

Research



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A perfectly matched layer–boundary integral equation method for wave scattering in a two-layer medium of a step-like interface

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This paper is concerned with wave scattering in a two-layer medium separated by a step-like interface, consisting of two half lines with different heights. For a plane-wave incidence, the two half lines generate parallel reflected and transmitted plane waves of different phases, posing a challenge in identifying the radiation behaviour of the scattered field at infinity. To tackle this difficulty, we introduce a transition curve that connects the reflection and transmission directions to divide the space into two unbounded regions. We propose that subtracting the corresponding plane waves from the scattered field in either region yields a piecewise-defined outgoing wave that satisfies the Sommerfeld radiation condition. We adopt a uniaxial perfectly matched layer (PML) to truncate the outgoing wave. Within each of the four bounded regions separated by the transition curve, the interface and the PML boundary, we use the PML-transformed Green's function to derive a boundary integral equation (BIE). A high-accuracy quadrature is adopted to discretize the four BIEs. Together with the interface conditions, they yield a final linear system with unknowns approximating the outgoing wave. Several numerical experiments are carried out to illustrate the validity of the radiation condition and the accuracy of the proposed solver.

This article is part of the theme issue 'Analytically grounded full-wave methods for advances in computational electromagnetics'.

1. Introduction

Wave scattering problems arise in areas such as acoustics, electromagnetics/optics and seismology. Modern technologies, including optical circuits, wireless communication, radar, sonar, geophysical prospecting, etc., pursue effective numerical solvers that can simulate related scattering problems fast and accurately. In realistic scenarios such as sea-surface scattering, air-ground scattering, optical waveguide scattering and so on, wave scattering in layered media has seen wide applications. In this paper, we study the problem of wave scattering in a two-layer medium.

Due to the unbounded interface between the two layers, understanding the radiation behaviour of the scattered wave becomes critical and essential not only in identifying the well-posedness of the problem but also in developing high-accuracy numerical solvers. For a planar interface with a local perturbation, the problem can be well-posed by enforcing that the part of the scattered wave due to the perturbation is outgoing at infinity, i.e. satisfying the Sommerfeld radiation condition (SRC) [1]. However, if the perturbation changes the global behaviour of the interface, it is more challenging to extract an outgoing wave from the scattered wave. Instead of the SRC, the angular spectral representation (ASR) condition has been proposed for the scattered wave to establish the well-posedness [2].

In the existing literature, numerical methods are more focused on wave scattering by locally perturbed planes, as the corresponding SRC condition is much easier to treat. Finite-difference methods [3] and finite-element methods [4], incorporating proper truncation techniques such as perfectly matched layer (PML) [5], discretize the whole truncated domain. They are versatile and simple to implement, but meet challenges in achieving high accuracy while maintaining efficiency. Boundary integral equation (BIE) methods, taking advantage of the homogeneous feature in each layer, establish equations on the interface only so that the whole dimensionality is reduced by one and thus are more competitive. Nevertheless, their performance rests heavily on the treatment of the unbounded interface. If the background Green's function is adopted, one derives BIEs on the bounded perturbed part of the interface, but the involved sophisticated Sommerfeld integrals can be costly to evaluate [6]. If Green's functions for the two homogeneous media are used instead, BIEs are defined on the unbounded interface. One has to truncate the interface first before discretizing the BIEs. Readers are referred to tapering methods [7], windowed Green's function methods [8] and the approximate truncation method [9] for various truncation techniques. Nevertheless, to meet a desired accuracy, hundreds or even significantly more wavelengths are required, often to truncate the interface. In our previous work [10], combining the two advanced techniques, PML and BIE method, we firstly proposed the so-called PML–BIE method to study electromagnetic wave scattering in a two-dimensional two-layer medium. The method uses the simple PML-transformed Green's functions to derive BIEs and can attain high accuracy with ease by using a two-wavelength-thick PML only to truncate the interface. This novel method has recently been extended to a variety of scattering problems [2,11–17].

This paper extends the PML–BIE method to a two-dimensional electromagnetic scattering problem in a two-layer medium of a step-like interface, which consists of two half lines of different heights on the two sides. Certainly, ASR condition can still be adopted to establish the well-posedness, but unfortunately cannot effectively guide the interface truncation as PML does. For incident plane waves, unlike locally perturbed planar interfaces, the two half lines generate two parallel reflected plane waves of different phases above the interface and two parallel transmitted plane waves below it, making the extraction of outgoing waves confusing and problematic. Inspired by our recent work [14], where a wave scattered in a half space bounded by a step-like surface was studied, we use a transition curve that joins the reflection and transmission directions to divide the whole domain into two regions. In each region, we enforce the SRC condition for the outgoing wave, defined as the difference between the scattered wave and the corresponding reflected and transmitted plane waves. We place a uniaxial PML to absorb the piecewise-defined outgoing wave and truncate the unbounded domain. PML-transformed Green's functions are used to derive BIEs on the boundaries of four bounded domains separated by the transition curve,

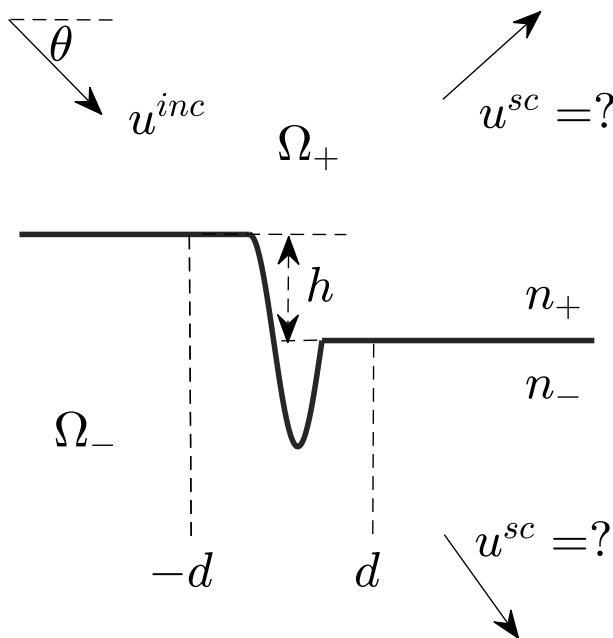


Figure 1. Profile of the scattering problem by a step-like surface.

the interface and the PML boundary. The high-accuracy quadrature developed in [10] is adopted to discretize the BIEs, which, together with the interface conditions, lead to the final linear system with unknowns approximating the outgoing wave. We carry out numerical experiments to validate the novel radiation condition and to illustrate the accuracy of the PML–BIE method.

2. Problem formulation

As shown in figure 1, in a two-dimensional space $\mathbb{R}^2$, let $\Gamma := \{x = (x_1, x_2) : x_2 = f(x_1)\}$ denote a step-like curve with

$$f(x_1) = \begin{cases} 0 & x_1 > d; \\ h & x_1 < -d, \end{cases}$$

which divides $\mathbb{R}^2$ into two half spaces $\Omega_{\pm}$; here, $d > 0$ denotes some constant and h denotes the height of the step. Throughout this paper, we assume that f is piecewise C^∞ for $|x_1| < d$ and shall use $x, y, \dots$ to denote two-dimensional points and $x_j, y_j, \dots$ to denote their i -th Cartesian coordinates for $j = 1, 2$.

Suppose two homogeneous media of refractive indices $n_{\pm}$ occupy the two domains $\Omega_{\pm}$. Let the free-space wavenumber be denoted by k_0 and write

$$n(x) = n_{\pm}, \quad x \in \Omega_{\pm}, \quad k_{\pm} = k_0 n_{\pm}.$$

Let a plane-wave $u^{\text{inc}} = e^{i(\alpha x_1 - \beta x_2)}$ in Ω_+ be incident upon the step-like surface Γ , where $\alpha = k_+ \cos \theta$ and $\beta = k_+ \sin \theta$ for some incident angle $\theta \in (0, \pi)$. Then, the total wavefield u^{tot} is governed by

$$\Delta u^{\text{tot}} + k_{\pm}^2 u^{\text{tot}} = 0, \quad \text{in } \Omega_{\pm}, \quad (2.1)$$

$$[u^{\text{tot}}]_{\Gamma} = 0, \quad [\gamma \partial_{\nu} u^{\text{tot}}]_{\Gamma} = 0, \quad (2.2)$$

where $\Delta = \partial_{x_1}^2 + \partial_{x_2}^2$ and $[\cdot]_\Gamma$ denotes the jump of the quantity across Γ . In real applications, equations (2.1) and (2.2) model the Transverse Electric (TE)- or Transverse Magnetic (TM)-polarized scattering problems. In TE polarization, u denotes the non-zero component of the electric field and $\gamma = 1$, while in TM polarization, u denotes the non-zero component of the magnetic field and $\gamma = 1/n^2(x)$. The well-posedness of the above-mentioned problem has been justified in [2]. The authors therein posed the ASR condition, a.k.a. the upward/downward propagation radiation condition (UDPRC), that is

$$u^{\text{sc}}(x) = \int_{x_2=\pm H} \frac{\partial \Phi_{\pm}(x; y)}{\partial \nu(y)} u^{\text{sc}}(y) ds(y), \quad \pm x_2 > H, \quad (2.3)$$

where $\Phi_{\pm}(x; y) = \frac{i}{4} H_0^{(1)}(k_{\pm}|x - y|)$ denotes the fundamental solution of the Helmholtz (2.1) with wavenumber $k_{\pm}$, and u^{sc} denotes the scattered wave defined by

$$u^{\text{sc}} := \begin{cases} u^{\text{tot}} - u^{\text{inc}}, & x \in \Omega_+; \\ u^{\text{tot}}, & x \in \Omega_-. \end{cases}$$

If a point-source incidence is specified at $x_* \in \Omega_+$, the total wavefield u^{tot} is exactly Green's function of the two-layer structure excited by the source point x_* . In this situation, (2.1) should be modified to

$$\Delta u^{\text{tot}} + k_{\pm}^2 u^{\text{tot}} = -\delta(x - x_*), \quad \text{in } \Omega_{\pm}, \quad (2.4)$$

and u^{tot} itself is proved to satisfy the UDPRC condition [2].

From a numerical perspective, a Sommerfeld-like radiation condition is highly preferred as the UDPRC cannot be directly used to effectively truncate the unbounded problem.

3. Sommerfeld radiation condition

In our previous two works [14,18], we have studied the problem of the same step-like structure but with the medium in Ω_- impenetrable. We have demonstrated that the scattered wave u^{sc} , after subtracting two reflected plane waves corresponding to the two half lines of Γ in two cone regions, respectively, becomes outgoing in all directions. Specifically, the two half lines on both sides of Γ produce two reflected plane waves of different phases given by

$$u_-^{\text{ref}}(x) := -e^{-2i\beta h} e^{i(\alpha x_1 + \beta x_2)}, \quad u_+^{\text{ref}}(x) := -e^{i(\alpha x_1 + \beta x_2)}.$$

Then, we justified in [18] that

$$u^{\text{og}} := \begin{cases} u^{\text{sc}} - u_-^{\text{ref}}, & \text{in } \{x \in \Omega_+ : x_2 > x_1 \tan \theta\}; \\ u^{\text{sc}} - u_+^{\text{ref}}, & \text{in } \{x \in \Omega_+ : x_2 < x_1 \tan \theta\}, \end{cases}$$

is outgoing in the sense that it satisfies, in place of the UDPRC condition, the following integral form of the SRC

$$\lim_{R \rightarrow \infty} \int_{\partial B(R) \cap \Omega_+} |\partial_r u^{\text{og}}(x) - i k_+ u^{\text{og}}|^2 ds(r) = 0. \quad (3.1)$$

In [14], we further adopted the Wiener–Hopf approach to derive Green's function for the Helmholtz equation in a cracked half plane $\{x : x_2 > 0\} \setminus \{x : x_2 = h, x_1 \leq 0\}$, a special background for the half-space scattering problem; by analysing the radiation behaviour of the Green function, we strictly proved that u^{og} satisfies the pointwise SRC

$$\lim_{r \rightarrow \infty} r^{1/2} [\partial_r u^{\text{og}}(x) - i k_+ u^{\text{og}}] = 0, \quad (3.2)$$

uniformly in all directions in Ω_+ . The SRC conditions (3.1) and (3.2) lead us to use PML to terminate u^{og} , and the PML-based BIE method [10] was then adopted to accurately solve the scattering problem [14].

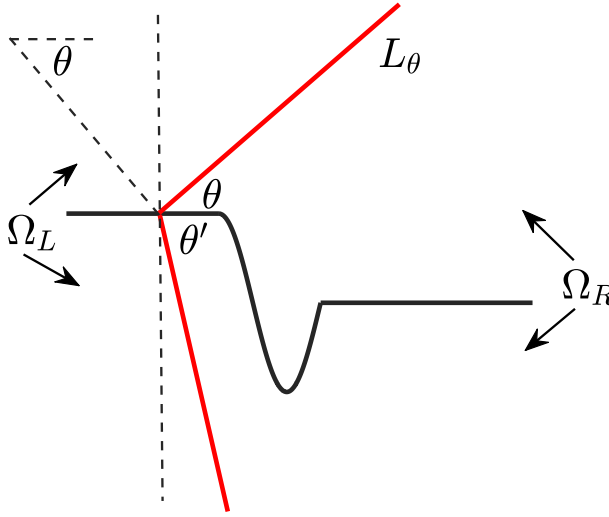


Figure 2. The transition curve L_θ .

Inspired by the half-space scattering problem with the same step-like surface Γ , we expect that an outgoing wave can also be extracted from the total field u^{tot} in the two homogeneous media $\Omega_\pm$. We assume $n_- < n_+$ for simplicity. Let u_-^{tot} be the solution of the same two-layer scattering problem but for the line interface $\Gamma_- = \{x : x_2 = h\}$, related to the left-most part of Γ , and u_+^{tot} for $\Gamma_+ = \{x : x_2 = 0\}$. It is deduced from Snell's law that

$$u_-^{\text{tot}}(x) = \begin{cases} u^{\text{inc}}(x) + R_- u^{\text{ref}}(x), & x_2 > h; \\ T_- u^{\text{tra}}(x), & x_2 < h, \end{cases} \quad u_+^{\text{tot}}(x) = \begin{cases} u^{\text{inc}}(x) + R_+ u^{\text{ref}}(x), & x_2 > 0; \\ T_+ u^{\text{tra}}(x), & x_2 < 0, \end{cases} \quad (3.3)$$

where $u^{\text{ref}}(x) = e^{i(\alpha x_1 + \beta x_2)}$ and $u^{\text{tra}}(x) = e^{i(\alpha x_1 - \beta^* x_2)}$ are the corresponding reflected plane waves and transmitted waves, respectively, $\beta^* = \sqrt{k_-^2 - \alpha^2} > 0$, and

$$R_- = \frac{\beta - \beta^*}{\beta + \beta^*} e^{-2i\beta h}, \quad T_- = \frac{2\beta}{\beta + \beta^*} e^{-i(\beta - \beta^*)h}, \quad (3.4)$$

$$R_+ = \frac{\beta - \beta^*}{\beta + \beta^*}, \quad T_+ = \frac{2\beta}{\beta + \beta^*}. \quad (3.5)$$

From the above, the refracted angle is given by $\theta' = \arctan \frac{\beta^*}{\alpha}$. We introduce a curve L_θ that is parallel to both the reflection and transmission directions at the two sides. For example, one may take

$$L_\theta := \{x : x_2 = h + (x_1 + d) \tan \theta, x_2 > 0, x_2 = h - (x_1 + d) \tan \theta', x_2 < 0\},$$

as illustrated in figure 2. It splits $\mathbb{R}^2$ into two unbounded domains Ω_L and Ω_R . We call L_θ a ‘transition curve’ to highlight the different radiation behaviours of u^{tot} in Ω_L and Ω_R . Following [14], the step-like structure suggests that the total field u^{tot} , after extracting u_L^{tot} in Ω_L and u_R^{tot} in Ω_R , becomes an outgoing wave with discontinuities across L_θ . In other words, we expect that the following wavefield

$$u^{\text{og}}(x) := \begin{cases} u^{\text{tot}}(x) - u_-^{\text{tot}}(x) & \text{for } x \in \Omega_L; \\ u^{\text{tot}}(x) - u_+^{\text{tot}}(x) & \text{for } x \in \Omega_R, \end{cases} \quad (3.6)$$

satisfies the SRC

$$\lim_{R \rightarrow \infty} \sum_{j=+,-} \int_{\partial B(R) \cap \Omega_j} |\partial_r u^{\text{og}}(x) - \mathbf{i} k_j u^{\text{og}}|^2 ds(r) = 0. \quad (3.7)$$

It is not hard to derive the governing equations of u^{og} given by

$$\Delta u^{\text{og}} + k^2 n_{\pm}^2 u^{\text{og}} = 0, \quad \text{in } \Omega_{\pm}/L_{\theta}, \quad (3.8)$$

$$[u^{\text{og}}]_I = T_{\pm} u^{\text{tra}} - u^{\text{inc}} - R_{\pm} u^{\text{ref}}, \quad [\partial_{\nu} u^{\text{og}}]_I = T_{\pm} \partial_{\nu} u^{\text{tra}} - \partial_{\nu} u^{\text{inc}} - R_{\pm} \partial_{\nu} u^{\text{ref}}, \quad (3.9)$$

$$[u^{\text{og}}]_{L_{\theta}} = u_{-}^{\text{tot}}|_{L_{\theta}} - u_{+}^{\text{tot}}|_{L_{\theta}}, \quad [\partial_{\nu} u^{\text{og}}]_{L_{\theta}} = \partial_{\nu} u_{-}^{\text{tot}}|_{L_{\theta}} - \partial_{\nu} u_{+}^{\text{tot}}|_{L_{\theta}}. \quad (3.10)$$

With the new condition (3.7), we are able to use PML to terminate u^{og} and to turn the scattering problem into a boundary value problem.

Before proceeding with our numerical solver, we make some remarks about a significant difficulty arising from the bottom penetrable medium in Ω_{-} . For the half-space scattering problem in [14], the Wiener–Hopf approach can be adopted to explicitly construct an associated Green’s function for a cracked half space, a background structure. Unfortunately, we are unable to find such a background structure that would allow an analytic approach to derive an explicit form of the Green’s function. The consequence is twofold. First, as a background, Green’s function is not available, nor is its asymptotic behaviour at infinity, therefore Green’s representation theorem cannot be used to characterize the radiation behaviour of u^{og} . Thus, it is questionable whether u^{og} satisfies a pointwise SRC. The justification of the integral-form SRC (3.7) is still possible by following the idea in [18] and [19], where an explicit form of the Green’s function is not required. Second and more critically, without an explicit form, it is challenging to analyse the asymptotic behaviour of the Green’s function in the PML, which is crucial in characterizing the truncation error introduced by the PML [16,20]. We shall leave the theoretical justification of the radiation condition (3.7) and also a rigorous convergence theory of PML to a future work, as these are not the main purpose of the current paper.

To conclude this section, we briefly discuss the point-source incidence case. At infinity, u^{tot} itself is supposed to satisfy the SRC (3.7). Thus, PML can be directly used to terminate u^{tot} , and hence the point-source incidence is much easier to handle numerically. In the following, we shall focus only on the plane-wave incidence.

4. The perfectly matched layer–boundary integral equation method

In this section, we present the PML–BIE method to solve the scattering problem. The basic idea follows mainly from the two previous works [10,14].

(a) Perfectly matched layer and boundary integral equations

We choose a uniaxial PML to absorb the outgoing wave u^{og} in (3.6). Mathematically, it introduces the following complexified coordinate transformation [5,21]

$$\tilde{x}_j = x_j + \mathbf{i} \int_0^{x_j} \sigma_j(t) dt, \quad j = 1, 2,$$

where the non-negative absorbing function $\sigma_j(x_j)$ is zero for $|x_j| < L_j$ and is positive otherwise for $j = 1, 2$; in the following, we shall use the tilde notation $\tilde{x}, \tilde{y}, \dots$ to denote the complexified points of $x, y, \dots$. As illustrated in figure 3, the shaded region with non-zero σ_j are called the PMLs. Let

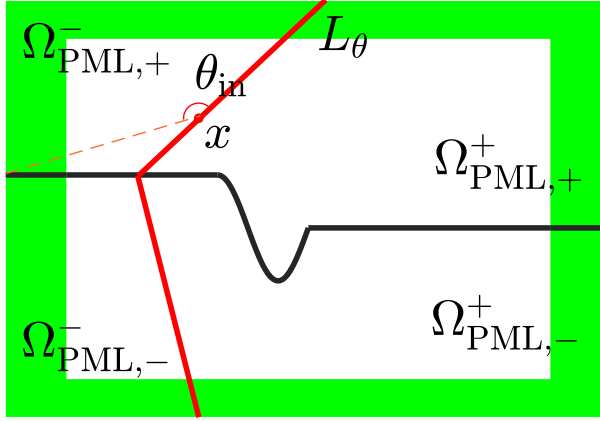


Figure 3. Configuration of an uniaxial PML.

$\tilde{u}^{\text{og}}(x) = u^{\text{og}}(\tilde{x}(x))$. We expect that $\tilde{u}^{\text{og}}$ decays exponentially in the PML and hence impose a zero boundary condition on the four edges $x_j = L_j + d_j$ for $d_j > 0$, the boundary of the truncated domain $\Omega_{\text{PML}} = \{x = (x_1, x_2) : |x_j| < L_j + d_j, j = 1, 2\}$, i.e. $\tilde{u}^{\text{og}} = 0$, on $\partial\Omega_{\text{PML}}$. In the above, $d_j, j = 1, 2$ are called the thicknesses of the PML. As illustrated in figure 3, the interface Γ divides Ω_{PML} into two subdomains $\Omega_{\text{PML},\pm} = \Omega_{\pm} \cap \Omega_{\text{PML}}$, and the transition curve L_{θ} further divides $\Omega_{\text{PML},\pm}$ into four domains given by

$$\Omega_{\text{PML},+}^{\pm} := \Omega_{\text{PML},+} \cap \{x : \pm(x_2 \cos \theta - x_1 \sin \theta) > 0\}. \quad (4.1)$$

$$\Omega_{\text{PML},-}^{\pm} := \Omega_{\text{PML},-} \cap \{x : \pm(x_2 \cos \theta' + x_1 \sin \theta') > 0\}. \quad (4.2)$$

By the chain rule, we obtain the governing equations of $\tilde{u}^{\text{og}}$, as what follows:

$$\nabla \cdot (\mathbf{A}(x) \nabla \tilde{u}^{\text{og}}) + k^2 J(x) n_{\pm}^2 \tilde{u}^{\text{og}} = 0, \quad \text{in } \Omega_{\text{PML},\pm} \setminus L_{\theta}, \quad (4.3)$$

$$\tilde{u}^{\text{og}} = 0, \quad \text{on } \partial\Omega_{\text{PML}}, \quad (4.4)$$

$$[\tilde{u}^{\text{og}}]_{\Gamma} = T_{\pm} \tilde{u}^{\text{tra}} - \tilde{u}^{\text{inc}} - R_{\pm} \tilde{u}^{\text{ref}}, \quad [\partial_{\nu_c} \tilde{u}^{\text{og}}]_{\Gamma} = T_{\pm} \partial_{\nu_c} \tilde{u}^{\text{tra}} - \partial_{\nu_c} \tilde{u}^{\text{inc}} - R_{\pm} \partial_{\nu_c} \tilde{u}^{\text{ref}}, \quad (4.5)$$

$$[\tilde{u}^{\text{og}}]_{L_{\theta}} = \tilde{u}_{-}^{\text{tot}}|_{L_{\theta}} - \tilde{u}_{+}^{\text{tot}}|_{L_{\theta}}, \quad [\partial_{\nu_c} \tilde{u}^{\text{og}}]_{L_{\theta}} = \partial_{\nu_c} \tilde{u}_{-}^{\text{tot}}|_{L_{\theta}} - \partial_{\nu_c} \tilde{u}_{+}^{\text{tot}}|_{L_{\theta}}, \quad (4.6)$$

where $\mathbf{A}(x) = \text{diag}\{\alpha_2/\alpha_1, \alpha_1/\alpha_2\}$, $J(x) = \alpha_1\alpha_2$ and $\alpha_j = 1 + \mathbf{i}\sigma_j(x)$.

We now present the BIEs for $\tilde{u}^{\text{og}}$ in the four domains $\Omega_{\text{PML},\pm}^{\pm}$. We consider $\Omega_{\text{PML},+}^+$ only. According to [10], $\tilde{u}^{\text{og}}$ and $\partial_{\nu_c} \tilde{u}^{\text{og}}$ satisfy the following BIE:

$$(\mathcal{K} - \mathcal{K}_0[1])[\tilde{u}^{\text{og}}] = \mathcal{S}[\partial_{\nu_c} \tilde{u}^{\text{og}}], \quad (4.7)$$

where $\mathcal{S}$ and $\mathcal{K}$ are the single- and double-layer potentials defined by

$$\mathcal{S}[\phi](x) = 2 \int_{\partial\Omega_{\text{PML},+}^+} \tilde{\Phi}_{+}(x; y) \phi(y) ds(y), \quad (4.8)$$

$$\mathcal{K}[\phi](x) = 2 \int_{\partial\Omega_{\text{PML},+}^+} \partial_{\nu_c(y)} \tilde{\Phi}_{+}(x; y) \phi(y) ds(y), \quad (4.9)$$

$\tilde{\Phi}_{+}(x; y) = \frac{\mathbf{i}}{4} H_0^{(1)}(k_{+} \text{dist}(\tilde{x}, \tilde{y}))$ is the fundamental solution of the complexified Helmholtz equation (4.3) in Ω^{+} , $\text{dist}(\tilde{x}, \tilde{y}) = \sqrt{(\tilde{x}_1 - \tilde{y}_1)^2 + (\tilde{x}_2 - \tilde{y}_2)^2}$ is the complex-valued distance function and K_0 is the double-layer potential

$$\mathcal{K}_0[\phi](x) = 2 \int_{\partial\Omega_{\text{PML},+}^+} \partial_{\nu_c(y)} \tilde{\Phi}_0(x; y) \phi(y) ds(y),$$

for the complexified Laplace equation $\nabla(\cdot \mathbf{A} \nabla \tilde{u}) = 0$, with the fundamental solution $\tilde{\Phi}_0(x; y) = \frac{1}{2\pi} \log \text{dist}(\tilde{x}, \tilde{y})$. Here and hereafter, the branch cut of the square-root function $\sqrt{\cdot}$ is chosen as the negative real axis such that its argument lies in $(-\pi/2, \pi/2]$.

Although we have only assumed the zero Dirichlet boundary condition (4.4), it turns out that simultaneously enforcing the Neumann boundary condition $\partial_{\nu_c} \tilde{u}^{\text{og}} \approx 0$ on $\partial\Omega_{\text{PML}}$ is more advantageous in numerically discretizing (4.7), as we expect that $\tilde{u}^{\text{og}}$ and its gradient $\nabla \tilde{u}^{\text{og}}$ both decay exponentially in the PML. Consequently, the BIE (4.7) on the closed curve $\partial\Omega_{\text{PML},+}^+$ is truncated onto the open curve $\Gamma_+^+ := \partial\Omega_{\text{PML},+}^+ \setminus \overline{\partial\Omega_{\text{PML}}}$, that is,

$$\left(\mathcal{K}_+^+ - \mathcal{K}_{0,+}^+[1] + 1 - \frac{\theta_{\text{in}}}{\pi} \right) [\tilde{u}^{\text{og}}] \approx \mathcal{S}_+^+ [\partial_{\nu_c} \tilde{u}^{\text{og}}], \quad (4.10)$$

where all integral operators are defined on the open curve Γ_+^+ now, and θ_{in} denotes the interior angle at point $x \in \Gamma_+^+$ as has been indicated in figure 3. Note that here we have used the following identity

$$2 \int_{\partial\Omega_{\text{PML},+}^+ \cap \partial\Omega_{\text{PML}}} \partial_{\nu_c(y)} \tilde{\Phi}_0(x; y) ds(y) = -1 + \frac{\theta_{\text{in}}(x)}{\pi},$$

to truncate the integration domain of the integral operator $\mathcal{K}_0$ onto Γ_+^+ .

On solving (4.10), we obtain the Neumann-to-Dirichlet (NtD) operator

$$\mathcal{N}_+^+ := \left(\mathcal{K}_+^+ - \mathcal{K}_{0,+}^+[1] + 1 - \frac{\theta_{\text{in}}}{\pi} \right)^{-1} \mathcal{S}_+^+ \quad (4.11)$$

that maps $\tilde{u}^{\text{og}}$ to $\partial_{\nu_c} \tilde{u}^{\text{og}}$ on Γ_+^+ . One similarly obtains the other three NtD maps $\mathcal{N}_+^-$ and $\mathcal{N}_\pm^\pm$ defined, respectively, on Γ_+^- and $\Gamma_\pm^\pm$. To establish the governing operator equations, it is more convenient to express each $\mathcal{N}_l^m$, $l, m = \pm$, as a 2×2 matrix of four operators $\mathcal{N}_l^{m,ij}$, $i, j = 1, 2$ based on the splitting $\Gamma_l^m = (\Gamma_l^m \cap \Gamma) \cup (\Gamma_l^m \cap L_\theta)$, i.e.

$$\begin{bmatrix} \tilde{u}^{\text{og}}|_{\Gamma_l^{m,1}} \\ \tilde{u}^{\text{og}}|_{\Gamma_l^{m,2}} \end{bmatrix} = \begin{bmatrix} \mathcal{N}_l^{m,11} & \mathcal{N}_l^{m,12} \\ \mathcal{N}_l^{m,21} & \mathcal{N}_l^{m,22} \end{bmatrix} \begin{bmatrix} \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_l^{m,1}} \\ \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_l^{m,2}} \end{bmatrix}, \quad l, m = \pm, \quad (4.12)$$

where $\Gamma_l^{m,1}$ and $\Gamma_l^{m,2}$ denote the sets of interior points of $\Gamma_l^m \cap \Gamma$ and $\Gamma_l^m \cap L_\theta$, respectively. For the two NtD operators $\mathcal{N}_+^\pm$ above Γ , the interface condition (4.6) can be used to get

$$\begin{aligned} \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_+^{-2}} = & -(\mathcal{N}_+^{+,22} - \mathcal{N}_+^{-,22})^{-1} \mathcal{N}_+^{+,21} \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_+^{+,1}} + (\mathcal{N}_+^{+,22} - \mathcal{N}_+^{-,22})^{-1} \mathcal{N}_+^{-,21} \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_+^{-,1}} \\ & + (\mathcal{N}_+^{+,22} - \mathcal{N}_+^{-,22})^{-1} ([\tilde{u}^{\text{og}}]_{L_\theta} - \mathcal{N}_+^{+,22} [\partial_{\nu_c} \tilde{u}^{\text{og}}]_{L_\theta}). \end{aligned} \quad (4.13)$$

This gives rise to an inhomogeneous equation on Γ as follows:

$$\begin{bmatrix} \tilde{u}^{\text{og}}|_{\Gamma_+^{+,1}} \\ \tilde{u}^{\text{og}}|_{\Gamma_+^{-,1}} \end{bmatrix} = \begin{bmatrix} \mathcal{N}_+^{11} & \mathcal{N}_+^{12} \\ \mathcal{N}_+^{21} & \mathcal{N}_+^{22} \end{bmatrix} \begin{bmatrix} \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_+^{+,1}} \\ \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_+^{-,1}} \end{bmatrix} + \begin{bmatrix} f_+ \\ g_+ \end{bmatrix}, \quad (4.14)$$

where

$$\begin{aligned} \mathcal{N}_+^{11} &= \mathcal{N}_+^{+,11} - \mathcal{N}_+^{+,12} (\mathcal{N}_+^{+,22} - \mathcal{N}_+^{-,22})^{-1} \mathcal{N}_+^{+,21}, & \mathcal{N}_+^{12} &= \mathcal{N}_+^{+,12} (\mathcal{N}_+^{+,22} - \mathcal{N}_+^{-,22})^{-1} \mathcal{N}_+^{-,21}, \\ \mathcal{N}_+^{21} &= -\mathcal{N}_+^{-,12} (\mathcal{N}_+^{+,22} - \mathcal{N}_+^{-,22})^{-1} \mathcal{N}_+^{+,21}, & \mathcal{N}_+^{22} &= \mathcal{N}_+^{-,11} + \mathcal{N}_+^{-,12} (\mathcal{N}_+^{+,22} - \mathcal{N}_+^{-,22})^{-1} \mathcal{N}_+^{-,21}, \\ f_+ &= \mathcal{N}_+^{+,12} (\mathcal{N}_+^{+,22} - \mathcal{N}_+^{-,22})^{-1} ([\tilde{u}^{\text{og}}]_{L_\theta} - \mathcal{N}_+^{+,22} [\partial_{\nu_c} \tilde{u}^{\text{og}}]_{L_\theta}) + \mathcal{N}_+^{+,12} [\partial_{\nu_c} \tilde{u}^{\text{og}}]_{L_\theta}, \\ g_+ &= \mathcal{N}_+^{-,12} (\mathcal{N}_+^{+,22} - \mathcal{N}_+^{-,22})^{-1} ([\tilde{u}^{\text{og}}]_{L_\theta} - \mathcal{N}_+^{+,22} [\partial_{\nu_c} \tilde{u}^{\text{og}}]_{L_\theta}). \end{aligned}$$

One similarly obtains the other equation on Γ based on the two bottom NtD operators $N^\pm$ and the interface condition (4.6)

$$\begin{bmatrix} \tilde{u}^{\text{og}}|_{\Gamma^{+,1}} \\ \tilde{u}^{\text{og}}|_{\Gamma^{-,1}} \end{bmatrix} = \begin{bmatrix} \mathcal{N}_-^{11} & \mathcal{N}_-^{12} \\ \mathcal{N}_-^{21} & \mathcal{N}_-^{22} \end{bmatrix} \begin{bmatrix} \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma^{+,1}} \\ \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma^{-,1}} \end{bmatrix} + \begin{bmatrix} f_- \\ g_- \end{bmatrix}. \quad (4.15)$$

Subtracting the two equations (4.14) and (4.15) and then using the interface condition (4.5), we obtain the final system of operator equations

$$\begin{aligned} & \begin{bmatrix} \mathcal{N}_+^{11} - \mathcal{N}_-^{11} & \mathcal{N}_+^{12} - \mathcal{N}_-^{12} \\ \mathcal{N}_+^{21} - \mathcal{N}_-^{21} & \mathcal{N}_+^{22} - \mathcal{N}_-^{22} \end{bmatrix} \begin{bmatrix} \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_+^{+,1}} \\ \partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_+^{-,1}} \end{bmatrix} \\ &= \begin{bmatrix} f_- \\ g_- \end{bmatrix} - \begin{bmatrix} f_+ \\ g_+ \end{bmatrix} + [\tilde{u}^{\text{og}}]_\Gamma - \begin{bmatrix} \mathcal{N}_-^{11} & \mathcal{N}_-^{12} \\ \mathcal{N}_-^{21} & \mathcal{N}_-^{22} \end{bmatrix} [\partial_{\nu_c} \tilde{u}^{\text{og}}]_\Gamma. \end{aligned} \quad (4.16)$$

We would like to point out that the above is not a second-kind Fredholm equation, but can basically be regarded as a first-kind one. In fact, the matrix operators $\mathcal{N}_\pm = [\mathcal{N}_\pm^{ij}]$ are exactly the NtD operators for $\tilde{u}^{\text{og}}$ in $\Omega^\pm$ if both $\tilde{u}^{\text{og}}$ and its normal derivative $\partial_{\nu_c} \tilde{u}^{\text{og}}$ are continuous across L_θ . Thus, analogous to (4.11), $\mathcal{N}_\pm$ can be expressed exactly in the same form but with the single- and double-layer potentials defined on Γ_{PML} instead, which are just single-layer integral operators with inverses of Fredholm-type operators as the left multipliers. More or less the same as inverting single-layer integral operators, such a formulation is still competitive, compared with second-kind integral equations, in two perspectives. First, to deal with scattering problems in layered media, Muller's formulation, to our best knowledge, seems to be the only approach that formulates second-kind integral equations [8]. However, SRC (3.7) brings an extra interface, the transition curve L_θ , making Muller's formulation more challenging to develop. Second, our formulation does not involve the discretization of hypersingular operators or their differences and thus is much simpler to use in practice.

Once we get $\partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_+^{\pm,1}}$ from (4.16), $\partial_{\nu_c} \tilde{u}^{\text{og}}|_{\Gamma_-^{\pm,1}}$ can be obtained from the interface condition (4.6). The two inhomogeneous equations (4.14) and (4.15) give $\tilde{u}^{\text{go}}|_{\Gamma_+^{\pm,1}}$, which, together with (4.13), make the field $\tilde{u}^{\text{og}}$ and its normal derivative $\partial_{\nu_c} \tilde{u}^{\text{og}}$ available on $\Gamma \cup L_\theta$. Finally, we adopt Green's representation formulae in all four domains $\Omega_{\text{PML},\pm}^\pm$ to get $\tilde{u}^{\text{og}}$ in the physical domain of Ω_{PML} . Throughout the entire procedure, the key step in the numerical implementation is the approximation of the four NtD operators $\mathcal{N}_\pm^\pm$, and this relies closely on the discretization of the single- and double-layer integral operators $\mathcal{S}_\pm^\pm$ and $\mathcal{K}_\pm^\pm$. We shall present the details in the next subsection.

(b) Discretizations of integral operators $\mathcal{S}_\pm^\pm$ and $\mathcal{K}_\pm^\pm$

Without loss of generality, we only discuss the discretizations of $\mathcal{S}_+^\pm$ and $\mathcal{K}_+^\pm$ defined on $\Gamma_+^\pm$. The key procedures follow our previous work [10]. For the sake of completeness, we present the basic idea below.

Suppose $\Gamma_+^\pm$ is parameterized by $x(s) = (x_1(s), x_2(s))$ for some proper parameter $s \in [0, L]$, e.g. the arclength parameter, where the two endpoints correspond to $s = 0, L$, respectively. Then, $\mathcal{S}_+^\pm$ and $\mathcal{K}_+^\pm$ are parameterized by

$$\mathcal{S}_+^\pm[\partial_{\nu_c} \tilde{u}^{\text{og}}](x(s)) = \int_0^L \frac{i}{2} H_0^{(1)}(k_+ \text{dist}(x(s), x(\tilde{s}))) \partial_{\nu_c} \tilde{u}^{\text{og}}(x(\tilde{s})) |x'(\tilde{s})| d\tilde{s} \quad (4.17)$$

$$\mathcal{K}_+^\pm[\tilde{u}^{\text{og}}](x(s)) = \int_0^L -\frac{ik_+}{2} \frac{\kappa(x(s), x(\tilde{s}))}{\text{dist}(x(s), x(\tilde{s}))} H_1^{(1)}(k_+ \text{dist}(x(s), x(\tilde{s}))) \tilde{u}^{\text{og}}(x(\tilde{s})) d\tilde{s}, \quad (4.18)$$

where $\kappa(x(s), x(\tilde{s})) = \tilde{x}_2'(\tilde{s})(\tilde{x}_1(s) - \tilde{x}_1(\tilde{s})) - \tilde{x}_1'(\tilde{s})(\tilde{x}_2(s) - \tilde{x}_2(\tilde{s}))$. We focus only on $\mathcal{S}_+^\pm$ in the following. As $\partial_{\nu_c} \tilde{u}^{\text{og}}$ is singular at corners of $\Gamma_+^\pm$, we introduce a sigmoid function $s = w(t)$, $0 \leq t \leq 1$ with

Table 1. Parameters for the sixth-order Alpert's quadrature rule.

k	δ_k	γ_k
1	$4.004884194926570 \times 10^{-3}$	$1.671879691147102 \times 10^{-2}$
2	$7.745655373336686 \times 10^{-2}$	$1.636958371447360 \times 10^{-1}$
3	$3.972849993523248 \times 10^{-1}$	$4.981856569770637 \times 10^{-1}$
4	$1.075673352915104 \times 10^0$	$8.372266245578912 \times 10^{-1}$
5	$2.003796927111872 \times 10^0$	$9.841730844088381 \times 10^{-1}$

$w(0) = 0$ and $w(1) = L$ to smoothen $\partial_{v_c} \tilde{u}^{\text{og}}$ first [1]. For each smooth part of Γ_+^+ , say, $s \in [s^1, s^2] \subset [0, L]$, we specify two constants $t^j \in [0, 1]$ such that $w(t^j) = s^j$ for $j = 1, 2$ and set for $t \in [t^1, t^2]$, [1, eq. (3.104)]

$$s = w(t) = \frac{s^1 w_1^p + s^2 w_2^p}{w_1^p + w_2^p}, \quad t \in [t^0, t^1], \quad (4.19)$$

where p is a positive integer that ensures $w^{(i)}(t_j) = 0$ for $i = 1, \dots, p$, and

$$w_1 = \left(\frac{1}{2} - \frac{1}{p}\right) \xi^3 + \frac{\xi}{p} + \frac{1}{2}, \quad w_2 = 1 - w_1, \quad \xi = \frac{2t - (t^1 + t^2)}{t^2 - t^1}.$$

Then, the operator $\mathcal{S}_+^+$ can be rewritten as

$$\mathcal{S}_+^+[\phi](t) := \mathcal{S}_+^+[\partial_{v_c} \tilde{u}^{\text{og}}](x(t)) = \int_0^1 \mathcal{S}_+^+(t, \tilde{t}) \phi(\tilde{t}) d\tilde{t}, \quad (4.20)$$

where we write $x(t)$ for $x(w(t))$ for simplicity, $\mathcal{S}_+^+(t, \tilde{t}) = \frac{1}{2} H_0^{(1)}(\text{kdist}(x(t), x(\tilde{t})))$ and $\phi(\tilde{t}) = \partial_{v_c} \tilde{u}^{\text{og}}(x(\tilde{t})) |x'(\tilde{t})|$. We use ϕ in place of $\partial_{v_c} \tilde{u}^{\text{og}}$ because it is significantly smoother, even at corners; moreover, binding $|x'|$ to $\partial_{v_c} \tilde{u}^{\text{og}}$ significantly reduces the condition number of the approximate matrix of the single-layer operator $\mathcal{S}_+^+$ [22,23]. Since ϕ decays exponentially in the PML, it can be treated as a smooth, 1-periodic function.

To treat the logarithmic singularity of the kernel function $S(t, \tilde{t})$ at $t = \tilde{t}$, we adopt Alpert's sixth-order quadrature rule to discretize the integral (4.20). Let $\{t_l := lh\}_{l=0}^{N-1}$ be N evenly spaced points on $[0, 1]$ with $h = 1/N$. Then, we approximate

$$\begin{aligned} \mathcal{S}_+^+(\phi)(t_l) &\approx \sum_{j=1}^5 \gamma_j h [\mathcal{S}_+^+(t_l, t_l + \delta_j h) \phi(t_l + \delta_j h) + \mathcal{S}_+^+(t_l, t_l + 1 - \delta_j h) \phi(t_l + 1 - \delta_j h)] \\ &\quad + \sum_{j=3}^{N-3} h \mathcal{S}_+^+(t_l, t_l + t_j) \phi(t_l + t_j), \quad l = 0, \dots, N-1, \end{aligned} \quad (4.21)$$

where $\{\delta_j, \gamma_j\}_{j=1}^5$ are given in table 1; note that $\phi(t)$ is naturally extended onto $\mathbb{R}$ by its periodicity. Readers are referred to [24] for potentially higher-order quadratures. Moreover, the trigonometric interpolation of ϕ can be adopted to rewrite the r.h.s. of (4.21) in terms of $\{\phi(t_j)\}_{j=0}^{N-1}$. Consequently, we find an $N \times N$ matrix $\mathbf{S}_+^+$ that satisfies

$$\mathcal{S}_+^+[\phi](\mathbf{t}) \approx \mathbf{S}_+^+ \boldsymbol{\phi}, \quad (4.22)$$

where $\mathbf{t} = [t_0, \dots, t_{N-1}]^T$, $\boldsymbol{\phi} = [\phi(t_0), \dots, \phi(t_{N-1})]^T$ and $\mathcal{S}_+^+[\phi](\mathbf{t})$ is a column vector of the N elements $\mathcal{S}_+^+[\phi](t_j)$. Similarly, one obtains an approximate $N \times N$ matrix $\mathbf{K}_+^+$ of $\mathcal{K}_+^+$ that satisfies

$$\mathcal{K}_+^+[\tilde{u}^{\text{og}}](\mathbf{t}) \approx \mathbf{K}_+^+ \tilde{\mathbf{u}}^{\text{og}}, \quad (4.23)$$

and also an $N \times N$ diagonal matrix for $\mathcal{K}_{0,+}^+$ [1]. Consequently, the NtD operator $\mathcal{N}_+^+$ in (4.11) can be approximated by an $N \times N$ matrix N_+^+ that maps ϕ to $\tilde{u}^{og}$. We note that, in the evaluation of the two functions $\text{dist}(x(s), x(\bar{s}))$ and $\kappa(x(s), x(\bar{s}))$ in (4.17) and (4.18), the stabilizing technique in [10] must be adopted to reduce round-off errors that are significant when the two points $x(s)$ and $x(\bar{s})$ are sufficiently close to each other (see [10] for details).

Repeating the above-mentioned procedures for the other three domains Ω_+^- and $\Omega_-^\pm$, we obtain the other three $N \times N$ matrices N_+^- and $N_-^\pm$, which, respectively, approximate $\mathcal{N}_+^-$ and $\mathcal{N}_-^\pm$. Correspondingly, the operators in equations (4.12)–(4.16) can be approximated accurately by matrices. These give rise to accurate approximations of the wavefield $\tilde{u}^{og}$ and its scaled normal derivative $\partial_{\nu_c} \tilde{u}^{og} |x'|$ on the step-like interface Γ and the transition curve L_θ . Consequently, Green's representation formula is adopted to numerically compute $\tilde{u}^{og}$ in each of the four domains $\Omega_\pm^\pm$, and $\tilde{u}^{og}$ outside of the PML region can be regarded as a numerical approximation of u^{og} in the physical domain.

5. Numerical examples

In this section, we carry out two numerical experiments to validate the newly proposed SRC (3.7) and to illustrate the efficiency and accuracy of the proposed PML–BIE method. In both of the examples, the physical region is defined as $\{(x_1, x_2) | |x_i| \leq L/2, i = 1, 2\}$, while the PML region is defined as $\{(x_1, x_2) | L/2 \leq |x_i| \leq L/2 + D, i = 1, 2, D > 0\}$ with thickness D . We choose the following parameters: $\lambda = 1$ so that $k_0 = 2\pi$, the incident angle $\theta = \frac{\pi}{3}$, refractive index $n_+ = 1, n_- = 2$ and $L = 5$. We adopt the following PML absorbing function:

$$\sigma_j(x_j) = \begin{cases} \frac{2Sf_1^6}{f_1^6 + f_2^6}, & L/2 \leq x_1 \leq L/2 + D, \\ S, & x_1 > L/2 + D \\ \sigma_j(-x_1), & x_1 \leq -L/2, \end{cases}$$

where

$$f_1 = \left(\frac{1}{2} - \frac{1}{8}\right) \bar{x}_j^3 + \frac{\bar{x}_j}{8} + \frac{1}{2}, \quad f_2 = 1 - f_1, \quad \bar{x}_j = \frac{x_j - (L/2 + D)}{D},$$

and $S > 0$ determines the magnitude of σ_j so that it can be used to adjust the absorbing strength of the PML. The boundary of the surface Γ consists of three parts $\Gamma = \Gamma_L \cup \Gamma_h \cup \Gamma_R$, where Γ_L, Γ_R and Γ_h , respectively, represent the left, right and step part of Γ . To achieve a high-order accuracy, we take $p = 6$ in the sigmoid function $s = w(t)$. We consider the TE polarization only.

Since the exact solution is not available, it is reasonable to evaluate the numerical accuracy of the methodology combined with the convergence curve of relative error. Particularly, we choose $N_p = 500$ as the number of grid points on each smooth segment of $(\Gamma \cup L_\theta) \cap \Omega_{\text{PML}}$ to ensure that the discretization error is sufficiently small so that the truncation error due to PML becomes dominant. To quantify the truncation error, we regard the numerical solution for $D = 2$ and $S = 2$ as our reference solution $u_{\text{ref}}^{\text{tot}}$ and compute the relative error

$$E_{\text{rel}} = \frac{\|\mathbf{u}^{\text{tot}} - \mathbf{u}_{\text{ref}}^{\text{tot}}\|_\infty}{\|\mathbf{u}_{\text{ref}}^{\text{tot}}\|_\infty}$$

at different values of D and S , where $\mathbf{u}^{\text{tot}}$ and $\mathbf{u}_{\text{ref}}^{\text{tot}}$ denote the vector of u^{tot} and $u_{\text{ref}}^{\text{tot}}$ at grid points on the physical part of Γ_h .

In the first example, $\Gamma = \Gamma_L \cup \Gamma_h \cup \Gamma_R$, where $\Gamma_L = \{(x_1, x_2) | x_1 < 0, x_2 = 0\}$, $\Gamma_R = \{(x_1, x_2) | x_1 > 0, x_2 = -1\}$ and $\Gamma_h = \{(0, x_2) | -1 \leq x_2 \leq 0\}$. The real part of the reference solution of u^{tot} is plotted in figure 4a. We show the convergence curves for $S = 2$ and D varying from 0.1 to 1.9 in

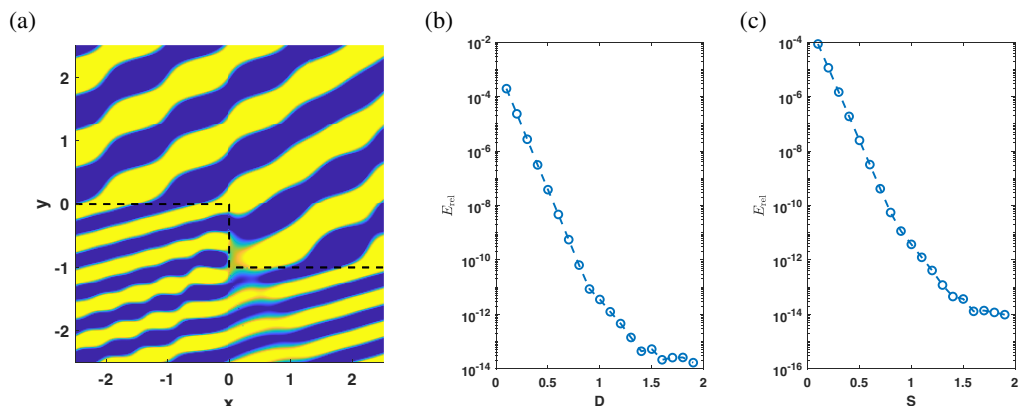


Figure 4. Example 1: (a) real part of the total field u^{tot} ; (b) convergence curve of relative error against PML thickness D ; (c) convergence curve of relative error against PML absorbing constant S . The dashed lines in (a) indicate the scattering interface Γ .

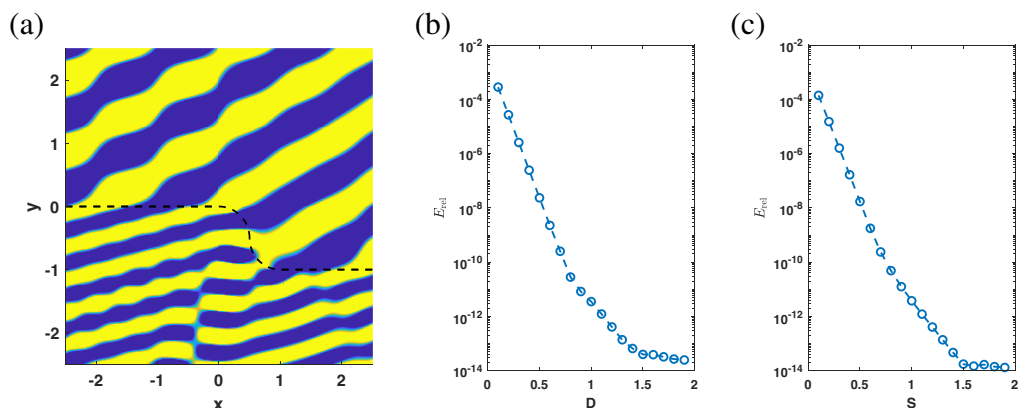


Figure 5. Example 2: (a) real part of the total field u^{tot} ; (b) convergence curve of relative error against PML thickness D ; (c) convergence curve of relative error against PML absorbing constant S . The dashed lines in (a) indicate the scattering interface Γ .

figure 4b and for $D=2$ and S varying from 0.1 to 1.9 in figure 4c, respectively, where the vertical axes are logarithmically scaled. We observe that E_{rel} decays exponentially as D or S increases until the discretization/round-off error dominates; at least 12 significant digits are obtained by the proposed method.

In the second example, Γ consists of two rays and two quarter circles of radius $1/2$. The real part of the reference solution of u^{tot} is plotted in figure 5a. We show the convergence curves for $S=2$ and D varying from 0.1 to 1.9 in figure 5b and for $D=2$ and S varying from 0.1 to 1.9 in figure 5c, respectively, where the vertical axes are logarithmically scaled. We observe that E_{rel} decays exponentially as D or S increases until discretization/round-off error dominates; at least 12 significant digits are obtained by the proposed method.

Data accessibility. This article has no additional data.

Declaration of AI use. We have not used AI-assisted technologies in creating this article.

Authors' contributions. W.L.: conceptualization, funding acquisition, methodology, project administration, writing—original draft, writing—review and editing; Z.L.: investigation, validation.

Both authors gave final approval for publication and agreed to be held accountable for the work performed therein

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