

Fast Boundary Element Methods Beyond Homogeneous Media: Challenges Towards Realistic Wave Propagation Simulations

Stéphanie Chaillat^[0000-0001-8478-4647]

1 Fast Boundary Element Methods for waves in unbounded domains

Wave propagation can be simulated using various numerical methods, including the finite element method, finite difference schemes, spectral element methods, and the Boundary Element Method (BEM). The BEM relies on the numerical solution of boundary integral equations [5]. The Green's function, used to reformulate the PDE into a boundary integral equation, determines both the advantages and limitations of the method. In particular, BEM is efficient only in configurations where the Green's function can be computed at low computational cost. However, this requirement is naturally satisfied for homogeneous, unbounded domains, since the free-space Green's function automatically satisfies the radiation conditions at infinity, making BEM particularly well suited for such problems. Possible applications include acoustic wave propagation in the air (Fig. 1a) or in the ocean (Fig. 1b), seismic wave propagation in sedimentary basins modeled as piecewise homogeneous layered media, or the modeling of curtains of gas bubbles in marine environments.

Another important drawback of the boundary integral formulation is that it leads to a linear system with a dense, non-symmetric matrix. Direct solvers, which factorize the system matrix, have a computational complexity of order $O(N^3)$ in time and $O(N^2)$ in memory, where N is the number of degrees of freedom on the boundary. They therefore become impractical as soon as N is large. Iterative solvers, on the other hand, construct a sequence that converges to the solution, with a complexity of order $O(n_{\text{iter}} \times N^2)$ in time and $O(N^2)$ in memory. These memory requirements and computational costs make BEMs challenging to apply to realistic configurations (in terms of geometry, heterogeneity, or wavelength). To overcome these limitations, fast BEM techniques have been developed.

Stéphanie Chaillat
Laboratoire POEMS, CNRS-ENSTA-INRIA, Institut Polytechnique de Paris, 828 bd des
Maréchaux, 91 120 Palaiseau, France, e-mail: stephanie.chaillat@ensta.fr

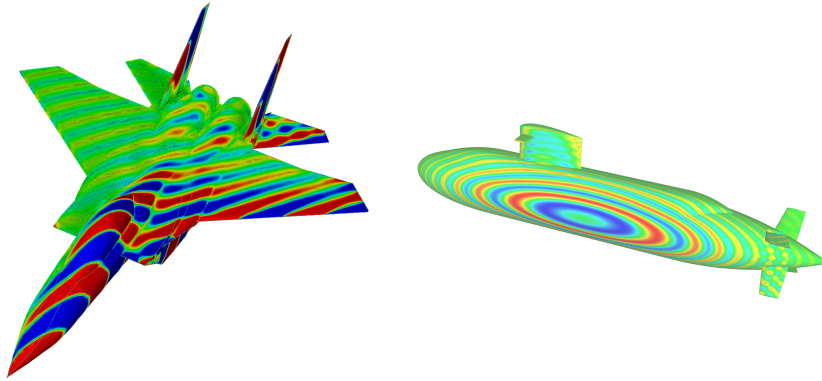


Fig. 1 Illustrations of three-dimensional acoustic diffraction problems solved using fast Boundary Element Methods: FM-BEM code developed at the POEMS laboratory (COFFEE).

The principle of a fast BEM is to accelerate the evaluation of the integral operators and to construct a data-sparse approximation of the system matrix, thereby reducing both the time per iteration and the memory footprint. The main fast BEMs are based on hierarchical (\mathcal{H})-matrices and the Fast Multipole Method (FMM).

\mathcal{H} -matrix techniques [29] approximate the dense BEM matrix by a *data-sparse* matrix, i.e., a matrix that is formally full but stores information in a compressed form. When used in conjunction with an efficient rank estimation algorithm, such as the Adaptive Cross Approximation (ACA), they yield a memory-efficient approximation of the BEM matrix. \mathcal{H} -matrix BEMs are a purely algebraic tool. They were originally designed for asymptotically smooth problems, such as Laplace or elastostatic equations. However, as shown in [16], although these methods are not theoretically optimal for wave propagation, they remain an efficient option for accelerating BEMs.

The optimal complexity for wave propagation problems is achieved with the FMM. Originally developed for N -body problems [27], the method has since been adapted to many fields, including wave propagation [26, 10]. The idea is to reformulate the Green's function, i.e., $G(\mathbf{x}, \mathbf{y}) = \frac{\exp(ik|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}$ for the Helmholtz equation or derivatives for elastodynamics, in terms of plane wave expansions to separate the variables \mathbf{x} and \mathbf{y} in the integral. It is no longer necessary to recompute the Green's function for each pair of points on the boundary of the object, and the integrations over \mathbf{x} can be reused. The mutual contributions between all points \mathbf{x} and \mathbf{y} are thus reduced to a few contributions between clusters of points \mathbf{x} and distant clusters of points \mathbf{y} (Figure 2). Moreover, to reduce memory usage and the computational cost of the matrix-vector product, the system matrix is never explicitly assembled, in contrast to the classical BEM. The FMM achieves a computational complexity of order $O(N \log N)$ for the matrix-vector product.

Both FM-BEM (BEM accelerated with the Fast Multipole Method) and \mathcal{H} -BEM (BEM accelerated with \mathcal{H} -matrices) have demonstrated their potential for modeling

not only acoustic wave propagation but also seismic waves in the ground [10, 16, 23, 25]. Early efforts focused on the efficient simulation of wave propagation in homogeneous domains in the frequency domain. As this area has matured, current challenges lie in extending these approaches to more complex settings, such as time-domain simulations (Section 2), piecewise homogeneous media (Section 4), and multiphysics problems (Section 2). The successful realization of these developments relies on methodologies that have been well established in the context of domain decomposition (DD) methods.

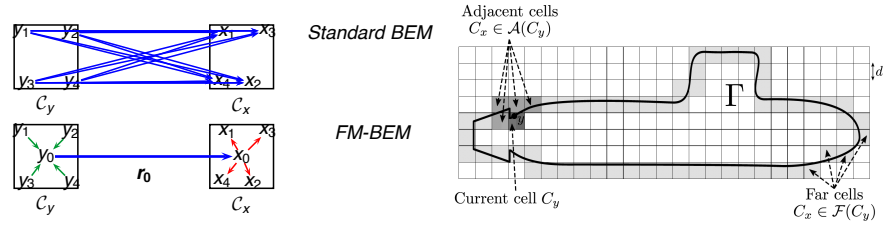


Fig. 2 Principle of the Fast Multipole Method. Left: clustering of boundary points to approximate far-field interactions using plane wave expansions of the Green's function. Right: geometric decomposition separating near-field interactions, evaluated with the standard approach, from far-field interactions, accelerated using the FMM. Image from [38].

2 Optimal non-intrusive coupling for multi-physics problems

Fast BEMs make the method particularly well suited for modeling acoustic wave propagation from underwater explosions in the ocean, where the fluid is well approximated by a homogeneous linear acoustic medium. When such waves interact with immersed structures, such as submarines, accurately modeling fluid–structure interaction effects becomes essential for efficient vessel design (Figure 3). In this context, the elastic response of the structure, potentially involving nonlinear behavior, is most effectively captured using the Finite Element Method (FEM). A key feature of this acoustic-elastic BEM-FEM coupling is that it does not involve junction points, which simplifies the design of efficient coupling algorithms. However, it requires the coupling of FEM and BEM in the time domain, raising new theoretical and numerical challenges for the domain decomposition community. This work has been done in collaboration with M. Bonnet (POEMS), D. Mavaleix-Marchessoux (former PhD student), A. Nassor (former PhD student, now at IFPEN) and B. Leblé (Naval Group).

The first challenge for this study is to propose a fast wave propagation solver in the time domain based on the BEM. Various approaches exist. One possibility is to use retarded potentials [28] based on time-domain Green's functions. But these approaches does not enable the use of the major advances made on fast BEMs in the

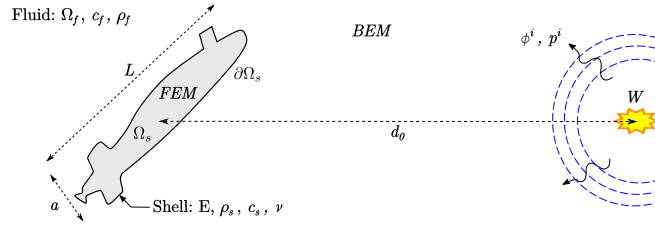


Fig. 3 Submarine subjected to a distant underwater explosion. Image from [38].

frequency domain. An alternative is to use Fast Fourier or Laplace Transform but these methods provide an approximation of the response at discrete time instances, which, however, does not reproduce the action of a time-stepping numerical scheme applied to the differential equation. Another approach allows one to benefit both from the advantages of operational calculus (in particular, the derivation of well-posed boundary value problems) and from obtaining the solution at discrete time steps resulting from a time integration scheme. It consists of (i) approximating the differential equation by a discrete-time integration scheme, and then (ii) applying to the resulting discrete-time evolution problem a \mathcal{Z} -transform [31] (the discrete-time analogue of the Laplace transform). For a review of time-domain approaches based on the \mathcal{Z} -transform, and a discussion of their differences with approaches based on convolution quadrature methods [35, 36, 3, 2], see [6].

While the \mathcal{Z} -BEM combined with FM-BEM yields a highly efficient method, it remains impractical for a large number of time steps (e.g., 10^5), as each time step requires solving a complex frequency-domain problem. To handle rapid excitations, additional acceleration is achieved via high-frequency approximations, reducing the number of frequencies needed. Numerical tests show that acceptable time-domain accuracy can be obtained with only a few hundred frequencies. This approach also allows flexible high- or low-fidelity simulations depending on computational resources. The performance of this \mathcal{Z} -based FM-BEM procedure (combined with high-frequency approximations) is validated, and its effectiveness is demonstrated on complex submarine geometries under realistic excitation conditions (see [39] and Figure 4 for an illustration).

The second challenge is to propose a non-intrusive acoustic-elastic coupling adapted to the specificities of our time-domain FEM and BEM solvers. The developed method is inspired by classical optimized Schwarz waveform relaxation techniques and previous works for Helmholtz equations [22]. It relies on the use of suitably designed transmission conditions in each subdomain. We established solvability results for the transient fluid-structure interaction problem [8], demonstrating the continuous dependence of solutions on the data and characterizing the correspondence between input and output regularity.

Exploiting these properties, we introduced a first global-in-time iterative method based on Neumann subproblems. Theoretical analysis revealed a loss of regularity in the space-time trace of the solution at the interface, which explains the lack

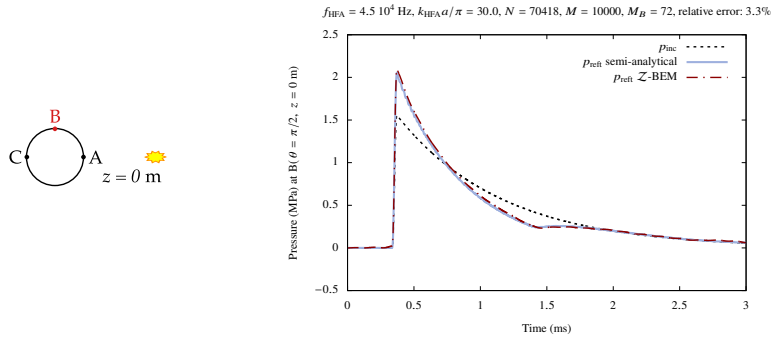


Fig. 4 Scattering by a small cylinder: comparison between the \mathcal{Z} -BEM (out of 10000 frequencies required, only 72 are solved using BEM, while the remaining frequencies are approximated with high frequency approximations) and semi-analytical solutions for the total field p_{refl} on the $z = 0$ plane, at the orthogonal point B. The incident field at this point is also shown. Result from [39].

of convergence observed numerically. To overcome this difficulty, we developed a second approach based on Robin evolution problems. Unlike the former, this formulation preserves the space-time regularity of the interface trace, thereby guaranteeing convergence. Numerical experiments were conducted to assess convergence and to optimize the coupling parameters of the Robin transmission conditions. We demonstrated how this FEM/ \mathcal{Z} -BEM approach can be applied to complex and realistic underwater explosion simulations [7]. A practical challenge arises from the reliance on non-homogeneous Robin boundary conditions in acoustics and elastodynamics, which are not always available in industrial software. To circumvent this limitation, we proposed a variant of the global-in-time iterative coupling that does not require elastic Robin boundary conditions. This alternative approach relies on a modified domain decomposition strategy in which the coupling interface is shifted into the acoustic medium, so that it no longer coincides with the fluid-structure boundary. At each iteration, one then solves a purely acoustic subproblem and a coupled acoustic-elastic subproblem. This reformulation preserves convergence while significantly broadening the applicability of the coupling strategy.

These results highlight the efficiency of BEMs in complex multiphysics contexts driven by industrial applications. However, the configurations presented thus far have been limited to homogeneous domains for the BEM components. This leads us to consider the question of recent advances in BEM formulations for piecewise homogeneous media.

3 Preconditioners for multiple scattering problems

We have illustrated the interest of drawing inspiration from DD methods for FEM–BEM coupling. However, very few DD approaches have been tailored for

BEMs, leaving significant room for improvement in this area. The main challenges involve designing methods that enable efficient parallelization of BEMs, while minimizing communications, a difficult task given the dense nature of the resulting matrices and the boundary-condensed information. Additionally, a key objective is to reduce the number of iterations in the iterative DD process.

As a first step, we focus on multiple scattering problems [37], a configuration that is well suited to DDMs and has the additional advantage of avoiding junction points. This work is conducted in collaboration with Marion Darbas (Université Sorbonne Paris Nord), Martin Gander (Université de Genève) and Laurence Halpern (Université Sorbonne Paris Nord). We consider a collection of I disjoint bounded open sets $\{O_i\}_{1 \leq i \leq I}$ of \mathbb{R}^d with smooth boundaries $\{\Gamma_i\}_{1 \leq i \leq I}$ and note $\Omega = \mathbb{R}^d \setminus \bigcup_{i=1}^I O_i$ the associated propagation domain (see Fig. 5 for the notations). In Ω , the problem writes:

$$\begin{cases} \Delta u + k^2 u = 0 & \text{in } \Omega, \\ u|_{\Gamma_i} = g_i = -u_{\text{inc}}|_{\Gamma_i}, & i = 1, \dots, I, \\ \text{Radiation condition.} \end{cases} \quad (1)$$

It can be naturally formulated as a system of boundary integral equations and solved using BEMs. For instance, if we consider a formulation based solely on the single-layer potential, we obtain the system:

$$\begin{pmatrix} S_{11} & S_{12} & \cdots & S_{1I} \\ \vdots & \vdots & \ddots & \vdots \\ S_{I1} & S_{I2} & \cdots & S_{II} \end{pmatrix} \begin{pmatrix} q_1 \\ \vdots \\ q_I \end{pmatrix} = \begin{pmatrix} g_1 \\ \vdots \\ g_I \end{pmatrix}.$$

Here, each block S_{ij} represents the discretized interaction between obstacles i and j . The vector q_i approximates the unknown potential on obstacle i , while g_i corresponds to the discretized boundary data associated with obstacle i . Formulating the linear system is intuitive, but its resolution is computationally intensive due to the non-symmetric and dense block matrix.

The Method of Reflections [18, 33] is a DD approach with a natural partitioning for multiple scattering problems. At the continuous level, this approach relies on decomposing the total scattered field into contributions associated with individual obstacles. Iteratively, the scattering problem is solved independently for every obstacle, with the incident field defined as the superposition of the original incident wave and the scattered fields produced by the remaining obstacles in the previous (or current, depending on the variant) iteration. A simpler way to understand the sequential Method of Reflection is at the matrix level, where it corresponds to applying a Gauss-Seidel decomposition to solve the global linear system. The sequential Method of Reflections can be interpreted as a Multiplicative Schwarz DD [13]. A parallel version of the method arises naturally by using a Jacobi algorithm, which leads to the Additive Schwarz method.

The method does not depend on the numerical method used to solve each single scattering problem but due to the homogeneous nature of the exterior problem, it

is particularly well suited to Boundary Element discretizations. It is thus a way to propose boundary domain decomposition methods. The key component is to understand the convergence of the iterative method. For waves problems, it can depend on the frequency and the geometric configuration, especially the distance between obstacles. In [13], we study the Method of Reflections for Helmholtz problems in detail. Our results show that both the sequential and parallel forms of the Method of Reflections, when based on boundary integral equations, provide an efficient and wavenumber-robust way to solve multiple scattering problems. However, we also observe that small distances between scatterers can significantly slow down the Method of Reflections, and in some cases prevent the parallel version from converging.

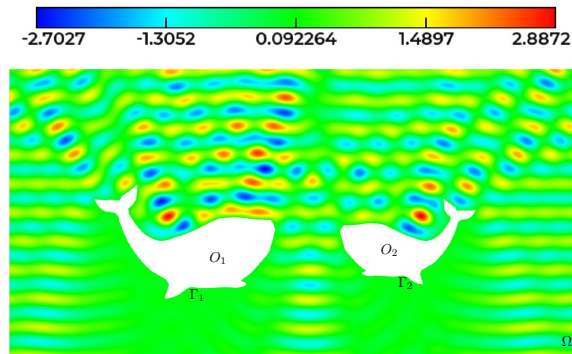


Fig. 5 Illustration of the convergence of the Method of Reflections. Diffraction of an incident plane wave. Real part of the scattered field at $k = 4\pi$. In this example, GMRES applied to the full system converges in 3620 iterations, the sequential Method of Reflections in 10 iterations, and GMRES preconditioned with this method in only 5 iterations to reach a residual below 10^{-8} .

To address this issue, using the connection between the Method of Reflections in boundary integral equation form and algebraic Schwarz methods, we introduce overlaps and coarse spaces, which substantially improve performance. Importantly, the main strength of the new approach lies not in its performance as a solver per se, but in its effectiveness as a preconditioner for Krylov methods, providing a computationally efficient way to reduce iteration counts (see Fig. 5). In [14], we extend the approach to 3D elastodynamics and show that it also very efficient.

These works have paved the way for new boundary domain decomposition strategies. Several important questions remain, including the choice of the most effective boundary integral formulations and the connection with analytic preconditioners [23, 24, 15]. Another key question concerns the optimal definition of overlapping domains. Finally, we plan to extend these techniques to transmission problems, in order to develop an efficient method for solving piecewise homogeneous domains without junction points.

4 Towards piecewise homogeneous domains

As illustrated in the previous section, the transfer of DDM techniques to BEMs is effective, even for multiple obstacles in homogeneous media. We conclude this review by outlining the key challenges that remain for BEMs to efficiently handle heterogeneous configurations, such as layered homogeneous media, based on some ongoing research.

4.1 Optimal discretization of layered domains: Boundary Mesh adaptation

The first challenge in addressing layered problems lies in discretizing the interfaces between media. Indeed, in integral equation discretization methods, all unknowns are condensed on these interfaces. Optimizing their discretization is therefore essential to achieve the highest possible computational efficiency. We are working on this challenge in collaboration with C. Tsogka (UC Merced), E. Cortes (UC Merced), and C. Carvalho (INSA Lyon).

For BEMs applied to wave propagation problems, a standard practice is to use meshes with around 10 points per wavelength. However, when dealing with problems involving multiple interfaces, a critical question arises: which wavelength should be used? To ensure robustness, the most restrictive wavelength is often adopted. Yet, from a physical standpoint, the field remains continuous at the interface, making excessive refinement unnecessary.

In [9], we start by investigating what could be learned from a circular configuration for which an analytical solution is available. We compare the sound-hard case with the transmission case for different configurations having the same interior/exterior contrast, but swapping the largest wavenumber, for instance with exterior/interior wavenumbers $k_{\text{ext}} = 2$ (resp. 6) and $k_{\text{int}} = 6$ (resp. 2). By examining the analytical solutions (Fig. 6), it becomes clear that they are very different, and therefore there is no reason to use the same mesh in all cases. As an additional illustration, to achieve an accuracy of 10^{-6} on the boundary, the sound-hard case indicates that 6 points per wavelength are required. However, when this criterion is applied to the transmission case, it leads to a number of boundary points that is significantly larger than what we observe in practice when using a trial-and-error approach on this analytic example.

It is clear from these examples that there is no simple *a priori* rule to determine the optimal number of discretization points on the interface. The only viable way to optimize the discretization, and thus reduce computational costs, is to rely on automatic mesh adaptation. While such techniques are well established for FEMs, they are much less developed for BEMs. Existing works [32] are either rather theoretical [1] or based on *a priori* strategies, but there is currently no approach that is unanimously adopted for BEMs. One possible direction is to rely on metric-based mesh adaptation [34].

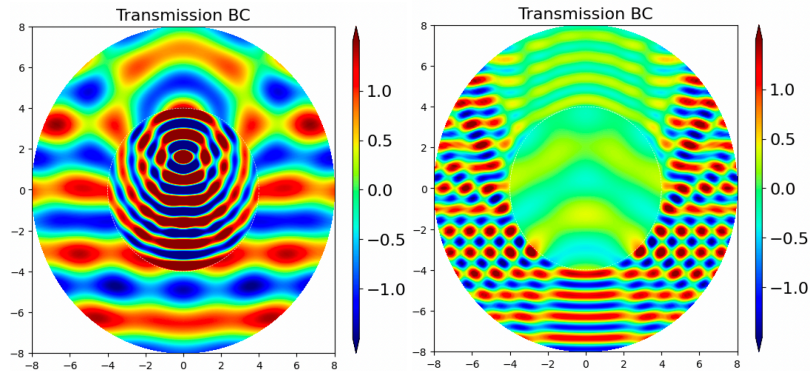


Fig. 6 Comparison of the real part of the total field analytic solutions for two contrasts. Left $k_{\text{ext}} = 2$ and $k_{\text{int}} = 6$. Right $k_{\text{ext}} = 6$ and $k_{\text{int}} = 2$. Result from [9].

Metric-based mesh adaptation can be formulated as the following optimization problem: find the optimal mesh with N vertices that minimizes the interpolation error. However, this problem is intractable in its direct form. For volumetric problems, it has been shown that this error can be minimized by leveraging the Hessian of the solution. By defining a new inner product, a direct relationship between the Hessian and the metric is established. The mesh adaptation process is ultimately a nonlinear problem. To solve it, an iterative procedure is employed, coupling the mesh and the solution at each step. In [17], we extended these techniques to 3D Helmholtz BEMs, demonstrating both their theoretical robustness and numerical efficiency, especially for complex geometries with singularities.

Despite the fact that BEMs primarily involve solving integral equations on interfaces, the optimal mesh for integral representation remains crucial, particularly in layered media. Given that simple *a priori* rules fail to capture the complexity of such configurations, we apply a metric-based mesh adaptation strategy. To accurately capture the intricate behavior of wave propagation between layers, we introduce a volumetric mesh. This approach highlights the influence of volume propagation on the optimal mesh at interfaces, demonstrating the necessity for an automatic mesh adaptation method. Validation against analytical solutions confirms the robustness of our approach for layered configurations [9]. Furthermore, this work underscores a specific need within the BEM community: the precise calculation of nearly singular integrals for accurate evaluation of boundary integral representations.

4.2 Multi-trace formalism

While significant progress has been made in addressing piecewise homogeneous wave propagation problems using BEMs, this review highlights that further advance-

ments are still required to develop efficient and scalable solutions for large-scale and realistic applications. In this final section, we discuss promising avenues to achieve these goals.

At the interfaces between domains, two conditions must be enforced: the continuity of the field and the compatibility of its Neumann trace (or traction in elasticity). A common approach is to use a P_0 discretization for the Neumann trace and a P_1 discretization for the Dirichlet trace. However, this choice introduces challenges in formulating the coupled system. For instance, collocation-based discretizations result in non-symmetric systems. While linear combinations of rows can restore a square system, not all combinations are equivalent, as discussed in [11].

The Multi-Trace Formulation (MTF), introduced a decade ago [20, 30], addresses these challenges by decoupling unknowns at interfaces to retain a square system. Although this approach requires additional computations, it provides a rigorous theoretical framework, optimizing convergence and iteration counts while enabling the design of effective preconditioners [40]. It enforces Calderón identities locally and imposes transmission conditions weakly across interfaces, offering compatibility with operator preconditioning techniques and facilitating multiphysics coupling. However, its adoption remains limited to the applied mathematics community due to its complex theoretical foundations and the intricacies of implementation. Recent works have made significant strides in bridging this gap. In [19], a clear link between MTF and DDMs was established, while in [12], we demonstrate, using a 1D didactic example, the various steps of the method and extend it to 2D elastodynamics.

Another critical issue in piecewise homogeneous domains is the treatment of junction points, which the MTF formalism elegantly addresses. Recent publications have further advanced this area, applying the MTF to Optimized Schwarz Methods [21] and FEM-BEM coupling [4]. Looking ahead, a critical priority for the community is the development of robust, user-friendly libraries, similar to those established in the DDM community. These libraries would not only democratize access to MTF methods but also catalyze practical research into optimizing preconditioners and adaptive mesh techniques for BEMs in layered homogeneous domains.

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