An overlapping decomposition framework for wave propagation in heterogeneous and unbounded media: Formulation, analysis, algorithm, and simulation

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Abstract

Finite element methods (FEM) are widely used for bounded heterogeneous media models, and boundary element methods (BEM) are efficient for simulating wave propagation in unbounded homogeneous media. A natural medium for wave propagation comprises a coupled bounded heterogeneous region and an unbounded homogeneous free space. Frequency-domain wave propagation models in the medium, such as the variable coefficient Helmholtz equation, include a faraway decay radiation condition (RC). The FEM wave propagation models are based on truncating the unbounded region and approximating the RC. The BEM models do not take into account of the heterogeneity in the medium. It is desirable to develop algorithms that incorporate the full physics of the heterogeneous and unbounded medium wave propagation model, and avoid approximation of the RC.

In this work we first present and analyze an overlapping decomposition framework that is equivalent to a two- or three-dimensional full space continuous model, governed by the Helmholtz equation with a spatially dependent refractive index and the Sommerfeld RC (SRC). Consequently we develop a novel overlapping FEM-BEM algorithm to simulate the equivalent coupled heterogeneous and unbounded medium system, modeling acoustic or electromagnetic wave propagation in two dimensions. Our FEM-BEM framework incorporates the SRC exactly and includes high-order FEM and BEM discretizations, respectively, in bounded and unbounded regions. In the overlapping bounded domain, in which we compute both FEM and BEM solutions, we impose appropriate constraints. Our numerical experiments demonstrate efficiency of the FEM-BEM framework, for models with heterogeneous media comprising smooth and complex non-smooth regions.

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1 Introduction

Wave propagation simulations are fundamental for numerous applications [6, 21]. The main focus of the book [6], and references therein, is on efficient simulation of scattering of waves in \textit{unbounded homogeneous} region exterior to a domain $\Omega_0 \subset \mathbb{R}^m$ ($m = 2, 3$), using boundary element methods (BEM). For a large class of applications, wave propagation also occurs inside the domain $\Omega_0$. In general, because of the heterogeneity of $\Omega_0$, the interior domain waves crucially depend on the spatially dependent refractive index function defined on $\Omega_0$. The main focus of the book [21], and literature therein, is on efficient simulation of the interior acoustic waves in the \textit{bounded heterogeneous} medium $\Omega_0$, using finite element methods (FEM).

Following the above large literature published over a decade ago, there has been substantial research activity in developing algorithms for efficient simulations of the interior and exterior acoustic wave propagation, modeled by the Helmholtz partial differential equation (PDE), see for example [14, 25, 29] and references therein for algorithms and software developments. The exterior wave propagation BEM models lead to dense complex algebraic systems, and standard interior wave FEM models lead to sparse complex systems with their eigenvalues taking values on the left half of the complex plane [17, 25]. Developing efficient preconditioned iterative solvers for such systems also dominated research activities over the last two decades [12], in conjunction with efficient implementation using multigrid and domain decomposition techniques, see [16, 18] and references therein.

For applications that require solving both interior heterogeneous and exterior homogeneous problems, various coupling of the FEM and BEM algorithms with appropriate conditions on \textit{polygonal interfaces} have also been investigated in the literature [3, 4, 20]. The review article [28] describes theoretical validation of the coupling approaches considered in the earlier literature and delicate choices of the coupling interface. The coupling methods in [3, 4, 20, 28] and references therein lead to very large algebraic systems with both dense and sparse structures. For wave propagation models, given the complexity involved in even separately solving the FEM and BEM algebraic systems, it is efficient to avoid large combined dense and sparse structured systems arising from coupling methods surveyed in [28].

Such complicated structured coupled large scale systems can be avoided, for the Helmholtz PDE interior and exterior problem, by using the approach proposed in [22] and recently further explored in [15] using high-order elements for a class of applications with complex heterogeneous structures. The FEM-BEM algorithms in [15, 22] is based on the idea of using a non-overlapping \textit{smooth interface} to couple the interior and exterior solutions. As described in [15, Section 6], there are several open mathematical analysis problems remain to be solved in the coupling and FEM-BEM framework of [15, 22].

The choice of smooth interface in the FEM-BEM algorithms of [15, 22] is crucial because the methods require solving several interior and exterior wave problems to setup the interface condition. In particular the number of FEM and BEM problems to be solved is equal to twice degrees of freedom (DoF) required to approximate the unknown interface function. The interface function can be approximated by a few degrees of freedom only on smooth interfaces. Efficient high-order BEM algorithms have been developed for simulating scattered waves exterior to smooth domains in two and three dimensional domains [6, 13]. However for standard interior FEM algorithms, it is desirable to have polygonal/polyhedral boundaries and
in particular those with right angles that facilitate easier development and implementation of high-order FEM algorithms.

To this end, it is desirable to develop an equivalent framework for the heterogeneous and unbounded region wave propagation model with two artificial interfaces. In particular, our novel FEM-BEM framework is based on an interior smooth interface $\Gamma$ for simulating exterior waves using a high-order BEM, and an exterior polygonal/polyhedral interface $\Sigma$ for efficient high-order FEM simulation of the interior waves. In Figure 1 we sketch the resulting overlapped decomposition of a heterogeneous and unbounded medium in which wave propagation is induced by an incident wave $u^i$.

The decomposition facilitates development of easy to implement efficient high-order FEM algorithms in the interior polygonal/polyhedral region $\Omega_2$, that contains the heterogenous domain $\Omega_0 \subset \Omega_1$. The exterior region $\mathbb{R}^m \setminus \Omega_1$ does not include the heterogeneity and has a smooth boundary $\Gamma$. It therefore facilitates application of high-order BEM algorithms to simulate exterior waves and exactly preserves the Sommerfeld radiation condition (SRC), even in the computational model. In addition, the decomposition framework provides an analytical representation of the far-field and hence using our high-order FEM-BEM model provides accurate computation of the far-field arising from the heterogeneous model. For inverse wave models [6], efficient computation of the far-field plays a crucial role in identification of unknown sources from far-field measurements.

Our approach in this article is related to some ideas presented in [5,8,9]. The choice of two artificial boundaries lead to two bounded domains $\Omega_0 \subset \Omega_1 \subset \Omega_2$ and an overlapping region between $\Omega_{12} = \mathbb{R}^m \setminus \Omega_1$ and $\Omega_2$. We show that, with appropriate restriction in the overlapping region $\Omega_{12} := \Omega_1 \cap \Omega_2$, our decomposed model is equivalent to the original Helmholtz model in the full space $\mathbb{R}^m$. The unknowns in our decomposed problem are: (a) the trace of the scattered wave in $\Gamma$ that will yield the density in the unbounded domain $\Omega_1$, through a boundary layer potential ansatz; (b) the trace of the total wave in the boundary $\Sigma$ of $\Omega_2$, that provides the Dirichlet data to determine the total wave in the bounded domain $\Omega_2$. These properties will play crucial role in designing and implementation of our high-order FEM-BEM algorithm.

The numerical algorithm can be discerned at this point: It comprises approximating the solution in a finite dimensional space using an FEM spline ansatz in the bounded domain, and by a BEM ansatz in the unbounded domain and these (numerically) coincide on the boundary of the common domain $\Omega_{12}$. Since the artificial boundaries can be freely chosen, we can ensure to have a bounded polygonal/polyhedral domain, more suitable for FEM, and unbounded smooth
domain for the BEM solution, facilitating best of the two numerical words. In particular, the framework provides easier application of high-order methods for both problems.

The algorithmic construction and solving of the linear system which determines key unknowns of the model – ansatz coefficients of the trace of the FEM and BEM solutions – is challenging. However, important properties of the continuous problem, such as compact perturbation of the identity, are inherited by the numerical scheme. In particular, the system matrix is very well conditioned. Such properties and in conjunction with cheaper matrix-vector multiplication for the underlying matrix support the use of iterative solvers such as GMRES [26,27] to compute the ansatz coefficients. Major computational aspects of our high-order FEM and BEM discretizations in the framework are independent and hence the underlying linear systems can be solved, a priori, by iterative Krylov methods. We show that the number of GMRES iterations is low, and also independent of various levels of discretizations for a chosen frequency of the model, to attain convergence independently of the level of discretization For increasing frequencies, we also demonstrate that the growth of GMRES iterations is lower than the frequency growth.

Instead of using an iterative scheme for the Schur complement system arising in our algorithm one may also consider, somewhat memory expensive, construction and storage of the matrix and use a direct solve for the system. The advantage of the latter is that it will facilitate reuse of the matrix for numerous incident input waves that occur in many practical applications to compute monostatic cross sections, and also for developing appropriate reduced order model (ROM) [14] versions of our algorithm. The matrix arising in our in our complement system is small because of the high-order accuracy of our algorithms and the system involves only unknowns on the artificial interface boundaries. Hence, post-processing such as the calculation of the far-field can be done quickly and efficiently. Far-field output plays a crucial role in developing stable ROMs for wave propagation models [14].

The paper is organized as follows. In Section 2 we present a decomposition framework and prove that, under very weak assumptions, the decomposition is well-posed and is equivalent to the full heterogeneous and unbounded medium wave propagation model. In Section 3 we present a numerical discretization for two dimensional case, combining high-order finite elements with spectrally accurate convergent boundary elements [23] and describe algebraic and implementation details. In Section 4 we demonstrate efficient of the FEM-BEM algorithm to simulate wave propagation in two distinct classes of (smooth and non-smooth) heterogenous media.

2 Decomposition framework and well-posedness analysis

Let $\Omega_0 \subset \mathbb{R}^m, m = 2, 3,$ be a bounded domain. The speed of wave propagation inside the heterogeneous (and not necessarily connected) region $\Omega_0$ and on its free-space exterior $\Omega_0^c := \mathbb{R}^m \setminus \overline{\Omega_0}$ is described through the index refraction function that we assume in this article to be piecewise smooth with $1 - n$ having compact support in $\overline{\Omega_0}$ (i.e, $n|_{\overline{\Omega_0}} \equiv 1$).

The main focus of this article is to study propagation in $\mathbb{R}^m$, induced by impinging of an incident wave $u^{inc}$, say, a plane wave with wavenumber $k > 0$. More precisely, the continuous wave propagation model is to study the total field $u := u^s + u^{inc} \in H_{\text{loc}}^1(\mathbb{R}^m)$ that satisfies the system

$$\begin{align*}
\Delta u + k^2 n u &= 0, \quad \text{in } \mathbb{R}^m, \\
\partial_r u^s - ik u^s &= o(|r|^{-\frac{n+1}{2}}), \quad \text{as } |r| \to \infty,
\end{align*}$$

(2.1)
It is well known that (2.1) is uniquely solvable [23]. (Later in this section, we introduce the classical Sobolev spaces $H^s$, for $s \geq 0$, with appropriate norms.)

2.1 A decomposition framework

The heterogeneous-homogeneous model problem (2.1) is decomposed by introducing two artificial curves/surfaces $\Gamma$ and $\Sigma$ with interior $\Omega_1$ and $\Omega_2$ respectively satisfying $\Omega_0 \subset \Omega_1 \subset \Omega_1 \subset \Omega_2$. We assume from now on that $\Gamma$ is smooth and $\Sigma$ is a polygonal/polyhedral boundary. A sketch of the different domains is displayed in Figure 1. Henceforth, $\Omega_i^c := \mathbb{R}^m \setminus \overline{\Omega}_i$, $i = 0, 1, 2$.

We introduce the following decomposed heterogeneous and homogeneous media auxiliary models:

- For a given function $f_{\Sigma}^{\text{inp}} \in H^{1/2}(\Sigma)$, we seek a propagating field $w \in H^1(\mathbb{R}^m)$ so that $w$ and its trace $\gamma_{\Sigma} w$ on the boundary $\Sigma$ satisfy

\[
\begin{align*}
\Delta w + k^2 n w &= 0, \text{ in } \Omega_2, \\
\gamma_{\Sigma} w &= f_{\Sigma}^{\text{inp}}.
\end{align*}
\] (2.2)

Throughout the article, we assume that this problem is uniquely solvable. We introduce the following operator notation for the heterogeneous auxiliary model: For any Lipschitz $m$- or $(m-1)$-dimensional (domain or manifold) $D \subset \Omega_2$, we define the solution operator $K_{D\Sigma}$ associated with the auxiliary model (2.2) as

\[
K_{D\Sigma} f_{\Sigma}^{\text{inp}} := w|_D.
\] (2.3)

Two cases will be of particular interest for us: $K_{\Omega_2\Sigma} f_{\Sigma}$, which is nothing but $w$ satisfying (2.2), and $K_{\Gamma\Sigma} f_{\Sigma}^{\text{inp}} = \gamma_{\Gamma} w$, the trace of the solution $\omega$ of (2.2) on $\Gamma \subset \Omega_2$.

- In the exterior unbounded homogeneous medium $\Omega^c := \mathbb{R}^m \setminus \Omega_1$, for a given function $f_{\Gamma}^{\text{inp}} \in H^{1/2}(\Gamma)$ we seek a scattered field $\tilde{\omega}$ satisfying

\[
\begin{align*}
\Delta \tilde{\omega} + k^2 \tilde{\omega} &= 0, \text{ in } \Omega^c_1, \\
\gamma_{\Gamma} \tilde{\omega} &= f_{\Gamma}^{\text{inp}}, \\
\partial_r \tilde{\omega} - ik \tilde{\omega} &= o(|r|^{(m-1)/2}).
\end{align*}
\] (2.4)

Unlike problem (2.2), (2.4) is always uniquely solvable [23]. We define the associated solution operator $K_{D\Gamma}$ as

\[
K_{D\Gamma} f_{\Gamma}^{\text{inp}} := \tilde{\omega}|_D,
\] (2.5)

with special attention to $K_{\Omega_1\Gamma} f_{\Gamma}$ and $K_{\Sigma\Gamma} f_{\Gamma}$, namely the scattered field $\tilde{\omega}$ satisfying (2.4) and its trace $\gamma_{\Sigma} \tilde{\omega}$.

The decomposition framework, we propose, for the continuous problem is the following:

1. Solve the interface boundary integral system to find $(f_{\Sigma}, f_{\Gamma})$, using data $(\gamma_{\Sigma} u^{\text{inc}}, \gamma_{\Gamma} u^{\text{inc}})$:

\[
\begin{align*}
(f_{\Sigma}, f_{\Gamma}) &\in H^{1/2}(\Sigma) \times H^{1/2}(\Gamma) \\
f_{\Sigma} - K_{\Sigma\Gamma} f_{\Gamma} &= \gamma_{\Sigma} u^{\text{inc}} \\
-K_{\Gamma\Sigma} f_{\Sigma} + f_{\Gamma} &= -\gamma_{\Gamma} u^{\text{inc}}
\end{align*}
\] (2.6a)
2. Construct the total field for the model problem (2.1) using the solution \((f_\Sigma, f_\Gamma)\) of (2.6a), by solving the auxiliary models (2.2) and (2.4):

\[
  u := \begin{cases} 
  K_{\Omega_2} f_\Sigma, & \text{in } \Omega_2, \\
  K_{\Omega_1} f_\Gamma + u^{inc}, & \text{in } \Omega_1^c.
  \end{cases}
\]  

(2.6b)

We claim that, provided that (2.6a) is solvable, the decomposed framework based field \(u\) defined in (2.6b) is the solution of (2.1). Notice that we are implicitly assuming in (2.6b) that

\[
  K_{\Omega_{12}} f_\Sigma = u^{inc}|_{\Omega_{12}} + K_{\Omega_{12}} f_\Gamma, \quad \Omega_{12} := \Omega_1^c \cap \Omega_2.
\]  

(2.7)

Indeed, in view of (2.6a), both functions in (2.7) agree on \(\Sigma \cup \Gamma\) (the boundary of \(\Omega_{12}\)). Assuming, as we will do from now on, that the only solution to the homogeneous system

\[
  \begin{align*}
    \Delta v + k^2 v &= 0, \quad \text{in } \Omega_{12}, \\
    \gamma_\Gamma v &= 0, \quad \gamma_\Sigma v = 0
  \end{align*}
\]  

(2.8)

is the trivial one and noticing that \(n|_{\Omega_{12}} \equiv 1\), we can conclude that (2.7) holds. Since \(u\) defined in (2.6b) belongs to \(H^1_{\text{loc}}(\mathbb{R}^d)\), it is simple to check that this function is the solution of (2.1).

We remark that the hypothesis we have taken on the artificial boundaries/domains, i.e. the well-posedness of problems (2.2) and (2.8) are not very restrictive in practice: \(\Sigma\) or \(\Gamma\) can be modified if needed. Alternatively, one can consider different boundary conditions on \(\Gamma\) and \(\Sigma\) (such as Robin), redefining \(K_{D\Sigma}\) and \(K_{D\Gamma}\) accordingly which will lead to a variant of the method that we analyze in this article. In a future work we shall explore other boundary conditions on the interfaces and analysis of resulting variant models.

### 2.2 Well-posedness of the decomposed continuous problem

The aim of this subsection is to prove that the system of equations (2.6a), under the above stated hypothesis, has a unique solution. Consequently, we can conclude the decomposition for the exact solution presented in (2.6b) exists and it is unique. To this end, we first derive some regularity results related to the operators \(K_{D\Sigma}\) and \(K_{D\Gamma}\) in Sobolev spaces. For references on the Sobolev spaces topic, we refer [1, 24].

#### 2.2.1 Functional spaces

Let \(D \subset \mathbb{R}^m\) be a Lipschitz domain. For any non-negative integer \(s\), we denote

\[
  \|f\|_{H^s(D)}^2 := \sum_{|\alpha| \leq s} \int_D |\partial_\alpha f|^2
\]

the Sobolev norm, where the summation includes the standard multi-index notation in \(\mathbb{R}^m\).

For \(s = s_0 + \beta\) with \(s_0\) a non-negative integer and \(\beta \in (0, 1)\), we set

\[
  \|f\|_{H^s(D)}^2 := \|f\|_{H^{s_0}(D)}^2 + \sum_{|\alpha| \leq s_0} \int_D \int_D \frac{|\partial_\alpha f(x) - \partial_\alpha f(y)|^2}{|x - y|^{m+2\beta}} \, dx \, dy.
\]
The Sobolev space $H^s(\Omega)$ ($s \geq 0$) can be introduced as,

$$H^s(D) := \{ f \in L^2(D) : \| f \|_{H^s(D)} < \infty \},$$

endowed with the above natural norm.

If $\partial D$ denotes the boundary of $D$, we can introduce $H^s(\partial D)$ with a similar construction using local charts: Let $\{ \partial D^j, \mu^j, \mathbf{x}^j \}_{j=1}^J$ be an atlas of $\partial D$, that is, $\{ \partial D \}_j$ is an open covering of $\partial D$, $\{ \mu^j \}$ a subordinated Lipschitz partition of unity on $\partial D$, and $\mathbf{x}^j : \mathbb{R}^{m-1} \to \partial D$ being Lipschitz and injective with $\partial D^j \subset \text{Im} \mathbf{x}^j$, then we define

$$\| \varphi \|_{H^s(\partial D)} := \sum_{j=1}^J \| (\mu^j \varphi) \circ \mathbf{x}^j \|_{H^s(\mathbb{R}^{m-1})}^2.$$

We note that $(\mu^j \varphi) \circ \mathbf{x}^j$ can be extended by zero outside of the image of $\mathbf{x}^j$. We then set

$$H^s(\partial D) := \{ \varphi \in L^2(\partial D) : \| \varphi \|_{H^s(\partial D)} < \infty \}.$$

The space $H^s(\partial D)$ is well defined for $s \in [0, 1]$: Any choice $\{ \partial D^j, \mu^j, \mathbf{x}^j \}$ gives rise to an equivalent norm (and inner product). If $\partial D$ is a $C^m$-boundary, such as the smooth $\Gamma$ in Figure 1, this construction can be set up for $s \in [0, m]$ by taking $\{ \mathbf{x}^j, \omega^j \}$ to be $C^m$ as well. In particular, if $\partial D$ is smooth we can set the full scale $H^s(\partial D)$ for any $s \geq 0$. The space $H^{-s}(\partial D)$ can be defined as the realization of the dual space of $H^s(\partial D)$ when the integral product is taken a representation of the duality pairing.

It is a classical result that the trace operator $\gamma_{\partial D} u := u|_{\partial D}$ define a continuous onto mapping from $H^{s+1/2}(D)$ into $H^s(\partial D)$ for any $s \in (0, 1)$. Actually, if $\partial D$ is smooth, $s \in (0, \infty)$. In these cases, we can alternatively define

$$H^s(\partial D) := \{ \gamma_{\partial D} u : u \in H^{s+1/2}(D) \}$$

endowed with the image norm:

$$\| \varphi \|_{H^s(\partial D)} := \inf_{\varphi = \gamma_{\partial D} u} \| u \|_{H^{s+1/2}(D)}, \quad (2.9)$$

We will use this definition to extend $H^s(\partial D)$ for $s > 1$ in the Lipschitz case. Notice that with this definition, the trace operator, from $H^{s+1/2}(D)$ into $H^s(\partial D)$, is continuous for any $s > 0$.

### 2.2.2 Boundary potentials and integral operators

Let $\Phi_k$ be the fundamental solution for the two- or three-dimensional constant coefficient Helmholtz operator $(\Delta + k^2 I)$ equation, defined for $x, y \in \mathbb{R}^m$ with $r := |x - y|$ as

$$\Phi_k(x, y) := \begin{cases} \frac{i}{4 \pi} H_0^{(1)}(kr), & x, y \in \mathbb{R}^2, \\ \frac{1}{4 \pi r} \exp(i kr), & x, y \in \mathbb{R}^3, \end{cases} \quad (2.10)$$

where $H_0^{(1)}$ denotes the first kind Hankel function of order $n$. For a smooth curve/surface $\Gamma$, with outward unit normal $\nu$ and normal derivative at $y \in \Gamma$ denoted by $\partial_\nu(y)$, let

$$(\text{SL}_k \varphi)(x) := \int_{\Gamma} \Phi_k(x-y) \varphi(y) \, d\sigma_y, \quad (\text{DL}_k g)(x) := \int_{\Gamma} \partial_\nu(y) \Phi_k(x-y) g(y) \, d\sigma_y, \quad x \in \mathbb{R}^m \setminus \Gamma,$$
denote the single- and double-layer potentials, with density functions \( \varphi \) and \( g \), respectively.

The single- and double-layer boundary integral operators are then given, via the well-known jump relations [6] for the boundary layer potentials, by

\[
V_k \varphi := (\gamma_\Gamma S L_k) \varphi = \int_{\Gamma} \Phi_k(\cdot - y) \varphi(y) \, d\sigma_y
\]

(2.11)

\[
K_k g := \pm \frac{1}{2} g + (\gamma_\Gamma^\mp D L_k) g = \int_{\Gamma} \partial_{\nu(y)} \Phi_k(\cdot - y) g(y) \, d\sigma_y
\]

(2.12)

where \( \gamma_\Gamma^- \) and \( \gamma_\Gamma^+ \) are, respectively the trace operator on \( \Gamma \) from the interior \( \Omega_1 \) and exterior \( \Omega_1^c \). Given \( \sigma : \Gamma \to \mathbb{R} \) a real non-vanishing smooth function, and for any \( \phi \in H^s(\Gamma) \) with \( (V_k \sigma) \phi := V_k(\sigma \phi) \), we consider the combined field acoustic layer operator

\[
\frac{1}{2} I + K_k - i k V_k \sigma : H^s(\Gamma) \to H^s(\Gamma).
\]

(2.13)

The standard combined field operator used in the literature [6] is based on the choice \( \sigma \equiv 1 \). In this article, we do not restrict ourselves to the standard choice for reasons which will be fully explained later. Since \( K_k, V_k \sigma : H^s(\Gamma) \to H^{s+1}(\Gamma) \) are continuous, recalling that \( \Gamma \) is smooth, the operator in (2.13) is invertible as a consequence of the Fredholm alternative and the injectivity of (2.13) which follows from a very simple modification of the classical argument in [6, Th 3.33]).

Thus the inverse of the combined field integral operator

\[
\mathcal{L}_\sigma := \left( \frac{1}{2} I + K_k - i k V_k \sigma \right)^{-1} : H^s(\Gamma) \to H^s(\Gamma)
\]

(2.14)

is well defined. Further, using (2.11)-(2.12), we can write the solution operator occurring in the construction (2.6b) as

\[
K_{\Omega_1^c \Gamma} = (D L_k - i k S L_k \sigma) \mathcal{L}_\sigma.
\]

(2.15)

The above solution operator, a variant of the Brakhage-Werner formulation (BWF) [2,6], will be used in this article for both theoretical and computational purposes. The choice \( \sigma \equiv 1 \) reduces to the standard BWF [2,6].

### 2.2.3 Well-posedness analysis of the interface model

In this subsection, we first develop two key results before proving well-posedness of the boundary integral system (2.6a).

**Lemma 2.1.** The operator

\[
K_{\Omega_1^c \Gamma} : H^s(\Gamma) \to H^{s+1/2}_{\text{loc}}(\Omega_1^c)
\]

(2.16)

is continuous for any \( s \in [0, \infty) \). Further, for any bounded Lipschitz domain/manifold \( D \subset \Omega_1^c \) with \( \overline{D} \cap \Gamma = \emptyset \) the solution operator \( K_{D \Gamma} \) in (2.5), for the homogeneous media problem (2.4), satisfies the following mapping property for any \( s, r \in \mathbb{R} \)

\[
K_{D \Gamma} : H^s(\Gamma) \to H^r(D).
\]

(2.17)

In particular,

\[
K_{\Sigma \Gamma} : H^s(\Gamma) \to H^r(\Sigma)
\]

(2.18)

is continuous and compact, for \( s, r \in \mathbb{R} \).
Lemma 2.2. Furthermore, if \( \text{(2.3)} \). We recall the well known classical estimate [21]

\[
\| K_{\Omega_2 \Sigma} f_{\Sigma}^{\text{imp}} \|_{H^1(\Omega_2)} \leq C \| f_{\Sigma}^{\text{imp}} \|_{H^{1/2}(\Sigma)},
\]

with \( C > 0 \) being a constant independent of \( f_{\Sigma} \). Below, we generalize this to obtain a higher regularity, using boundary layers potentials and boundary integral operators defined in this case on barely Lipschitz curves/surfaces to improve this estimate for domains \( D \subset \Omega_2 \subset \Omega_0 \).

Next we consider the heterogeneous media model solution operator \( K_{\Omega_2 \Sigma} \), as defined in \( \text{(2.2)} \)-(2.3). We recall the well known classical estimate [21]

\[
\| K_{\Omega_2 \Sigma} f_{\Sigma}^{\text{imp}} \|_{H^{1/2}(\Omega_2)} \leq C \| f_{\Sigma}^{\text{imp}} \|_{H^{1/2}(\Sigma)},
\]

Furthermore, if \( D \subset \overline{D} \subset \Omega_2 \setminus \overline{\Omega}_1 \) the following solution operator mapping property holds for any \( r \in \mathbb{R} \)

\[
K_{D \Sigma} : H^0(\Sigma) \rightarrow H^r(D).
\]

Consequently,

\[
K_{\Gamma \Sigma} : H^0(\Sigma) \rightarrow H^r(\Gamma)
\]

is continuous and compact, for any \( r \in \mathbb{R} \).

Proof. Throughout this proof we let \( s \in [0,1] \) and, for notational convenience, we denote \( v := K_{\Omega_2 \Sigma} f_{\Sigma}^{\text{imp}} \). Since, by definition,

\[
\Delta v + k^2 v = k^2 (1 - n) v, \quad \gamma_{\Sigma} v = f_{\Sigma}^{\text{imp}}.
\]

by the third Green identity (see for instance [24, Th. 6.10]) we have the representation

\[
v = k^2 \int_{\Omega_0} \Phi_k (\cdot - y) g_n^{\Sigma}(y) \, dy + \text{SL}_{k \Sigma} \lambda_{\Sigma}^v - \text{DL}_{k \Sigma} f_{\Sigma}^{\text{imp}},
\]

with \( \text{supp} \, g_n^{\Sigma} \subset \Omega_0 \), where we have used the notation

\[
\lambda_{\Sigma}^v := \partial_n v, \quad g_n := (1 - n) v.
\]

In the expression above \( \text{SL}_{k \Sigma} \) and \( \text{DL}_{k \Sigma} \) denote respectively the single and double layer potential from the corresponding densities defined on \( \Sigma \) associated with the constant coefficient Helmholtz operator \( \Delta + k^2 I \). Next we prove now that

\[
\| \lambda_{\Sigma}^v \|_{H^{s-1}(\Sigma)} = \| \partial_n v \|_{H^{s-1}(\Sigma)} \leq C \| f_{\Sigma}^{\text{imp}} \|_{H^{s}(\Sigma)}.
\]

To this end, we start from the decomposition of \( v = v_1 + v_2 \) where harmonic \( v_1 \) and interior wave-field \( v_2 \) are solutions of

\[
\begin{align*}
\Delta v_1 &= 0, & \text{in } \Omega_2, \\
\gamma_{\Sigma} v_1 &= f_{\Sigma}^{\text{imp}}, \quad \text{and} \\
\Delta v_2 + k^2 v_2 &= -k^2 n v_1, & \text{in } \Omega_2, \\
\gamma_{\Sigma} v_2 &= 0.
\end{align*}
\]
Classical results on potential theory, see [24, Th 6.12] and the discussion which follows it (see also references therein) show that there exists $C > 0$ so that
\[ \|v_1\|_{H^{s+1/2} (\Omega_2)} \leq C \|f_{\Sigma}^{\text{inp}}\|_{H^s (\Sigma)}, \quad \|\partial_\nu v_1\|_{H^{s-1} (\Omega)} \leq C' \|f_{\Sigma}^{\text{inp}}\|_{H^s (\Sigma)}, \tag{2.24} \]
for any $f_{\Sigma}^{\text{inp}} \in H^s (\Sigma)$. On the other hand, following [19, Ch. 4] or [7] there exists $\varepsilon > 0$ and $C_\varepsilon > 0$ such that
\[ \|v_2\|_{H^{3/2+\varepsilon} (\Omega_2)} \leq C_\varepsilon \|v_1\|_{H^0 (\Omega)} \leq C_\varepsilon \|f_{\Sigma}^{\text{inp}}\|_{H^0 (\Sigma)}. \tag{2.25} \]
By the trace theorem (applied to $\nabla v_2$),
\[ \|\partial_\nu v_2\|_{H^{\frac{1}{2}+\varepsilon} (\Gamma)} \leq C' \|v_2\|_{H^{3/2+\varepsilon} (\Omega_2)} \leq C'' \|f_{\Sigma}^{\text{inp}}\|_{H^0 (\Sigma)}. \]
Combining these estimates with (2.23) we conclude that
\[ \|v\|_{H^{s+1/2} (\Omega_2)} \leq C_s \left( \|g\|_{L^2 (\Omega_0)} + \|\lambda_{\Sigma}^c\|_{H^{s-1} (\Sigma)} + \|f_{\Sigma}^{\text{inp}}\|_{H^s (\Sigma)} \right) \]
\[ \leq C_s' \left( \|v\|_{L^2 (\Omega_0)} + \|f_{\Sigma}^{\text{inp}}\|_{H^s (\Sigma)} \right) \]
\[ \leq C'' \|f_{\Sigma}^{\text{inp}}\|_{H^0 (\Sigma)}. \]
Notice also that if $D \subset \overline{D} \subset \Omega_2 \setminus \overline{\Omega}_1$, because the kernels of the potentials operators and the Newton potential are smooth in the corresponding variables, we gain from the extra smoothing properties of the underlying operators in (2.23) to derive
\[ \|v\|_{H^r (D)} \leq C \left( \|g\|_{L^2 (\Omega_0)} + \|\lambda_{\Sigma}^c\|_{H^{r-1} (\Sigma)} + \|f_{\Sigma}^{\text{inp}}\|_{H^r (\Sigma)} \right) \]
\[ \leq C' \|f_{\Sigma}^{\text{inp}}\|_{L^2 (\Sigma)}. \]

For deriving the main desired result of this section, it is convenient to define the following off-diagonal operator matrix
\[ \mathcal{K} := \begin{bmatrix} K_{\Sigma \Sigma} & K_{\Sigma \Gamma} \\ K_{\Sigma \Gamma} & K_{\Gamma \Gamma} \end{bmatrix}. \]
Then (2.6a) can be written in operator form as follows
\[ (I - \mathcal{K}) \begin{bmatrix} f_{\Sigma} \\ f_{\Gamma} \end{bmatrix} = \begin{bmatrix} \gamma_{\Sigma} u_{\text{inc}} \\ -\gamma_{\Gamma} u_{\text{inc}} \end{bmatrix}. \tag{2.26} \]
A simple consequence of Lemmas 2.1 and 2.2 is that
\[ I - \mathcal{K} : H^s (\Sigma) \times H^t (\Gamma) \to H^s (\Sigma) \times H^t (\Gamma) \]
is continuous for any $s, t \geq 0$. Next we prove that this operator is indeed an isomorphism:

**Theorem 2.3.**
\[ I - \mathcal{K} : H^s (\Sigma) \times H^s (\Gamma) \to H^s (\Sigma) \times H^s (\Gamma) \]
is an invertible compact perturbation of the identity operator.
Proof. The continuity of $K : H^0(\Sigma) \times H^0(\Gamma) \to H^s(\Sigma) \times H^s(\Gamma)$ for any $s \in \mathbb{R}$ has been already established in the two preceding lemmas. In particular, $K$ is compact. Moreover, the null space $I - K$ consists of smooth functions. For any $(g_\Sigma, g_\Gamma) \in N(I - K)$, we construct

$$v := K_{\Omega_2 \Sigma} g_\Sigma, \quad \vartheta := K_{\Omega_1 \Gamma} g_\Gamma.$$  

Note that $w := (v - \vartheta)$ defined, in principle, in $\Omega_{12} = \Omega_2 \cap \Omega_1^c$ satisfies

$$\Delta w + k^2 w = 0, \quad \text{in } \Omega_{12}, \quad \gamma_\Sigma w = \gamma_\Gamma w = 0.$$

By the well-posedness of problem (2.8), we have first $w = 0$ in $\Omega_{12}$. Extend $u$ to $\mathbb{R}^m$ as follows

$$u = \begin{cases} v, & \text{in } \Omega_2, \\ \vartheta, & \text{in } \Omega_1^c. \end{cases}$$

Note that $u$ is well defined in $\Omega_2 \cap \Omega_1^c$, and it is a solution of (2.1) with incident wave $u^{\text{inc}} = 0$. Therefore, $u = 0$ which implies that $\vartheta = 0$ in $\Omega_2^5$. The principle of analytic continuation yields that $\vartheta = 0$ also in $\Omega_1^c$ and therefore $g_\Gamma = \gamma_\Gamma \vartheta = 0$. Finally,

$$g_\Sigma = \gamma_\Sigma u = \gamma_\Sigma \vartheta = 0,$$

and hence the desired result follows.

\[\square\]

3 A FEM-BEM algorithm for decomposed model in 2-D

In this section we consider numerical discretizations of the proven equivalent decomposed system (2.6). In this article, we restrict to the two-dimensional (2-D) case. [The 3-D algorithms and analysis for (2.6) will be different to the 2-D, and in a future work we will investigate the 3-D case.] Briefly, the approach consists in replacing the continuous operators $K_{\Omega_2 \Sigma}$ and $K_{\partial \Gamma}$ with suitable high-order FEM and BEM procedures based discrete operators. The stability of such a discretization depends on the numerical methods chosen in each case.

For discretization of the differential operator $K_{\Omega_2 \Sigma}$ based heterogeneous domain model, we could consider a standard FEM with triangular, quadrilateral or even more complex elements. We will choose the first case, for the sake of simplicity, and we expect the analysis developed in this case could cover these other types of elements, with appropriate minor modifications.

The BEM procedure, for discretizing the exterior homogeneous medium associated $K_{\partial \Gamma}$ through boundary integral operators, is more open since an extensive range of methods is available in the literature. We will restrict ourselves to the high-order Nyström method [23] (see also [10]). This scheme provides a discretization of the four integral operators, of the associated Calderon calculus, and converges super-algebraically. In this article, we will make use of high-order discretizations of the Single and Double Layer operators that are easy to implement.

A key restriction of the standard Nyström method to achieve spectrally accurate convergence is the requirement smooth diffeomorphic parameterization of the boundary. This is because the method starts from appropriate decompositions and factorizations of the kernels of the operators to split the kernels into regular and singular parts. This is not a severe restriction in our case since $\Gamma$ is an auxiliary user-chosen smooth curve and therefore can be easily constructed and as detailed as necessary.

Next we briefly consider these two known numerical procedures and hence describe our combined FEM-BEM algorithm and implementation details.
3.1 The FEM procedure

Let \( \{ \mathcal{T}_h \}_h \) be a sequence of regular triangular meshes where \( h \) is the discrete mesh parameter, the diameter of the larger element of the grid. Hence we write \( h \to 0 \) to mean that the maximum of the diameters of the elements tends to 0. Using \( \mathcal{T}_h \), we construct the finite dimensional spline approximation space

\[
P_{h,d} := \{ v_h \in C^0(\Omega_2) : v_h|_{\mathcal{T}_h} \in \mathbb{P}_d \},
\]

where \( \mathbb{P}_d \) is the space of bivariate polynomial of degree \( d \). We define the FEM approximation \( K^h_{\Omega_2 \Sigma} \) to \( K_{\Omega_2 \Sigma} \) as follows: The FEM operator

\[
K^h_{\Omega_2 \Sigma} : \gamma_{\Sigma} \mathbb{P}_{h,d} \to \mathbb{P}_{h,d},
\]

for \( f^\text{imp} \in \gamma_{\Sigma} \mathbb{P}_{h,d} \), is constructed as \( w_h := K^h_{\Omega_2 \Sigma} f^\text{imp} \), where \( w_h \in \mathbb{P}_{h,d} \) is the solution of the discrete FEM equations:

\[
\begin{aligned}
&b_{k,n}(w_h, v_h) = 0, \quad \forall v_h \in \mathbb{P}_{h,d} \cap H^1_0(\Omega_2) \\
&\gamma_{\Sigma} w_h = f^\text{imp}, \\
b_{k,n}(u, v) = \int_{\Omega_2} \nabla u \cdot \nabla v - k^2 \int_{\Omega_2} n uv.
\end{aligned}
\]

(3.1)

The discrete FEM operator \( K^h_{\Omega_2 \Sigma} \) is well defined for sufficiently small \( h \).

3.2 The BEM procedure

Let

\[
x : \mathbb{R} \to \Gamma, \quad x(t) := (x_1(t), x_2(t)), \quad t \in \mathbb{R}
\]

be a smooth \( 2\pi \)-periodic regular parameterization of \( \Gamma \). We denote by the same symbol \( SL_k \), \( DL_k \), \( V_k \) and \( K_k \) the parameterized layer potentials and boundary layer operators:

\[
(SL_k \varphi)(z) = \int_0^{2\pi} \Phi_k(z - x(t)) \varphi(t) \, dt
\]

\[
(DL_k g)(z) = \int_0^{2\pi} \left( \nabla_y \Phi_k(z - y) \right) \bigg|_{y=x(t)} \cdot \mu(t) g(t) \, dt
\]

where \( \mu(t) := (x_2'(t), -x_1'(t)) = |x'(t)| \nu \circ x(t) \). Observe that \( |x'(t)| \) is incorporated to the density in \( SL_k \) and to the kernel in \( DL_k \). We follow the same convention for the single- and double-layer weakly singular boundary integral operators. For high-order approximations, it is important to efficiently take care of the singularities. In particular, for the high-order Nyström BEM solver, we use the following representations of the layer operators with smooth kernels \( A, B, C, D \) [6] and \( 2\pi \) bi-periodic:

\[
(V_k \varphi)(s) = \int_0^{2\pi} A(s, t) \log \sin^2 \frac{s-t}{2} \varphi(t) \, dt + \int_0^{2\pi} B(s, t) \varphi(t) \, dt,
\]

\[
(K_k g)(s) = \int_0^{2\pi} C(s, t) \log \sin^2 \frac{s-t}{2} g(t) \, dt + \int_0^{2\pi} D(s, t) g(t) \, dt.
\]

The Nyström method, based on a discrete positive integer parameter \( N \), starts with setting up a uniform grid

\[
t_j := \frac{\pi j}{N}, \quad j = -N + 1, \ldots, N,
\]

(3.3)
and the space of trigonometric polynomials of degree at most $N$

$$T_N := \text{span}\{\exp(\im \ell t) : \ell \in \mathbb{Z}_N\},$$

with $\mathbb{Z}_N = \{-N + 1, -N + 2, \ldots, N\}$. We next introduce the interpolation operator $Q_N$

$$T_N \ni Q_N \varphi \quad \text{s.t.} \quad (Q_N \varphi)(t_j) = \varphi(t_j), \quad j = -N + 1, \ldots, N,$$

to define discretizations of the single and double layer operators:

$$(V_k^N \varphi)(s) := \int_0^{2\pi} Q_N(A(s, \cdot)\varphi)(t) \log \sin^2 \frac{\pi t}{2} dt + \int_0^{2\pi} Q_N(B(s, \cdot)\varphi)(t) dt,$$

$$(K_k^N g)(s) := \int_0^{2\pi} Q_N(C(s, \cdot)g)(t) \log \sin^2 \frac{\pi t}{2} dt + \int_0^{2\pi} Q_N(D(s, \cdot)g)(t) dt.$$

We stress that the above integrals can be computed exactly using the identities:

$$-\frac{1}{2\pi} \int_0^{2\pi} \log \sin^2 \frac{t}{2} \exp(\im \ell t) dt = -\frac{1}{2\pi} \int_0^{2\pi} \log \sin^2 \frac{t}{2} \cos(\ell t) dt = \begin{cases} \log 4, & \ell = 0 \\ \frac{1}{|\ell|}, & \ell \neq 0 \end{cases}$$

and for $g_N \in T_N$,

$$\int_0^{2\pi} g_N(t) dt = \frac{\pi}{N} \sum_{j=0}^{N-1} g_N(t_j),$$

(3.6)

that are based on properties of the trapezoidal/rectangular rule for $2\pi -$periodic functions.

The high-order approximation evaluation of the potentials is achieved in a similar way:

$$(SL_k^N \varphi)(z) := \int_0^{2\pi} Q_N(\Phi_k(z - x(\cdot))\varphi)(t) dt,$$

$$(DL_k^N g)(z) := \int_0^{2\pi} Q_N((\nabla_y \Phi_k(z - y))|_{y=x(\cdot)} \cdot \nu(\cdot) g)(t) dt$$

(3.7)

leading to the rectangular rule approximation as in (3.6).

Now we are ready to describe the discrete operator $K_{\Omega \Gamma}^N$, that is a high-order approximation to the exterior homogeneous model continuous operator $K_{\Omega \Gamma}$. First, we introduce the parameterized counterpart of the continuous operator in (2.13),

$$L_k g := (\frac{1}{2}I + K_k - i k V_k)^{-1} g,$$

(3.8)

(which corresponds to $\sigma \circ x = \frac{1}{|\nu|}$). Then we define

$$K_{\Omega \Gamma}^N g := (DL_k^N - i k SL_k^N) L_k^N g, \quad \text{with} \quad L_k^N := (\frac{1}{2}I + K_k^N - i k V_k^N)^{-1}.$$  

(3.9)

We remark that the definition of $K_{\Omega \Gamma}^N$ requires only evaluation of input functions at the grid points. In particular it is well defined on continuous functions. Indeed, we have

$$\varphi = L_k^N g \iff Q_N \varphi = Q_N L_k^N Q_N g,$$

and since the discrete boundary layer operators only uses pointwise values of the density at the grid points (i.e., $Q_N \varphi$), evaluation of $K_{\Omega \Gamma}^N g$ requires only values of $g$ at the grid nodes. So we can replace, when necessary,

$$K_{\Omega \Gamma}^N g = K_{\Omega \Gamma}^N Q_N g.$$  

(3.10)

The discrete operator $K_{\Omega \Gamma}^N g$ is defined accordingly by taking the trace of $K_{\Omega \Gamma}^N g$ on $\Sigma$. Thus our algorithm is based on the idea of taking the trace of FEM and BEM solutions on $\Gamma$ and $\Sigma$, respectively.
3.3 A FEM-BEM numerical method for decomposed model

In addition to the discrete operators defined above, we need one last discrete operator to describe the FEM-BEM algorithm. Let

\[ Q_h^\Sigma : C^0(\Sigma) \to \gamma_\Sigma F_{h,d}, \]  

(3.11)
denote the usual Lagrange interpolation operator on \( \gamma_\Sigma F_{h,d} \), the inherited finite element space on \( \Sigma \). Our full FEM-BEM algorithm is:

- **Step 1:** Solve the finite dimensional system

\[
(I - \begin{bmatrix} Q_h^\Sigma K_h^\Gamma & Q_h^\Sigma K_h^\Gamma \end{bmatrix}) \begin{bmatrix} f_h^\Sigma \\ f_h^\Gamma \end{bmatrix} = \begin{bmatrix} Q_h^\Sigma \gamma_\Sigma u_{\text{inc}} \\ -Q_h^\Sigma \gamma_\Gamma u_{\text{inc}} \end{bmatrix}. \]  

(3.12a)

- **Step 2:** Construct the FEM-BEM solution

\[
u_h := K_h^\Omega f_h^\Sigma, \quad \omega_N := K_h^\Omega f_h^\Gamma, \quad u_{h,N} := \begin{cases} u_h, & \text{in } \Omega_2, \\ \omega_N + u_{\text{inc}}, & \text{in } \Omega_1. \end{cases} \]  

(3.12b)

**Remark 3.1.** We have committed a slight abuse of notation in the right-hand-side of (3.12a) by writing \( Q_h^\Sigma \gamma_\Gamma u_{\text{inc}} \) instead of the correct, but more complex, form \( Q_h^\Sigma ((\gamma_\Gamma u_{\text{inc}}) \circ x) \). Similarly, \( Q_h^\Gamma ((K_h^\Gamma \cdot) \circ x) \) should be read in the lower extra-diagonal block of the matrix in (3.12a). Indeed this is equivalent to replacing a space on \( \Gamma \) with that obtained via the parameterization (3.2). Since both spaces are isomorphic, being strict in the notation for description of these operators is not absolutely necessary. In particular, we avoid complicated notation and use a compact way to describe the algorithm that will facilitate easier to understand associated theoretical results and proofs.

**Remark 3.2.** Complete numerical analysis of the FEM-BEM algorithm is beyond the scope of this article. In a future work, we will carry out a detailed numerical analysis of the FEM-BEM algorithm. Below we give the main results. In summary, the analysis is based on the following assumption on the mesh-grid:

**Assumption 1** There exists \( \varepsilon_0 > 0 \) such that the sequence of grids \( \{ T_h \}_h \) satisfies

\[
h_1^{1/2} h_D^{\varepsilon_0} \to 0 \]  

(3.13)

where \( D \subset \Omega_2 \setminus \overline{\Omega}_0 \) is an open neighborhood of \( \Gamma \), and \( h_D \), the maximum of the diameters of the elements of the grid \( T_h \) with non-empty intersection with \( D \).

We note that this assumption allows locally refined grids but introduce a very weak restriction on the ratio between the larger element in \( \Omega_2 \) and the smaller element in \( D \). However, since the exact solution is smooth on \( D \), the partial differential equation in this domain is just
the homogeneous Helmholtz equation, it is reasonable to expect that small elements are not going to be used in this subdomain.

Using Assumption 1, we will prove that the discrete system (3.12) is well-posed and also prove optimal convergence of the FEM-BEM solution. More precisely, after deriving convergence of the individual FEM and BEM approximations, we will prove the following convergence result, for any region \( \Omega_R \subset \mathbb{R}^d \setminus \overline{\Omega}_1 \), \( 0 < \varepsilon \leq \varepsilon_0 \), \( r \geq 0 \), \( t \geq d + 3/2 \)

\[
\|u - u_h\|_{H^1(\Omega_R)} + \|\omega - \omega_N\|_{H^r(\Omega_R)} \leq C (h_D^{d-\varepsilon} N^{-\varepsilon} + h_\Sigma^{d+1/2} + N^{-t} + h_D^d) \|u^{inc}\|_{H^{r+1}(\Omega_2)} + C \inf_{v_h \in \mathcal{P}_h,d} \|u - v_h\|_{H^r(\Omega_2)}, \quad (3.14)
\]

where \( h_D \) is as in (3.13) and \( h_\Sigma \) is the maximum distance between any two consecutive Dirichlet/constrained nodes in \( \mathcal{T}_h \); \( (u, \omega) = (K_{\Omega_2} f_\Sigma, K_{\Omega_1} \Gamma f_\Gamma) \) is the exact solution of (2.6); and \((u_h, \omega_N)\) is the unique solution of the numerical method (3.12).

Next we describe algebraic details required for implementation of the algorithm, followed by numerical experiments in Section 4 to demonstrate the FEM-BEM method to simulate wave propagation in heterogeneous unbounded media.

### 3.4 FEM-BEM algebraic systems and evaluation of wave fields

Simulation of approximate interior and exterior wave fields \( u_{h,N} \) using the representation in (3.12b) requires: (i) computing the interior solution \( w_h \) by once solving finite element system (3.1) using the Dirichlet data \( f_{\Sigma,h} \); and (ii) the exterior solution \( \omega_N \) in \( \Omega_1^c \) by evaluating the layer potential value \( (D_L^N - IS_L^N) \) using the approximation density \( I_L^N \in \mathbb{T}_N \).

Thus, using (3.4)–(3.7), the degrees of freedom (DoF) to evaluate \( \omega_N \) is same as the dimension \( 2N \) of \( \mathbb{T}_N \). We note that the dimension of \( \mathbb{T}_N \) is same as the number of interpolatory uniform grid points \( t_j, j = -N + 1, \ldots, N \) in (3.3) that determine the interpolatory operator \( \mathbb{Q}_N \) in (3.5). The linear algebraic system corresponding to the Dirichlet problem (3.1) for \( w_h \in \mathcal{P}_{h,d} \) is obtained by using an ansatz that is a linear combination of the basis functions that span \( \mathcal{P}_{h,d} \). Coefficients in the \( w_h \) ansatz are values of \( w_h \) at the nodes that determine \( \{\mathcal{T}_h\}_h \). The nodes include constrained/boundary Dirichlet nodes on \( \Sigma \) and free/interior non-Dirichlet nodes in \( \Omega_2 \). Let \( M \) be the number of Dirichlet nodes and \( L \) be the number of free-nodes.

Consequently, the FEM system (3.1) to compute \( w_h \) leads to an \( L \)-dimensional linear system for the unknown vector \( w_L \) (that are values of \( w_h \) at the interior nodes). The system is governed by a symmetric sparse matrix, say, \( A_L \). The matrix \( A_L \) is obtained by eliminating the row and column vectors associated at the boundary nodes. Let \( D_{L,M} \) be the \( L \times M \) matrix that is used to move the Dirichlet condition to the right-hand-side of the system. Thus for a given data vector \( \hat{f}_M \), we may theoretically write \( w_M = A_L^{-1} D_{L,M} \hat{g}_M \). Let \( T_{2N,L} \) be the \( 2N \times L \) sparse matrix so that \( T_{2N,L} w_M = (T_{2N,L} A_L^{-1} D_{L,M} \hat{f}_M) \) is the evaluation (trace) of the finite element solution \( w_h \) of (3.1) at the \( 2N \) interior points \( x(t_j) \in \Gamma, j = -N + 1, \ldots, N \) that are the BEM grid points.

For describing the full FEM-BEM system, using the above representation, it is convenient to defined the \( 2N \times M \) matrix

\[
\tilde{K}_{2N,M} := T_{2N,L} A_L^{-1} D_{L,M}. \quad (3.15)
\]

The matrix \( A_L^{-1} \) in (3.15), in general, should not be computed in practice. We may consider instead a \( L_L D_L L_L^t \) factorization \[11\] (for example, implemented in the Matlab command \texttt{ldl}),
where $D_L$ is a block diagonal matrix with $1 \times 1$ or $2 \times 2$ blocks and $L_L$ is a block (compatible) unit lower triangular matrix. Hence, each multiplication by $A_L^{-1}$ is reduced to solving two (block) triangular and one diagonal system which can be efficiently done, leading to evaluation of $\tilde{K}_{2N,M}$ on $M$ dimensional vectors. Of course the $L_L D_L L_L^\top$ factorization is a relatively expensive process, but worth to consider in our method to simulate the complex heterogeneous and unbounded domain model. (We further quantify this process using numerical experiments in Section 4.)

The ansatz for the unknown density $f^N_j \in \mathbb{T}_N$ is a linear combination of $2N$ basis functions $\exp(i\ell t)$, $\ell = -N+1, \ldots, N$ in (3.4) that span $\mathbb{T}_N$. The $2N$-dimensional BEM system for the unknown vector $f_{2N}$ (that are values of the unknown density at the Nyström node points $t_j$, $j = -N+1, \ldots, N$) is governed by a complex dense matrix and an input $2N$-dimensional vector $\tilde{g}_{2N}$ determined by the Dirichlet data on $\Gamma$ in the exterior homogeneous model (2.4) evaluated at $t_j$, $j = -N+1, \ldots, N$. We may theoretically write

$$\varphi_{2N} = B_{2N} \tilde{f}_{2N},$$

where $B_{2N}$ is the inverse of the $2N \times 2N$ Nyström matrix corresponding to the discrete boundary integral operator in (3.9). Similar to $T_{2N,L}$, let $P_{M,2N}$ be the matrix representation of the (discrete) combined potential generated by a density at the $M$ Dirichlet nodes of $\mathcal{T}_M$. That is, $P_{M,2N} \varphi_{2N}$ is the vector form of $Q^N_k \gamma_\Sigma (D\Sigma_k^N - ik \mathbb{S} \Sigma_k^N) \varphi$, following the BEM representation (3.9) for evaluation of the exterior field at the $M$ Dirichlet nodes on $\Sigma$. Similar to interior problem based matrix in (3.15), corresponding to the exterior field it is convenient to introduce the $M \times 2N$ matrix

$$\hat{K}_{M,2N} := P_{M,2N} B_{2N}. \quad (3.17)$$

Thanks to the choice of smooth boundary $\Gamma$, the standard Nyström BEM is spectrally accurate and hence in practice $2N << L$ and also the number of Dirichlet nodes $M > 2N$ (and we quantify this claim using numerical experiments in Section 4). Thus the cost of setting up an LU decomposition of the dense matrix $B_{2N}$ is relatively negligible and consequently the matrix $K_{M,2N}$ can be efficiently evaluated on any $2N$-dimensional vector.

The implementation procedure described above to compute the interior and exterior fields using (3.12b) requires $M$-dimensional the vector $\tilde{f}_M$ at the Dirichlet nodes on $\Sigma$ and the $2N$-dimensional $\tilde{f}_{2N}$ at the $2N$ uniform grid points $x(t_j)$, $j = -N+1, \ldots, N$ on $\Gamma$. Since $\Sigma$ and $\Gamma$ are artificially chosen boundaries for the decomposition of the original model, the vectors $\tilde{f}_M$, $\tilde{f}_{2N}$ are unknown. The interface system (3.12a), that uses the data $u^{inc}$ in the original model, completes the process to compute $\tilde{f}_M$, $\tilde{f}_{2N}$. In particular, for matrix-vector form description of (3.12a), we obtain input data vectors, say $\tilde{u}^{inc}_M$ and $\tilde{u}^{inc}_{2N}$, using the vector form representations of $Q^k_{\Sigma \Sigma} u^{inc}$ and $Q_N \gamma_T u^{inc}$, respectively.

More precisely, using (3.15)–(3.17), the matrix-vector algebraic system corresponding to (3.12a) takes the form

$$\begin{bmatrix}
    \mathbf{I}_M & -\hat{K}_{M,2N} \\
    -\hat{K}_{2N,M} & \mathbf{I}_{2N}
\end{bmatrix}
\begin{bmatrix}
    \tilde{f}_M \\
    \tilde{f}_{2N}
\end{bmatrix}
=\begin{bmatrix}
    \tilde{u}^{inc}_M \\
    -\tilde{u}^{inc}_{2N}
\end{bmatrix} \quad (3.18)$$

where $\mathbf{I}_M, \mathbf{I}_{2N}$ are, respectively, the $M \times M$ and $2N \times 2N$ identity matrices.

In our implementation, instead of solving the full linear system in (3.18) we work with the
Schur complement form of the system:

\[
\begin{pmatrix}
I_{2N} - \tilde{K}_{2N,M} \hat{K}_{M,2N}
\end{pmatrix}_{d_{\text{Sch}}} \tilde{f}_{2N} = -\tilde{u}^{\text{inc}}_{2N} + \tilde{K}_{2N,M} \hat{u}^{\text{inc}}_M
\]

(3.19a)

\[
\hat{f}_M = \hat{u}^{\text{inc}}_M + \hat{K}_{M,2N} \tilde{f}_{2N}.
\]

(3.19b)

After solving for \( \tilde{f}_{2N} \) in (3.19a), main computational cost for finding \( \hat{f}_M \) involves only the matrix-vector multiplication \( \hat{K}_{M,2N} f_{2N} \). The latter requires solving a BEM system and it can be carried out using a direct solve because of \( 2N \) being relatively small.

In our numerical experiments to compute \( \tilde{f}_{2N} \) in (3.19a), we solve the linear system using:

(i) iterative GMRES method with the (relative) residual set to be equal \( 10^{-8} \) in all the cases; and (b) direct Gaussian elimination solve which requires to construct the full matrix of the method \( A_{\text{Sch}} \). Both the approaches are compared in the numerical experiments Section 4. As an error indicator of our full FEM-BEM algorithm, we analyze the widely used quantity of interest (QoI) in numerous wave propagation applications: the far-field arising from both the interior and exterior fields induced by the incident field impinging from a direction. For a large class of inverse wave models [6], the far-field measured at several directions is fundamental to understand various properties of the wave propagation medium.

To computationally verify the quality of our FEM-BEM algorithm in Section 4, as an error indicator, we analyze the far-field at thousands of direction unit vectors \( z \). Using (3.16), we define a spectrally accurate approximation to the QoI as

\[
(F_N \varphi_{2N})(z) := \sqrt{\frac{k}{8\pi}} \exp \left( -\frac{1}{4} \pi i \right) \frac{\pi}{N} \sum_{j=-N+1}^N \exp(-ik(z \cdot x(t_j))) \left[ z \cdot (x'_2(t_j), x'_2(t_j)) + 1 \right] [\varphi_{2N}]_j.
\]

(3.20)

The exact representation of QoI is [6]

\[
(F \varphi)(z) := \sqrt{\frac{k}{8\pi}} \exp \left( -\frac{1}{4} \pi i \right) \int_0^{2\pi} \exp(-ik(z \cdot x(t))) \left[ z \cdot (x'_2(t), x'_2(t)) + 1 \right] \varphi(t) \, dt.
\]

(3.21)

In our numerical experiments, using angular representation of the direction vectors \( z \), we compute the approximate far-field at 1,000 uniformly distributed angles. We report the QoI errors for various grid parameters \( h, N \) and demonstrate high-order convergence of our FEM-BEM algorithm. The maximum of the estimated errors in the approximate QoI, using the values at the 1,000 uniform directions, are used in the next section to validate efficiency and high-order accuracy of the FEM-BEM algorithm.

4 Numerical experiments

In this section we consider two sets of numerical experiments to demonstrate the overlapping decomposition framework based FEM-BEM algorithm. In the first set of experiments the heterogeneous domain \( \Omega_0 \) with non-trivial curved boundaries and the refractive index function \( n \) on \( \Omega_0 \) are smooth; and in the second set \( \Omega_0 \) is a complex non-smooth structure and \( n \) is a discontinuous. For these two experiments, we consider the \( \mathbb{P}_d \) Lagrange Finite Elements with \( d = 2, 3, 4 \) for the interior FEM model with mesh values \( h \) and several values \( N \) to achieve spectral accuracy and make the BEM error less than that in the FEM discretizations. The
reported CPU times in the section are based on serial implementation of the algorithm in Matlab (02017b) and running our FEM-BEM software for the two sets of experiments on a desktop with a 10-core Xeon E5-2630 processor and 128GB RAM.

4.1 Star-shaped domain with five-star-pointed refractive index

In the first (Experiment 1) set, we choose $\Omega_0$ to be the star-shaped region sketched in the interior of the disk $\Omega_1$ in Figure 2, and the refractive index function $n$ is given in polar coordinates by

$$n(r, \theta) := 1 + 16\chi\left(\frac{1}{0.975}\left[\frac{r}{2 + 0.75 \sin(5\theta)} - 0.025\right]\right),$$

with

$$\chi(x) := \frac{1}{2}(\tilde{\chi}(x) + 1 - \tilde{\chi}(1 - x)), \quad \tilde{\chi}(x) := \begin{cases} 1, & \text{if } x \leq 0, \\ \exp\left(\frac{1}{\alpha}e^{-e^{1/x}}\right), & x \in (0, 1) \\ 0, & \text{if } x > 1, \end{cases}$$

Notice that $\tilde{\chi}(x)$ is a smooth cut-off function with $\text{supp} \chi = (-\infty, 1]$. Therefore, function $\chi$ is smooth and also symmetric around $1/2$: $\chi(1 - x) = 1 - \chi(x)$ for any $x$.

We have taken as $\Omega_2$ the rectangle $[-6, 6] \times [-8, 8]$ with boundary $\Sigma$ so that diameter of interior domain is 20. Thus the choice $k = \alpha\pi$ corresponds to interior heterogeneous model with wavelength $10\alpha$. For our numerical experiments we choose low ($\alpha = 1/4$) and medium frequency ($10$ and $40$ wavelength) models (with $k = \pi, 4\pi$). For the smooth, artificial boundary $\Gamma$ of $\Omega_1$, we have taken the circle centered at zero with radius 3.5 so that with $k = \alpha\pi$ the exterior model has wavelength $3.5\alpha$.

For interior FEM models, the initial grid consists of 2,654 triangles which is refined up to four times, in the usual way. We show the simulated far-field error results in Tables 1-2 for low...
frequency $k = \pi/4$ and medium frequency domain problems for $k = \pi$ and $4\pi$. In these tables an estimate of the (relative) maximum error in computing the QoI far-field is presented as well as the number (given within parentheses) of GMRES iterations needed to achieve convergence when the residual tolerance was set to be $10^{-8}$. Next we discuss some key aspects of the computed results reported in Tables 1-2.

To compute the errors, as an exact/truth solution we have taken that obtained using the FEM-BEM algorithm, with $N = 640$ and the next level of FEM mesh refinement to that in the tables. The fast spectrally accurate convergence of the Nyström BEM, after achieving a couple of digits of accuracy, can be observed by following the maximum errors in the last columns in Tables 1-2. In particular the last columns results, for FEM spline degree $d = 3, 4$ cases, demonstrate that relatively small DoF $2N$ is required, compared to the FEM DoF $L$, for Nyström BEM solutions accuracy to match that of the FEM solutions. The last rows in Tables 1-2 clearly demonstrate that higher values of $N$ are not useful because of the stagnation of error due to limitation of the FEM accuracy. Further, a closer analysis of results in Tables 1-2 shows that the far-field error in maximum-norm seems to achieve superconvergence $O(h^{2d})$.

In addition, in Figure 6 we demonstrate faster convergence of the total field in $H^1$-norm and compare with a non-smooth solution (Experiment 2) case.

In the Experiment 1 set, with smooth heterogeneous region $\Omega_0$ and smooth refractive index function $n$, it can be shown that the exact solution for the model problem is smooth. However, this fact alone is not sufficient to explain in detail the superconvergence of the far field. We may conjecture that some faster convergence is occurring in the background for the near field in some weak norms, and that the calculation of the far field is taking profit from this to achieve superconvergence. In a future work, we will explore the numerical analysis our FEM-BEM algorithm. In Figure 3, we illustrate convergence of GMRES iterations and show that as the frequency is increased four-fold, the number of iterations convergence within a $10^{-8}$ error tolerance increases at slower rate.
Table 1: Experiment 1: $\mathbb{P}_3$ Finite element space and $k = \pi/4, \pi, 4\pi$ (top, middle, bottom tables)

| N/L | 7,999 | 31,657 | 125,953 | 502,465 | 2,007,169 |
|-----|-------|--------|---------|---------|-----------|
| 010 | 3.1e-03 (012) | 6.6e-05 (012) | 2.2e-06 (012) | 1.2e-06 (012) | 1.2e-06 (012) |
| 020 | 3.1e-03 (012) | 6.5e-05 (012) | 2.0e-06 (012) | 2.5e-10 (012) | 4.7e-11 (012) |
| 040 | 3.1e-03 (012) | 6.5e-05 (012) | 2.0e-06 (012) | 1.8e-10 (012) | 1.4e-11 (012) |
| 080 | 3.1e-03 (012) | 6.4e-05 (012) | 2.0e-06 (012) | 1.5e-10 (012) | 9.0e-12 (012) |

N/L | 7,999 | 31,657 | 125,953 | 502,465 | 2,007,169 |
|-----|-------|--------|---------|---------|-----------|
| 010 | 4.3e-01 (020) | 9.4e-06 (012) | 1.4e-06 (012) | 1.2e-06 (012) | 1.2e-06 (012) |
| 020 | 1.8e+00 (040) | 1.4e+00 (040) | 1.1e+00 (040) | 1.4e+01 (040) | 4.0e+00 (040) |
| 040 | 3.5e-01 (031) | 1.6e-02 (031) | 3.3e-04 (031) | 7.3e-06 (031) | 5.2e-06 (031) |
| 080 | 3.5e-01 (031) | 1.6e-02 (031) | 3.3e-04 (031) | 6.0e-06 (031) | 3.5e-07 (031) |

N/L | 7,999 | 31,657 | 125,953 | 502,465 | 2,007,169 |
|-----|-------|--------|---------|---------|-----------|
| 010 | 2.0e-01 (020) | 1.8e-01 (020) | 1.8e-01 (020) | 1.8e-01 (020) | 1.8e-01 (020) |
| 020 | 6.9e-02 (031) | 7.1e-04 (031) | 6.9e-06 (031) | 5.4e-06 (031) | 5.4e-06 (031) |
| 040 | 6.9e-02 (031) | 7.1e-04 (031) | 3.9e-06 (031) | 4.7e-10 (031) | 4.7e-10 (031) |
| 080 | 6.9e-02 (031) | 7.1e-04 (031) | 4.0e-06 (031) | 4.0e-10 (031) | 4.0e-10 (031) |

Table 2: Experiment 1: $\mathbb{P}_4$ Finite element space and $k = \pi/4, \pi, 4\pi$ (top, middle, bottom tables)

| N/L | 14,145 | 56,129 | 223,617 | 892,673 | 3,567,105 |
|-----|--------|--------|---------|---------|-----------|
| 010 | 3.9e-04 (012) | 9.4e-06 (012) | 1.4e-06 (012) | 1.2e-06 (012) | 1.2e-06 (012) |
| 020 | 3.9e-04 (012) | 8.9e-06 (012) | 2.5e-07 (012) | 6.9e-10 (012) | 8.4e-11 (012) |
| 040 | 3.9e-04 (012) | 8.9e-06 (012) | 2.5e-07 (012) | 7.0e-10 (012) | 1.0e-10 (012) |
| 080 | 3.9e-04 (012) | 8.9e-06 (012) | 2.5e-07 (012) | 7.0e-10 (012) | 9.9e-11 (012) |

N/L | 14,145 | 56,129 | 223,617 | 892,673 | 3,567,105 |
|-----|--------|--------|---------|---------|-----------|
| 010 | 2.0e-01 (020) | 1.8e-01 (020) | 1.8e-01 (020) | 1.8e-01 (020) | 1.8e-01 (020) |
| 020 | 6.9e-02 (031) | 7.1e-04 (031) | 6.9e-06 (031) | 5.4e-06 (031) | 5.4e-06 (031) |
| 040 | 6.9e-02 (031) | 7.1e-04 (031) | 3.9e-06 (031) | 4.7e-10 (031) | 4.7e-10 (031) |
| 080 | 6.9e-02 (031) | 7.1e-04 (031) | 4.0e-06 (031) | 4.0e-10 (031) | 4.0e-10 (031) |

N/L | 14,145 | 56,129 | 223,617 | 892,673 | 3,567,105 |
|-----|--------|--------|---------|---------|-----------|
| 010 | 5.0e+00 (040) | 9.3e+00 (040) | 3.1e+00 (040) | 4.1e+00 (040) | 3.9e+00 (040) |
| 020 | 3.7e+00 (080) | 4.9e-01 (080) | 2.4e-01 (080) | 8.5e-02 (080) | 8.6e-02 (080) |
| 040 | 9.1e+00 (098) | 4.6e-01 (100) | 2.6e-01 (102) | 2.0e-03 (102) | 8.8e-06 (102) |
| 160 | 9.8e+00 (098) | 4.6e-01 (100) | 2.6e-01 (102) | 2.0e-03 (102) | 8.8e-06 (102) |
Figure 3: GMRES residual vector for $k = \pi/4$, $k = \pi$ and $k = 4\pi$ in Experiment 1 with $P_3$ finite element space on a grid with FEM DoF $L = 502,465$ and BEM DoF $2N = 160$.

4.2 Pikachu-shaped domain with non-smooth refractive index

In the second (Experiment 2) set of experiments, we consider a more complicated non-smooth heterogeneous region shown in the interior of the curved domain $\Omega_1$ in Figure 4. The region $\Omega_0$ is set to be a polygonal Pikachu-shaped domain with the refractive index function

$$n(x, y) = \begin{cases} 5 + 4\chi\left(\frac{1}{0.75\frac{r}{2-0.75\cos(0.4\theta)}} - 0.025\right), & (x, y) \in \Omega_0, \\ 1, & (x, y) \notin \Omega_0, \end{cases}$$

where $r = \sqrt{(x + 0.18)^2 + (y + 0.6)^2}$, $\theta = \arctan2((y + 0.6), (x + 0.18))$. The grids used in our computation is adapted to the region $\Omega_0$, in such a way that any triangle $\tau \in T_h$ is either contained or has empty intersection with $\Omega_0$. As the boundary of $\Omega_1$ and auxiliary curve $\Gamma$ for the exterior model, we took

$$x(t) = \frac{7\sqrt{2}}{4}(1 + \cos^2 t) \cos t + (1 + \sin^2 t) \sin t, (1 + \sin^2 t) \sin t - (1 + \cos^2 t) \cos t$$

For the interior FEM model, we choose $\Omega_2$ to be a polygonal domain as in Figure 4 with boundary $\Sigma$. We then proceed as in the previous experiment, using an initial grid with 8,634 triangles which is refined up to four times. The solution $u$ of the model is not smooth in $\Omega_0$ and $\overline{\Omega_0}$, because of the non-smoothness of the region $\Omega_0$ and the jump in the refractive index function. One may consider the use of graded mesh around the boundary of $\Omega_0$ to obtain faster
convergence, but we wanted to leave our code and comparisons easier. Using the size of $\Omega_2$, the choices $k = \alpha \pi, \alpha = 1/4, 1, 4$ lead to approximately 2.5, 10, and 40 wavelengths interior FEM model, respectively, for simulations in Experiment 2.

We observe from integer numbers (within in parentheses) in Tables 3-4 that the number of GMRES iterations grow slower compared to quadruple growth of the three frequencies considered in Experiment 2. The estimated (relative) maximum far-field errors for the non-smooth Experiment 2 model are given in Tables 3-4, demonstrating high-order accuracy of our FEM-BEM model as the finite element space degree, grid size, and the BEM DoF are increased. In Figure 6, for $d = 2, 3, 4$, we compare convergence of the total field in $H^1$-norm for smooth (Experiment 1) and non-smooth (Experiment 2) simulations.

In Figure 5 we depict the simulated wave field solution for $k = \pi$, with $P_4$ finite elements on a grid with 138, 144 triangles and $M = 1, 106, 385$ nodes for the FEM solution, and $N = 160$ for the BEM solution. Specifically, we plot the simulated absorbed and scattered field numerical solution $u_{h,N}$ inside $\Omega_2$ in Figure 5.
Table 3: Experiment 2: $\mathbb{P}_3$ Finite element space and $k = \pi/4, \pi, 4\pi$ (top, middle, bottom tables)

| N/L | 39,085 | 69,381 | 622,573 | 2,488,441 |
|-----|--------|--------|---------|-----------|
| 010 | 2.8e-03 (015) | 2.8e-03 (015) | 2.8e-03 (015) | 2.8e-03 (015) |
| 020 | 5.8e-05 (015) | 8.4e-07 (015) | 8.4e-07 (015) | 8.4e-07 (015) |
| 040 | 5.3e-05 (015) | 1.0e-07 (015) | 6.1e-09 (015) | 6.9e-10 (015) |
| 080 | 5.8e-05 (015) | 7.4e-08 (015) | 6.5e-09 (015) | 4.4e-10 (015) |

| N/L | 39,085 | 69,381 | 622,573 | 2,488,441 |
|-----|--------|--------|---------|-----------|
| 020 | 2.5e+00 (040) | 2.5e+00 (040) | 2.5e+00 (040) | 2.5e+00 (040) |
| 040 | 3.8e-03 (042) | 2.5e-04 (042) | 7.1e-05 (042) | 5.2e-05 (042) |
| 080 | 3.1e-03 (042) | 1.7e-04 (042) | 7.1e-06 (042) | 2.7e-07 (042) |
| 160 | 3.4e-03 (042) | 1.4e-04 (042) | 7.9e-06 (042) | 2.6e-07 (042) |

| N/L | 39,085 | 69,381 | 622,573 | 2,488,441 |
|-----|--------|--------|---------|-----------|
| 040 | 6.8e+00 (080) | 3.2e+00 (080) | 3.7e+00 (080) | 3.6e+00 (080) |
| 080 | 9.2e+00 (130) | 7.4e-01 (140) | 2.1e-00 (139) | 2.3e+00 (139) |
| 160 | 6.7e+00 (140) | 4.6e-01 (148) | 1.3e-02 (149) | 4.1e-04 (149) |
| 320 | 6.8e+00 (140) | 4.4e-01 (148) | 1.1e-02 (149) | 2.8e-04 (149) |

Table 4: Experiment 2: $\mathbb{P}_4$ Finite element space and $k = \pi/4, \pi, 4\pi$ (top, middle, bottom tables)

| N/L | 69,381 | 276,905 | 1,106,385 | 4,423,073 |
|-----|--------|---------|-----------|-----------|
| 010 | 2.8e-03 | 2.8e-03 (015) | 2.8e-03 (015) | 2.8e-03 (015) |
| 020 | 1.3e-06 (015) | 8.4e-07 (015) | 8.4e-07 (015) | 8.4e-07 (015) |
| 040 | 1.3e-06 (015) | 1.6e-07 (015) | 6.8e-10 (015) | 6.8e-10 (015) |
| 080 | 1.3e-06 (015) | 1.6e-07 (015) | 6.9e-10 (015) | 6.8e-10 (015) |

| N/L | 69,381 | 276,905 | 1,106,385 | 4,423,073 |
|-----|--------|---------|-----------|-----------|
| 020 | 2.5e+00 (040) | 2.5e+00 (040) | 2.5e+00 (040) | 2.5e+00 (040) |
| 040 | 2.8e-04 (042) | 4.7e-05 (042) | 5.3e-07 (042) | 5.2e-05 (042) |
| 080 | 1.9e-04 (042) | 2.2e-06 (042) | 1.8e-07 (042) | 6.9e-09 (042) |
| 160 | 1.6e-04 (042) | 1.1e-06 (042) | 6.3e-08 (042) | 3.3e-09 (042) |

| N/L | 69,381 | 276,905 | 1,106,385 | 4,423,073 |
|-----|--------|---------|-----------|-----------|
| 040 | 1.7e+00 (080) | 3.8e+00 (080) | 3.6e+00 (080) | 3.6e+00 (080) |
| 080 | 8.8e-01 (139) | 1.8e+00 (140) | 2.3e+00 (139) | 2.3e+00 (139) |
| 160 | 5.4e-01 (147) | 3.9e-02 (149) | 4.8e-04 (149) | 6.9e-05 (149) |
| 320 | 5.4e-01 (147) | 3.6e-02 (149) | 2.9e-04 (149) | 8.4e-06 (149) |
Figure 5: Real part of the total field FEM solution $u_h$ in $\Omega_2$ for $k = \pi$.

Figure 6: Comparisons of convergence of the FEM-BEM algorithm for the total field in $H^1(\Omega_2)$-norm for Experiment 1 and 2 using $P_2$, $P_3$ and $P_4$ elements with $N = 80$ and $k = \pi/4$. The bottom part of the figure shows the expected order of convergence, as given in (3.14).
4.3 Direct solver implementation and comparison with Iterative solver

In this subsection we discuss the direct solver implementation of our method and compare its performance with the iterative approach we have used for simulating results described earlier in the section. When computing the matrix in (3.19a), the main issue is concerned with the matrix \( \hat{\mathbf{K}}_{2N,M} \), which comprises the calculation of finite element solution followed by its evaluation at the nodes of the BEM. Because of the spectral accuracy of the Nyström BEM approximation, the DoF \( 2N \) is expected to be smaller, in practice, even compared to the number \( M \) of FEM boundary Dirichlet (constrained) nodes (that is, \( M > 2N \)). Accordingly, in our implementation we use instead the representation

\[
\hat{\mathbf{K}}_{2N,M}^\top = (\mathbf{T}_{2N,L} \mathbf{A}_L^{-1} \mathbf{D}_{L,M})^\top = \mathbf{D}_{L,M}^\top \mathbf{L}_L^{-1} \mathbf{L}_L^{-\top} \mathbf{T}_{2N,L}^\top,
\]

where we recall that \( \mathbf{A}_L = \mathbf{L}_L \mathbf{D}_L \mathbf{L}_L^\top \) is symmetric. This representation requires solving \( 2N \) (independent) finite element problems, one for each column of \( (\mathbf{K}_N^{\Sigma \Gamma})^\top \), i.e. for each row of \( \mathbf{K}_N^{\Sigma \Gamma} \), and a (sparse) matrix-vector multiplication. The first process, consumes the bulk of computation time (but is a naturally parallel task w.r.t. \( N \)) and can be carried out with wall-clock time similar to solving one FEM problem [15, Section 5.1.5].

The common CPU time for direct and iterative solver amounts to the assembly of the Finite element matrices \( \mathbf{A}_L \) and \( \mathbf{D}_{L,M} \), the \( \text{LDL}^\top \) factorization of the former, the Boundary Element matrix \( \mathbf{B}_{2N} \) and the auxiliary matrices \( \mathbf{T}_{2N,L} \) and \( \mathbf{D}_{M,2N} \). Consequently the major difference in computation between the two approach is: (i) construction and storage of the matrix in (3.19a), followed by exactly solving the linear system for the direct method; versus (ii) setting up the system (3.19a) for matrix-vector multiplication and approximately solving the linear system with GMRES. The former approach is faster especially if the number of GMRES iterations is not very low (in single-digits) because of modern fast multi-threaded implementation of direct solvers. However, the latter approach is memory efficient and needed especially for large scale 3-D models. The direct method is practical only if the available memory can store the matrix in (3.19a).

Currently, 128GB (and higher) RAM is standard workstation computers. Using such a computer (with 10 cores and 128GB), with the direct solver we were able to simulate the example 2-D models in Experiment 1 and 2, even with millions of FEM (sparse) DoF within our FEM-BEM framework. For one of the largest cases reported in Table 2, with \( \mathbb{P}_4 \) elements for the wavenumber \( k = 4\pi \) (40 wavelengths case), with

\[
N = 80, \quad L = 3, 567, 105 \quad \text{(with 445, 440 triangles)}, \quad M = 7, 168
\]

the GMRES approach demanded the system setup CPU time 172 seconds; and the direct approach a setup CPU time of 332 seconds. Because of requiring 102 GMRES iterations, the solve time to compute a converged iterative solution was \textbf{586 seconds}. However, because of very efficient multi-threaded direct solvers (in Matlab) the direct solve time to compute exact solution was only \textbf{0.014 seconds}. Thus we conclude that our FEM-BEM framework provides options to apply direct or iterative approaches to efficiently simulate wave propagation in heterogeneous and unbounded media. For 2-D low and medium frequency models with sufficient RAM, it seems to be efficient even to use direct solvers and for higher frequency cases iterative solvers are efficient because of the demonstrated well-conditioned property of the system.

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