldsymbol{x}, t)$, introduce its vector trace on Γ_t : $Tr_{\Gamma_t} w \stackrel{\text{def}}{=} (w, \frac{\partial w}{\partial n})|_{\Gamma_t}$. If $u = u(\boldsymbol{x}, t)$ satisfies (1a), then $u = P_{\tilde{\Omega}} Tr_{\Gamma_t} u$ on $\tilde{\Omega}$, and (4) becomes the classical Green's formula.

The Calderon's boundary projection is defined as the trace of the potential (4): $P_{\Gamma_t} \stackrel{\text{def}}{=} Tr_{\Gamma_t} P_{\tilde{\Omega}}$. The Calderon's boundary equation with projection (BEP)

$$P_{\Gamma_t}\xi_{\Gamma_t} = \xi_{\Gamma_t} \tag{5}$$

holds iff the density ξ_{Γ_t} coincides with the trace of a solution to (1a) on $\tilde{\Omega}$ subject to (1c). Then, one supplements the BEP (5) with the boundary condition (1b):

$$l_{\Gamma_t} \boldsymbol{\xi}_{\Gamma_t} = \boldsymbol{\phi}. \tag{6}$$

Equations (5)–(6) yield an equivalent reformulation of the IBVP (1) at the boundary Γ_t .

2.2. Partition in time

Let T_0 be fixed and $0 \le t \le K \cdot T_0 \equiv T$. Split Γ_T into *K* equal parts:

$$\Gamma_T = \Gamma_1 \cup \Gamma_2 \cup \dots \cup \Gamma_K, \quad \text{where} \quad \Gamma_k = \partial \Omega \times ((k-1)T_0, kT_0], \tag{7}$$

and represent $\boldsymbol{\xi}_{\Gamma_T}$ accordingly:

$$\boldsymbol{\xi}_{\Gamma_T} = \boldsymbol{\xi}_{\Gamma_1} + \boldsymbol{\xi}_{\Gamma_2} + \dots + \boldsymbol{\xi}_{\Gamma_K}, \text{ where } \boldsymbol{\xi}_{\Gamma_k}(\boldsymbol{x}, t) = \begin{cases} \boldsymbol{\xi}_{\Gamma_T}(\boldsymbol{x}, t), & (\boldsymbol{x}, t) \in \Gamma_k, \\ \boldsymbol{0}, & (\boldsymbol{x}, t) \in \Gamma_T \setminus \Gamma_k. \end{cases}$$

$$\tag{8}$$

One can recast (5)–(6) so as to determine ξ_{Γ_k} consecutively [24]. By computing ξ_{Γ_k} one after another for k = 1, ..., K, one can complete the solution for the entire time interval of length $T = KT_0$. In doing so, each ξ_{Γ_k} depends on all the previous partition elements. In particular, ξ_{Γ_k} depends on all ξ_{Γ_k} , k = 1, ..., K - 1, i.e., on the entire temporal history of the solution. Since, however, the wave equation satisfies the Huygens' principle, the dependence of ξ_{Γ_k} on ξ_{Γ_k} , k < K, can be truncated.

2.3. Huygens' principle

Let *f* be compactly supported in space-time. Then, the solution *u* of $\Box_c u = f$ has a lacuna [28], which is the intersection of the characteristic cones as their vertex sweeps the support of *f*:

$$u(x,t) \equiv 0 \text{ if } (x,t) \in \bigcap_{(x',t') \in \text{supp } f} \{(x,t) | |x-x'| < c(t-t'), t > t' \}.$$

Let $T_0 \ge \frac{1}{c} \operatorname{diam} \Omega$. Then, according to (4), for $(x, t) \in \Gamma_K$ there is no contribution from any ξ_{Γ_k} , $k \le K - 2$, because if the vertex of a characteristic cone belongs to Γ_K , then its surface doesn't intersect with Γ_k for $k \le K - 2$, see [24, Figure 2(a)], and may intersect only with Γ_{K-1} . In other words, for the sources on Γ_T below $t = T - 2T_0$, the domain Ω completely falls into the lacuna starting from $t = T - T_0$, see [24, Figure 2(b)]. Hence, from (5) we have:

$$P_{\Gamma_{T_0}}\boldsymbol{\xi}_{\Gamma_K} + \underbrace{Tr_{\Gamma_K}P_{\tilde{\Omega}}\boldsymbol{\xi}_{\Gamma_{K-1}}}_{\boldsymbol{R}_{\Gamma_{T_0}}\boldsymbol{\xi}_{\Gamma_{K-1}}} = \boldsymbol{\xi}_{\Gamma_K}.$$
(9)

Thus, ξ_{Γ_K} depends only on $\xi_{\Gamma_{K-1}}$ rather than on all ξ_{Γ_k} . Equation (9), combined with the boundary condition $l_{\Gamma_K} \xi_{\Gamma_K} = \phi$, allows one to solve for ξ_{Γ_K} given the data $\xi_{\Gamma_{K-1}}$ for K - 1 and ϕ for K. This procedure can be thought of as time stepping with step size T_0 performed along a (2+1)-dimensional lateral boundary, as opposed to the (3+1)-dimensional volumetric integration.

2.4. Spectral discretization on the surface and time marching

Introduce a basis of functions $\psi_{0,s} = (\psi_s, 0)$ and $\psi_{1,s} = (0, \psi_s)$ on Γ_K and Γ_{K-1} . Then,

$$\boldsymbol{\xi}_{\Gamma_{K-1}} = \sum_{s=1}^{N} c_{0,s}^{(K-1)} \boldsymbol{\psi}_{0,s} + c_{1,s}^{(K-1)} \boldsymbol{\psi}_{1,s}, \quad \boldsymbol{\xi}_{\Gamma_{K}} = \sum_{s=1}^{N} c_{0,s}^{(K)} \boldsymbol{\psi}_{0,s} + c_{1,s}^{(K)} \boldsymbol{\psi}_{1,s}.$$
(10)

The dimension N of the basis in (10) is finite. It is chosen so as to guarantee that the corresponding error will be smaller than the error in computing the discrete counterparts to Calderon's operators on the grid (see Sections 5.3 and 5.4 for detail).

Let $\boldsymbol{\xi}_{\Gamma_{K-1}}$, i.e., the coefficients $c_{0,s}^{(K-1)}$ and $c_{1,s}^{(K-1)}$, be known. Substitute (10) into (9):

$$\sum_{s} c_{0,s}^{(K)} \underbrace{\left\{ P_{\Gamma_{T_{0}}} - I \right\}}_{Q_{\Gamma_{T_{0}}}} \psi_{0,s} + c_{1,s}^{(K)} \underbrace{\left\{ P_{\Gamma_{T_{0}}} - I \right\}}_{Q_{\Gamma_{T_{0}}}} \psi_{1,s} = -\sum_{s} c_{0,s}^{(K-1)} R_{\Gamma_{T_{0}}} \psi_{0,s} + c_{1,s}^{(K-1)} R_{\Gamma_{T_{0}}} \psi_{1,s}, \tag{11}$$

where I is the identity operator. In addition, the boundary condition on Γ_K yields:

$$l_{\Gamma_{K}} \sum_{s} c_{0,s}^{(K)} \boldsymbol{\psi}_{0,s} + c_{1,s}^{(K)} \boldsymbol{\psi}_{1,s} = \phi \equiv \sum_{s} c_{s}^{(\phi,K)} \boldsymbol{\psi}_{s}.$$
(12)

The boundary condition (12) does not affect the reduction of the IBVP (1) to the BEP (9) and can be arbitrary. It is merely combined with the BEP to form the overall system.

In (11), (12), $c_{0,s}^{(K)}$, $c_{1,s}^{(K)}$ are the unknowns, and $c_{0,s}^{(K-1)}$, $c_{1,s}^{(K-1)}$, $c_s^{(\phi,K)}$ are the data. Neither the operators $Q_{\Gamma_{T_0}}$, $R_{\Gamma_{T_0}}$, $R_{\Gamma_{T_0}}$, $R_{\Gamma_{T_0}}\psi_{1,s}$, $R_{\Gamma_{T_0}}\psi_{1,s}$, $R_{\Gamma_{T_0}}\psi_{1,s}$, $R_{\Gamma_{T_0}}\psi_{1,s}$ remain the same for all K. This enables time marching with respect to K, which is done as follows.

First, (9), is solved for K = 1. Then, for $\boldsymbol{\xi}_{\Gamma_{K-1}} \equiv \boldsymbol{\xi}_{\Gamma_1}$ we obtain the coefficients $c_{0,s}^{(1)}$ and $c_{1,s}^{(1)}$ using (10). Next, we solve (11), (12) for the coefficients $c_{0,s}^{(2)}$ and $c_{1,s}^{(2)}$ that are attributed to $\boldsymbol{\xi}_{\Gamma_K} \equiv \boldsymbol{\xi}_{\Gamma_2}$. After that, we perform one time step by solving system (11), (12) again, for $c_{0,s}^{(3)}$ and $c_{1,s}^{(3)}$ of $\boldsymbol{\xi}_{\Gamma_K} \equiv \boldsymbol{\xi}_{\Gamma_3}$. The process continues for $K = 4, 5, \ldots$

2.5. Difference potentials

Let $\boldsymbol{\xi}_{\Gamma_t} = (\xi_0, \xi_1)$ be given and $w = w(\boldsymbol{x}, t), \ \boldsymbol{x} \in \tilde{\Omega}$, be such that $Tr_{\Gamma_t}w = \boldsymbol{\xi}_{\Gamma_t}$. The Calderon's potential $P_{\tilde{\Omega}}\boldsymbol{\xi}_{\Gamma_t}$ of (4) can be obtained as the solution v to the following initial value problem that we will subsequently refer to as the auxiliary problem (AP):

$$\frac{1}{c^2} \frac{\partial^2 v}{\partial t^2} - \Delta v = \begin{cases} \Box_c w, & x \in \Omega, \\ 0, & x \notin \Omega, \end{cases}$$

$$v|_{t=0} = \begin{cases} w|_{t=0}, & x \in \Omega, & \frac{\partial v}{\partial t}|_{t=0} = \begin{cases} \frac{\partial w}{\partial t}|_{t=0}, & x \in \Omega, \\ 0, & x \notin \Omega, & \frac{\partial t}{\partial t}|_{t=0} = \end{cases}$$
(13)

The AP (13) is formulated on the entire \mathbb{R}^3 , but both its initial data and source term are compactly supported on Ω . To compute the discrete counterparts to $Q_{\Gamma_{T_0}}$ and $R_{\Gamma_{T_0}}$ of (11), (9), it is sufficient to solve the AP (13) for $0 \le t \le 2T_0$. Hence, no treatment of artificial outer boundary is required as one can take a larger computational domain that would guarantee no reflection before the computation is terminated at $t = 2T_0$ (Section 5.2).

The AP (13) is discretized and solved by finite differences, in particular, one can use the fourth order compact scheme of [22] (see Section 5.2). This scheme is built on the Cartesian grid yet the shape of the boundary $\partial \Omega$ can be non-conforming. The grid boundary γ_t is constructed as follows. Consider the stencil of the scheme used to approximate the wave equation in (13) on the Cartesian grid. When this stencil is applied to every grid node inside Ω , some of the nodes of the stencil appear outside Ω . Conversely, when the stencil is applied to the exterior grid, some of its nodes appear inside Ω . Those nodes of the stencil that end up in the complementary domain on either side of the boundary γ_t . Since the shape of Ω does not change as the time elapses and the stencil of the scheme is also assumed fixed, the structure of the grid boundary γ_t remains the same for all time levels. Hereafter, we will denote by γ the grid boundary on any given time level. In Fig. 2, we are showing a 2D example of how the grid boundary γ may look like.

The difference boundary projection P_{γ_t} is an operator in the space of grid functions defined on γ_t . It is obtained by solving the discrete AP. The discrete BEP $P_{\gamma_t}\xi_{\gamma_t} = \xi_{\gamma_t}$ holds iff there is a solution $u^{(h)}$ of the discrete wave equation such that $u^{(h)}|_{\gamma_t} = \xi_{\gamma_t}$. The continuous and discrete density ξ_{Γ_t} and ξ_{γ_t} are coupled by the equation-based extension operator $Ex: \xi_{\gamma_t} = Ex\xi_{\Gamma_t}$ that we describe in Section 4.



Fig. 2. 2D schematic for the grid boundary at a given time.

A discrete counterpart of (11) is obtained by solving the AP (13) with finite differences for all $Ex\psi_{0,s}$ and $Ex\psi_{1,s}$:

$$\boldsymbol{Q}_{\gamma\tau_0}^{(0)} \boldsymbol{c}_0^{(K)} + \boldsymbol{Q}_{\gamma\tau_0}^{(1)} \boldsymbol{c}_1^{(K)} = -\boldsymbol{R}_{\gamma\tau_0}^{(0)} \boldsymbol{c}_0^{(K-1)} - \boldsymbol{R}_{\gamma\tau_0}^{(1)} \boldsymbol{c}_1^{(K-1)}.$$
(14a)

The boundary condition (12) is also recast as a system of linear equations

$$B_0 c_0^{(K)} + B_1 c_1^{(K)} = c^{(\phi, K)}.$$
(14b)

The linear system (14) with unknowns $c_0^{(K)} = \{c_{0,s}^{(K)}\}, c_1^{(K)} = \{c_{1,s}^{(K)}\}$ is solved by least squares:

$$\begin{bmatrix} c_0^{(K)} \\ c_1^{(K)} \end{bmatrix} = -\mathcal{R}^{-1} \mathcal{Q}^* \begin{bmatrix} \mathbf{R}_{\gamma T_0}^{(0)} & \mathbf{R}_{\gamma T_0}^{(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} c_0^{(K-1)} \\ c_1^{(K-1)} \\ c_1^{(\phi,K)} \end{bmatrix}.$$
(15)

The matrix on the right-hand side of (15) does not depend on K. It can be pre-computed after computing the discrete operators in (14a). The dimension of this matrix corresponds to the dimension N of the basis in (10). Remarkably, it does not depend on the dimension of the volumetric discretization grid. Consequently, advancing the solution along the boundary by the time step T_0 costs $\mathcal{O}(N^2)$ operations. This cost won't increase as the volumetric Cartesian grid is refined.

3. Representation of the scattering surface using NURBS

The scattering surface $\partial \Omega$ is a bounded 2D surface in \mathbb{R}^3 . We consider its partition into a number of non-overlapping patches: $\partial \Omega = P_1 \cup P_2 \cup ... \cup P_{N_p}$. Every patch P_j , $j = 1, ..., N_p$, is assumed to have a parametric representation of type (2) by means of a differentiable mapping $\hat{h}: \hat{\Omega} \mapsto P_j$ between a reference domain $\hat{\Omega} \subset \mathbb{R}^2$ and P_j . Henceforth, we will denote the parametric coordinates by $(s_1, s_2) \in \hat{\Omega}$ so that for a given patch, the mapping \hat{h} would yield $x = x(s_1, s_2) \in P_i$. In our implementation (see Section 5.1), \hat{h} will be a tensor product of high order spline functions.

A popular approach for surface representation in CAD systems is based on non-uniform rational B-splines (NURBS), see, e.g., [45]. A NURBS definition of a 2D surface requires two sequences of knots, $\{k_1, k_2, ..., k_{n_m+d_m+1}\}$, one per dimension m = 1, 2, two weight vectors $\{w_1, ..., w_{n_m}\}$, and a set of control points $A_{i_1i_2} \in \mathbb{R}^3$, $i_1 = 1, ..., n_1$, $i_2 = 1, ..., n_2$, with $n_m > d_m$. The first and last knots are repeated $d_m + 1$ times, i.e., $k_1 = k_2 = ... = k_{d_m+1}, k_{n_m+1} = k_{n_m+2} = ... = k_{n_m+d_m+1}, m = 1, 2$. The NURBS parametrization relies on B-splines of degree d, $\{B^{(i,d)}\}_{i=1}^n$, with respect to a knot sequence $\Theta_d = 0$

 $\{k_1, k_2, ..., k_{n+d+1}\}$. The B-splines of degree zero are defined as follows:

$$B^{(i,0)}(s) = \begin{cases} 1, & k_i \leq s < k_{i+1}, \\ 0, & \text{otherwise.} \end{cases}$$

A B-spline of degree *d* is obtained by the Cox-de Boor recurrence relation:

$$B^{(i,d)}(s) = \frac{s - k_i}{k_{i+d} - k_i} B^{(i,d-1)}(s) + \frac{k_{i+d+1} - s}{k_{i+d+1} - k_{i+1}} B^{(i+1,d-1)}(s).$$

A one-dimensional NURBS is then constructed as a weighted B-spline:

$$N^{(i,d)}(s) = \frac{w_i B^{(i,d)}(s)}{\sum_{j=1}^n w_j B^{(j,d)}(s)}.$$
(16)



Fig. 3. Surface-oriented monoclinic coordinate system.

Note that, if all $w_i = 1$ then the denominator in (16) is equal to one and the NURBS reduces to a B-spline. The choice of w_i is presented in Section 5.1.

A 2D surface is parametrized as linear combination of NURBS in each coordinate direction with the control points $A_{i_1i_2}$ as coefficients:

$$\boldsymbol{x} = \boldsymbol{x}(s_1, s_2) = \sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} A_{i_1 i_2} N^{(i_1, d_1)}(s_1) N^{(i_2, d_2)}(s_2).$$
(17)

Formula (17) is a realization of the mapping \hat{h} .

4. Equation based extension in surface-oriented coordinates

In this section, we construct the extension operator Ex first introduced in Section 2.5. Consider a point A near the surface $\partial\Omega$, see Fig. 3, and let O_A be the foot of a normal dropped from A to $\partial\Omega$. Then, the position vector x_A of the point A can be represented as the sum: $x_A = x'_A + zn_A$, where x'_A is the position vector of O_A , n_A is a unit normal to the surface $\partial\Omega$ at O_A , and z is a signed distance between O_A and A. As $x' \in \partial\Omega$, then it belongs to one of the patches P_j for a particular j. Hence, we have $x' = x'(s_1, s_2)$ and $n = n(s_1, s_2)$ in accordance with the parametrization (17). Therefore, every point in \mathbb{R}^3 near the surface is uniquely defined by a triplet of real numbers (s_1, s_2, z) , as long as |z| does not exceed the local radius of curvature. This representation of points near $\partial\Omega$ is called a surface-oriented locally monoclinic coordinate system, see [46]. The vector n needed to define the surface-oriented coordinates is given by the normalized cross-product of two tangential vectors: $n = \frac{\partial x'}{\partial s_1} \times \frac{\partial x'}{\partial s_2} / \|\frac{\partial x'}{\partial s_1} \times \frac{\partial x'}{\partial s_2}\|$. Let $A \in \gamma$, where γ is the grid boundary γ_t at any given moment of time, see Fig. 2. The goal is to extend the boundary

Let $A \in \gamma$, where γ is the grid boundary γ_t at any given moment of time, see Fig. 2. The goal is to extend the boundary data $(\xi_0, \xi_1) = (u, \frac{\partial u}{\partial \pi})$ from the point O_A to the point A. A natural way is to use the Taylor expansion in the surface-oriented coordinates:

$$u|_{A} \approx u|_{O_{A}} + z_{A} \frac{\partial u}{\partial z}\Big|_{O_{A}} + \frac{z_{A}^{2}}{2} \frac{\partial^{2} u}{\partial z^{2}}\Big|_{O_{A}} + \dots,$$
(18)

where $O_A = (s_1^A, s_2^A, 0)$ and z_A is the distance along n_A between O_A and A, see Fig. 3. For the purpose of building the extension Ex, the Dirichlet and Neumann data u and $\frac{\partial u}{\partial n} = \frac{\partial u}{\partial z}$ are assumed given as functions of (s_1, s_2) and the time t on the surface, so the first and second term on the right-hand side of (18) can be considered known. The second derivative $\frac{\partial^2 u}{\partial z^2}$ in (18) is not known and will be derived from the wave equation written in the surface-oriented coordinates at the point O_A , i.e., on the surface $\partial \Omega$ at z = 0:

$$\partial_t^2 u - \Delta u = \partial_t^2 u - g^{ij} \left(\partial_i \partial_j u - \Gamma^I_{ij} \partial_l u \right) = 0.$$
⁽¹⁹⁾

In equation (19), the indices (i, j, l) correspond to the coordinates (s_1, s_2, z) , g^{ij} is the inverse of the metric tensor (evaluated at z = 0, i.e., on the surface)

$$g_{ij} = \begin{pmatrix} \|\partial_{s_1} x'\|^2 & \partial_{s_1} x' \cdot \partial_{s_2} x' & 0\\ \partial_{s_1} x' \cdot \partial_{s_2} x' & \|\partial_{s_2} x'\|^2 & 0\\ 0 & 0 & 1 \end{pmatrix},$$
(20)

and $\Gamma_{ij}^{l} = \frac{1}{2}g^{lk}(\partial_{j}g_{ik} + \partial_{i}g_{jk} - \partial_{k}g_{ij})$ are the Christoffel symbols. The tangential vectors $\partial_{s_{1}}x'$, $\partial_{s_{2}}x'$ are not necessarily mutually orthogonal, yet both are orthogonal to the normal vector n by design of the latter, see the structure of the metric tensor (20). Summation is assumed over the repeated indices everywhere, so the second derivative $\frac{\partial^{2}u}{\partial z^{2}}|_{O_{A}}$ in (18) can be obtained from (19) at any moment of time via the tangential derivatives of the function u w.r.t. s_{1} and s_{2} , its normal



(a) A submarine-like scattering body

(b) Five patches marked with colors

Fig. 4. A CAD model of a submarine built with the help of Rhinoceros 3D[©]. In panel (a), the rectangular box represents the computational domain where the solution is sought.

derivative $\frac{\partial u}{\partial z}$, and its second time derivative $\frac{\partial^2 u}{\partial t^2}$. The normal derivative is known as a function of (s_1, s_2) and t on the surface, and the tangential and time derivatives can be computed because $u = u(s_1, s_2, t)$ is also known.

A fourth order algorithm requires two additional terms in expansion (18). The derivatives $\frac{\partial^3 u}{\partial z^3}\Big|_{O_A}$, $\frac{\partial^4 u}{\partial z^4}\Big|_{O_A}$ are obtained by differentiating equation (19) in *z* once and twice, respectively, and setting z = 0 afterwards. The results, again, are expressed via the derivatives of *u* and $\frac{\partial u}{\partial z}$ w.r.t. s_1 and s_2 , as well as the corresponding time derivatives. In doing so, one needs to differentiate g_{ij} and Γ_{ij}^l while taking into account the *z*-dependence of these quantities. The latter is simple as *z* enters the definition of the position vector $x_A = x'_A + zn_A$ linearly.

For technical reasons (see Section 5.1), we may also need to extend the boundary data from the point O_A to a point $A \in \gamma$ in a direction other than normal. Let this direction be defined by the vector l with the length ||l|| equal to the distance between the two points. Then, expansion (18) is replaced with

$$u|_{A} \approx u|_{O_{A}} + l^{i}\nabla_{i}u\Big|_{O_{A}} + \frac{1}{2!}l^{i}l^{j}\nabla_{i}\nabla_{j}u\Big|_{O_{A}} + \frac{1}{3!}l^{i}l^{j}l^{k}\nabla_{i}\nabla_{j}\nabla_{k}u\Big|_{O_{A}} + \dots,$$

$$(21)$$

where l^i are components of the vector l in the same non-orthogonal local frame of reference with the axes parallel to the tangential vectors $\frac{\partial x'}{\partial s_1}$, $\frac{\partial x'}{\partial s_2}$ and normal vector n (cross product of the two tangential vectors). The vector l is oblique with respect to the normal n. The operators ∇_i in (21) are the conventional covariant derivatives: $\nabla_i u = \partial_i u$, $\nabla_i \nabla_j u =$ $\partial_i \partial_j u - \Gamma_{ij}^l \nabla_l u$, etc. The idea of obtaining the unknown higher-order derivatives in z by differentiating equation (19) and then substituting into (21) remains unchanged.

As the expressions for higher-order derivatives quickly become cumbersome, in practice it is convenient to derive those with the help of a computer algebra system. For our implementation, we have used Maple©.

5. Test problem

5.1. Geometric model

We will be solving the IBVP (1) for the scattering body Ω shaped similar to a submarine, see Fig. 4. The model of a submarine (Fig. 4(a)) is composed of five patches (Fig. 4(b)) and built with the help of Rhinoceros 3D© CAD software. Every patch is defined by a one-to-one mapping $\hat{h} : (s_1, s_2) \mapsto x$ from the 2D parameter space to the surface of a 3D object, i.e., $\mathbb{R}^3 \ni x = x(s_1, s_2)$, see (17). For the current model, it is sufficient to use uniform splines, so the weights $w_i = 1$ in (16). Each of the five patches is topologically equivalent to a quadrilateral. Patches #1-4 that comprise the hull of a submarine use fifth degree B-splines and are periodic in the direction of revolution about the axis of symmetry (direction s_1). The tower (patch #5) is also periodic w.r.t. the parameter s_1 and uses first degree splines in the vertical direction s_2 , i.e., straight lines with no intermediate knots.

As discussed in Section 2.5, the grid boundary γ is a fringe of nodes that straddles the continuous boundary $\partial\Omega$, see Fig. 2. The extension operator Ex based on the Taylor's formula (18) defines u at a node $A \in \gamma$ by extending the data $\left(u, \frac{\partial u}{\partial n}\right)$ from the boundary point closest to A, which is the foot of the normal. Yet sometimes it may be more convenient to extend the data from a different point on the boundary $\partial\Omega$ rather than the foot of the normal. Then, the extension operator Ex employs the oblique Taylor's formula (21).

An oblique extension is warranted, in particular, when the foot of the normal appears very close to either front or rear tip of the submarine hull. Indeed, to provide the data at the foot of the normal, the corresponding patch (patch # 1 or parch # 4, see Fig. 4) would have to reach all the way to the tip. Then, one of its edges will converge to a single point, and the coefficients of the wave equation in surface-oriented coordinates will become singular (similar, e.g., to singularities in the coefficients of a Laplacian on the polar axis in cylindrical or polar coordinates). To avoid singularities and use the simplest topologically quadrilateral patches, we terminate patch # 1 and patch # 4 before they reach the front and rear tip of the



(a) Near the tip of the hull

(b) Near the top of the tower

Fig. 5. Oblique extension in accordance with equation (21). The direction of the extension is shown by orange line. The white points belong to set γ . (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

hull, respectively, and use the oblique extension (21) of the boundary data from the nearest point on the patch no closer than a small positive distance to its edge, see Fig. 5(a). The patches are terminated at a distance from the tip comparable to the grid size.

The nodes of γ that are projected onto the planar top of the tower may also warrant an oblique extension (see Fig. 5(b)) provided that there are relatively few of such nodes, i.e., if the discretization grid is not very fine. For finer grids, on the other hand, introducing an additional patch on the top of the tower could be justified. However, our simulations indicate that having too few nodes of γ that are projected onto a given patch may hamper the stability of simulations. Therefore, for the grids employed in the current work we use the oblique extension from patch # 5 to the nodes of γ above or below the top of the tower.

5.2. Computational domain, grids, and FD schemes

The scatterer (submarine) is illuminated by an external source and the scattered field needs to be known on a rectangular box around the scatterer, see Fig. 4(a). A larger rectangular computational domain is introduced for solving the auxiliary problem (13), terminated with the simplest homogeneous boundary conditions. Its size is taken such that the waves reflected from the outer boundary will not reach the domain of interest (box in Fig. 4(a)) during the time interval on which we solve the AP (13).

In Section 2.5, we have indicated that the AP (13) is to be solved on the time interval of length $2T_0$ to enable the time stepping at the boundary with step size T_0 , see equation (9). Yet to reduce the size of the domain of the AP, it may be convenient to time march with a smaller step \mathcal{T} . In doing so, the key time interval T_0 remains unchanged. It determines how soon the scatterer Ω falls into the lacuna. Hence, it cannot be taken shorter than $\frac{1}{c} \operatorname{diam} \Omega$, see Section 2.3. However, we can further partition T_0 into \mathcal{N} subintervals of size \mathcal{T} : $T_0 = \mathcal{N} \cdot \mathcal{T}$, and time march along the boundary with step size \mathcal{T} rather than the full T_0 . Then, all the Γ_k will have duration \mathcal{T} rather than T_0 (cf. Section 2.2), ξ_{Γ_k} will be defined accordingly, and instead of equation (9) for a given K we will have:

$$P_{\Gamma_{\mathcal{T}}} \boldsymbol{\xi}_{\Gamma_{\mathcal{K}}} + \sum_{k=1}^{\mathcal{N}} \underbrace{Tr_{\Gamma_{\mathcal{K}}} P_{\tilde{\Omega}} \boldsymbol{\xi}_{\Gamma_{\mathcal{K}-k}}}_{R_{\Gamma_{\mathcal{N}}}^{(k)} \boldsymbol{\xi}_{\Gamma_{\mathcal{K}-k}}} = \boldsymbol{\xi}_{\Gamma_{\mathcal{K}}}.$$
(22)

Equation (22) takes into account that the extent of backward dependence of the solution on time is still controlled by T_0 . Hence, ξ_{Γ_K} depends not on one but on \mathcal{N} previous partition elements $\xi_{\Gamma_{K-k}}$, $k = 1, ..., \mathcal{N}$, of the proportionally smaller size $\mathcal{T} = T_0/\mathcal{N}$. The discrete equation (14a) that is derived from (9) is modified accordingly for equation (22).

For the boundary time marching in the sense of equation (22) rather than equation (9), the AP (13) needs to be solved on the time interval of duration $T_0 + \mathcal{T}$ rather than $2T_0$. In the current work, we choose $\mathcal{T} \approx \frac{L/c}{3.5} < T_0$. Then, the size of the domain of the AP for which the waves reflected from its outer boundary won't contaminate the solution on the domain of interest (Fig. 4(a)) can be reduced because for the solution interval we have $T_0 + \mathcal{T} < 2T_0$. In what follows, the domain of the AP is $[-1.4L, 1.4L] \times [-0.85L, 0.85L] \times [-0.85L, 0.85L]$, where *L* is the length of the submarine hull. This domain is discretized with a 107 × 64 × 68 Cartesian grid referred to as Grid 1x (see Fig. 9). To study the convergence, this grid is subsequently refined by a factor of 2 (Grid 2x), see Section 5.4. Additional benefits of choosing $\mathcal{T} < T_0$ are discussed in Section 5.3.



(a) Trace of the incident field (b) Error of the expasion

Fig. 6. Spectral representation of the incident plane wave on the scattering surface for $L/\lambda \approx 8$.

To demonstrate the performance of our algorithm, we use two different schemes for the AP (13): a standard second order central difference explicit scheme and a compact fourth order implicit scheme of [22] on the $3 \times 3 \times 3 \times 3$ space-time stencil (81 nodes). The fourth order scheme first builds the discretization in time:

$$\Delta u^{n+1} - \frac{u^{n+1}}{\theta \tau^2 c^2} = 2\left(\Delta u^n - \frac{u^n}{\theta \tau^2 c^2}\right) - \left(\Delta u^{n-1} - \frac{u^{n-1}}{\theta \tau^2 c^2}\right) - \frac{1}{\theta} \Delta u^n,\tag{23}$$

where $\theta = \frac{1}{12}$. Equation (23) is a modified Helmholtz equation $\Delta u^{n+1} - \kappa^2 u^{n+1} = f^{n+1}$ on the upper time level, which is discretized by fourth order compact finite differences in space [22].

5.3. Spectral representation of the boundary data

In this section, we study the approximation of the boundary data by a finite series, see formulae (10), for the chosen geometry. Specifically, consider a plane wave $\cos(\omega t - kx)$ impinging on the scatterer, Fig. 6(a), at an angle defined by the wave vector $k = |k|(1, 1, 1)/\sqrt{3}$. The parametrization $x = x(s_1, s_2)$ on every patch P_i , j = 1, 2, ..., 5, renders the plane wave a function of s_1, s_2 , and t. To represent this trivariate function on patch $\#_j$, we use the following finite basis:

- 1. Basis in $s_1 \in [0, 2\pi]$ (periodic direction of the patch): 1, $\cos s_1$, $\sin s_1$, $\cos 2s_1$, $\sin 2s_1$,..., $\cos N_1^{(j)}s_1$, $\sin N_1^{(j)}s_1$. 2. Basis in $s_2 \in [-1, 1]$ (non-periodic direction): $T_0(s_2)$, $T_1(s_2)$, ..., $T_{N_2^{(j)}}(s_2)$, where $T_k(s_2)$ is a Chebyshev polynomial of order k.
- 3. For the time dependence on the interval $t \in [t_0, t_1]$, $t_1 t_0 = \mathcal{T}$, we use a Chebyshev expansion w.r.t. $T_0(t'), T_1(t'), ..., T_{N_3}(t'), t' = \frac{2(t-t_0)-\mathcal{T}}{\mathcal{T}} \in [-1, 1]$.

The expansion of the plane wave in this basis on patch P_i reads:

$$\cos(\omega t - kx(s_1, s_2)) \approx \sum_{n_3=0}^{N_3^{(j)}} \sum_{n_2=0}^{N_2^{(j)}} \sum_{n_1=0}^{N_1^{(j)}} C_{n_1 n_2 n_3}^{\{\cos, \sin\}} \left\{ \frac{\cos n_1 s_1}{\sin n_1 s_1} \right\} T_{n_2}(s_2) T_{n_3}(t').$$
(24)

We use the same basis to represent the normal derivative of the field as well. The overall expansion (10) then becomes a combination of expansions (24) for the function and its normal derivative for all the patches. The dimension of the basis on patch P_j is equal to $(N_3 + 1)(2N_1^{(j)} + 1)(N_2^{(j)} + 1)$. Hence, the total number of terms in each expansion (10) that yields the number of the APs to be solved is $N = (N_3 + 1)\sum_{j=1}^{5}(2N_1^{(j)} + 1)(N_2^{(j)} + 1)$. The relative error of the series representation (24) and that for the normal derivative in ∞ -norm over the surface of

the submarine for the time interval \mathcal{T} is shown in Tables 1–5. The first column in each table shows the ratio of the length of the hull L to the wavelength $\lambda = 2\pi/k = 2\pi c/\omega$. As the frequency increases (the wavelength decreases), the basis dimension is increased accordingly so that the expansion error is kept approximately constant at about 10%. A snapshot of the error distribution over the surface of the submarine is presented in Fig. 6(b) for a particular $t \in [0, \mathcal{T}]$. The growth of the dimension of the basis in time N_3 could be offset to some extent by choosing a smaller step \mathcal{T} of time marching at the boundary, as discussed in Section 5.2. Indeed, the same number of Chebyshev polynomials on a shorter interval will help maintain the same accuracy of the truncated expansion for a higher frequency. Otherwise, the effect of varying the frequency is discussed in Section 5.5.

Table 1		
Error of	he expansion at the boundary for patch	h # 1

L/λ	$N_{1}^{(1)}$	$N_{2}^{(1)}$	N_3	# APs	Error u	Error $\frac{\partial u}{\partial n}$
pprox 6	4	5	8	486	0.11	0.099
pprox 8	6	7	10	1040	0.11	0.11
≈ 11	8	8	12	1836	0.14	0.079
≈ 17	10	11	16	4284	0.17	0.13

Table 2		
Error of the expansion	at the boundary for patch $\#$ 2.	

L/λ	$N_{1}^{(2)}$	$N_{2}^{(2)}$	N_3	# APs	Error u	Error $\frac{\partial u}{\partial n}$
pprox 6	4	5	8	486	0.070	0.10
pprox 8	6	7	10	1040	0.046	0.054
≈ 11	8	8	12	1836	0.047	0.056
≈ 17	10	9	16	3570	0.083	0.072

Table 3

Error of the expansion at the boundary for patch # 3.

L/λ	$N_{1}^{(3)}$	$N_{2}^{(3)}$	N_3	# APs	Error u	Error $\frac{\partial u}{\partial n}$
pprox 6	4	5	8	486	0.070	0.092
pprox 8	6	7	10	1040	0.053	0.054
≈ 11	8	8	12	1836	0.11	0.067
pprox 17	10	11	16	4284	0.18	0.18

Table 4

Error of the expansion at the boundary for patch # 4.

L/λ	$N_{1}^{(4)}$	$N_{2}^{(4)}$	N_3	# APs	Error u	Error $\frac{\partial u}{\partial n}$
pprox 6	3	6	8	392	0.097	0.15
≈ 8	4	8	10	810	0.12	0.11
≈ 11	8	12	12	2448	0.088	0.085
≈ 17	11	13	16	5474	0.18	0.18

Table 5

Error of the expansion at the boundary for patch # 5.

L/λ	$N_{1}^{(5)}$	$N_{2}^{(5)}$	N_3	# APs	Error u	Error $\frac{\partial u}{\partial n}$
pprox 6	3	4	8	280	0.13	0.27
pprox 8	5	4	10	550	0.084	0.17
≈ 11	6	5	12	780	0.083	0.15
pprox 17	7	6	16	1680	0.15	0.21

In addition, in Table 6 we show the convergence of the expansion at the boundary (i.e., the reduction of the error) as the dimension of the basis is doubled while all other parameters remain unchanged. The error drops by a factor of 10 to 1000 depending on the patch. As expected, the slowest decrease of the error corresponds to the patches where the surface curvature is the largest, in particular, the tower (# 5) and the nose patch (# 1).

Note that, Table 6 only shows the error for the spatial factors $\cos kx$ and $\sin kx$. The reason is that, the convergence in space is affected by the representation of the surface by means of splines (Section 3), while for the convergence in time this is not the case. Indeed, for each patch the function $\cos kx(s_1, s_2)$ is defined on $(s_1, s_2) \in [0, 2\pi] \times [-1, 1]$ through the mapping $\hat{h} : (s_1, s_2) \mapsto x \in \partial \Omega$. The latter has discontinuities in high order derivatives at the knots of the spline. As we use splines of fifth degree, the fifth derivative is discontinuous. It is well known that, the rate of convergence of a Fourier or Chebyshev series depends on the smoothness of the function that is expanded. It is faster for the functions with higher regularity and slower for the functions with lower regularity. Therefore, the jumps of the derivatives of a particular order will limit the rate of convergence. These considerations do not apply to the temporal part of the expansion because no parameterization by splines of a given fixed regularity is involved.

5.4. Grid convergence

To study the grid convergence of the algorithm we use a reference solution in the form of an outgoing spherical wave generated by an artificial point source located at some $x_0 \in \Omega$ underneath the tower:

Table 6

Reduction of the error as the dimension of the basis increases. Basis 1: $[N_1^{(1)}, ..., N_1^{(5)}] \times [N_2^{(1)}, ..., N_2^{(5)}] = [4, 4, 4, 3, 3] \times [5, 5, 5, 6, 4]$, where $N_1^{(j)}$ and $N_2^{(j)}$ are dimensions in the directions s_1 and s_2 , respectively, for patch # *j*. Basis 2 is twice as large in either dimensions for every patch.

Patch #	Basis 1		Basis 2	Basis 2		
	error $u _{\Gamma}$	error $\frac{\partial u}{\partial n}\Big _{\Gamma}$	error $u _{\Gamma}$	error $\frac{\partial u}{\partial n} _{\Gamma}$		
1	$1.1 \cdot 10^{-1}$	$9.9 \cdot 10^{-2}$	$7.6 \cdot 10^{-3}$	$1.3 \cdot 10^{-2}$		
2	$0.7 \cdot 10^{-1}$	$1.0 \cdot 10^{-1}$	$8.1 \cdot 10^{-5}$	$2.1 \cdot 10^{-4}$		
3	$6.9 \cdot 10^{-2}$	$9.2 \cdot 10^{-2}$	$1.4 \cdot 10^{-4}$	$2.6 \cdot 10^{-4}$		
4	$9.7 \cdot 10^{-2}$	$1.5 \cdot 10^{-1}$	$6.5 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$		
5	$1.3 \cdot 10^{-1}$	$2.7 \cdot 10^{-1}$	$1.6 \cdot 10^{-2}$	$7.0 \cdot 10^{-2}$		



Fig. 7. Binary logarithm of the error as a function of time for the second order central difference scheme. Grid 2x is obtained from Grid 1x by halving both the space and time steps. The frequency ω corresponds to $L/\lambda = 6$. Basis dimensions for the coarse and fine grids are $[2, 2, 2, 3, 2] \times [5, 5, 6, 7, 3] \times 7$ and $[2, 2, 2, 4, 3] \times [7, 6, 6, 9, 4] \times 8$, respectively.

$$u(x,t) = \frac{1}{4\pi |x - x_0|} \cos(k(x - x_0) - \omega t).$$
(25)

The trace of u given by (25) on $\partial\Omega$ and trace of its normal derivative are used as boundary data for the Dirichlet and Neumann problems, respectively. The error history of the computed solution in ∞ -norm on two successive grids is shown in Fig. 7 for the second order central difference scheme and in Fig. 8 for the fourth order compact scheme (23). A sample computed solution is visualized in Fig. 9(a).

As indicated in Section 2.4, the dimension of the basis at the boundary should be chosen so as to have the accuracy of the spectral representation of the data the same or better than the accuracy of the solution computed on the grid. To study the grid convergence, one could choose a sufficiently large dimension of the basis ahead of time to guarantee an a priori superior accuracy at the boundary compared to that on all grids. Alternatively, one can increase the dimension of the basis as the grid is refined. The latter strategy was employed for the computations presented in Figs. 7 and 8.

One can clearly see in Figs. 7 and 8 that the numerical solution converges to the reference solution with the design rate. The error drops by a factor of 4 and 16 for the second and fourth order scheme, respectively. Moreover, the simulations are stable over a long time interval $T_{sim} \approx 350L/c$, where L is the length of the submarine hull.

5.5. Scaling with frequency and numerical pollution

It is well known for both the steady-state and time-dependent problems [17,47] that, the error of a finite difference solution remains constant as long as $k^{p+1}h^p = \text{const.}$ Here *k* is the wavenumber, *h* the grid size (in the time-dependent case, the time step $\tau \propto h$) and *p* is the order of accuracy of the finite difference scheme. For a fourth order scheme, p = 4, halving the grid size $h \rightarrow h/2$ allows one to increase the frequency by a factor of $\sqrt[5]{16} \approx 1.74$ with no reduction of accuracy of the numerical solution. For a second order scheme, p = 2, one can only increase the frequency by a factor of $\sqrt[3]{4} \approx 1.59$ in order to keep the accuracy unchanged as the grid size is halved. In Tables 7 and 8, we corroborate these theoretical results by computations. The reference solution is the same as described in Section 5.4.

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(a) Dirichlet problem

(b) Neumann problem

Fig. 8. Binary logarithm of the error as a function of time for the fourth order compact scheme (23). Grid 2x is obtained from Grid 1x by halving both the space and time steps. The frequency ω corresponds to $L/\lambda = 6$. Basis dimensions for the coarse and fine grids are $[2, 2, 2, 3, 2] \times [5, 5, 6, 7, 3] \times 7$ and $[2, 2, 2, 2, 6] \times [12, 10, 10, 12, 5] \times 10$, respectively.

Table 7

Error on two successive grids as the frequency increases according to the law $k^3h^2 = \text{const}$ (second order scheme). Also shown are the error of the series representation at the boundary for all patches, dimensions of the bases, the number of APs to be solved, and CPU time (in seconds) per one step of boundary marching.

L/λ	Error on	two grids	Error $u _{\Gamma}$	Basis	APs	CPU time
	$1 \times$	2×				
6	0.27	-	$[11, 7, 7, 10, 13] \cdot 10^{-2}$	$[2, 2, 2, 2, 3] \times [7, 6, 6, 9, 4] \times 8$	1755	$4.5\cdot 10^{-4}$
$6\sqrt[3]{4}$	-	0.24	$[11, 2, 10, 7, 10] \cdot 10^{-2}$	$\begin{array}{l} [3,3,3,3,4] \times \\ [9,6,8,12,3] \times 10 \end{array}$	3399	$1.7 \cdot 10^{-3}$

Table 8

The same as in Table 7 for the fourth order scheme with the scaling $k^5h^4 = \text{const.}$

L/λ	Error c	on two grids	Error $u _{\Gamma}$	Basis	APs	CPU time
	1×	2×				
6	0.27	-	$[11, 7, 7, 10, 13] \cdot 10^{-2}$	$[2, 2, 2, 3, 2] \times [5, 5, 6, 7, 3] \times 7$	1368	$5.7\cdot 10^{-4}$
6∜16	-	0.32	$[18, 12, 11, 17, 14] \cdot 10^{-2}$	$\begin{matrix} [4,4,4,4,8] \times \\ [8,8,10,12,4] \times 11 \end{matrix}$	5556	$2.4\cdot 10^{-3}$

5.6. Scattering of a plane wave

The field scattered about the submarine for the incident plane wave described in Section 5.3 is visualized in Fig. 9(b).

5.7. CPU times

The CPU times presented in Tables 7 and 8 account for making one step of length $\mathcal{T} = \frac{L/c}{3.5}$ (see Section 5.2) of the boundary time marching. These times do not depend on the grid. For example, in the case of a second order accurate scheme (Table 7) and $L/\lambda = 6$, the CPU time needed to advance the solution by \mathcal{T} along the boundary is $4.5 \cdot 10^{-4}$ seconds on either Grid 1x or Grid 2x. The computations were conducted on a Dell PowerEdge server with two Intel[®] Xeon[®] E5-2698 processors. Moreover, the computation of the discrete counterparts of operators $P_{\Gamma_{\mathcal{T}}}$ and $R_{\Gamma_{\mathcal{N}}}^{(k)}$ in equation (22), which are similar to those in equation (14a), adds a separate upfront cost. This computation requires solving a total number of APs specific to each scenario (also presented in Tables 7 and 8). In particular, in the case of a second order accurate scheme (Table 7), $L/\lambda = 6$, and Grid 1x, the associated CPU time for solving 1755 APs is 669 seconds. Note that, this one-time upfront cost covers subsequent solution of all possible exterior IBVPs for a given shape. For example, the solutions



(a) Artificial point source inside Ω , see (25) (b) Incident plane wave, $\mathbf{k} = |\mathbf{k}|(1,1,1)/\sqrt{3}$

Fig. 9. Scattered field around a submarine computed on Grid 1x (Section 5.2).

presented in Fig. 9(a) (artificial source inside the hull) and Fig. 9(b) (scattering of an incident plane wave) were computed based on the same set of discrete operators $P_{\Gamma_{T}}$ and $R_{\Gamma_{N}}^{(k)}$.

6. Conclusions

We have developed and tested a high-order accurate finite difference algorithm for the simulation of 3D unsteady scattering problems governed by the scalar wave equation. The key advantages of our approach include a stable and accurate treatment of complex non-conforming scattering shapes on simple rectangular grids, universal handling of the boundary conditions, and reduction of the problem from the domain to the boundary with the help of the MDP, which enables an efficient time marching with grid-independent complexity. Our approach also provides an exact treatment of the outgoing waves with no artificial reflections.

An important issue that needs to be further explored and improved upon is the convergence of the series that represents the trace of the solution on the surface of the scatterer. The faster the convergence the smaller the dimension of the basis can be and hence, fewer auxiliary problems will need to be solved. The convergence rate is limited by the smoothness of the splines employed for the surface representation. For higher-order splines, one can expect that it will be faster. On the other hand, we have observed that the convergence may slow down for a patch that contains regions with high curvature such as bends, corners, etc., neighboring with the flat parts of the patch. The boundary data as a function of the variables s_1 and s_2 will vary more rapidly on those regions requiring more basis functions to provide an acceptable error. A number of techniques could be tried to circumvent this difficulty such as stretching reparametrization [43] in the regions of high curvature, splitting the patch into smaller ones so as to cover a high curvature region separately, knot redistribution over the parameter space, making use of the NURBS with weights $w_i \neq 1$, and some others.

Subsequent objectives will include methods to accommodate open two-sided surfaces such as keels or rudders and a generalization of the algorithm to vector models such as Maxwell's equations of electromagnetism.

CRediT authorship contribution statement

Sergey Petropavlovsky: Conceptualization, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **Semyon Tsynkov:** Conceptualization, Formal analysis, Funding acquisition, Methodology, Supervision, Writing – original draft, Writing – review & editing. **Eli Turkel:** Conceptualization, Funding acquisition, Methodology, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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