

# A Class of Iterative Solvers for the Helmholtz Equation: Factorizations, Sweeping Preconditioners, Source Transfer, Single Layer Potentials, Polarized Traces, and Optimized Schwarz Methods\*

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**Abstract.** Solving time-harmonic wave propagation problems by iterative methods is a difficult task, and over the last two decades an important research effort has gone into developing preconditioners for the simplest representative of such wave propagation problems, the Helmholtz equation. A specific class of these new preconditioners is considered here. They were developed by researchers with various backgrounds using formulations and notations that are very different, and all are among the most promising preconditioners for the Helmholtz equation.

The goal of the present article is to show that this class of preconditioners is based on a common mathematical principle, and that they can all be formulated in the context of domain decomposition methods known as optimized Schwarz methods. This common formulation allows us to explain in detail how and why all these methods work. The domain decomposition formulation also allows us to avoid technicalities in the implementation description we give of these recent methods.

The equivalence of these methods with optimized Schwarz methods translates at the discrete level into equivalence with approximate block LU decomposition preconditioners, and in each case we give the algebraic version, including a detailed description of the approximations used. While we choose to use the Helmholtz equation for which these methods were developed, our notation is completely general and the algorithms we give are written for an arbitrary second-order elliptic operator. The algebraic versions are even more general, assuming only a connectivity pattern in the discretization matrix.

All the new methods studied here are based on sequential decomposition of the problem in space into a sequence of subproblems, and they have in their optimal form the property to lead to nilpotent iterations, like an exact block LU factorization. Using our domain decomposition formulation, we finally present an algorithm for two-dimensional decompositions, i.e., decompositions that contain cross points, which is still nilpotent in its optimal form. Its approximation is currently an active area of research, and it would have been difficult to discover such an algorithm without the domain decomposition framework.

**Key words.** Helmholtz, iterative, preconditioner, factorization, sweeping, Schwarz

**AMS subject classifications.** 65N55, 65N22, 65F10

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\*Received by the editors October 7, 2016; accepted for publication (in revised form) January 29, 2018; published electronically February 7, 2019.

<http://www.siam.org/journals/sirev/61-1/M109781.html>

**Funding:** The work of the first author was supported by the Swiss National Science Foundation SNF (200020.168999/1). The work of the second author was supported by Zhejiang Provincial Natural Science Foundation of China (LY17A010014), Natural Science Foundation of China (11671074, 11771313, 11771398), and research start funding of Zhejiang Ocean University.

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**I. Introduction.** Solving the Helmholtz equation numerically for moderate to high wavenumbers is a difficult task, and very different from solving Laplace-like problems. This is due to three main reasons: First, Helmholtz problems are often posed on unbounded domains, which have to be artificially truncated to perform computations on finite computers, or by using Green's functions; see, e.g., [21, 134]. Second, one needs to have a much higher mesh resolution than what would usually be required to represent the solution because of the so-called pollution effect [5, 106, 182]. Finally, one must then solve the resulting very large scale system of linear equations, for which classical iterative methods are not suitable [55, 59]. Our focus here is on a class of recently developed novel iterative solvers for the Helmholtz equation based on sequential decompositions in space. Many research groups around the world have focused on developing such solvers, and for practitioners, and even specialists, it is

not easy to keep up with these developments and to grasp important novelties in these methods. The main reason for this is that these new methods are sometimes formulated at the continuous level, sometimes at the discrete level, sometimes using integral formulations, and sometimes using volume discretizations, and the groups developing these methods come from different backgrounds and use different motivations, intuitions, and notation when formulating their methods. Furthermore, most of these new methods require absorbing boundary conditions or perfectly matched layers for their formulation, which are ingredients that are not commonly encountered in classical iterative methods for Laplace-like problems.

The purpose of this article is to first describe in simple terms the main underlying fundamental algorithms for the new class of methods based on sequential decompositions in space. At the continuous level, the underlying algorithms are optimal and optimized Schwarz methods, and at the discrete level, the underlying algorithms are exact and approximate block LU factorizations. This first, relatively short part gives the main insight needed to understand the new Helmholtz solvers in a simplified and nontechnical setting. In the second, main part, we then rigorously show how members of this new class of Helmholtz solvers are tightly related. To do so, we introduce a compact notation that allows us to formulate all these new techniques, and we give for each one first the original formulation given by the authors, and then equivalent formulations at the continuous and discrete levels in the form of the fundamental underlying algorithms, for which we can prove equivalence results. We hope that our article will help people working in this challenging area of numerical analysis to rapidly understand this new class of algorithms and their potential.

**2. Underlying Fundamental Algorithms.** We start by explaining two fundamental algorithms which are very much related, one at the discrete level and one at the continuous level. These algorithms are the key ingredient in all the recent iterative methods proposed for the Helmholtz equation. Even though these algorithms can be formulated for other partial differential equations (PDEs) and all our equivalence results still hold, we use first the Helmholtz equation in its simplest form to explain them, namely,

$$(1) \quad (\Delta + k^2)u = f \quad \text{in } \Omega := (0, 1) \times (0, 1),$$

with suitable boundary conditions to make the problem well-posed.<sup>1</sup> Discretizing (1) using a standard five point finite difference discretization for the Laplacian on an equidistant grid leads to the linear system of equations

$$(2) \quad \begin{bmatrix} D_1 & U_1 & & \\ L_1 & D_2 & U_2 & \\ & \ddots & \ddots & \ddots \\ & & L_{J-2} & D_{J-1} & U_{J-1} \\ & & & L_{J-1} & D_J \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{J-1} \\ u_J \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{J-1} \\ f_J \end{bmatrix},$$

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<sup>1</sup>We use this simplest form of the Helmholtz equation to start with, then treat in the main part of the article the more complete formulation given in (11).

where  $D_j = \text{tridiag}(\frac{1}{h^2}, -\frac{4}{h^2} + k^2, \frac{1}{h^2})$ ,<sup>2</sup>  $L_j = U_j = \text{diag}(\frac{1}{h^2})$ . The block LU factorization of the coefficient matrix in (2) is given by

$$(3) \quad A = \begin{bmatrix} T_1 & & & \\ L_1 & T_2 & & \\ & \ddots & \ddots & & \\ & & L_{J-2} & T_{J-1} & \\ & & & L_{J-1} & T_J \end{bmatrix} \begin{bmatrix} I_1 & T_1^{-1}U_1 & & & \\ & I_2 & T_2^{-1}U_2 & & \\ & & \ddots & \ddots & \\ & & & I_{J-1} & T_{J-1}^{-1}U_{J-1} \\ & & & & I_J \end{bmatrix},$$

where the  $T_j$ 's are the Schur complements<sup>3</sup> that satisfy the recurrence relation

$$(4) \quad T_1 = D_1, \quad T_j = D_j - L_{j-1}T_{j-1}^{-1}U_{j-1} \quad \text{for } j \geq 2,$$

as one can see by simply multiplying the two factors in (3) and comparing with the original matrix in (2). Using this factorization, we can solve (2) by first solving by forward substitution the block lower triangular system

$$(5) \quad \begin{bmatrix} T_1 & & & \\ L_1 & T_2 & & \\ & \ddots & \ddots & & \\ & & L_{J-2} & T_{J-1} & \\ & & & L_{J-1} & T_J \end{bmatrix} \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \vdots \\ \mathbf{v}_{J-1} \\ \mathbf{v}_J \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_{J-1} \\ \mathbf{f}_J \end{bmatrix},$$

and then solving by backward substitution the block upper triangular system

$$(6) \quad \begin{bmatrix} I_1 & T_1^{-1}U_1 & & & \\ & I_2 & T_2^{-1}U_2 & & \\ & & \ddots & \ddots & & \\ & & & I_{J-1} & T_{J-1}^{-1}U_{J-1} & \\ & & & & I_J & \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_{J-1} \\ \mathbf{u}_J \end{bmatrix} = \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \vdots \\ \mathbf{v}_{J-1} \\ \mathbf{v}_J \end{bmatrix}.$$

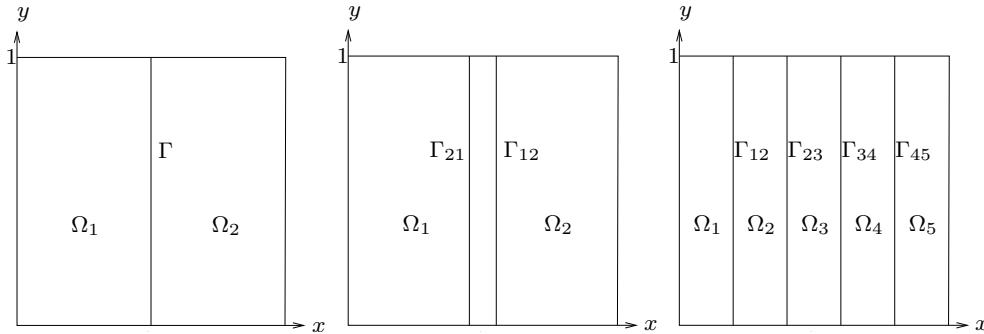
This shows that one forward sweep (forward substitution) and one backward sweep (backward substitution) are enough to solve the linear system, and this is the fundamental underlying idea of the new “sweeping algorithms” for the Helmholtz equation mentioned in the title. This becomes a preconditioner if the block LU factorization is approximated by using approximate Schur complement matrices instead of the exact matrices. If we use the exact matrices, then the iteration converges in one step and thus the iteration matrix is nilpotent of degree (or index) one. One can, however, already see another one of the new algorithms here by taking a closer look at the forward substitution in (5): solving the first equation, and substituting the result into the second one, and the result obtained into the third one, and so on, we find

$$(7) \quad \begin{aligned} \mathbf{v}_1 &= T_1^{-1}\mathbf{f}_1, \\ \mathbf{v}_2 &= T_2^{-1}(\mathbf{f}_2 - L_1\mathbf{v}_1) = T_2^{-1}(\mathbf{f}_2 - L_1T_1^{-1}\mathbf{f}_1) =: T_2^{-1}\tilde{\mathbf{f}}_2, \\ \mathbf{v}_3 &= T_3^{-1}(\mathbf{f}_3 - L_2\mathbf{v}_2) = T_3^{-1}(\mathbf{f}_3 - L_2T_2^{-1}\tilde{\mathbf{f}}_2) =: T_3^{-1}\tilde{\mathbf{f}}_3, \\ &\vdots && \vdots && \vdots \end{aligned}$$

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<sup>2</sup>We assume homogeneous Dirichlet boundary conditions and well-posedness for simplicity to start with; see section 4 for more information.

<sup>3</sup>For now, we also assume here for simplicity that the  $T_j$ 's are invertible.



**Fig. 1** Domain decompositions of the unit square: without or with overlap, and many subdomains.

where we introduced new source terms  $\tilde{f}_2 := f_2 - L_1 T_1^{-1} f_1$ ,  $\tilde{f}_3 := f_3 - L_2 T_2^{-1} \tilde{f}_2, \dots$  to make the solve for  $v_2, v_3, \dots$  look like the first solve for  $v_1$ . These new source terms contain a transferred source term from the previous line,

$$\tilde{f}_j := f_j - L_{j-1} T_{j-1}^{-1} \tilde{f}_{j-1},$$

which is the feature that led to the so-called source transfer methods mentioned in the title. Note that  $v_J = u_J$ , so after the forward substitution, the last set of unknowns is already the exact solution, a property that will be used later by some algorithms.

In the form in which we presented the block LU decomposition, the diagonal blocks only contained one grid line of unknowns, but one could also collect several grid lines into one block. This suggests looking at the problem at the continuous level, where we decompose the domain into subdomains, as illustrated in Figure 1. For the first decomposition on the left, which would correspond to only two large diagonal blocks at the discrete level, an optimal parallel Schwarz algorithm is given by the iterative method (see [53, 133]) for arbitrary initial guess  $u_1^0, u_2^0$ ,

$$(8) \quad \begin{aligned} (\Delta + k^2)u_1^n &= f && \text{in } \Omega_1, \\ \partial_{\mathbf{n}_1} u_1^n + \text{DtN}_1(u_1^n) &= \partial_{\mathbf{n}_1} u_2^{n-1} + \text{DtN}_1(u_2^{n-1}) && \text{on } \Gamma, \\ (\Delta + k^2)u_2^n &= f && \text{in } \Omega_2, \\ \partial_{\mathbf{n}_2} u_2^n + \text{DtN}_2(u_2^n) &= \partial_{\mathbf{n}_2} u_1^{n-1} + \text{DtN}_2(u_1^{n-1}) && \text{on } \Gamma, \end{aligned}$$

where  $\partial_{\mathbf{n}_j}$  denotes the outward normal derivative for subdomain  $\Omega_j$ , and  $\text{DtN}_j$  is the *Dirichlet-to-Neumann* (DtN) operator taking Dirichlet interface data on the interface  $\Gamma$  and returning the outward normal derivative of the corresponding solution of the Helmholtz equation on the exterior of the subdomain  $\Omega_j$ . This algorithm converges in two iterations, and thus the iteration operator is nilpotent of degree two, as one can easily understand as follows: Denoting by  $e_j^n := u - u_j^n$  the error at iteration  $n$ , this error satisfies by linearity the same equation as  $u_j^n$ , but with zero right hand side (r.h.s.),  $f = 0$ . Since, after the first iteration, the error  $e_j^1$  satisfies the equation in subdomain  $\Omega_j$ , its normal derivative at the interface will be exactly canceled by the DtN operator result when evaluating the r.h.s. on the interface  $\Gamma$  for the second iteration.<sup>4</sup> The error  $e_j^2$  then satisfies the equation in  $\Omega_j$  with homogeneous data and thus by uniqueness is zero, and so the algorithm has converged.

<sup>4</sup>The r.h.s. on the interface is in fact an exact or transparent boundary condition for the neighboring subdomain.

The optimal parallel Schwarz algorithm in (8) can also be run with overlap, as indicated in Figure 1 (middle), i.e.,

$$(9) \quad \begin{aligned} (\Delta + k^2)u_1^n &= f && \text{in } \Omega_1, \\ \partial_{\mathbf{n}_1} u_1^n + \text{DtN}_1(u_1^n) &= \partial_{\mathbf{n}_1} u_2^{n-1} + \text{DtN}_1(u_2^{n-1}) && \text{on } \Gamma_{12}, \\ (\Delta + k^2)u_2^n &= f && \text{in } \Omega_2, \\ \partial_{\mathbf{n}_2} u_2^n + \text{DtN}_2(u_2^n) &= \partial_{\mathbf{n}_2} u_1^{n-1} + \text{DtN}_2(u_1^{n-1}) && \text{on } \Gamma_{21}. \end{aligned}$$

The overlap has no influence on the two-step convergence property of the optimal parallel Schwarz method.<sup>5</sup> With  $J$  subdomains, as indicated in Figure 1 (right), the corresponding optimal parallel Schwarz algorithm

$$(10) \quad \begin{aligned} (\Delta + k^2)u_j^n &= f && \text{in } \Omega_j, \\ \partial_{\mathbf{n}_j} u_j^n + \text{DtN}_j(u_j^n) &= \partial_{\mathbf{n}_j} u_{j+1}^{n-1} + \text{DtN}_j(u_{j+1}^{n-1}) && \text{on } \Gamma_{j,j+1}, \\ \partial_{\mathbf{n}_j} u_j^n + \text{DtN}_j(u_j^n) &= \partial_{\mathbf{n}_j} u_{j-1}^{n-1} + \text{DtN}_j(u_{j-1}^{n-1}) && \text{on } \Gamma_{j,j-1}, \end{aligned}$$

converges in  $J$  iterations [133], and thus the iteration operator is nilpotent of degree  $J$ . At the discrete level, this result was also presented by F.-X. Roux at the IMACS conference in 2001. If, however, we organize the solves in sweeps, starting on the leftmost subdomain and going to the rightmost subdomain and back, i.e., sweeping once forward and once backward, the algorithm converges in one such double sweep, independent of the number of subdomains  $J$ , and thus the sweeping iteration operator becomes nilpotent of degree one. This algorithm is in fact the continuous analogue of the block LU factorization, with just the small modification that the DtN transmission condition on the right is replaced by the Dirichlet condition, as we will see later in section 7. Optimized Schwarz methods use approximations of the DtN operator and thus approximations of the transparent boundary condition, in the same spirit that approximate block LU factorizations use approximations to the Schur complement matrices. Well-known approximations of this type are *absorbing boundary conditions* (ABCs; cf. [49, 50, 96, 101]) and *perfectly matched layers* (PMLs; cf. [13, 31, 44, 99]).

**3. The Helmholtz Equation.** To be able to explain the details of recent iterative solvers for the Helmholtz equation, we need to consider a slightly more general Helmholtz equation than the simple model problem in (1), namely,

$$(11) \quad \mathcal{L}u := -\nabla^T(\alpha\nabla u) - \frac{\omega^2}{\kappa}u = f \text{ in } \Omega, \quad \mathcal{B}u = g \text{ on } \partial\Omega,$$

where  $\omega \in \mathbb{C}$ ,  $\Omega \subset \mathbb{R}^d$ ,  $d = 2, 3$ , is a bounded Lipschitz domain, the coefficient matrix  $\alpha$ , the scalar field  $\kappa$ , and the source  $f$  are all given complex-valued quantities varying on  $\Omega$ , and the unknown function  $u$  on  $\Omega$  is to be sought. In addition to the truly physical part, the domain  $\Omega$  may also contain artificial layers, for example, representing PMLs. The boundary condition  $\mathcal{B}u = g$  is piecewise defined on  $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_R \cup \overline{\Gamma}_V$  as follows:<sup>6</sup>

$$(12) \quad u = g_D \quad \text{on } \Gamma_D,$$

$$(13) \quad \mathbf{n}^T(\alpha\nabla u) + p_0 u = g_R \quad \text{on } \Gamma_R,$$

$$(14) \quad \mathbf{n}^T(\alpha\nabla u) + p_0 u + p_1 \mathbf{n}^T(\alpha\nabla_S u) - \nabla_S^T(q_1 \Pi_S(\alpha\mathbf{n})u + p_2 \alpha\nabla_S u) = g_V \quad \text{on } \Gamma_V,$$

<sup>5</sup>This will be different if one uses approximations of the DtN operators, as we will see.

<sup>6</sup>For simplicity, we assume either  $\Gamma_V = \emptyset$  or  $\Gamma_R = \emptyset$  and that  $\Gamma_V$  has no edges and corners.

where  $\mathbf{n}$  is the unit outer normal vector,  $\nabla_S$  is the surface gradient,  $p_0, p_1, q_1, p_2$  are complex-valued functions, and  $\Pi_S$  is the orthogonal projection onto the tangential plane of the surface. Besides acoustic waves, the Helmholtz equation (11) is also used to describe electromagnetics, where it can be derived from Maxwell's equations; see [134].

*Example 1.* In a typical geophysical application,  $\Omega$  is a rectangle in  $\mathbb{R}^2$  or a box in  $\mathbb{R}^3$ , obtained from truncation of the free space problem. The original time domain equation in free space is given by

$$\frac{1}{c^2} \frac{\partial^2 \tilde{u}}{\partial t^2} - \rho \nabla_{\mathbf{x}}^T \left( \frac{1}{\rho} \nabla_{\mathbf{x}} \tilde{u} \right) = \tilde{f},$$

where  $c$  is the wave speed and  $\rho$  is the mass density, both dependent only on space,  $\tilde{u}$  is the pressure, and  $\tilde{f}$  is the space-time source term with compact support in  $\Omega^{phy} \subset \Omega$  at all times.  $\Omega^{phy}$  is the domain in which the solution is of interest. We make the ansatz that  $\tilde{f}(\mathbf{x}, t)$  is a superposition of the time-harmonic sources  $\rho(\mathbf{x}) f(\mathbf{x}, \omega) e^{-i\omega t}$ . Then, for each  $\omega$ , the corresponding mode  $u(\mathbf{x}, \omega) e^{-i\omega t}$  satisfies

$$-\frac{\omega^2}{\rho c^2} u - \nabla_{\mathbf{x}}^T \left( \frac{1}{\rho} \nabla_{\mathbf{x}} u \right) = f.$$

The time domain solution  $\tilde{u}(\mathbf{x}, t)$  is the sum of the time-harmonic modes  $u(x, \omega)$  over all possible values of  $\omega$ . Note that  $\omega$  is the time *frequency*,  $k := \frac{\omega}{c}$  is called the *wavenumber*, and the *wavelength* is  $\lambda = \frac{2\pi}{k}$ . A certain boundary condition along infinity is imposed to exclude energy incoming from infinity and to allow energy outgoing to infinity, viewed from  $\Omega^{phy}$ . An example is the Sommerfeld radiation condition (cf. [154, p. 189]) in a homogeneous medium,

$$(15) \quad \lim_{|\mathbf{x}| \rightarrow \infty} |\mathbf{x}|^{\frac{d-1}{2}} (\partial_{|\mathbf{x}|} u - i k u) = 0.$$

Since we are interested in only the near-field solution (i.e., in  $\Omega^{phy}$ ), the free space model is truncated to  $\Omega^{phy}$  by imposing on  $\partial\Omega^{phy}$  artificial boundary conditions or artificial layers, which leads to (11).

*Example 2.* Some models have physical boundaries from special materials, which leads directly to a boundary condition, e.g., Dirichlet for sound soft and Neumann for sound hard matter in acoustics. As a simple model, one can consider a parallel pipe open in one dimension and closed with walls in the other dimensions on which Dirichlet, Neumann, or artificial boundary conditions (layers) are imposed. We further truncate the open dimension to obtain (11). The truncated dimension is typically still much larger than the other dimensions such as for optical waveguides; see [125].

*Example 3.* An important class of models is that of the so-called scattering problems which are posed on an unbounded domain exterior to obstacles delimited by physical boundaries. A given incident wave then hits the obstacles and is scattered. The sum of the incident wave and the scattered wave gives the total wave field which satisfies homogeneous Dirichlet, Neumann, or impedance boundary conditions as shown in (12) and (13) on the physical boundaries. The scattered wave field satisfies the homogeneous Helmholtz equation and some condition along infinity. Usually, this is the Sommerfeld radiation condition given in (15) based on the assumption that the

medium is homogeneous outside a bounded region. The unbounded domain is truncated to a bounded region near the obstacles, which results in (11). Once the Dirichlet and Neumann traces of the solution are known on some surface, the solution in the far-field, i.e., far away from the obstacles, can be recovered using a representation formula; see [134].

*Remark 4.* The algorithms to be discussed in this paper are applicable not only to the model (11) but also to more complicated cases as long as the PDE and the boundary conditions are defined locally in space such that they make sense in subsets of  $\Omega$  and  $\partial\Omega$ . For instance, we can supplement (14) with edge and corner conditions (see [7]) or use high-order absorbing boundary conditions localized with auxiliary unknowns (see [33, 97]) which can also be viewed as semidiscretized PMLs (see [45, 92]), and solve other PDEs (see, e.g., [130]). This will become clearer in the following sections.

We will occasionally need the weak formulation of (11) in appropriate function spaces; see, e.g., Lemma 10. Multiplying both sides of (11) with the complex conjugate of an arbitrary function  $v$  and integrating by parts in  $\Omega$ , we find formally

$$\int_{\Omega} (\alpha \nabla u)^T \nabla \bar{v} - \frac{\omega^2}{\kappa} u \bar{v} - \int_{\partial\Omega} \mathbf{n}^T (\alpha \nabla u) \bar{v} = \int_{\Omega} f \bar{v}.$$

Substituting the boundary conditions from (12)–(14) into the above equation leads us to the following weak formulation of (11):

$$(16) \quad \text{find } u - \mathcal{E}g_D \in V, \text{ such that } a(u, v) + b(u, v) = c(v) \quad \forall v \in V,$$

where  $\mathcal{E}g_D$  is an extension of  $g_D$  and

$$\begin{aligned} V &:= \{v \in H^1(\Omega) : v|_{\Gamma_D} = 0, v|_{\Gamma_V} \in H^1(\Gamma_V)\}, \quad \|v\|_V = \sqrt{\|v\|_{H^1(\Omega)}^2 + \|v\|_{H^1(\Gamma_V)}^2}, \\ a(u, v) &:= \int_{\Omega} (\alpha \nabla u)^T \nabla \bar{v} - \frac{\omega^2}{\kappa} u \bar{v}, \\ b(u, v) &:= \int_{\Gamma_R \cup \Gamma_V} p_0 u \bar{v} + \int_{\Gamma_V} p_1 \mathbf{n}^T (\alpha \nabla_S u) \bar{v} + \int_{\Gamma_V} (q_1 \Pi_S(\alpha \mathbf{n}) u + p_2 \alpha \nabla_S u)^T \nabla_S \bar{v}, \\ c(v) &:= V' \langle f, v \rangle_V + {}_{H^{-\frac{1}{2}}} \langle g_R, v|_{\Gamma_R} \rangle_{H^{\frac{1}{2}}} + {}_{H^{-\frac{1}{2}}} \langle g_V, v|_{\Gamma_V} \rangle_{H^{\frac{1}{2}}}. \end{aligned}$$

The well-posedness of (16) can be ensured by the following simultaneous assumptions:

- (i)  $\alpha, \frac{\omega^2}{\kappa}$  are uniformly bounded in  $\Omega$ , and so are  $p_0, p_1, q_1, p_2$  in their domains;
- (ii) there exist constants  $C_1, C_2, C_3 > 0$  independent of  $u$  such that

$$\left| \int_{\Omega} (\alpha \nabla u)^T \nabla \bar{u} + \int_{\Gamma_V} p_2 (\alpha \nabla_S u)^T \nabla_S \bar{u} + C_2 \int_{\Omega} |u|^2 + C_3 \int_{\Gamma_V \cup \Gamma_R} |u|^2 \right| \geq C_1 \|u\|_V^2;$$

(iii)  $a(u, u) + b(u, u) = 0$  and  $g_D \equiv 0$  together imply  $u \equiv 0$ ;

(iv)  $f \in V'$ ,  $g_D \in H_{00}^{\frac{1}{2}}(\Gamma_D)$ ,  $g_R \in H^{-\frac{1}{2}}(\Gamma_R)$ ,  $g_V \in H^{-\frac{1}{2}}(\Gamma_V)$ .

We refer the reader to [164] for the definitions of the function spaces and the well-posedness, which is based on the Lax–Milgram lemma and the Fredholm alternative.

**4. Direct and Iterative Solvers.** After discretization of (11), we obtain the linear system

$$(17) \quad A\mathbf{u} = \mathbf{f},$$

where  $A$  is an  $N$ -by- $N$  matrix,  $\mathbf{u}$  is the solution to be sought, and  $\mathbf{f}$  is given.

Gaussian elimination is probably the oldest<sup>7</sup> and the most fundamental solver for linear algebraic systems like (17). Its modern form consists in first computing the LU factorization  $A = RPLUQ$  with  $R$  a row scaling diagonal matrix,  $L$  ( $U$ ) being lower (upper) triangular, and  $P$  ( $Q$ ) being row (column) permutations, and then solving  $L\mathbf{v} = P(R^{-1}\mathbf{f})$  and  $U(Q\mathbf{u}) = \mathbf{v}$ . For a dense matrix  $A$ , e.g., from boundary element or spectral discretizations, the factorization requires  $\mathcal{O}(N^3)$  flops and  $\mathcal{O}(N^2)$  storage, and the triangular solves cost  $\mathcal{O}(N^2)$  flops. For a sparse matrix  $A$ , e.g., from a low-order finite element discretization, one can benefit from the nonzero structure of the entries of  $A$  by ordering the eliminations such that as few nonzeros as possible are generated in  $L$  and  $U$ , because the number of nonzeros determines the storage and time complexities of the triangular solves; see, e.g., [39, 47]. Doing so on two-dimensional regular meshes, we need  $\mathcal{O}(N^{3/2})$  flops for a sparse factorization, and the  $L, U$  factors one obtains have  $\mathcal{O}(N \log N)$  nonzeros; see [86, 104]. On three-dimensional regular meshes, we need  $\mathcal{O}(N^2)$  flops and get  $\mathcal{O}(N^{4/3})$  nonzeros in  $L, U$ ; see [39, p. 143]. Significant progress has been made on reducing the actual constants hidden in the asymptotic complexities which is nowadays coded in widely used software packages like UMFPACK [38], PARDISO [150], SuperLU [117], and MUMPS [2]. The classical, factorization-based direct solvers aim at the exact solution and introduce no error in the algorithms other than round-off errors due to finite precision arithmetic. They have been proved in practice to be robust for various problems, and they are robust with respect to problem parameters. Moreover, they are very advantageous for multiple r.h.s., because the factorization can be reused for different r.h.s. just performing triangular solves, which is much faster than the factorization stage.

The drawbacks of direct solvers are the superlinear complexities they have in time and storage requirements, and also the important communication overhead in a parallel environment in both the factorization and the triangular solution stages.

A recent trend of direct solvers is their introducing low rank truncation of some off-diagonal dense blocks arising in the process of factorization. This is accomplished by  $\mathcal{H}$ -matrix techniques [8, 9, 10, 11, 93, 94] and related approaches [22, 88, 103, 126, 127, 170, 171, 172, 173, 175]. The numerical low rank property depends on the Green's function of the underlying PDE. In particular, for the Helmholtz equation, the numerical rank can be shown to grow in specific geometric conditions in two dimensions only logarithmically with the wavenumber (see [51, 127]). In general, however, as indicated in [9, p. 157], the growth seems to be linear in the wavenumber. In [95], the author says that there are two types of off-diagonal blocks: one type is small and can be treated easily by  $\mathcal{H}$ -matrix arithmetic, and the other type is large and is better treated by a multipole expansion; see [8] for more details. Recently, [54] gave lower and upper bounds for the separability of Green's function. Nearly linear complexities for two-dimensional Helmholtz problems have been presented in, e.g., [8, 88, 103, 126, 127, 170, 175], with fixed or increasing wavenumbers. For three-dimensional Helmholtz problems, although considerable improvements over classical direct solvers have been made using  $\mathcal{H}$ -matrix techniques, the numerical experiments

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<sup>7</sup>Gaussian elimination can even be found in ancient Chinese scripts [122].

in [171, 173] show that the time complexity of factorization tends to  $\mathcal{O}(N^{5/3}) \sim \mathcal{O}(N^2)$  at high wavenumber on proportionally refined meshes.

In contrast to direct solvers which deliver very accurate solutions in a finite number of operations, iterative solvers start from an initial guess and improve the accuracy successively by iteration. Iterative solvers have become a core area of research in numerical analysis.<sup>8</sup> The central issue in designing an iterative solver is finding an approximation of  $A^{-1}$  which is called *preconditioner*. In this sense, the direct solvers with low rank truncation mentioned in the previous paragraph can be used as preconditioners; see, e.g., [8, 51, 175]. The simplest way to use a preconditioner  $M^{-1} \approx A^{-1}$  is iterative refinement, also called Richardson iteration<sup>9</sup> or deferred correction:  $\mathbf{u} \leftarrow \mathbf{u} + M^{-1}(\mathbf{f} - A\mathbf{u})$ . More advanced are Krylov subspace methods; see [91, 145] for general introductions to iterative methods for linear systems. It is particularly difficult to design a fast iterative solver for the Helmholtz equation; see, e.g., the review papers [3, 55, 59]. The main challenge is to accomplish  $\mathcal{O}(N)$  time complexity for increasing frequency  $\omega$  of (11) on appropriately refined meshes; an easier goal is the linear complexity under mesh refinement for fixed frequency, because this does not add more propagating waves to the solution. To tackle the special difficulties of the Helmholtz equation, many techniques have been developed and integrated into three major frameworks: incomplete factorizations, (algebraic) multigrid, and domain decomposition. We will now briefly review some of these techniques.

The shifted-Laplace preconditioner  $M_\epsilon^{-1}$ , proposed in [58, 109], introduces an imaginary shift  $\epsilon$  to the frequency  $\omega$  or  $\omega^2$  in the continuous problem given in (11), and  $M_\epsilon$  is obtained from a discretization of the shifted operator. The analyses in [32, 37, 59, 66, 166, 167] collectively exhibit a gap between the requirements that the shifted operator is close to the original operator and yet cheap to solve. In practice,  $\mathcal{O}(\omega^2)$  imaginary shifts to  $\omega^2$  are often used. In this case, it is easy to find an iterative solver  $\tilde{M}_\epsilon^{-1}$  of  $\mathcal{O}(N)$  complexity for  $M_\epsilon$  for any  $\omega$ ; but  $M_\epsilon$  deviates from the original matrix  $A$  more and more as  $\omega$  increases, so that the iteration numbers for the original system with the preconditioner  $\tilde{M}_\epsilon^{-1}$  also grow with  $\omega$  and can be  $\mathcal{O}(\omega)$  for the truncated free space problem or even  $\mathcal{O}(\omega^2)$  in the case of a waveguide [32]. In the former case, we observed from numerical experiments in [14, 26, 36, 57, 90] that for two-dimensional problems with  $N = \mathcal{O}(\omega^2)$  the overall time complexity becomes  $\mathcal{O}(N^{3/2})$ , and in [20, 36, 144] that for three-dimensional problems with  $N = \mathcal{O}(\omega^3)$  it seems to be  $\mathcal{O}(N^{4/3})$ . Even though not optimal, for three-dimensional models and  $\mathcal{O}(1)$  r.h.s. these iterative solvers can be faster than a complete factorization.

To accelerate convergence of iterations, an important idea is identifying the slowly convergent components of the errors and the corresponding residuals, and projecting them out from the iterates by solving the original problem restricted to the corresponding subspace. This is called coarse correction or deflation. When these slowly convergent coarse components are, however, based on a grid discretization, then for the Helmholtz equation the coarse problem for projection needs to be *fine* enough, typically of dimension  $\mathcal{O}(\omega^2)$  in two dimensions and  $\mathcal{O}(\omega^3)$  in three dimensions, to keep the convergence independent of  $\omega$ ; see, e.g., [19, 116] for convergence theory with such rich coarse problems. This excessive requirement manifests inadequacy of the basic iterations presumed in  $\mathcal{O}(N)$  time for oscillatory waves. Of course, the more time we

<sup>8</sup>Trefethen [165]: “The name of the new game is *iteration with preconditioning*. Increasingly often it is not optimal to try to solve a problem exactly in one pass; instead, solve it approximately, then iterate.”

<sup>9</sup>The method Richardson proposed is much more sophisticated, including a relaxation parameter that changes with each iteration and is chosen to lead to an optimized polynomial [143].

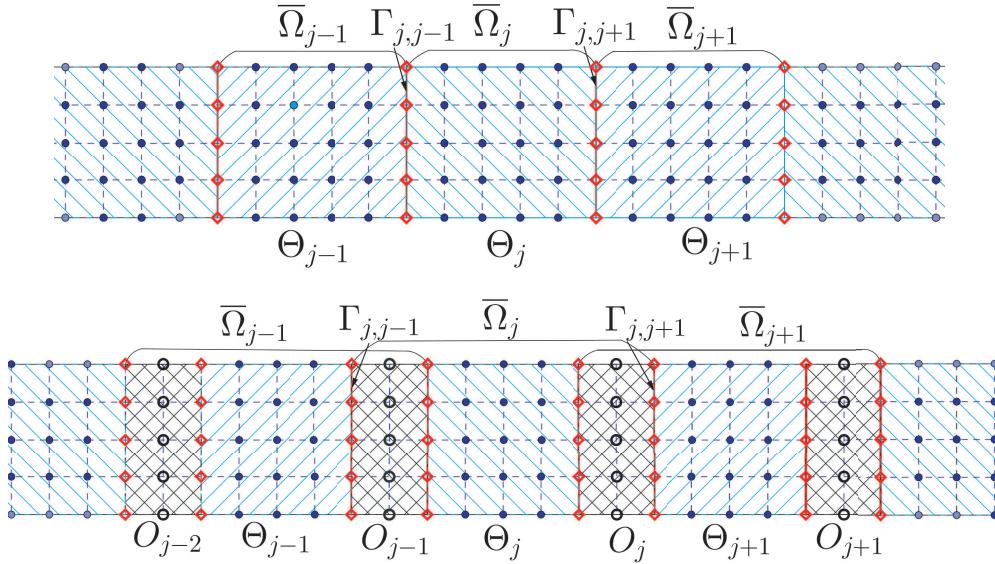
allocate to the basic underlying iteration, the smaller the coarse problem will be that we need to compensate for inadequacies of the basic iteration. Another approach is to try to develop an efficient solver for the coarse problem. For the shifted-Laplace preconditioner, multilevel Krylov with multigrid deflation was studied in [56, 152], and it was seen that the first coarse level (with mesh size twice as coarse as the finest level) needs to be solved more and more accurately to keep iteration numbers from growing as  $\omega$  increases. Another direction is to seek more efficient coarse problems. Those based on wave-ray or plane waves that originated from [16, 161] in the context of multigrid have become popular in algebraic multigrid methods (see, e.g., [136, 168]) and in domain decomposition methods (see, e.g., [40, 61, 81, 105]). Some recent developments include the bootstrap trick [123] to discover the slowly convergent subspace, the local eigenspaces [35] for heterogeneous media, and improvement in stability of the coarse problems [24, 159]. Complex-symmetric least squares formulations [89, 123, 136], numerical-asymptotic hybridization [138], and block Krylov methods for multiple r.h.s. [114] have also given further insight in the search for a scalable Helmholtz solver.

When applying domain decomposition methods (see, e.g., [42, 63, 115, 141, 153, 164]) to the Helmholtz equation, an immediate obstacle is the use of the usual Dirichlet or Neumann boundary conditions on subdomain interfaces. In particular, taking a diagonal block of  $A$ , one cannot ensure that it is nonsingular. For example, in the unit square  $(0, 1)^2$  with homogeneous Dirichlet boundary conditions, the negative Laplace operator  $-\Delta = -\partial_{xx} - \partial_{yy}$  has eigenvalues  $(n^2 + m^2)\pi^2$  ( $n, m = 1, 2, \dots$ ), so the Helmholtz operator  $-\Delta - k^2$  is singular if  $k^2$  is equal to one of these eigenvalues. This will not happen if a subdomain is sufficiently small, because the minimal eigenvalue will then be larger than the given  $k^2 \in \mathbb{R}$ : for example, in the square  $(0, H)^2$ , the minimal eigenvalue is  $2\pi^2/H^2$ , which can be made bigger than any given real number  $k^2$  when  $H$  is sufficiently small. This strategy was adopted in [19, 61, 116], but the coarse problems then become very large to maintain scalability with so many subdomains. Another natural treatment is regularization of subdomain problems with ABCs (or layers), which helps verify assumption (iii) in section 3. For example, letting  $\Delta u + k^2 u = 0$  in  $\Omega$  ( $k \in \mathbb{R}$ ) and  $\partial_n u + pu = 0$  on  $\partial\Omega$ , we have  $\int_{\Omega} |\nabla u|^2 - k^2 |u|^2 + \int_{\partial\Omega} p|u|^2 = 0$ ; if  $\text{Im } p \neq 0$ , we obtain  $\partial_n u = u = 0$  on  $\partial\Omega$  which implies  $u \equiv 0$  in  $\Omega$  by the unique continuation property (see [174]). The well-posedness of high-order ABCs can be found in, e.g., [166]. Regularization with a zeroth-order absorbing condition was first used by B. Després in his thesis [41] and later in, e.g., [17, 40, 62]. See [128] for a parallel numerical study with application to scattering problems. Actually, one gets even more from this choice: compared to the classical Schwarz method that uses Dirichlet transmission conditions, faster convergence was observed. This can be understood in the ideal case with *transparent* transmission conditions as we have seen in section 2 for the optimal Schwarz method [53, 133] motivated by the numerical study in [98]. Based on this principle, optimized Schwarz methods (see, e.g., [64] for an introduction, [67, 124, 140] for analyses, and [79, 80] for geometry-dependent optimization) leverage various approximations, i.e., absorbing transmission conditions or PMLs for fast convergence. For Helmholtz problems, the second-order Taylor expansion was used in [43], square-root based nonlocal conditions were studied in [34, 87], best approximations of zero and second order were sought in [30, 69, 76, 83, 84, 160], Padé approximants with complex-shifted wavenumbers were used in [15], PMLs were first employed in [148, 163], and recently some rational interpolants were tested in [110] for waveguide problems. For a numerical comparison of low-order and high-order transmission conditions for the overlapping Schwarz methods, we refer to [84].

Parallel to the development of optimized Schwarz methods, absorbing transmission conditions have also found use in the *analytic incomplete LU* (AILU) preconditioner; see [77, 78]. The idea is based on the identification of the DtN-based transparent transmission condition with the Schur complements arising in the block LU factorization we saw in section 2. An important improvement to the AILU preconditioner was made by the independent development in [52] using PML instead of the second-order approximation used in [78]. This triggered more studies on exploiting PML for the iterative solution of the Helmholtz equation in a forward and backward sweeping fashion; see, e.g., [28, 29, 60, 111, 139, 157, 169, 179, 180]. A recursive version that solves the two-dimensional subproblems in a three-dimensional domain recursively by decomposing them into one-dimensional lines and sweeping can be found in [120]; see also [178] for a similar idea. A recursive sweeping algorithm with low-order ABCs was proposed earlier [1]. Another double sweep process that extends the Dirichlet–Neumann alternating method [141] to many subdomains is proposed in [25]. In all these sweeping methods, there is little parallelism across the block solves, since the blocks (or subdomains) are passed through one by one, but in return an expensive coarse problem for connecting the blocks is avoided. Hence, the parallelism and the complexity within each block become crucial. In [139] for three-dimensional models, each block is kept quasi-two-dimensional with fixed thickness, and a tailored parallel direct solver for the quasi-two-dimensional problems is used. The sequential complexity was shown to be  $\mathcal{O}(\delta^2 N^{4/3})$  for the setup and  $\mathcal{O}(\delta N \log N)$  for the solve, where  $\delta = \delta(k)$  is the thickness of the discrete PML on one side of each block. Instead of PML, hierarchical matrix approximations can also be used; see [6, 51]. More recently, in an effort to parallelize the sweeping preconditioner, the authors of [119] proposed decomposing the source term into subdomains and then simulating its influence on the other subdomains by sweeping from that subdomain toward the first and the last subdomains. The final approximation is then obtained by adding the solutions corresponding to the different subdomain sources. The sweeping methods have also been combined with a two-level method in [158], and with the sparsifying preconditioner [176] for a volume integral reformulation of the Helmholtz equation in [121, 181].

The methods above based on approximation of transparent boundary conditions are currently among the most promising iterative methods for the Helmholtz equation and more general wave propagation phenomena. In the following sections, we will explain how these methods were invented while following various paths from very different starting points, and we give a formulation of each method in a common notation that allows us to prove that each of these methods is in fact a special optimized Schwarz method distinct only in transmission conditions, overlaps, and/or implementation. A first such relation between the source transfer method and an optimized Schwarz method was discovered in the proceedings paper [27], and further relations were pointed out in [82].

**5. Notation.** To make the analogy we have seen between the block LU factorization and the optimal Schwarz algorithm mathematically rigorous, and then to show precisely how all the new Helmholtz solvers are related to one another, requires a common notation that works for all formulations. This formulation must permit the simultaneous use of overlapping and nonoverlapping blocks or subdomains, Green’s function formulations and volume discretizations, and very general transmission conditions including ABCs and PMLs, and all this for both continuous and discrete formulations. We introduce the reader to this notation in this section, as we intro-



**Fig. 2** Nonoverlapping and overlapping domain decomposition,  $\bullet \in \Theta_*$ ,  $\circ \in O_*$ ,  $\diamond \in \Gamma_{*,\#}$ .

duce the fundamental concepts common to all algorithms step by step. The first steps in learning the notation will be hard, but it will be rewarding to be able to understand the details of all these new Helmholtz solvers and their tight relationships.

**5.1. Domain Decomposition.** As we have seen, the algorithms are based on a decomposition, and we introduce this decomposition for the original domain  $\Omega$  on which (11) is posed. We decompose  $\bar{\Omega}$  into serially connected subdomains  $\bar{\Omega}_j, j = 1, \dots, J$ , such that

$$(18) \quad \bar{\Omega} = \cup_{j=1}^J \bar{\Omega}_j, \quad \bar{\Omega}_j \cap \bar{\Omega}_l = \emptyset \text{ if } |j - l| > 1.$$

To simplify the notation for the algorithms, we also introduce at each end an empty subdomain,  $\Omega_0 = \Omega_{J+1} = \emptyset$ . We denote the overlap between the subdomains by  $O_j := \bar{\Omega}_j \cap \bar{\Omega}_{j+1}, j = 1, \dots, J-1$ , the interfaces by  $\Gamma_{j,j\pm 1} := \partial\Omega_j \cap \partial(\Omega_{j\pm 1} - \Omega_j)$ ,  $j, j \pm 1 \in \{1, \dots, J\}$ , and the nonoverlapping region within each subdomain by  $\Theta_j := \bar{\Omega}_j - (\bar{\Omega}_{j-1} \cup \bar{\Omega}_{j+1}), j = 1, \dots, J$ , as indicated in Figure 2. Note that this partition can be considered either for the continuous domain or for the discretized domain. At the discrete level, the domain decomposition is a partition of the d.o.f.  $\mathbf{u}$  of (17). Corresponding to that partition, we introduce the notion of index sets as shown in Table 1, which we chose to make it easier to remember them: for example, in the nonoverlapping case, we have for subdomain  $\Omega_j$  on the left boundary  $\mathbf{u}_{j\langle} = \mathbf{u}_{j]} = \mathbf{u}_{j\langle}$ , and similarly on the right boundary  $\mathbf{u}_{j\rangle} = \mathbf{u}_{j[} = \mathbf{u}_{j\rangle}$ , and the unknowns interior to subdomain  $\Omega_j$  are  $\mathbf{u}_{j\langle} = \mathbf{u}_{j\rangle}$ , where a dot always means only the interior unknowns, and we have equality because the overlap is empty. As another example, if  $\Theta_j \neq \emptyset$  in the overlapping case, we have  $\mathbf{u}_{j\langle} = [\mathbf{u}_{j\langle}; \mathbf{u}_{j\langle}; \mathbf{u}_{j\langle}; \mathbf{u}_{j\langle}; \mathbf{u}_{j\langle}]$ .<sup>10</sup> We denote by  $I_*^\#$  the 0-1 restriction or extension matrix from the set of d.o.f. indicated by  $\#$  to the

<sup>10</sup>We use MATLAB notation for concatenating column vectors vertically to avoid having to use the transpose symbol  $^T$ .

**Table I** Meaning of the subscripted vector  $\mathbf{v}_*$ .

Subscript *	Meaning of the vector $\mathbf{v}_*$
$j\langle$ or $j\langle$	$\bar{\Omega}_j$ : all the d.o.f. on the $j$ th subdomain $\bar{\Omega}_j$
$j\langle$	left interface of $\Omega_j$ : restriction of $\mathbf{v}_j$ to the interface $\Gamma_{j,j-1}$
$j\rangle$	right interface of $\Omega_j$ : restriction of $\mathbf{v}_j$ to the interface $\Gamma_{j,j+1}$
$j\langle\langle$	left overlap of $\Omega_j$ : restriction of $\mathbf{v}_j$ to the overlap $\bar{\Omega}_j \cap \bar{\Omega}_{j-1}$
$j\rangle\rangle$	right overlap of $\Omega_j$ : restriction of $\mathbf{v}_j$ to the overlap $\bar{\Omega}_j \cap \bar{\Omega}_{j+1}$
$j]$	end of left overlap in $\Omega_j$ : restriction of $\mathbf{v}_j$ to $\Gamma_{j-1,j}$
$j[$	end of right overlap in $\Omega_j$ : restriction of $\mathbf{v}_j$ to $\Gamma_{j+1,j}$
$j\langle\langle$ or $j\bullet$	interior unknowns of $\Omega_j$ : after removing $\mathbf{v}_{j\langle\langle}$ and $\mathbf{v}_{j\rangle}$ from $\mathbf{v}_{j\langle}$
$j\langle\bullet$	interior of left overlap of $\Omega_j$ : after removing $\mathbf{v}_{j\langle\langle}$ and $\mathbf{v}_{j]}$ from $\mathbf{v}_{j\langle}$
$j\rangle\bullet$	interior of right overlap of $\Omega_j$ : after removing $\mathbf{v}_{j[}$ and $\mathbf{v}_{j\rangle}$ from $\mathbf{v}_{j\rangle}$
$j\bullet\bullet$	interior without overlaps of $\Omega_j$ : after removing $\mathbf{v}_{j\langle\langle}$ and $\mathbf{v}_{j\rangle\rangle}$ from $\mathbf{v}_{j\langle}$
$\sim j$	everything to the left of $\Omega_j$ , i.e., all the d.o.f. in $(\cup_{m=1}^{j-1} \bar{\Omega}_m) - \bar{\Omega}_j$
$j\sim$	everything to the right of $\Omega_j$ , i.e., all the d.o.f. in $(\cup_{m=j+1}^J \bar{\Omega}_m) - \bar{\Omega}_j$

set indicated by \*. For example,  $I_{j\langle}^{j-1}$  is the restriction from  $\bar{\Omega}_{j-1}$  to  $\Gamma_{j,j-1}$ . For the identity matrix  $I_*^*$  we simply write  $I_*$ . A common restriction operator we will often use is  $R_* := I_*^{1,\dots,J}$ . Note that by  $\mathbf{v}_l$  and  $\mathbf{v}_j$  we do not mean in general the restriction  $\mathbf{v}_l = R_l \mathbf{v}$  and  $\mathbf{v}_j = R_j \mathbf{v}$  of a common  $\mathbf{v}$ , but that the components of  $\mathbf{v}_j$  correspond to the d.o.f. on  $\bar{\Omega}_j$ . Hence,  $I_{j\rangle}^j \mathbf{v}_j$  can be different from  $I_{j+1\langle}^{j+1} \mathbf{v}_{j+1}$ . Only for the exact solution  $\mathbf{u}$  and the r.h.s.  $\mathbf{f}$  of (17) do we use  $\mathbf{u}_j$  and  $\mathbf{f}_j$  for  $R_j \mathbf{u}$  and  $R_j \mathbf{f}$ . For submatrices of  $A$ , we also use the subscripts  $j[$  interchangeably with  $j+1\langle$  because they refer to the same index set in the global case, and similarly for  $j]$  and  $j-1\rangle$ .

If  $\Theta_j \neq \emptyset$  for  $j = 1, \dots, J$ , we assume that (17) has block tridiagonal structure<sup>11</sup> when the vector of unknowns is partitioned as  $\mathbf{u} = [\mathbf{u}_{1\bullet}; \mathbf{u}_{1\rangle}; \dots; \mathbf{u}_{J-1\rangle}; \mathbf{u}_{J\bullet}]$ , i.e.,

$$(19) \quad \begin{bmatrix} A_{1\bullet} & A_{1\bullet 1\langle} \\ A_{1\rangle 1\bullet} & A_{1\rangle} & A_{1\rangle 2\bullet} \\ \ddots & \ddots & \ddots \\ & A_{J-1\rangle J-1\bullet} & A_{J-1\rangle} & A_{J-1\rangle J\bullet} \\ & & A_{J\bullet J-1\bullet} & A_{J\bullet} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{1\bullet} \\ \mathbf{u}_{1\rangle} \\ \vdots \\ \mathbf{u}_{J-1\rangle} \\ \mathbf{u}_{J\bullet} \end{bmatrix} = \mathbf{f}.$$

For overlapping decompositions (i.e.,  $O_j \neq \emptyset$ ), we can also partition the overlap,  $\mathbf{u}_{j\rangle} = [\mathbf{u}_{j\langle}; \mathbf{u}_{j\rangle\bullet}; \mathbf{u}_{j\rangle}]$ , and similar to the block tridiagonal assumption, we assume that there are no direct interactions between d.o.f. across the interfaces, e.g.,

$$A_{j\rangle j\bullet} = 0, \quad A_{j\rangle j\langle} = 0, \quad A_{j[j+1\bullet]} = 0, \quad A_{j\rangle j+1\bullet} = 0.$$

In the nonoverlapping case we also use  $j\rangle$  for  $j\rangle$ , since the index sets  $\rangle$  and  $\rangle$  coincide in that case, and the same holds for  $\langle$  and  $\langle$ .

<sup>11</sup>This holds naturally for classical finite difference and finite element discretizations which approximate derivatives by only looking at neighboring nodes.

*Remark 5.* When  $\Theta_1, \Theta_J \neq \emptyset$ ,  $\Theta_j = \emptyset$  for  $j = 2, \dots, J - 1$ , and  $O_j \neq \emptyset$  for  $j = 1, \dots, J - 1$ , we assume (17) is block tridiagonal under the partition

$$\mathbf{u} = [\mathbf{u}_{1\langle}; \mathbf{u}_{1\langle}; \mathbf{u}_{1\langle}; \mathbf{u}_{1\rangle}; \mathbf{u}_{2\langle}; \mathbf{u}_{2\rangle}; \dots; \mathbf{u}_{J-1\langle}; \mathbf{u}_{J\langle}].$$

Then all our subsequent discussions on (19) can be adapted to this case without essential difference. This case corresponds to what is called *generous overlap* in domain decomposition, i.e., almost every subdomain consists of overlaps with neighbors:  $\Omega_j = O_{j-1} \cup \Gamma_{j-1,j} \cup O_j$  and  $\Gamma_{j+1,j} = \Gamma_{j-1,j}$  for  $j = 2, \dots, J - 1$ . For convenience, we will also denote  $O_0 := \Theta_1$  and  $O_J := \Theta_J$  for later use in subsection 8.1.

*Remark 6.* The algorithms we will discuss below also permit  $A_{j\langle l\rangle} \neq 0$  for  $|j-l|=1$ , which can happen, for example, for spectral element discretizations with only one spectral element over the entire subdomain width. However, we exclude this situation for simplicity in what follows.

*Remark 7.* The block tridiagonal form we assumed in (19) is natural if the d.o.f. in the overlap  $\overline{O}_j$  including its boundaries are the same and shared by  $\Omega_j$  and  $\Omega_{j+1}$ , i.e., the problem stems from a globally assembled problem. In domain decomposition, however, nonmatching grids are also common, and we may have two sets of d.o.f. in  $\overline{O}_j$ , one set  $\mathbf{u}_{j\langle}$  for  $\Omega_j$  and another set  $\mathbf{u}_{j+1\langle}$  for  $\Omega_{j+1}$ . In this case, when  $O_j \neq \emptyset$  we may assume (17) has the form of the *augmented system*

$$\left[ \begin{array}{cccccc} A_{1\langle} & A_{1\langle 1\rangle} & & & & \\ A_{1\langle 1\rangle} & A_{1\rangle} & A_{1\rangle 2\langle} & \boxed{A_{1\rangle 2\rangle}} & & \\ \boxed{A_{2\langle 1\rangle}} & A_{2\langle 1\rangle} & A_{2\rangle} & A_{2\rangle 2\langle} & & \\ & \ddots & \ddots & \ddots & \boxed{A_{J-1\rangle J\langle}} & \\ & & & & \boxed{A_{J\rangle J-1\langle}} & A_{J\rangle J-1\rangle} & A_{J\rangle} & A_{J\rangle J\langle} & A_{J\rangle J\langle} \\ & & & & & A_{J\langle J\langle} & A_{J\langle J\rangle} & A_{J\langle} & A_{J\langle} \end{array} \right] \begin{bmatrix} \mathbf{u}_{1\langle} \\ \mathbf{u}_{1\rangle} \\ \mathbf{u}_{2\langle} \\ \vdots \\ \mathbf{u}_{J\langle} \\ \mathbf{u}_{J\rangle} \end{bmatrix} = \mathbf{f},$$

which would be block tridiagonal if we removed the boxed blocks. This form also arises naturally from nonconforming discretizations in the overlaps and on the interfaces, e.g., from certain discontinuous Galerkin methods (see, e.g., [4]). It is possible to generalize our discussions to this case, but we would not gain more insight and will thus not do so here to avoid further complications in the notation.

**5.2. Transmission Conditions.** We now present the three fundamental types of transmission conditions used by the algorithms: Dirichlet, Neumann, and generalized Robin conditions. For the Dirichlet condition, based on the assumptions in subsection 5.1, if we take the rows for  $\mathbf{u}_{j\bullet}$  from (17), we find  $A_{j\bullet}\mathbf{u}_{j\bullet} = \mathbf{f}_{j\bullet} - A_{j\bullet j\langle}\mathbf{u}_{j\langle} - A_{j\bullet j\rangle}\mathbf{u}_{j\rangle}$ . We rewrite this as a linear system for  $\mathbf{u}_j$  with the interface data  $\mathbf{u}_{j\langle}$  and  $\mathbf{u}_{j\rangle}$  provided by the neighboring subdomains,

$$(20) \quad \begin{bmatrix} I_{j\langle} & & \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} \\ & I_{j\rangle} & \end{bmatrix} \begin{bmatrix} \mathbf{u}_{j\langle} \\ \mathbf{u}_{j\bullet} \\ \mathbf{u}_{j\rangle} \end{bmatrix} = \begin{bmatrix} \mathbf{u}_{j-1\langle} \\ \mathbf{f}_{j\bullet} \\ \mathbf{u}_{j+1\rangle} \end{bmatrix}.$$

At the continuous level, this corresponds to (11) localized to  $\Omega_j$  with Dirichlet transmission conditions on the interfaces,

$$(21) \quad \begin{aligned} \mathcal{L} u_j &= f && \text{in } \Omega_j, \\ \mathcal{B} u_j &= g && \text{on } \partial\Omega_j \cap \partial\Omega, \\ u_j &= u_{j-1} && \text{on } \Gamma_{j,j-1}, \\ u_j &= u_{j+1} && \text{on } \Gamma_{j,j+1}, \end{aligned}$$

where  $u_l := u|_{\Omega_l}$  ( $l = j, j \pm 1$ ). As mentioned before, the subdomain problem in (21) might not be well-posed if we replace  $u_j$  by  $v_j$  and then try to solve (21) for  $v_j$ . Similarly, the matrix in (20) might not be invertible.

For the Neumann condition, we split the diagonal block of  $A$  corresponding to the interface  $\Gamma_{j,j-1}$  into two parts as would arise naturally from the splitting of the bilinear forms in (16) in a conforming finite element method:  $A_{j\langle} = A_{j\langle}^{\rangle} + A_{j\langle}^{\langle}$ , where  $A_{j\langle}^{\rangle}$  is the contribution from the left side of  $\Gamma_{j,j-1}$  and  $A_{j\langle}^{\langle}$  is the contribution from the right side of  $\Gamma_{j,j-1}$ . The reader might wonder why we use the superscript  $\rangle$  here (`\rangleangle!`) for the contribution from the left and the superscript  $\langle$  for the contribution from the right. The reason is that the contribution from the right will be used on the left of the corresponding subdomain that uses it, and vice versa, and based on the assumptions in subsection 5.1, the rows from (17) for  $\mathbf{u}_j$  can then be written similar to the Dirichlet case in the form

$$(22) \quad \begin{bmatrix} A_{j\langle}^{\langle} & A_{j\langle}j\bullet & \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} \\ & A_{j\rangle j\bullet} & A_{j\rangle}^{\rangle} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{j\langle} \\ \mathbf{u}_{j\bullet} \\ \mathbf{u}_{j\rangle} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{j\langle} - A_{j\langle}j-1\bullet \mathbf{u}_{j-1\bullet} - A_{j\langle}^{\rangle} \mathbf{u}_{j-1\lceil} \\ \mathbf{f}_{j\bullet} \\ \mathbf{f}_{j\rangle} - A_{j\rangle}j+1\bullet \mathbf{u}_{j+1\bullet} - A_{j\rangle}^{\langle} \mathbf{u}_{j+1\lceil} \end{bmatrix},$$

and now the superscript looks very natural and easy to remember. Equation (22) corresponds to (11) localized to  $\Omega_j$  with Neumann transmission conditions on the interfaces,

$$(23) \quad \begin{aligned} \mathcal{L} u_j &= f && \text{in } \Omega_j, \\ \mathcal{B} u_j &= g && \text{on } \partial\Omega_j \cap \partial\Omega, \\ \mathbf{n}_j^T(\alpha \nabla u_j) &= \mathbf{n}_j^T(\alpha \nabla u_{j-1}) && \text{on } \Gamma_{j,j-1}, \\ \mathbf{n}_j^T(\alpha \nabla u_j) &= \mathbf{n}_j^T(\alpha \nabla u_{j+1}) && \text{on } \Gamma_{j,j+1}. \end{aligned}$$

In particular, we note that the discretization of  $-\mathbf{n}_j^T(\alpha \nabla u_j)$  on  $\Gamma_{j,j-1}$  gives  $\mathbf{f}_{j\langle}^{\langle} - A_{j\langle}^{\langle} \mathbf{u}_{j\langle} - A_{j\langle}j\bullet \mathbf{u}_{j\bullet}$  and the discretization of  $\mathbf{n}_j^T(\alpha \nabla u_{j-1})$  on  $\Gamma_{j,j-1}$  gives  $\mathbf{f}_{j\langle}^{\rangle} - A_{j\langle}^{\rangle} \mathbf{u}_{j-1\lceil} - A_{j\langle}j-1\bullet \mathbf{u}_{j-1\bullet}$ , where  $f_{j\langle} = f_{j\langle}^{\rangle} + f_{j\langle}^{\langle}$  is again the splitting of the contribution from the two sides of  $\Gamma_{j,j-1}$ . Note that as in the case of Dirichlet conditions, if we replace  $u_j$  by  $v_j$  in (23), the resulting subdomain problem might not be well-posed, and the matrix in (22) might not be invertible.

By generalized Robin transmission conditions, we mean the generalized linear combination of Dirichlet and Neumann conditions, i.e.,

$$(24) \quad \mathcal{Q}(\mathbf{n}_j^T(\alpha \nabla u_j)) + \mathcal{P}u_j = \mathcal{Q}(\mathbf{n}_j^T(\alpha \nabla u_l)) + \mathcal{P}u_l \text{ on } \Gamma_{j,l},$$

where  $\mathcal{Q}$  and  $\mathcal{P}$  are linear, possibly nonlocal operators along  $\Gamma_{j,l}$ ,  $l = j \pm 1$ . At the discrete level, this corresponds to a generalized linear combination of the interface

rows of (20) and (22), while the interior rows are unchanged, i.e.,

$$(25) \quad \begin{aligned} & \left[ \begin{array}{cc} Q_{j\langle}^{\langle} A_{j\langle}^{\langle} + P_{j\langle}^{\langle} & Q_{j\langle}^{\langle} A_{j\langle j\bullet} \\ A_{j\bullet j\langle} & A_{j\bullet} \\ Q_{j\rangle}^{\rangle} A_{j\rangle j\bullet} & Q_{j\rangle}^{\rangle} A_{j\rangle}^{\rangle} + P_{j\rangle}^{\rangle} \end{array} \right] \begin{bmatrix} \mathbf{u}_{j\langle} \\ \mathbf{u}_{j\bullet} \\ \mathbf{u}_{j\rangle} \end{bmatrix} \\ & = \begin{bmatrix} Q_{j\langle}^{\langle} (\mathbf{f}_{j\langle} - A_{j\langle j-1} \mathbf{u}_{j-1}) + (P_{j\langle}^{\langle} - Q_{j\langle}^{\langle} A_{j\langle}^{\langle}) \mathbf{u}_{j-1} \\ \mathbf{f}_{j\bullet} \\ Q_{j\rangle}^{\rangle} (\mathbf{f}_{j\rangle} - A_{j\rangle j+1} \mathbf{u}_{j+1}) + (P_{j\rangle}^{\rangle} - Q_{j\rangle}^{\rangle} A_{j\rangle}^{\rangle}) \mathbf{u}_{j+1} \end{bmatrix}. \end{aligned}$$

If  $Q_{j\langle}^{\langle} = I_{j\langle}$  and  $Q_{j\rangle}^{\rangle} = I_{j\rangle}$ , we can also rewrite (25) without the explicit splitting of  $A_{j\langle}$  and  $A_{j\rangle}$ ,

$$(26) \quad \begin{bmatrix} \tilde{S}_{j\langle}^{\langle} & A_{j\langle j\bullet} \\ A_{j\bullet j\langle} & A_{j\bullet} \\ A_{j\rangle j\bullet} & \tilde{S}_{j\rangle}^{\rangle} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{j\langle} \\ \mathbf{u}_{j\bullet} \\ \mathbf{u}_{j\rangle} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{j\langle} - A_{j\langle j-1} \mathbf{u}_{j-1} + (\tilde{S}_{j\langle}^{\langle} - A_{j\langle}^{\langle}) \mathbf{u}_{j-1} \\ \mathbf{f}_{j\bullet} \\ \mathbf{f}_{j\rangle} - A_{j\rangle j+1} \mathbf{u}_{j+1} + (\tilde{S}_{j\rangle}^{\rangle} - A_{j\rangle}^{\rangle}) \mathbf{u}_{j+1} \end{bmatrix},$$

where  $\tilde{S}_{j\langle}^{\langle} = A_{j\langle}^{\langle} + P_{j\langle}^{\langle}$  and  $\tilde{S}_{j\rangle}^{\rangle} = A_{j\rangle}^{\rangle} + P_{j\rangle}^{\rangle}$ . If we first specify  $\tilde{S}_{j\langle}^{\langle}$  and  $\tilde{S}_{j\rangle}^{\rangle}$ , then it is not necessary to introduce a splitting of  $A_{j\langle}$  and  $A_{j\rangle}$  to use (26).

We now consider a special case of (11): we assume that the data  $f$  and  $g$  are supported only on  $\bar{\Omega}_j$  and vanish elsewhere. Suppose we are interested in the solution of (11) in  $\Omega_j$  only. Then it would be desirable to have a problem equivalent to the original problem in (11) but defined just on the truncated domain  $\Omega_j$ . This can be done by setting a *transparent boundary condition* on the truncation boundary  $\partial\Omega_j - \partial\Omega$  and solving

$$(27) \quad \begin{aligned} \mathcal{L} u_j &= f && \text{in } \Omega_j, \\ \mathcal{B} u_j &= g && \text{on } \partial\Omega_j \cap \partial\Omega, \\ \mathbf{n}_j^T (\alpha \nabla u_j) + \text{DtN}_j u_j &= 0 && \text{on } \partial\Omega_j - \partial\Omega, \end{aligned}$$

where  $\text{DtN}_j$  is a linear operator defined as follows.

**DEFINITION 8.** *The Dirichlet-to-Neumann (DtN) operator exterior to  $\Omega_j \subset \Omega$  for (11) is*

$$(28) \quad \begin{aligned} \text{DtN}_j : d &\rightarrow -\mathbf{n}_j^T (\alpha \nabla v), \quad s.t. \quad \mathcal{L} v = 0 \quad \text{in } \Omega - \Omega_j, \\ &\quad \mathcal{B} v = 0 \quad \text{on } \partial\Omega - \partial\Omega_j, \\ &\quad v = d \quad \text{on } \partial\Omega_j - \partial\Omega, \end{aligned}$$

where  $\mathbf{n}_j$  is the unit outward normal vector of  $\Omega_j$ .

**Remark 9.** The DtN operator is an example of a Poincaré–Steklov operator referring to maps between different boundary data. According to [108, p. VI], this class of operators was first studied by V. A. Steklov [156] and H. Poincaré [137]. They are also related to the Calderon projectors; see, e.g., [134].

**LEMMA 10.** *Assume that  $f$  and  $g$  in (11) vanish outside  $\bar{\Omega}_j$ . If (28) has a unique solution  $v \in H^1(\Omega - \Omega_j)$  for  $d \in H^{1/2}(\partial\Omega_j - \partial\Omega)$  and (11) has a unique solution  $u \in H^1(\Omega)$ , then (27) also has a unique solution  $u_j \in H^1(\Omega_j)$ , and  $u_j = u|_{\Omega_j}$ .*

*Proof.* In Definition 8, we substitute  $u_j|_{\partial\Omega_j-\partial\Omega}$  for  $d$  and combine it with (27) to find

$$(29) \quad \begin{aligned} \mathcal{L}u_j &= f & \text{in } \Omega_j, & \mathcal{L}v = 0 & \text{in } \Omega - \Omega_j, \\ \mathcal{B}u_j &= g & \text{on } \partial\Omega_j \cap \partial\Omega, & \mathcal{B}v = 0 & \text{on } \partial\Omega - \partial\Omega_j, \\ \mathbf{n}_j^T(\alpha\nabla u_j) &= \mathbf{n}_j^T(\alpha\nabla v) & \text{on } \partial\Omega_j - \partial\Omega, & v = u_j & \text{on } \partial\Omega_j - \partial\Omega. \end{aligned}$$

This coupled system for  $(u_j, v)$  has at least one solution  $(u|_{\Omega_j}, u|_{\Omega-\Omega_j})$ . For uniqueness, we set  $f := 0$  and  $g := 0$  and show that  $u_j \equiv 0$  if  $u_j \in H^1(\Omega_j)$ : similar to (16), we test the PDE satisfied by  $u_j$  and  $v$  separately with arbitrary  $w \in V$ ,

$$\begin{aligned} a_j(u_j, w) + b_j(u_j, w) &= \int_{\partial\Omega_j - \partial\Omega} \mathbf{n}_j^T(\alpha\nabla u_j) \bar{w}, \\ a_j^c(v, w) + b_j^c(v, w) &= \int_{\partial\Omega_j - \partial\Omega} -\mathbf{n}_j^T(\alpha\nabla v) \bar{w}, \end{aligned}$$

where the bilinear forms  $a_j$  and  $b_j$  correspond to  $a$  and  $b$  in (16) with the integration domains restricted to  $\overline{\Omega}_j$ , and similarly for  $a_j^c$  and  $b_j^c$  with the corresponding restriction to  $\overline{\Omega} - \Omega_j$ . Adding the two equations above and using the Neumann transmission condition from (29), the integral terms cancel and we obtain

$$a_j(u_j, w) + a_j^c(v, w) + b_j(u_j, w) + b_j^c(v, w) = 0.$$

Now we need to recombine these bilinear forms into the entire forms defined on the original function space on  $\Omega$ . Given  $u_j \in H^1(\Omega_j)$  and  $u_j|_{\partial\Omega_j-\partial\Omega} \in H^{1/2}$ , we have  $v \in H^1(\Omega - \Omega_j)$  by assumption. If we define  $\tilde{u} := u_j$  in  $\Omega_j$  and  $\tilde{u} := v$  in  $\Omega - \Omega_j$ , we know that  $\tilde{u} \in H^1(\Omega)$  because  $u_j = v$  on  $\partial\Omega_j - \partial\Omega$  from (29). Hence, we have found a  $\tilde{u} \in H^1(\Omega)$  satisfying  $a(\tilde{u}, w) + b(\tilde{u}, w) = 0$ . By uniqueness of the solution of (11), we then conclude that  $\tilde{u} \equiv 0$ .  $\square$

The matrix analogue of the exact truncation is simply Gaussian elimination: if we consider (19) with  $\mathbf{f}$  nonzero *only* in  $\mathbf{f}_j$ , then we can rewrite (19) as

$$(30) \quad \left[ \begin{array}{ccccc} A_{\sim j} & A_{\sim j,j\langle} & & & \\ A_{j\langle,\sim j} & A_{j\langle} & A_{j\langle,j\bullet} & & \\ & A_{j\bullet,j\langle} & A_{j\bullet} & A_{j\bullet,j\langle} & \\ & & A_{j\bullet,j\bullet} & A_{j\bullet,j\bullet} & \\ & & A_{j\rangle,j\bullet} & A_{j\rangle} & A_{j\rangle,j\sim} \\ & & & A_{j\sim,j\rangle} & A_{j\sim} \end{array} \right] \left[ \begin{array}{c} \mathbf{u}_{\sim j} \\ \mathbf{u}_{j\langle} \\ \mathbf{u}_{j\bullet} \\ \mathbf{u}_{j\rangle} \\ \mathbf{u}_{j\sim} \end{array} \right] = \left[ \begin{array}{c} 0 \\ \mathbf{f}_{j\langle} \\ \mathbf{f}_{j\bullet} \\ \mathbf{f}_{j\rangle} \\ 0 \end{array} \right].$$

To obtain the truncated model for  $\mathbf{u}_j$  only, we eliminate  $\mathbf{u}_{\sim j}$  and  $\mathbf{u}_{j\sim}$  and find

$$(31) \quad \left[ \begin{array}{ccc} S_{j\langle}^{\langle} & A_{j\langle,j\bullet} & A_{j\bullet,j\langle} \\ A_{j\bullet,j\langle} & A_{j\bullet} & A_{j\bullet,j\bullet} \\ A_{j\rangle,j\bullet} & A_{j\rangle,j\bullet} & S_{j\rangle}^{\rangle} \end{array} \right] \left[ \begin{array}{c} \mathbf{u}_{j\langle} \\ \mathbf{u}_{j\bullet} \\ \mathbf{u}_{j\rangle} \end{array} \right] = \left[ \begin{array}{c} \mathbf{f}_{j\langle} \\ \mathbf{f}_{j\bullet} \\ \mathbf{f}_{j\rangle} \end{array} \right],$$

where  $S_{j\langle}^{\langle} = A_{j\langle} - A_{j\langle,\sim j} A_{\sim j}^{-1} A_{\sim j,j\langle}$  and  $S_{j\rangle}^{\rangle} = A_{j\rangle} - A_{j\rangle,j\sim} A_{j\sim}^{-1} A_{j\sim,j\rangle}$  are known as Schur complements, which are usually dense matrices. Similar to Lemma 10, we have the following lemma.

LEMMA 11. *If in (30) the coefficient matrix and the diagonal blocks  $A_{\sim j}$ ,  $A_{j\sim}$  are invertible, then (31) is uniquely solvable and its solution is part of the solution of (30).*

*Remark 12.* If  $j = 1$ , then there is no  $\mathbf{u}_{j\langle}$ , and similarly if  $j = J$ , then there is no  $\mathbf{u}_{j\rangle}$ , so the corresponding rows and columns in (30) and (31) should be deleted. In this case, Lemma 11 still holds. From now on, we will treat  $j = 1$  and  $j = J$  like the other  $j$ 's and just assume that the nonexistent blocks are deleted.

Recalling the splitting  $A_{j\langle} = A_{j\langle}^{\rangle} + A_{j\langle}^{\langle}$ , we can interpret (31) as containing generalized Robin boundary conditions similar to (25) by writing  $S_{j\langle}^{\langle} = A_{j\langle}^{\langle} + P_{j\langle}^{\langle}$  and  $S_{j\rangle}^{\rangle} = A_{j\rangle}^{\rangle} + P_{j\rangle}^{\rangle}$  with

$$(32) \quad P_{j\langle}^{\langle} := A_{j\langle}^{\rangle} - A_{j\langle,\sim j} A_{\sim j}^{-1} A_{\sim j,j\langle}, \quad P_{j\rangle}^{\rangle} := A_{j\rangle}^{\rangle} - A_{j\rangle,j\sim} A_{j\sim}^{-1} A_{j\sim,j\rangle}.$$

Comparing (27) and (31), both for the exact truncation, we find  $P_{j\langle}^{\langle}$  should be the analogue of the Dirichlet-to-Neumann operator  $\text{DtN}_j$  restricted to its input argument on  $\Gamma_{j,j-1}$ . We can also observe directly from (32) that  $P_{j\langle}^{\langle}$  acts on Dirichlet data  $\mathbf{v}_{j\langle}$  by  $-A_{\sim j,j\langle}$  (negative sign for moving to the r.h.s.), solves for  $\mathbf{v}_{\sim j}$  in the exterior by  $A_{\sim j}^{-1}$  and then evaluates the Neumann data by  $A_{j\langle}^{\rangle} \mathbf{v}_{j\langle} + A_{j\langle,\sim j} \mathbf{v}_{\sim j}$ .

*Remark 13.* PML is a popular technique to approximate the transparent boundary condition, and it is appropriate to make a connection here between the practical implementation of PML and our present discussion. The PML technique replaces the original problem exterior to  $\Omega_j$  by a modified one on another exterior domain  $\Omega_j^{pml}$  surrounding  $\Omega_j$  along the truncation boundary  $\partial\Omega_j - \partial\Omega$ . A DtN operator for the modified problem in  $\Omega_j^{pml}$  can be defined as<sup>12</sup>

$$(33) \quad \begin{aligned} \text{DtN}_j^{pml} : (d_1, d_2) &\rightarrow -\mathbf{n}_j^T (\tilde{\alpha} \nabla v) && \text{on } (\Gamma_{j,j-1}, \Gamma_{j,j+1}), \\ \text{s.t.} \quad \tilde{\mathcal{L}} v &= 0 && \text{in } \Omega_j^{pml}, \\ \tilde{\mathcal{B}} v &= 0 && \text{on } \partial\Omega_j^{pml} - \partial\Omega_j, \\ v &= d_1 && \text{on } \Gamma_{j,j-1} \subset (\partial\Omega_j^{pml} \cap \partial\Omega_j), \\ v &= d_2 && \text{on } \Gamma_{j,j+1} \subset (\partial\Omega_j^{pml} \cap \partial\Omega_j), \end{aligned}$$

where  $\tilde{\mathcal{L}} := -\nabla^T \tilde{\alpha} \nabla - \omega^2 / \tilde{\kappa}$ . Then an approximate transparent boundary condition can be used in the case stated in Lemma 10 to obtain  $\tilde{u}_j \approx u_j$ :

$$(34) \quad \begin{aligned} \mathcal{L} \tilde{u}_j &= f && \text{in } \Omega_j, \\ \mathcal{B} \tilde{u}_j &= g && \text{on } \partial\Omega_j \cap \partial\Omega, \\ \mathbf{n}_j^T (\alpha \nabla \tilde{u}_j) + \text{DtN}_j^{pml} \tilde{u}_j &= 0 && \text{on } \partial\Omega_j - \partial\Omega. \end{aligned}$$

To actually solve (34), as we did in the proof of Lemma 10, we substitute with (33) and compose a problem defined on  $\tilde{\Omega}_j := \overline{\Omega}_j \cup \overline{\Omega}_j^{pml}$ ,

$$\begin{aligned} \tilde{\mathcal{L}} \tilde{u}_j &= \tilde{f} && \text{in } \tilde{\Omega}_j, \\ \tilde{\mathcal{B}} \tilde{u}_j &= \tilde{g} && \text{on } \partial\tilde{\Omega}_j, \end{aligned}$$

where  $\tilde{\mathcal{L}} = \mathcal{L}$  in  $\Omega_j$ ,  $\tilde{\mathcal{B}} = \mathcal{B}$  on  $\partial\Omega_j \cap \partial\Omega$ , and  $\tilde{f}, \tilde{g}$  are the zero extensions of  $f, g$ .

<sup>12</sup>In our setting, except for  $j = 1, J$ ,  $\Omega_j^{pml}$  has two disconnected parts, one on the left side of  $\Gamma_{j,j-1}$  and one on the right side of  $\Gamma_{j,j+1}$ . So  $\text{DtN}_j^{pml}$  is block diagonal in the sense that  $\mathbf{n}_j^T (\tilde{\alpha} \nabla v)$  on  $\Gamma_{j,j-1}$  depends only on  $d_1$ , and on  $\Gamma_{j,j+1}$  it depends only on  $d_2$ .

*Remark 14.* At the matrix level, the PML technique corresponds to replacing (30) with

$$(35) \quad \begin{bmatrix} \tilde{A}_{\sim j} & \tilde{A}_{\sim j, j\langle} & & \\ \tilde{A}_{j\langle, \sim j} & \tilde{A}_{j\langle} & A_{j\langle j\bullet} & \\ & A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} \\ & & A_{j\rangle j\bullet} & \tilde{A}_{j\rangle} \\ & & & \tilde{A}_{j\rangle, j\sim} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{u}}_{\sim j} \\ \mathbf{u}_{j\langle} \\ \mathbf{u}_{j\bullet} \\ \mathbf{u}_{j\rangle} \\ \tilde{\mathbf{u}}_{j\sim} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{f}_{j\langle} \\ \mathbf{f}_{j\bullet} \\ \mathbf{f}_{j\rangle} \\ 0 \end{bmatrix},$$

where the entries with tildes (except  $\tilde{A}_{j\langle}$  and  $\tilde{A}_{j\rangle}$ ) are typically of much smaller dimension than the original ones. The Schur complemented system of (35), intended to approximate (31), is

$$(36) \quad \begin{bmatrix} \tilde{S}_{j\langle}^{\langle} & A_{j\langle j\bullet} & \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} \\ A_{j\rangle j\bullet} & \tilde{S}_{j\rangle}^{\rangle} & \end{bmatrix} \begin{bmatrix} \mathbf{u}_{j\langle} \\ \mathbf{u}_{j\bullet} \\ \mathbf{u}_{j\rangle} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{j\langle} \\ \mathbf{f}_{j\bullet} \\ \mathbf{f}_{j\rangle} \end{bmatrix},$$

where  $\tilde{S}_{j\langle}^{\langle} := \tilde{A}_{j\langle} - \tilde{A}_{j\langle, j\sim} \tilde{A}_{j\sim, j\langle}^{-1} \tilde{A}_{j\sim, j\langle}$  and  $\tilde{S}_{j\rangle}^{\rangle} := \tilde{A}_{j\rangle} - \tilde{A}_{j\rangle, j\sim} \tilde{A}_{j\sim, j\rangle}^{-1} \tilde{A}_{j\sim, j\rangle}$ . As before, we see that  $\tilde{P}_{j\langle}^{\langle} := \tilde{S}_{j\langle}^{\langle} - A_{j\langle}^{\langle}$  is the matrix version of the PML-DtN operator  $\text{DtN}_j^{pml}$  restricted to its input argument on  $\Gamma_{j,j-1}$ . For implementation, one usually does not solve (36) directly, but instead solves (35).

**5.3. Green's Function.** So far we have prepared the reader for the new Helmholtz solvers based only on the concepts of domain decomposition and transmission conditions. However, there are also formulations of these new Helmholtz solvers based on Green's functions, which we introduce next. By definition, a fundamental solution  $G(\mathbf{x}, \mathbf{y})$  of the partial differential operator  $\mathcal{M}$  is a solution of the PDE in a domain  $Y$  without consideration of boundary conditions,

$$\mathcal{M}_y G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{y} - \mathbf{x}) \quad \forall \mathbf{x} \in X \subseteq Y,$$

where  $\mathcal{M}_y$  is the operator  $\mathcal{M}$  acting on the  $\mathbf{y}$  variable and  $\delta(\mathbf{y} - \mathbf{x})$  is the Dirac delta function representing a point source and satisfying  $\int_Y \delta(\mathbf{y} - \mathbf{x}) v(\mathbf{y}) d\mathbf{y} = v(\mathbf{x})$ . Let  $u$  be a solution of  $\mathcal{L}u = f$  in  $Y$  (see (11) without boundary condition), and  $\mathcal{M} := -\nabla^T(\alpha^T \nabla \cdot) - \frac{\omega^2}{\kappa}$ . Using integration by parts, we have formally for  $\mathbf{x} \in X - \partial Y$

$$(37) \quad u(\mathbf{x}) = \int_Y G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y} + \int_{\partial Y} \mathbf{n}_y^T (\alpha \nabla u(\mathbf{y})) G(\mathbf{x}, \mathbf{y}) - \mathbf{n}_y^T (\alpha^T \nabla_y G(\mathbf{x}, \mathbf{y})) u(\mathbf{y}) d\sigma(\mathbf{y}),$$

which is a representation formula for the solution, and the three summands are called volume potential, single layer potential, and double layer potential; see [134]. A justification of (37) involves existence, regularity, and singularity of the fundamental solution and the solution, which can be found in the literature if  $\alpha$ ,  $\kappa$ ,  $f$ , and  $\partial X$  are bounded and smooth; see, e.g., [142, 147]. We note that the r.h.s. of (37) uses both Neumann and Dirichlet traces of  $u$ , while a well-posed boundary condition usually only tells us one of them or a generalized linear combination of them. For example, let  $u = 0$  on  $\partial Y$ . To obtain a usable representation, we can require  $G$  to also satisfy  $G(\mathbf{x}, \mathbf{y}) = 0$  for  $\mathbf{y} \in \partial Y$ ,  $\mathbf{x} \in X$ . Then the single layer and the double layer potentials in (37) vanish, and we obtain the simple representation formula

$$(38) \quad u(\mathbf{x}) = \int_Y G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}.$$

We call a *fundamental solution* satisfying a homogeneous boundary condition *Green's function*. However, the two terms are sometimes used in an exchangeable way.

*Remark 15.* If  $u$  satisfies an inhomogeneous boundary condition  $\mathcal{B}u|_{\partial Y} = g$ , we can lift (extend) the boundary data into  $Y$ , i.e., find a function  $v$  on  $Y$  such that  $\mathcal{B}v|_{\partial Y} = g$ , and subtract it from  $u$  so that the boundary condition becomes homogeneous for the new unknown  $\tilde{u} := u - v$ . (We will see that this trick is useful also for the implementation of the transmission condition in (24).) For the Green's function  $G$ , we impose  $\mathcal{B}_y^T G(\mathbf{x}, \mathbf{y}) = 0$ , where  $\mathcal{B}^T$  corresponds to  $\mathcal{B}$  but with  $\alpha$  replaced by  $\alpha^T$ .

*Remark 16.* Another convention is to define the Green's function  $G(\mathbf{x}, \mathbf{y})$  through  $\mathcal{L}_x G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y})$  equipped with homogeneous boundary conditions as for  $u$ . Then (38) can be obtained by the superposition principle. Similarly, we may define  $H(\mathbf{x}, \mathbf{y})$  through  $\mathcal{L}_y H(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{y} - \mathbf{x})$ . We then have  $H(\mathbf{y}, \mathbf{x}) = G(\mathbf{x}, \mathbf{y})$ . Furthermore, if  $\alpha = \alpha^T$ , we have  $G(\mathbf{x}, \mathbf{y}) = G(\mathbf{y}, \mathbf{x})$ .

We now point out an analogy between (38) and the solution  $\mathbf{u} = A^{-1}\mathbf{f}$  of (17). For a particular value of  $\mathbf{x}$ ,  $u(\mathbf{x})$  in (38) corresponds to a particular (say, the  $m$ th) entry of  $\mathbf{u}$ , and  $G(\mathbf{x}, \mathbf{y})$  then also corresponds to the  $m$ th row of  $A^{-1}$ , and the integral in (38) becomes the inner product of the row of  $A^{-1}$  with  $\mathbf{f}$ . Similarly, for a particular  $\mathbf{y}$ ,  $G(\mathbf{x}, \mathbf{y})$  corresponds to a particular column of  $A^{-1}$ . We now take a closer look at the Schur complement  $S_{j\langle}^{\langle}$  in (31), which is essentially derived from the 2-by-2 block matrix by Gaussian elimination,

$$(39) \quad \begin{bmatrix} A_{\sim j} & A_{\sim j, j\langle} \\ A_{j\langle, \sim j} & A_{j\langle} \end{bmatrix} = \begin{bmatrix} I_{\sim j} & \\ A_{j\langle, \sim j} A_{\sim j}^{-1} & I_{j\langle} \end{bmatrix} \begin{bmatrix} A_{\sim j} & A_{\sim j, j\langle} \\ & S_{j\langle}^{\langle} \end{bmatrix}.$$

Taking the inverse of both sides, we find

$$= \begin{bmatrix} A_{\sim j} & A_{\sim j, j\langle} \\ A_{j\langle, \sim j} & A_{j\langle} \end{bmatrix}^{-1} = \begin{bmatrix} A_{\sim j} & A_{\sim j, j\langle} \\ & S_{j\langle}^{\langle} \end{bmatrix}^{-1} \begin{bmatrix} I_{\sim j} & \\ -A_{j\langle, \sim j} A_{\sim j}^{-1} & I_{j\langle} \end{bmatrix} = \begin{bmatrix} * & * \\ * & S_{j\langle}^{\langle} \end{bmatrix},$$

where we omit the terms marked by \*. Recalling the analogy between the matrix inverse and the Green's function, we can identify  $S_{j\langle}^{\langle} \^{-1}$  as a diagonal part of the Green's function  $G(\mathbf{x}, \mathbf{y})$ . Here,  $G$  satisfies for  $\mathbf{x}, \mathbf{y} \in \Omega_{\sim j}^{+h}$

$$\begin{aligned} \mathcal{M}_y G(\mathbf{x}, \mathbf{y}) &= \delta(\mathbf{y} - \mathbf{x}) && \text{in } \Omega_{\sim j}^{+h}, \\ \mathcal{B}_y^T G(\mathbf{x}, \mathbf{y}) &= 0 && \text{on } \partial\Omega \cap \partial\Omega_{\sim j}^{+h}, \\ G(\mathbf{x}, \mathbf{y}) &= 0 && \text{on } \Gamma_{j,j-1}^{+h}, \end{aligned}$$

where  $\Omega_{\sim j}^{+h}$  is the domain covering the left part of  $\Omega - \Omega_j$  but with one grid layer further into  $\Omega_j$ , and  $\Gamma_{j,j-1}^{+h}$  is the interface of  $\Omega_{\sim j}^{+h}$  in  $\Omega_j$ . We see that  $S_{j\langle}^{\langle} \^{-1}$  corresponds to  $G(\mathbf{x}, \mathbf{y})$  with  $\mathbf{x}, \mathbf{y}$  both restricted to  $\Gamma_{j,j-1}$ . This identification was first given in [51, 52].

**6. Optimized Schwarz Methods.** If we have  $u_j = u|_{\Omega_j}$ ,  $j = 1, \dots, J$ , with  $u$  the solution of (11), we must have consistency: (a)  $u_j$  and  $u_l$  matching<sup>13</sup> on  $\overline{\Omega}_j \cap \overline{\Omega}_l$ , and (b) the original equations are satisfied in neighborhoods of interfaces  $\partial\Omega_j \cap \overline{\Omega}_l$  for all  $j \neq l$ ,  $j, l \in \{1, \dots, J\}$ . Conversely, if  $u_j$ ,  $j = 1, \dots, J$ , solves (11) restricted to  $\overline{\Omega}_j$ , then (a) and (b) together imply  $u_j = u|_{\Omega_j}$ . For second-order elliptic PDEs like (11), (b) is equivalent to saying the Neumann traces  $\mathbf{n}^T \alpha \nabla u_j$ ,  $\mathbf{n}^T \alpha \nabla u_l$  match<sup>14</sup> on  $\partial\Omega_j \cap \overline{\Omega}_l$  for all  $j, l \in \{1, \dots, J\}$ . Hence, when  $\{\Omega_j\}_{j=1}^J$  are nonoverlapping, (a) and (b) reduce to both Dirichlet and Neumann (or any other equivalent pair of) traces to match on every interface. If the subdomains  $\{\Omega_j\}_{j=1}^J$  overlap, (a) and (b) as a whole can be further condensed as (a') one transmission condition (matching one of Dirichlet/Neumann/generalized Robin traces) on every interface, and (b') the transmission conditions ensure  $u_j = u_l$  on  $\overline{\Omega}_j \cap \overline{\Omega}_l$  if  $u_j$  and  $u_l$  both solve the original equations restricted to overlaps. Therefore, no matter whether the decomposition is overlapping or nonoverlapping, the original problem can be rewritten as a system of subdomain problems coupled through transmission conditions on interfaces; cf. [141].

Schwarz methods split the coupling between subdomains by taking the interface data from the already available iterates and solving subdomain problems to obtain the new iterate.<sup>15</sup> Historically, the first Schwarz method was the *alternating Schwarz method* introduced by Schwarz himself [151], where one subdomain is solved at a time and then the newest data is passed on to the neighboring subdomains. This is analogous to the Gauss–Seidel iteration in linear algebra. More than a century later, Lions introduced the so-called *parallel Schwarz method* [118], where each subdomain solves its local problem at the same time and data is only exchanged afterward. This is analogous to the Jacobi iteration in linear algebra. In the alternating Schwarz method in the presence of many subdomains, one also needs to specify an ordering, and for the Helmholtz solvers we are interested in here with the decomposition into a one-dimensional sequence of subdomains, the particular ordering of sweeping from the first subdomain to the last one and then back, like in the symmetrized Gauss–Seidel iteration in linear algebra, is important, and we call these “double sweep” methods.

One also has to decide upon which unknowns are used to write the iteration: one can choose subdomain approximations (for the equivalent coupled system), global approximations (for the original problem), interface data, and residuals. We explain now in detail these formulations and their relations.

**6.1. Subdomain Transmission Form of Schwarz Methods.** In this formulation, the iterates represent approximate solutions on the subdomains. The corresponding *double sweep optimized Schwarz method* (DOSM) was first proposed in [129, 130]. Based on the decomposition defined in (18), we state the DOSM in Algorithm 1 at the PDE level for (11) and in Algorithm 2 at the matrix level for (19). Note that the transmission conditions on the interfaces can be changed in the process, e.g., from the forward sweep to the backward sweep or from one iteration to the next. Note

<sup>13</sup>Usually, “match” means “coincide.” But there are exceptions; e.g., the original problem can enforce a jump of the solution across a surface, or at the discrete level nonconforming discretization is used in overlaps and interfaces.

<sup>14</sup>We assume all surface/line/point sources on the interface have been split and incorporated into subdomain problems.

<sup>15</sup>Our description is also applicable to single-trace methods such as BDD, FETI, and FETI-H, which are based on nonoverlapping decompositions and use the same data for neighboring subdomains on each interface. In contrast, for Schwarz methods each subdomain is equipped with its own interface data which is provided by (but not used by) the other subdomains.

**Algorithm 1.** DOSM in the **subdomain transmission** form at the **PDE** level.

Given the last iterate  $\{u_j^{(n-1)} \text{ in } \Omega_j, j = 1, \dots, J\}$ , solve successively for  $j = 1, \dots, J-1$ ,

$$\begin{aligned} \mathcal{L} u_j^{(n-\frac{1}{2})} &= f && \text{in } \Omega_j, \\ \mathcal{B} u_j^{(n-\frac{1}{2})} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathcal{Q}_j^{\langle} \left( \mathbf{n}_j^T \alpha \nabla u_j^{(n-\frac{1}{2})} \right) + \mathcal{P}_j^{\langle} u_j^{(n-\frac{1}{2})} &= \mathcal{Q}_j^{\langle} \left( \mathbf{n}_j^T \alpha \nabla u_{j-1}^{(n-\frac{1}{2})} \right) + \mathcal{P}_j^{\langle} u_{j-1}^{(n-\frac{1}{2})} && \text{on } \Gamma_{j,j-1}, \\ \mathcal{Q}_j^{\rangle} \left( \mathbf{n}_j^T \alpha \nabla u_j^{(n-\frac{1}{2})} \right) + \mathcal{P}_j^{\rangle} u_j^{(n-\frac{1}{2})} &= \mathcal{Q}_j^{\rangle} \left( \mathbf{n}_j^T \alpha \nabla u_{j+1}^{(n-1)} \right) + \mathcal{P}_j^{\rangle} u_{j+1}^{(n-1)} && \text{on } \Gamma_{j,j+1}, \end{aligned}$$

where  $\mathcal{Q}_j^{\langle}$ ,  $\mathcal{P}_j^{\langle}$  and  $\mathcal{Q}_j^{\rangle}$ ,  $\mathcal{P}_j^{\rangle}$  are some possibly nonlocal operators on the interfaces  $\Gamma_{j,j-1}$  and  $\Gamma_{j,j+1}$ , and  $\mathbf{n}_j$  is the unit outward normal vector of  $\Omega_j$ . We call this process the forward sweep.

Then the backward sweep consists in solving successively for  $j = J, \dots, 1$ ,

$$\begin{aligned} \mathcal{L} u_j^{(n)} &= f && \text{in } \Omega_j, \\ \mathcal{B} u_j^{(n)} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathcal{Q}_j^{\langle} \left( \mathbf{n}_j^T \alpha \nabla u_j^{(n)} \right) + \mathcal{P}_j^{\langle} u_j^{(n)} &= \mathcal{Q}_j^{\langle} \left( \mathbf{n}_j^T \alpha \nabla u_{j-1}^{(n-\frac{1}{2})} \right) + \mathcal{P}_j^{\langle} u_{j-1}^{(n-\frac{1}{2})} && \text{on } \Gamma_{j,j-1}, \\ \mathcal{Q}_j^{\rangle} \left( \mathbf{n}_j^T \alpha \nabla u_j^{(n)} \right) + \mathcal{P}_j^{\rangle} u_j^{(n)} &= \mathcal{Q}_j^{\rangle} \left( \mathbf{n}_j^T \alpha \nabla u_{j+1}^{(n)} \right) + \mathcal{P}_j^{\rangle} u_{j+1}^{(n)} && \text{on } \Gamma_{j,j+1}. \end{aligned}$$

**Algorithm 2.** DOSM in the **subdomain transmission** form at the **matrix** level.

Given the last iterate  $\{\mathbf{u}_j^{(n-1)}, j = 1, \dots, J\}$ , solve successively for  $j = 1, \dots, J-1$ ,

$$= \begin{bmatrix} Q_{j\langle}^{\langle} A_{j\langle}^{\langle} + P_{j\langle}^{\langle} & Q_{j\langle}^{\langle} A_{j\langle} j\bullet & & \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} & \\ & Q_{j\rangle}^{\rangle} A_{j\rangle j\bullet} & Q_{j\rangle}^{\rangle} A_{j\rangle}^{\rangle} + P_{j\rangle}^{\rangle} & \\ Q_{j\langle}^{\langle} \left( \mathbf{f}_{j\langle} - A_{j\langle j-1} \mathbf{u}_{j-1}^{(n-\frac{1}{2})} \right) + \left( P_{j\langle}^{\langle} - Q_{j\langle}^{\langle} A_{j\langle}^{\langle} \right) \mathbf{u}_{j-1}^{(n-\frac{1}{2})} & & \\ & \mathbf{f}_{j\bullet} & \\ Q_{j\rangle}^{\rangle} \left( \mathbf{f}_{j\rangle} - A_{j\rangle j+1} \mathbf{u}_{j+1}^{(n-1)} \right) + \left( P_{j\rangle}^{\rangle} - Q_{j\rangle}^{\rangle} A_{j\rangle}^{\rangle} \right) \mathbf{u}_{j+1}^{(n-1)} & \end{bmatrix},$$

which constitutes the forward sweep.

Then perform the backward sweep: solve successively for  $j = J, \dots, 1$ ,

$$= \begin{bmatrix} Q_{j\langle}^{\langle} A_{j\langle}^{\langle} + P_{j\langle}^{\langle} & Q_{j\langle}^{\langle} A_{j\langle} j\bullet & & \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} & \\ & Q_{j\rangle}^{\rangle} A_{j\rangle j\bullet} & Q_{j\rangle}^{\rangle} A_{j\rangle}^{\rangle} + P_{j\rangle}^{\rangle} & \\ Q_{j\langle}^{\langle} \left( \mathbf{f}_{j\langle} - A_{j\langle j-1} \mathbf{u}_{j-1}^{(n-\frac{1}{2})} \right) + \left( P_{j\langle}^{\langle} - Q_{j\langle}^{\langle} A_{j\langle}^{\langle} \right) \mathbf{u}_{j-1}^{(n-\frac{1}{2})} & & \\ & \mathbf{f}_{j\bullet} & \\ Q_{j\rangle}^{\rangle} \left( \mathbf{f}_{j\rangle} - A_{j\rangle j+1} \mathbf{u}_{j+1}^{(n-1)} \right) + \left( P_{j\rangle}^{\rangle} - Q_{j\rangle}^{\rangle} A_{j\rangle}^{\rangle} \right) \mathbf{u}_{j+1}^{(n-1)} & \end{bmatrix}.$$

If  $Q_{j\langle}^{\langle} = I$  and  $Q_{j\rangle}^{\rangle} = I$ , one can rewrite the subproblems as in (26).

also that in the double sweep, the subproblem on the last subdomain  $\Omega_J$  is solved only once. If the transmission conditions on  $\Gamma_{1,2}$  are the same in the forward and the backward sweeps, we find the same problem on  $\Omega_1$  is solved in the backward sweep of the current iteration and in the forward sweep of the next iteration, so one can also solve it only once.

For the *parallel optimized Schwarz method* (POSM), where all subdomains are solved simultaneously and data is exchanged afterward, it was shown in [133] that if optimal transmission conditions based on the DtN operators are used, then the algorithm converges in a finite number of steps, equal to the number of subdomains, and thus the iteration operator is nilpotent of degree equal to the number of subdomains. We present now an optimal choice for the DOSM, where the operators  $\mathcal{Q}_j^\langle$  and  $\mathcal{P}_j^\rangle$  can still be arbitrary, as long as the subdomain problems are well-posed.

**THEOREM 17.** *If in the forward and the backward sweeps  $\mathcal{Q}_j^\langle$  is the identity,  $\mathcal{P}_j^\rangle = \text{DtN}_j^\langle := \text{DtN}_j|_{\Gamma_{j,j-1}}$  is well-defined for  $j = 2, \dots, J$  as in Definition 8, and the original problem in (11) and the subdomain problems in Algorithm 1 are uniquely solvable, then Algorithm 1 converges in one double sweep for an arbitrary initial guess, and  $u_j^{(1)} = u|_{\Omega_j}$ ,  $j = 1, \dots, J$ , with  $u$  the solution of (11). This means that the iteration operator of the DOSM is nilpotent of degree one.*

*Proof.* We note that the subdomain problems in Algorithm 1 are satisfied by the solution  $u$ . By linearity, it is thus sufficient to prove  $u_j^{(1)} \equiv 0$  when  $f \equiv 0$  and  $g \equiv 0$ . We first consider  $u_2^{(\frac{1}{2})}$ , which satisfies the transmission condition

$$(40) \quad \mathbf{n}_2^T \alpha \nabla u_2^{(\frac{1}{2})} + \text{DtN}_2^\langle u_2^{(\frac{1}{2})} = \mathbf{n}_2^T \alpha \nabla u_1^{(\frac{1}{2})} + \text{DtN}_2^\langle u_1^{(\frac{1}{2})} \text{ on } \Gamma_{2,1}.$$

Since  $\mathcal{L}u_1^{(\frac{1}{2})} = 0$  in  $\Omega_1 \supset \Omega_{\sim 2}$  and  $\mathcal{B}u_1^{(\frac{1}{2})} = 0$  on  $(\partial\Omega \cap \partial\Omega_1) \supset (\partial\Omega \cap \partial\Omega_{\sim 2})$ , from Definition 8 we have  $\text{DtN}_2^\langle u_1^{(\frac{1}{2})} = -\mathbf{n}_2^T \alpha \nabla u_1^{(\frac{1}{2})}$ . Substituting this into (40) we obtain

$$\mathbf{n}_2^T \alpha \nabla u_2^{(\frac{1}{2})} + \text{DtN}_2^\langle u_2^{(\frac{1}{2})} = 0 \text{ on } \Gamma_{2,1}.$$

Now assuming that

$$(41) \quad \mathbf{n}_j^T \alpha \nabla u_j^{(\frac{1}{2})} + \text{DtN}_j^\langle u_j^{(\frac{1}{2})} = 0 \text{ on } \Gamma_{j,j-1},$$

we will show that this also holds for  $j+1$  instead of  $j$ . In fact, by the assumption that  $\text{DtN}_{j+1}^\langle$  is well-defined, we have a unique solution  $v_{\sim j+1}$  of the problem

$$\begin{aligned} \mathcal{L}v_{\sim j+1} &= 0 && \text{in } \Omega_{\sim j+1}, \\ \mathcal{B}v_{\sim j+1} &= 0 && \text{on } \partial\Omega \cap \partial\Omega_{\sim j+1}, \\ v_{\sim j+1} &= u_j^{(\frac{1}{2})} && \text{on } \Gamma_{j+1,j}. \end{aligned}$$

By Lemma 10, we have from (41) that  $u_j^{(\frac{1}{2})} = v_{\sim j+1}$  in  $\Omega_j \cap \Omega_{\sim j+1}$ . Therefore,  $\text{DtN}_{j+1}^\langle u_j^{(\frac{1}{2})} = -\mathbf{n}_{j+1}^T \alpha \nabla v_{\sim j+1} = -\mathbf{n}_{j+1}^T \alpha \nabla u_j^{(\frac{1}{2})}$  on  $\Gamma_{j+1,j}$ . Substituting this into the transmission condition for  $u_{j+1}^{(\frac{1}{2})}$  we find

$$\mathbf{n}_{j+1}^T \alpha \nabla u_{j+1}^{(\frac{1}{2})} + \text{DtN}_{j+1}^\langle u_{j+1}^{(\frac{1}{2})} = 0 \text{ on } \Gamma_{j+1,j}.$$

By induction, (41) holds for all  $j = 2, \dots, J - 1$  and also  $j = J$  except that we write  $u_J^{(1)}$  instead of  $u_J^{(\frac{1}{2})}$ . By Lemma 10, and recalling that  $f \equiv 0$  and  $g \equiv 0$ , we obtain  $u_J^{(1)} = u|_{\Omega_J} \equiv 0$ . Now assuming that

$$(42) \quad u_{j+1}^{(1)} \equiv 0 \text{ in } \Omega_{j+1},$$

we have to show that  $u_j \equiv 0$  in  $\Omega_j$ . This follows directly from (42) and (41), which imply that all the data in the problem for  $u_j^{(1)}$  vanish, and from the assumption that the subdomain problem is uniquely solvable.  $\square$

We also have the equivalent result of convergence in one step for the discrete case.

**THEOREM 18.** *If in the forward and the backward sweeps  $Q_{j\langle}^{\langle} = I_{j\langle}$ ,  $P_{j\langle}^{\langle} = A_{j\langle}^{\rangle} - A_{j\langle} \sim_j A_{\sim j}^{-1} A_{\sim j,j\langle}$  is well-defined for  $j = 2, \dots, J$ , and the original problem in (19) and the subdomain problems in Algorithm 2 are uniquely solvable, then Algorithm 2 converges in one step and  $\mathbf{u}_j^{(1)} = R_j \mathbf{u}$  with  $\mathbf{u}$  the solution of (19). This means the iteration matrix of the DOSM is nilpotent of degree one.*

*Proof.* First, the subdomain problems are consistent, i.e., neglecting the iteration numbers and substituting  $\mathbf{u}_j = R_j \mathbf{u}$ , we find the equations are satisfied by  $\mathbf{u}$ . Hence, by considering the errors, we only need to show that  $\mathbf{u}_j^{(1)} = 0$  if  $\mathbf{f} = 0$ . In the problem for  $\mathbf{u}_2^{(\frac{1}{2})}$ , the r.h.s. corresponding to  $\Gamma_{2,1}$  becomes

$$-A_{2\langle 1\rangle} \mathbf{u}_{1\langle}^{(\frac{1}{2})} - A_{2\langle 1\rangle} A_{1\langle}^{-1} A_{1\langle 2\rangle} \mathbf{u}_{1\langle}^{(\frac{1}{2})} = -A_{2\langle 1\rangle} \left( \mathbf{u}_{1\langle}^{(\frac{1}{2})} - A_{1\langle}^{-1} A_{1\langle 2\rangle} \mathbf{u}_{1\langle}^{(\frac{1}{2})} \right) = 0,$$

since  $\mathbf{u}_1^{(\frac{1}{2})}$  satisfies  $A_{1\langle} \mathbf{u}_{1\langle}^{(\frac{1}{2})} + A_{1\langle 2\rangle} \mathbf{u}_{1\langle}^{(\frac{1}{2})} = 0$ . In other words, we have for  $j = 2$ ,

$$(43) \quad S_{j\langle}^{\langle} \mathbf{u}_{j\langle}^{(\frac{1}{2})} + A_{j\langle j\bullet} \mathbf{u}_{j\bullet}^{(\frac{1}{2})} = 0.$$

Assuming (43) holds for one  $j$  in  $\{2, \dots, J - 1\}$ , we will show it will also hold for  $j + 1$  instead of  $j$ . In the theorem we are proving, we have assumed that  $A_{\sim j+1}$  is invertible, so we can introduce  $\mathbf{v}_{\sim j+1} := [\mathbf{v}_{\sim j}; \mathbf{v}_{j-1\rangle}; \mathbf{v}_{j\langle}]$  as the solution of

$$\begin{bmatrix} A_{\sim j} & A_{\sim j,j-1\rangle} & A_{j-1\rangle j\langle} \\ A_{j-1\rangle \sim j} & A_{j-1\rangle} & A_{j-1\rangle j\langle} \\ A_{j\langle j-1\rangle} & A_{j\langle} & A_{j\langle} \end{bmatrix} \begin{bmatrix} \mathbf{v}_{\sim j} \\ \mathbf{v}_{j-1\rangle} \\ \mathbf{v}_{j\langle} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -A_{j\langle,j+1\rangle} \mathbf{u}_{j\langle}^{(\frac{1}{2})} \end{bmatrix}.$$

By Gaussian elimination, we have

$$\begin{bmatrix} S_{j-1\rangle}^{\langle} & A_{j-1\rangle j\langle} \\ A_{j\langle j-1\rangle} & A_{j\langle} \end{bmatrix} \begin{bmatrix} \mathbf{v}_{j-1\rangle} \\ \mathbf{v}_{j\langle} \end{bmatrix} = \begin{bmatrix} 0 \\ -A_{\sim j+1,j+1\rangle} \mathbf{u}_{j\langle}^{(\frac{1}{2})} \end{bmatrix},$$

which is also satisfied by the restriction of  $\mathbf{u}_j^{(\frac{1}{2})}$  because of (43),  $\mathbf{f} \equiv 0$ , and Algorithm 2. By Lemma 11, we have that  $\mathbf{v}_{j-1\rangle} = \mathbf{u}_{j\langle}^{(\frac{1}{2})}$  and  $\mathbf{v}_{j\langle} = \mathbf{u}_{j\langle}^{(\frac{1}{2})}$ . In Algorithm 2,

the r.h.s. for  $\mathbf{u}_{j+1\langle}^{(\frac{1}{2})}$  then becomes

$$\begin{aligned} & -A_{j+1\langle} \mathbf{u}_{j\langle}^{(\frac{1}{2})} - A_{j+1\langle, \sim j+1} A_{\sim j+1}^{-1} A_{\sim j+1, j+1\langle} \mathbf{u}_{j\lceil}^{(\frac{1}{2})} \\ &= -A_{j+1\langle} \mathbf{u}_{j\langle}^{(\frac{1}{2})} + A_{j+1\langle, \sim j+1} \mathbf{v}_{\sim j+1} \\ &= -A_{j+1\langle} \mathbf{u}_{j\langle}^{(\frac{1}{2})} + A_{j+1\langle} \mathbf{v}_j \\ &= -A_{j+1\langle} \mathbf{u}_{j\langle}^{(\frac{1}{2})} + A_{j+1\langle} \mathbf{u}_{j\langle}^{(\frac{1}{2})} = 0. \end{aligned}$$

Now we know that (43) holds for  $j = 2, \dots, J-1$  and  $j = J$ , except that we write  $\mathbf{u}_J^{(1)}$  instead of  $\mathbf{u}_J^{(\frac{1}{2})}$ , and we see that the r.h.s. for  $\mathbf{u}_J^{(1)}$  vanishes, so  $\mathbf{u}_J^{(1)} = 0$ . In the backward sweep, the r.h.s. on  $\Gamma_{j,j-1}$  for  $\mathbf{u}_j^{(1)}$  is by Algorithm 2, as it is for  $\mathbf{u}_j^{(\frac{1}{2})}$ , and hence is zero by (43), and the r.h.s. on  $\Gamma_{j,j+1}$  vanishes, given  $\mathbf{u}_{j+1}^{(1)} = 0$ . By induction, we thus conclude that  $\mathbf{u}_j^{(1)} = 0$ ,  $j = 1, \dots, J$ .  $\square$

Algorithms 1 and 2 use the subdomain approximations as iterates. If we want to have a global approximation for the original problem as a final result, we can just glue together subdomain approximations after stopping the iteration. This can be done by setting  $u^{(n)} := \sum_{j=1}^J \mathcal{E}_j(\phi_j u_j^{(n)})$  at the PDE level and  $\mathbf{u}^{(n)} = \sum_{j=1}^J R_j^T \Phi_j \mathbf{u}_j^{(n)}$  at the matrix level, where  $\mathcal{E}_j$  is the extension by zero from  $\Omega_j$  to  $\Omega$  and  $\phi_j$  is a weighting function and, correspondingly,  $\Phi_j$  a diagonal matrix. For consistency, when  $u_j^{(n)} = u|_{\Omega_j}$  with  $u$  the solution of the original problem, we want  $u^{(n)} = u$ , or  $\sum_{j=1}^J \mathcal{E}_j(\phi_j u|_{\Omega_j}) = \sum_{j=1}^J (\mathcal{E}_j \phi_j) u = u$ . To ensure this for arbitrary data of (11), we must have  $\sum_{j=1}^J \mathcal{E}_j \phi_j \equiv 1$ . At the matrix level, we must have  $\sum_{j=1}^J R_j^T \Phi_j R_j = I$ . In particular, for a nonoverlapping decomposition, we must have  $\phi_j \equiv 1$  in  $\Omega_j$ .

**6.2. Global Deferred Correction Form of Schwarz Methods.** If we want to use global approximations as iterates, i.e., input the last iterate  $u^{(n-1)}$  to the DOSM and get  $u^{(n)}$  as output, we need to be very careful with the weighting functions introduced in the last paragraph. This is because Algorithm 1 relies essentially on the interface data, and when inputting  $u^{(n-1)}$  instead of  $\{u_j^{(n-1)}\}$ , we must ensure that the values of  $\{u_j^{(n-1)}\}$  necessary for the evaluation of the interface data in Algorithm 1 can still be found in  $u^{(n-1)}$ . We thus need a variant of Algorithm 1 that generates the iterate  $u^{(n)}$  without storing  $u_j^{(n-1)}$  (just storing  $u^{(n-1)}$ ), and satisfying  $u^{(n)} = \sum_{j=1}^J \mathcal{E}_j \phi_j u_j^{(n)}$ , given that this relation holds for  $n = 0$ . The result of this algorithm should be identical to the glued result from the iterates  $\{u_j^{(n)}\}$  generated by Algorithm 1. The equivalence of the new variant to Algorithm 1, and Algorithm 2 at the discrete level, is important, because then Theorem 17, and Theorem 18 at the discrete level, will also hold for the variant. We present the DOSM version with global approximations as iterates in Algorithm 3 at the continuous level and in Algorithm 4 for the discrete case. For the parallel form of the algorithms, i.e., the POSM, the situation is even more delicate and has been studied at length in [48, 155]. For example, the well-known preconditioner [46], called the *additive Schwarz method* (AS), is designed to be symmetric but then loses any equivalence to the POSM. The AS also cannot be used as a standalone iterative method, since it is not convergent; for a discussion, see [48, 65].

*Remark 19.* Algorithms 3 and 4 require the weighting functions to take values either 0 or 1, and to constitute a partition of unity. The resulting way of gluing sub-

**Algorithm 3.** DOSM in the **global deferred correction** form at the **PDE level**.

Given the last iterate  $u^{(n-1)}$ , solve successively for  $j = 1, \dots, J-1$ ,

$$\begin{aligned} \mathcal{L} v_j^{(n-\frac{1}{2})} &= f - \mathcal{L} u^{(n-1+\frac{j-1}{2J-1})} && \text{in } \Omega_j, \\ \mathcal{B} v_j^{(n-\frac{1}{2})} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathcal{Q}_j^{\langle} \left( \mathbf{n}_j^T \alpha \nabla v_j^{(n-\frac{1}{2})} \right) + \mathcal{P}_j^{\langle} v_j^{(n-\frac{1}{2})} &= 0 && \text{on } \Gamma_{j,j-1}, \\ \mathcal{Q}_j^{\rangle} \left( \mathbf{n}_j^T \alpha \nabla v_j^{(n-\frac{1}{2})} \right) + \mathcal{P}_j^{\rangle} v_j^{(n-\frac{1}{2})} &= 0 && \text{on } \Gamma_{j,j+1}, \end{aligned}$$

with each solve followed by  $u^{(n-1+\frac{j}{2J-1})} \leftarrow u^{(n-1+\frac{j-1}{2J-1})} + \mathcal{E}_j(\phi_j v_j^{(n-\frac{1}{2})})$  with  $\mathcal{E}_j \phi_j$  forming a nonoverlapping partition of unity of  $\Omega$ , i.e.,  $\phi_j = 1$  in its support contained in  $\bar{\Omega}_j$ ,  $(\mathcal{E}_j \phi_j)(\mathcal{E}_l \phi_l) \equiv 0$  for  $j \neq l$  and  $\sum_{j=1}^J \mathcal{E}_j \phi_j \equiv 1$  in  $\Omega$ .

Then in the backward sweep solve successively for  $j = J, \dots, 1$ ,

$$\begin{aligned} \mathcal{L} v_j^{(n)} &= f - \mathcal{L} u^{(n-1+\frac{2J-j-1}{2J-1})} && \text{in } \Omega_j, \\ \mathcal{B} v_j^{(n)} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathcal{Q}_j^{\langle} \left( \mathbf{n}_j^T \alpha \nabla v_j^{(n)} \right) + \mathcal{P}_j^{\langle} v_j^{(n)} &= 0 && \text{on } \Gamma_{j,j-1}, \\ \mathcal{Q}_j^{\rangle} \left( \mathbf{n}_j^T \alpha \nabla v_j^{(n)} \right) + \mathcal{P}_j^{\rangle} v_j^{(n)} &= 0 && \text{on } \Gamma_{j,j+1}, \end{aligned}$$

with each solve followed by  $u^{(n-1+\frac{2J-j}{2J-1})} \leftarrow u^{(n-1+\frac{2J-j-1}{2J-1})} + \mathcal{E}_j(\phi_j v_j^{(n)})$ .

**Algorithm 4.** DOSM in the **global deferred correction** form at the **matrix level**.

Given the last iterate  $\mathbf{u}^{(n-1)}$ , solve successively for  $j = 1, \dots, J-1$  (note that  $\mathbf{v}_j$  changes with  $n$ ),

$$(44) \quad \begin{bmatrix} Q_{j\langle}^{\langle} A_{j\langle}^{\langle} + P_{j\langle}^{\langle} & Q_{j\langle}^{\langle} A_{j\langle j\bullet} & \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} \\ Q_{j\rangle}^{\rangle} A_{j\rangle j\bullet} & Q_{j\rangle}^{\rangle} A_{j\rangle}^{\rangle} + P_{j\rangle}^{\rangle} & \end{bmatrix} \begin{bmatrix} \mathbf{v}_{j\langle} \\ \mathbf{v}_{j\bullet} \\ \mathbf{v}_{j\rangle} \end{bmatrix} = \begin{bmatrix} Q_{j\langle}^{\langle} \\ I_{j\bullet} \\ Q_{j\rangle}^{\rangle} \end{bmatrix} R_j \left( \mathbf{f} - A \mathbf{u}^{(n-1+\frac{j-1}{2J-1})} \right),$$

with each solve followed by

$$(45) \quad \mathbf{u}^{(n-1+\frac{j}{2J-1})} \leftarrow \mathbf{u}^{(n-1+\frac{j-1}{2J-1})} + R_j^T \Phi_j \mathbf{v}_j$$

with the following constraints:  $\Phi_j$  is a diagonal matrix with its diagonal containing ones on  $\Theta_j \cup \Gamma_{j+1,j}$  and zeros on  $\Gamma_{j,j-1}$ ,  $(R_j^T \Phi_j) R_j (R_l^T \Phi_l) = 0$  as  $j \neq l$ , and  $\sum_{j=1}^J R_j^T \Phi_j R_j = I_{1,\dots,J}$ .

Then solve successively for  $j = J, \dots, 1$ ,

$$\begin{bmatrix} Q_{j\langle}^{\langle} A_{j\langle}^{\langle} + P_{j\langle}^{\langle} & Q_{j\langle}^{\langle} A_{j\langle j\bullet} & \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} \\ Q_{j\rangle}^{\rangle} A_{j\rangle j\bullet} & Q_{j\rangle}^{\rangle} A_{j\rangle}^{\rangle} + P_{j\rangle}^{\rangle} & \end{bmatrix} \begin{bmatrix} \mathbf{v}_{j\langle} \\ \mathbf{v}_{j\bullet} \\ \mathbf{v}_{j\rangle} \end{bmatrix} = \begin{bmatrix} Q_{j\langle}^{\langle} \\ I_{j\bullet} \\ Q_{j\rangle}^{\rangle} \end{bmatrix} R_j \left( \mathbf{f} - A \mathbf{u}^{(n-1+\frac{2J-j-1}{2J-1})} \right),$$

with each solve followed by  $\mathbf{u}^{(n-1+\frac{j}{2J-1})} \leftarrow \mathbf{u}^{(n-1+\frac{j-1}{2J-1})} + R_j^T \Phi_j \mathbf{v}_j$ . This time the diagonal matrix  $\Phi_j$  has as its diagonal values ones on  $\Theta_j \cup \Gamma_{j-1,j}$  and zeros on  $\Gamma_{j,j+1}$ , and the last two constraints are the same as before.

domain approximations into a global approximation was introduced in [18] under the name *restricted additive Schwarz method* (RAS), and this made the method equivalent to the underlying parallel Schwarz method, but at the price of sacrificing symmetry. The restricted weighting never adds two subdomain approximations at the same location so that the current subdomain approximation can be subtracted and updated through a correction. One can then use a global deferred correction at every substep. One could also evaluate the global residual at the beginning of the  $n$ th iteration and do the gluing and the global correction at the end of the  $n$ th iteration, while carrying out the intermediate substeps in the subdomain transmission form or a local deferred correction form (see subsection 8.1). Then, weighting functions from the backward sweep of Algorithm 4 without the restricted constraint  $(R_j^T \Phi_j) R_j (R_l^T \Phi_l) = 0$  could be used for gluing the global correction.

*Remark 20.* Algorithm 3 (Algorithm 4) uses a restricted extension  $\mathcal{E}_j \phi_j$  ( $R_j^T \Phi_j$ ) of the local approximations, but a full restriction  $\cdot|_{\Omega_j}$  ( $R_j$ ) of the global residuals. A variant of each algorithm can be obtained by using a restricted restriction  $\cdot|_{\Omega_j} \phi_j$  ( $\Phi_j R_j$ ) of the global residuals but a full extension  $\mathcal{E}_j$  ( $R_j^T$ ) of the local approximations. For example, in Algorithm 4,  $\Phi_j$  could be moved from the right of  $R_j^T$  in (45) to the left of  $R_j$  in (44). This idea was first introduced in [18] to transform RAS into the *additive Schwarz method with harmonic extension* (ASH), and later adopted and studied in [113] for optimized Schwarz methods with overlap. In [113], a close relation was proved between the iterates of the optimized ASH and the POSM. Moreover, the harmonic extension variant of Algorithms 3 and 4 can be shown to converge in one step under the assumptions of Theorems 17 and 18. When the coefficient matrices of the original problem and the subproblems are complex symmetric (i.e.,  $A^T = A$ ), then the RAS and the ASH lead to preconditioned systems that are the transpose of each other, and hence they have the same spectra.

**THEOREM 21.** Suppose the subproblems in Algorithm 3 are well-posed. For an overlapping decomposition, if  $\phi_j$  of Algorithm 3 also satisfies  $\mathbf{n}_j^T \alpha \nabla \phi_j = 0$  on  $\Gamma_{j \pm 1, j}$ ,  $j = 1, \dots, J$ , then Algorithm 3 is equivalent to Algorithm 1. That is, given  $u^{(0)} = \sum_{j=1}^J \mathcal{E}_j(\phi_j u_j^{(0)})$ , the iterates generated by the two algorithms satisfy for all  $n$  that  $u^{(n)} = \sum_{l=1}^J \mathcal{E}_l(\phi_l u_l^{(n)})$ .

*Proof.* Suppose  $u^{(0)} = \sum_{j=1}^J \mathcal{E}_j(\phi_j u_j^{(0)})$  and the sequence  $u^{(*)}$  is generated by Algorithm 3, and the sequence  $u_j^{(*)}$  is generated by Algorithm 1. Assuming that  $u^{(n-1+\frac{j-1}{2J-1})} = \sum_{l=1}^{j-1} \mathcal{E}_l(\phi_l u_l^{(n-\frac{1}{2})}) + \sum_{l=j}^J \mathcal{E}_l(\phi_l u_l^{(n-1)})$ , we will show that the same relation also holds for  $j+1$  instead of  $j$ . First, we have  $u^{(n-1+\frac{j-1}{2J-1})} = u_{j-1}^{(n-\frac{1}{2})}$  on  $\Gamma_{j,j-1}$  because  $\phi_{j-1} = 1$  in  $\Theta_{j-1}$  and  $\phi_j$  is compactly supported in  $\Omega_j$ . Second, we have  $\mathbf{n}_j^T \alpha \nabla u^{(n-1+\frac{j-1}{2J-1})} = \mathbf{n}_j^T \alpha \nabla u_{j-1}^{(n-\frac{1}{2})}$  on  $\Gamma_{j,j-1}$  because  $\phi_{j-1} = 1$  in  $\Theta_{j-1}$ ,  $\phi_j$  is compactly supported in  $\Omega_j$ ,  $\phi_{j-1}$  is smooth, and  $\mathbf{n}_j^T \alpha \nabla \phi_{j-1} = 0$  on  $\Gamma_{j,j-1}$ . Combining the two traces, we have that the transmission condition on  $\Gamma_{j,j-1}$  in Algorithm 1 is equivalent to

$$\mathcal{Q}_j^\langle \left( \mathbf{n}_j^T \alpha \nabla u_j^{(n-\frac{1}{2})} \right) + \mathcal{P}_j^\langle u_j^{(n-\frac{1}{2})} = \mathcal{Q}_j^\langle \left( \mathbf{n}_j^T \alpha \nabla u^{(n-1+\frac{j-1}{2J-1})} \right) + \mathcal{P}_j^\langle u^{(n-1+\frac{j-1}{2J-1})}.$$

By the same argument, the other transmission condition in the forward sweep can also be rewritten using  $u^{(n-1+\frac{j-1}{2J-1})}$ . We introduce  $\tilde{v}_j := u_j^{(n-\frac{1}{2})} - u^{(n-1+\frac{j-1}{2J-1})}|_{\Omega_j}$  and we find from Algorithm 1 that  $\tilde{v}_j$  solves the forward sweeping problem of Algorithm 3.

Hence,  $v_j^{(n-\frac{1}{2})} = \tilde{v}_j = u_j^{(n-\frac{1}{2})} - u^{(n-1+\frac{j-1}{2J-1})}|_{\Omega_j}$ . By this equation, Algorithm 3, and our assumptions, we obtain

$$\begin{aligned} u^{(n-1+\frac{j}{2J-1})} &= u^{(n-1+\frac{j-1}{2J-1})} + \mathcal{E}_j(\phi_j v_j^{(n-\frac{1}{2})}) \\ &= (1 - \mathcal{E}_j \phi_j) u^{(n-1+\frac{j-1}{2J-1})} + \mathcal{E}_j(\phi_j u_j^{(n-\frac{1}{2})}) \\ &= \sum_{s \neq j} \mathcal{E}_s \phi_s \left( \sum_{l=1}^{j-1} \mathcal{E}_l(\phi_l u_l^{(n-\frac{1}{2})}) + \sum_{l=j}^J \mathcal{E}_l(\phi_l u_l^{(n-1)}) \right) + \mathcal{E}_j(\phi_j u_j^{(n-\frac{1}{2})}) \\ &= \sum_{l=1}^j \mathcal{E}_l(\phi_l u_l^{(n-\frac{1}{2})}) + \sum_{l=j+1}^J \mathcal{E}_l(\phi_l u_l^{(n-1)}). \end{aligned}$$

By induction, we know this holds for all  $j = 1, \dots, J-1$ . Similarly, we can prove for the backward sweep

$$u^{(n-1+\frac{2J-j}{2J-1})} = \sum_{l=1}^{j-1} \mathcal{E}_l(\phi_l u_l^{(n-\frac{1}{2})}) + \sum_{l=j}^J \mathcal{E}_l(\phi_l u_l^{(n)}) \text{ for all } j = J, \dots, 1.$$

In particular,  $u^{(n)} = \sum_{l=1}^J \mathcal{E}_l(\phi_l u_l^{(n)})$ , and the result follows by induction.  $\square$

*Remark 22.* The assumption that  $\mathbf{n}_j^T \alpha \nabla \phi_j = 0$  on  $\Gamma_{j\pm 1,j}$  was first introduced in [28]. We think this assumption can be removed from Theorem 21. In the matrix version (see Theorem 23) we find no counterpart of this assumption. For the same reason, we think that Theorem 21 also holds for nonoverlapping decompositions. There are, however, some difficulties for the justification at the PDE level: as noted in [157], “ $u^{(*)}$  is generally discontinuous at the interface  $\Gamma_{j,j-1}$ , which results in a most singular residual, and the restriction of the residual to the subdomain  $\Omega_j$  is not well defined.”

**THEOREM 23.** *If the subproblems in Algorithm 4 are well-posed, Algorithm 4 is equivalent to Algorithm 2. That is, given  $\mathbf{u}^{(0)} = \sum_{j=1}^J R_j^T \Phi_j \mathbf{u}_j^{(0)}$ , the iterates generated by the two algorithms satisfy  $\mathbf{u}^{(n)} = \sum_{l=1}^J R_l^T \Phi_l \mathbf{u}_l^{(n)}$  for all  $n$ .*

*Proof.* Suppose  $\mathbf{u}^{(0)} = \sum_{j=1}^J R_j^T \Phi_j \mathbf{u}_j^{(0)}$  and the iterates  $\mathbf{u}^{(*)}$  are generated by Algorithm 4, and the iterates  $\mathbf{u}_j^*$ ,  $j = 1, \dots, J$ , by Algorithm 2. Assuming that

$$(46) \quad \mathbf{u}^{(n-1+\frac{j-1}{2J-1})} = \sum_{l=1}^{j-1} R_l^T \Phi_l \mathbf{u}_l^{(n-\frac{1}{2})} + \sum_{l=j}^J R_l^T \Phi_l \mathbf{u}_l^{(n-1)},$$

we will show that the same relation also holds for  $j+1$  instead of  $j$ . By (46) and the constraints on  $\Phi_l$ , we have

$$\begin{aligned} R_j \langle \mathbf{u}^{(n-1+\frac{j-1}{2J-1})} \rangle &= \mathbf{u}_{j-1[\frac{1}{2}]}^{(n-\frac{1}{2})}, & R_{j-1} \langle \mathbf{u}^{(n-1+\frac{j-1}{2J-1})} \rangle &= \mathbf{u}_{j-1[\frac{1}{2}]}^{(n-\frac{1}{2})}, \\ R_j \langle \mathbf{u}^{(n-1+\frac{j-1}{2J-1})} \rangle &= \mathbf{u}_{j+1[\frac{1}{2}]}^{(n-1)}, & R_{j+1} \langle \mathbf{u}^{(n-1+\frac{j-1}{2J-1})} \rangle &= \mathbf{u}_{j+1[\frac{1}{2}]}^{(n-1)}. \end{aligned}$$

Substituting these into the forward sweep problem in Algorithm 2, we find  $\mathbf{u}_j^{(n-\frac{1}{2})} - R_j \mathbf{u}^{(n-1+\frac{j-1}{2J-1})}$  solves the forward sweep problem of Algorithm 4, i.e.,  $\mathbf{v}_j = \mathbf{u}_j^{(n-\frac{1}{2})} - R_j \mathbf{u}^{(n-1+\frac{j-1}{2J-1})}$ . Substituting this into the update relation of Algorithm 4 and using

the constraints on  $\Phi_l$ , we obtain

$$\begin{aligned}\mathbf{u}^{(n-1+\frac{j}{2J-1})} &= (I - R_j^T \Phi_j R_j) \mathbf{u}^{(n-1+\frac{j-1}{2J-1})} + R_j^T \Phi_j \mathbf{u}_j^{(n-\frac{1}{2})} \\ &= \sum_{s \neq j} R_s^T \Phi_s R_s \left( \sum_{l=1}^{j-1} R_l^T \Phi_l \mathbf{u}_l^{(n-\frac{1}{2})} + \sum_{l=j}^J R_l^T \Phi_l \mathbf{u}_l^{(n-1)} \right) + R_j^T \Phi_j \mathbf{u}_j^{(n-\frac{1}{2})} \\ &= \sum_{l=1}^j R_l^T \Phi_l \mathbf{u}_l^{(n-\frac{1}{2})} + \sum_{l=j+1}^J R_l^T \Phi_l \mathbf{u}_l^{(n-1)}.\end{aligned}$$

By induction, we know this holds for all  $j = 1, \dots, J-1$ . Similarly, the backward sweep gives

$$\mathbf{u}^{(n-1+\frac{2J-j}{2J-1})} = \sum_{l=1}^{j-1} R_l^T \Phi_l \mathbf{u}_l^{(n-\frac{1}{2})} + \sum_{l=j}^J R_l^T \Phi_l \mathbf{u}_l^{(n)} \quad \forall j = J, \dots, 1.$$

In particular, we have  $\mathbf{u}^{(n)} = \sum_{l=1}^J R_l^T \Phi_l \mathbf{u}_l^{(n)}$ , and the result follows by induction.  $\square$

*Remark 24.* The DOSM can be used also as a preconditioner for the original problem. The DOSM preconditioner as a linear operator acts on a given r.h.s. and outputs an approximate solution by one or multiple steps of the DOSM iteration with *zero* initial guess. As we showed above, choosing an appropriate gluing scheme is very important for the preconditioned Richardson iteration  $\mathbf{u}^{(l)} = \mathbf{u}^{(l-1)} + M^{-1}(\mathbf{f} - A\mathbf{u}^{(l-1)})$  to be equivalent to the DOSM in the subdomain transmission form. If we use the preconditioner with a Krylov method, e.g., GMRES, the convergence cannot be slower than the Richardson iteration. Hence, the equivalence tells us that if the optimal DOSM from Theorem 18 is used as a preconditioner for a Krylov method, the latter also converges in one step. This is not the case for the gluing scheme of the AS, which uses for the weights all ones on each subdomain. Another advantage of using the DOSM as a *preconditioner* is that even if one uses inexact subdomain solves, i.e.,  $\tilde{M}^{-1} \approx M^{-1}$ , the global consistency is retained, i.e., the converged iterate is always the solution of the original problem, while the *plain* DOSM iterates have a consistency error.

*Remark 25.* From the subdomain transmission form (Algorithm 1 or 2) to the deferred correction form (Algorithm 3 or Algorithm 4), we see that the interface conditions become homogeneous and the evaluation of the r.h.s. becomes unrelated to the transmission operators  $\mathcal{P}, \mathcal{Q}$  or  $P, Q$ . This can be an advantage when the action of those operators is expensive. For example, the PML technique (see Remark 13) leads to the choice  $\mathcal{Q} = \mathcal{I}$ ,  $\mathcal{P} = \text{DtN}_j^{pml}$  on  $\Gamma_{j,j\pm 1}$ . In this case, the action of  $\mathcal{P}$  involves solving a problem in  $\Omega_j^{pml}$  which one might want to avoid. In the deferred correction form, the action of  $\mathcal{P}$  is not required for the evaluation of the r.h.s., but  $\mathcal{P}$  still appears as acting on the unknown function in the interface condition

$$\mathbf{n}_j^T \alpha \nabla v_j + \text{DtN}_j^{pml} v_j = 0 \quad \text{on } \Gamma_{j,j\pm 1},$$

where we have omitted the superscripts for simplicity. For the implementation, one usually unfolds the PML-DtN operator and composes a bigger problem defined in  $\Omega_j \cup \Omega_j^{pml}$ , as explained in Remark 13. The first use of PML in a Schwarz method is due to Toselli (see [163]), who seemed to use the full extension including the PML regions for updating the global iterates, so that his algorithm deviates from the optimized Schwarz method and may be interpreted as an overlapping Schwarz method with the

PML equations used in the overlap. This resembles in the overlap the shifted-Laplace based Schwarz method recently proposed and studied in [90].

*Remark 26.* There are many other ways of implementing the PML transmission conditions. One was proposed in [148, 149]. First, we rewrite the condition as

$$\mathbf{n}_j^T \alpha \nabla u_j + \text{DtN}_j^{pml}(u_j - u_{j-1}) = \mathbf{n}_j^T \alpha \nabla u_{j-1} \quad \text{on } \Gamma_{j,j-1}.$$

Then, we unfold  $\text{DtN}_j^{pml}$  and compose a coupled problem in  $\Omega_j \cup \Omega_j^{pml}$  as follows:

$$\begin{aligned} \mathcal{L}u_j &= f && \text{in } \Omega_j, \\ \mathcal{B}u_j &= g && \text{on } \partial\Omega_j \cap \partial\Omega, \\ \mathbf{n}_j^T \alpha \nabla u_j - \mathbf{n}_j^T \alpha \nabla v &= \mathbf{n}_j^T \alpha \nabla u_{j-1} && \text{on } \partial\Omega_j - \partial\Omega, \\ \tilde{\mathcal{L}}v &= 0 && \text{in } \Omega_j^{pml}, \\ \tilde{\mathcal{B}}v &= 0 && \text{on } \partial\Omega_j^{pml} - \partial\Omega_j, \\ v - u_j &= -u_{j-1} && \text{on } \partial\Omega_j^{pml} - \partial\Omega. \end{aligned}$$

A straightforward discretization requires two sets of d.o.f. on the interfaces  $\Gamma_{j,j\pm 1}$ , one for  $u_j$  and the other for  $v$ . In this way, we need only to solve one coupled problem in  $\Omega_j \cup \Omega_j^{pml}$  and we avoid solving an extra problem in  $\Omega_j^{pml}$ . We can further remove the Dirichlet jump from the coupled problem by extending (lifting)  $u_{j-1}$  from the interfaces into  $\Omega_j^{pml}$ . Let the extended function be  $\tilde{u}_{j-1}^{j,pml}$ . We change the unknown in the PML to  $\tilde{v} := v + \tilde{u}_{j-1}^{j,pml}$  so that the coupled problem for  $(u_j, \tilde{v})$  enforces no jump of Dirichlet traces across the interfaces.

**6.3. Substructured Form of Schwarz Methods.** The substructured form of the optimized Schwarz method consists in taking interface data as iterates (unknowns).<sup>16</sup> These iterates are substantially smaller than the volume iterates and thus can save memory and flops for Krylov subspace methods. This form was first introduced in [132] for one-way domain decompositions like in Figure 2. In particular, for Helmholtz problems, it was used in [30, 76]. Later, the substructured form was generalized to the case of domain decompositions with cross points (points shared by three or more subdomains); see, e.g., [12, 62, 73, 81, 124] for various approaches (some are called FETI-2LM). Here, we consider only the sequential one-way domain decomposition from Figure 2. The substructured form of the DOSM is given in Algorithm 5 at the PDE level and in Algorithm 6 at the matrix level. Theorems 27 and 28 give the equivalence of the substructured formulations to the formulations with subdomain iterates. Their proofs are simple and we thus omit them here.

**THEOREM 27.** *Algorithm 5 is equivalent to Algorithm 1. That is, given  $\lambda_{j\rangle}^{(0)} = \mathcal{Q}_j^\rangle(\mathbf{n}_j^T \alpha \nabla u_j^{(0)}) + \mathcal{P}_j^\rangle u_j^{(0)}$ , the iterates generated by the two algorithms satisfy  $\lambda_{j\rangle}^{(n)} = \mathcal{Q}_j^\rangle(\mathbf{n}_j^T \alpha \nabla u_j^{(n)}) + \mathcal{P}_j^\rangle u_j^{(n)}$ .*

**THEOREM 28.** *Algorithm 6 is equivalent to Algorithm 2. That is, given  $\boldsymbol{\lambda}_{j\rangle}^{(0)} = (\mathcal{Q}_{j\rangle}^\rangle A_{j\rangle}^\rangle + \mathcal{P}_{j\rangle}^\rangle) \mathbf{u}_{j\rangle}^{(0)} + \mathcal{Q}_{j\rangle}^\rangle A_{j\rangle j\bullet} \mathbf{u}_{j\bullet}^{(0)} - \mathcal{Q}_{j\rangle}^\rangle \mathbf{f}_{j\rangle}^\rangle$ , the iterates generated by the two algorithms satisfy  $\boldsymbol{\lambda}_{j\rangle}^{(n)} = (\mathcal{Q}_{j\rangle}^\rangle A_{j\rangle}^\rangle + \mathcal{P}_{j\rangle}^\rangle) \mathbf{u}_{j\rangle}^{(n)} + \mathcal{Q}_{j\rangle}^\rangle A_{j\rangle j\bullet} \mathbf{u}_{j\bullet}^{(n)} - \mathcal{Q}_{j\rangle}^\rangle \mathbf{f}_{j\rangle}^\rangle$ .*

<sup>16</sup>If exact subdomain solvers are used, the glued global approximation has compact residual for the original problem near interfaces. Making use of this property leads to yet another substructured form; see Algorithm 12 in subsection 8.2.

**Algorithm 5.** DOSM in the **substructured** form at the **PDE** level.

Given the last iterate  $\lambda_j^{(n-1)} = \{\lambda_{j\langle}^{(n-1)}\}_{j=1,\dots,J-1}$ , solve successively for  $j = 1, \dots, J-1$ ,

$$\begin{aligned}\mathcal{L} u_j^{(n-\frac{1}{2})} &= f && \text{in } \Omega_j, \\ \mathcal{B} u_j^{(n-\frac{1}{2})} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathcal{Q}_j^{\langle} \left( \mathbf{n}_j^T \alpha \nabla u_j^{(n-\frac{1}{2})} \right) + \mathcal{P}_j^{\langle} u_j^{(n-\frac{1}{2})} &= \lambda_{j\langle}^{(n)} && \text{on } \Gamma_{j,j-1}, \\ \mathcal{Q}_j^{\rangle} \left( \mathbf{n}_j^T \alpha \nabla u_j^{(n-\frac{1}{2})} \right) + \mathcal{P}_j^{\rangle} u_j^{(n-\frac{1}{2})} &= \lambda_{j\rangle}^{(n-1)} && \text{on } \Gamma_{j,j+1},\end{aligned}$$

with each solve followed by  $\lambda_{j+1\langle}^{(n)} \leftarrow \mathcal{Q}_{j+1}^{\langle} \left( \mathbf{n}_{j+1}^T \alpha \nabla u_j^{(n-\frac{1}{2})} \right) + \mathcal{P}_{j+1}^{\langle} u_j^{(n-\frac{1}{2})}$ .

Then solve successively for  $j = J, \dots, 1$ ,

$$\begin{aligned}\mathcal{L} u_j^{(n)} &= f && \text{in } \Omega_j, \\ \mathcal{B} u_j^{(n)} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathcal{Q}_j^{\langle} \left( \mathbf{n}_j^T \alpha \nabla u_j^{(n)} \right) + \mathcal{P}_j^{\langle} u_j^{(n)} &= \lambda_{j\langle}^{(n)} && \text{on } \Gamma_{j,j-1}, \\ \mathcal{Q}_j^{\rangle} \left( \mathbf{n}_j^T \alpha \nabla u_j^{(n)} \right) + \mathcal{P}_j^{\rangle} u_j^{(n)} &= \lambda_{j\rangle}^{(n)} && \text{on } \Gamma_{j,j+1},\end{aligned}$$

with each solve followed by  $\lambda_{j-1\rangle}^{(n)} \leftarrow \mathcal{Q}_{j-1}^{\rangle} \left( \mathbf{n}_{j-1}^T \alpha \nabla u_j^{(n)} \right) + \mathcal{P}_{j-1}^{\rangle} u_j^{(n)}$ .

We obtain  $\lambda_j^{(n)} \leftarrow \{\lambda_{j\rangle}^{(n)} \text{ on } \Gamma_{j,j+1}, j = 1, \dots, J-1\}$ .

To explain how to use Krylov acceleration for the substructured formulations, we denote  $\lambda_{\langle}^{(n)} := \{\lambda_{j\langle}^{(n)}, j = 2, \dots, J\}$ . The forward and backward sweeps of Algorithm 5 define a linear forward map  $\mathcal{F}_{\langle}$  and a backward map  $\mathcal{F}_{\rangle}$  such that  $\lambda_{\langle}^{(n)} = \mathcal{F}_{\langle}(\lambda_{\rangle}^{(n-1)}, f, g)$  and  $\lambda_{\rangle}^{(n)} = \mathcal{F}_{\rangle}(\lambda_{\langle}^{(n)}, f, g)$ . The corresponding fixed point equation  $\lambda_{\rangle} = \mathcal{F}_{\rangle}(\mathcal{F}_{\langle}(\lambda_{\rangle}, f, g), f, g)$  can be rewritten as a linear system

$$(\mathcal{I} - \mathcal{F}_{\rangle}(\mathcal{F}_{\langle}(\cdot, 0, 0), 0, 0)) \lambda_{\rangle} = \mathcal{F}_{\rangle}(\mathcal{F}_{\langle}(0, f, g), f, g),$$

which can now be solved by polynomial methods, e.g., Chebyshev iterations and/or Krylov methods.

*Remark 29.* If we look at each solve and the following update, we have a linear map  $\mathcal{F}_{j+1\langle}$  such that  $\lambda_{j+1\langle}^{(n)} = \mathcal{F}_{j+1\langle}(\lambda_{j\langle}^{(n)}, \lambda_{j\rangle}^{(n-1)}, f, g)$  and  $\mathcal{F}_{j-1\rangle}$  such that  $\lambda_{j-1\rangle}^{(n)} = \mathcal{F}_{j-1\rangle}(\lambda_{j\langle}^{(n)}, \lambda_{j\rangle}^{(n)}, f, g)$ . Considering the converged solution (i.e., removing the superscripts), we find the linear system

$$\left[ \begin{array}{cc|cc} 1 & & -\mathfrak{b}_1^- & \\ -\mathfrak{a}_1^- & 1 & -\mathfrak{b}_2^- & \\ \ddots & \ddots & \ddots & \\ -\mathfrak{a}_{J-2}^- & 1 & -\mathfrak{b}_{J-1}^- & \\ \hline -\mathfrak{b}_1^+ & & 1 & -\mathfrak{a}_1^+ \\ -\mathfrak{b}_2^+ & & 1 & \ddots \\ \ddots & & \ddots & -\mathfrak{a}_{J-2}^+ \\ -\mathfrak{b}_{J-1}^+ & & & 1 \end{array} \right] \begin{bmatrix} \lambda_{2\langle} \\ \lambda_{3\langle} \\ \vdots \\ \lambda_{J\langle} \\ \hline \lambda_{1\rangle} \\ \lambda_{2\rangle} \\ \vdots \\ \lambda_{J-1\rangle} \end{bmatrix} = \begin{bmatrix} \mathfrak{g}_{2\langle} \\ \mathfrak{g}_{3\langle} \\ \vdots \\ \mathfrak{g}_{J\langle} \\ \hline \mathfrak{g}_{1\rangle} \\ \mathfrak{g}_{2\rangle} \\ \vdots \\ \mathfrak{g}_{J-1\rangle} \end{bmatrix},$$

---

**Algorithm 6.** DOSM in the **substructured** form at the **matrix** level.

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Given the last iterate  $\lambda_j^{(n-1)} = \{\lambda_j^{(n-1)}, j = 1, \dots, J-1\}$ , solve successively for  $j = 1, \dots, J-1$ ,

$$\begin{bmatrix} Q_j^{\langle} A_{j\langle}^{\langle} + P_j^{\langle} & Q_j^{\langle} A_{j\langle} \bullet \\ A_{j\bullet j\langle} & A_{j\bullet} \\ Q_j^{\rangle} A_{j\rangle j\bullet} & Q_j^{\rangle} A_{j\rangle}^{\rangle} + P_j^{\rangle} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{j\langle}^{(n-\frac{1}{2})} \\ \mathbf{u}_{j\bullet}^{(n-\frac{1}{2})} \\ \mathbf{u}_{j\rangle}^{(n-\frac{1}{2})} \end{bmatrix} = \begin{bmatrix} Q_j^{\langle} \mathbf{f}_{j\langle}^{\langle} + \lambda_j^{(n)} \\ \mathbf{f}_{j\bullet} \\ Q_j^{\rangle} \mathbf{f}_{j\rangle}^{\rangle} + \lambda_j^{(n-1)} \end{bmatrix},$$

with each solve followed by

$$\lambda_{j+1\langle}^{(n)} \leftarrow Q_{j+1\langle}^{\langle} \left( \mathbf{f}_{j+1\langle}^{\langle} - A_{j+1\langle} j\bullet \mathbf{u}_{j\bullet}^{(n-\frac{1}{2})} \right) + \left( P_{j+1\langle}^{\langle} - Q_{j+1\langle}^{\langle} A_{j+1\langle}^{\langle} \right) \mathbf{u}_{j\langle}^{(n-\frac{1}{2})}.$$

Note that it does not matter which splits  $\mathbf{f}_{j\langle} = \mathbf{f}_{j\langle}^{\langle} + \mathbf{f}_{j\langle}^{\rangle}$  and  $\mathbf{f}_{j\rangle} = \mathbf{f}_{j\rangle}^{\langle} + \mathbf{f}_{j\rangle}^{\rangle}$  are used, the only difference will be the definition of the interface data. For example, one can use the simple splits  $\mathbf{f}_{j\langle}^{\rangle} = 0$  and  $\mathbf{f}_{j\rangle}^{\langle} = 0$ .

Then solve successively for  $j = J, \dots, 1$ ,

$$\begin{bmatrix} Q_j^{\langle} A_{j\langle}^{\langle} + P_j^{\langle} & Q_j^{\langle} A_{j\langle} \bullet \\ A_{j\bullet j\langle} & A_{j\bullet} \\ Q_j^{\rangle} A_{j\rangle j\bullet} & Q_j^{\rangle} A_{j\rangle}^{\rangle} + P_j^{\rangle} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{j\langle}^{(n)} \\ \mathbf{u}_{j\bullet}^{(n)} \\ \mathbf{u}_{j\rangle}^{(n)} \end{bmatrix} = \begin{bmatrix} Q_j^{\langle} \mathbf{f}_{j\langle}^{\langle} + \lambda_j^{(n)} \\ \mathbf{f}_{j\bullet} \\ Q_j^{\rangle} \mathbf{f}_{j\rangle}^{\rangle} + \lambda_j^{(n)} \end{bmatrix},$$

with each solve followed by

$$\lambda_{j-1\rangle}^{(n)} \leftarrow Q_{j-1\rangle}^{\rangle} \left( \mathbf{f}_{j-1\rangle}^{\rangle} - A_{j-1\rangle} j\bullet \mathbf{u}_{j\bullet}^{(n)} \right) + \left( P_{j-1\rangle}^{\rangle} - Q_{j-1\rangle}^{\rangle} A_{j-1\rangle}^{\rangle} \right) \mathbf{u}_{j\rangle}^{(n)}.$$

We obtain  $\lambda_j^{(n)} = \{\lambda_j^{(n)}, j = 1, \dots, J-1\}$ .

---

where  $\mathbf{1}$ 's are the identity operators,  $\mathbf{a}_j^- := \mathcal{F}_{j+2\langle}(\cdot, 0, 0, 0)$ ,  $\mathbf{b}_j^- := \mathcal{F}_{j+1\langle}(0, \cdot, 0, 0)$ ,  $\mathbf{a}_j^+ := \mathcal{F}_{j\rangle}(0, \cdot, 0, 0)$ ,  $\mathbf{b}_j^+ := \mathcal{F}_{j\rangle}(\cdot, 0, 0, 0)$ , and  $\mathbf{g}_* = \mathcal{F}_*(0, 0, f, g)$ . If we regard the above system as a 2-by-2 block system, the block Gauss–Seidel method (see Remark 39 for block Jacobi) leads to Algorithm 5 with each block solved exactly by forward or backward substitution. The operators  $\mathbf{a}_j$  and  $\mathbf{b}_j$  can also be represented using Green's functions based on (37), which we will see in more detail in section 8.

**7. AILU and Sweeping Preconditioners.** We now explain the AILU and sweeping preconditioners. To do so, we denote in (19)  $\mathbf{u}_1 := \mathbf{u}_{1\bullet}$ ,  $\mathbf{f}_1 := \mathbf{f}_{1\bullet}$ ,  $D_1 := A_{1\bullet}$ ,  $L_1 := [A_{1\bullet} 0]$ ,  $U_1 := [A_{1\bullet} 0]$ , and, for  $j \geq 2$ ,  $\mathbf{u}_j := [\mathbf{u}_{j-1\bullet}; \mathbf{u}_{j\bullet}]$ ,  $\mathbf{f}_j := [\mathbf{f}_{j-1\bullet}; \mathbf{f}_{j\bullet}]$ ,

$$D_j := \begin{bmatrix} A_{j-1\rangle} & A_{j-1\rangle j\bullet} \\ A_{j\bullet j-1\rangle} & A_{j\bullet} \end{bmatrix}, \quad L_j := \begin{bmatrix} 0 & A_{j\rangle j\bullet} \\ 0 & 0 \end{bmatrix}, \quad U_j := \begin{bmatrix} 0 & 0 \\ A_{j\bullet j\bullet} & 0 \end{bmatrix}.$$

With this notation, (19) becomes (2). Then, based on the factorization given in (3), we can solve (5) and (6) by forward and backward substitution, which leads to Algorithm 7.

**THEOREM 30.** *If  $T_j$ ,  $j = 1, \dots, J$ , are invertible, then Algorithm 7 is equivalent to Algorithm 2 with a nonoverlapping decomposition, zero initial guess, and  $Q_j^{\langle} = I_{j\langle}$ ,*

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**Algorithm 7.** Block LU solve for the block tridiagonal system in (2).

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Compute  $T_j$ 's according to (4).

Forward sweep: solve successively the subproblems

$$\begin{aligned} T_1 \mathbf{v}_1 &= \mathbf{f}_1, \\ T_j \mathbf{v}_j &= \mathbf{f}_j - L_{j-1} \mathbf{v}_{j-1}, \quad j = 2, \dots, J. \end{aligned}$$

Backward sweep: let  $\mathbf{u}_J \leftarrow \mathbf{v}_J$ ; solve successively the subproblems

$$T_j \mathbf{u}_j = T_j \mathbf{v}_j - U_j \mathbf{u}_{j+1}, \quad j = J-1, \dots, 1.$$


---

$P_{j\langle}^{\langle} = A_{j\langle}^{\rangle} - A_{j\langle, \sim j} A_{\sim j}^{-1} A_{\sim j, j\langle}$ ,  $Q_{j\rangle}^{\rangle} = 0$ ,  $P_{j\rangle}^{\rangle} = I_{j\rangle}$ . That is, the iterates generated by the two algorithms satisfy  $\mathbf{v}_j = [\mathbf{u}_{j\langle}^{(\frac{1}{2})}; \mathbf{u}_{j\rangle}^{(\frac{1}{2})}]$  and  $\mathbf{u}_j = [\mathbf{u}_{j\langle}^{(1)}; \mathbf{u}_{j\rangle}^{(1)}]$ .

*Proof.* We first show that the  $T_j$ 's defined by (4) satisfy for  $j \geq 2$ ,

$$(47) \quad T_j = D_j - \tilde{L}_{j-1} A_{\sim j}^{-1} \tilde{U}_{j-1},$$

where  $\tilde{L}_1 := L_1$ ,  $\tilde{U}_1 := U_1$ ,  $\tilde{L}_{j-1} := [0, L_{j-1}]$ , and  $\tilde{U}_{j-1} := [0; U_{j-1}]$  for  $j \geq 3$ . The case of  $j = 2$  follows directly by definition. Assuming (47) holds for one  $j$ , we now show that it also holds for  $j + 1$  instead of  $j$ . First, by Gaussian elimination we have from (47) that

$$A_{\sim j+1}^{-1} = \begin{bmatrix} A_{\sim j} & \tilde{U}_{j-1} \\ \tilde{L}_{j-1} & D_j \end{bmatrix}^{-1} = \begin{bmatrix} * & * \\ * & T_j^{-1} \end{bmatrix},$$

where  $*$  represents terms not interesting to us. Therefore,

$$D_{j+1} - \tilde{L}_j A_{\sim j+1}^{-1} \tilde{U}_j = D_{j+1} - [0 \quad L_j] \begin{bmatrix} * & * \\ * & T_j^{-1} \end{bmatrix} \begin{bmatrix} 0 \\ U_j \end{bmatrix} = T_{j+1},$$

which is (47) with  $j$  replaced by  $j + 1$ . By induction, (47) holds for all  $j \geq 2$ . Note that we are considering a nonoverlapping decomposition so we can write

$$\tilde{L}_{j-1} = \begin{bmatrix} A_{j\langle, \sim j} \\ 0 \end{bmatrix}, \quad \tilde{U}_{j-1} = \begin{bmatrix} A_{\sim j, j\langle} & 0 \end{bmatrix}, \quad D_j = \begin{bmatrix} A_{j\langle} & A_{j\langle j\bullet} \\ A_{j\bullet j\langle} & A_{j\bullet} \end{bmatrix}.$$

Substituting the above equations into (47), we obtain for  $j \geq 2$ ,

$$(48) \quad T_j = \begin{bmatrix} A_{j\langle} - A_{j\langle, \sim j} A_{\sim j}^{-1} A_{\sim j, j\langle} & A_{j\langle j\bullet} \\ A_{j\bullet j\langle} & A_{j\bullet} \end{bmatrix}.$$

Let the initial guess of Algorithm 2 be  $\mathbf{u}_j^{(0)} = 0$ ,  $j = 1, \dots, J$ . Substituting this and the specified matrices  $P$  and  $Q$  into Algorithm 2, we find

$$(49) \quad \begin{bmatrix} A_{1\bullet} & A_{1\bullet 1\rangle} \\ 0 & I_{1\rangle} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{1\bullet}^{(\frac{1}{2})} \\ \mathbf{u}_{1\rangle}^{(\frac{1}{2})} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{1\bullet} \\ 0 \end{bmatrix}.$$

By definition, we know  $T_1 = D_1 = A_{1\bullet} = A_{1\bullet}$  and  $\mathbf{f}_1 = \mathbf{f}_{1\bullet}$ . Hence, from (49), we have  $T_1 \mathbf{u}_{1\bullet}^{(\frac{1}{2})} = \mathbf{f}_1$ , which is satisfied also by  $\mathbf{v}_1$  of Algorithm 7. Since  $T_1$  is invertible and

from the fact that the decomposition is nonoverlapping, we have  $\mathbf{v}_1 = \mathbf{u}_{1\bullet}^{(\frac{1}{2})} = \mathbf{u}_{1\overline{\bullet}}^{(\frac{1}{2})}$ . From (49) and again using the fact that the decomposition is nonoverlapping, we have  $\mathbf{u}_{1[\cdot]}^{(\frac{1}{2})} = \mathbf{u}_{1\rangle}^{(\frac{1}{2})} = 0$ . Now assume that<sup>17</sup>

$$(50) \quad \mathbf{v}_{j-1} = \left[ \mathbf{u}_{j-1\langle}^{(\frac{1}{2})}; \mathbf{u}_{j-1\overline{\bullet}}^{(\frac{1}{2})} \right], \quad \mathbf{u}_{j-1[\cdot]}^{(\frac{1}{2})} = 0,$$

with  $\mathbf{v}_{j-1}$  obtained by Algorithm 7 and  $\mathbf{u}_{j-1}^{(\frac{1}{2})}$  obtained by Algorithm 2. In the next substep of Algorithm 2, we substitute the specified matrices  $P$  and  $Q$ , and the second equation of (50), to find

$$(51) \quad \left[ \begin{array}{cc|c} A_{j\langle} - A_{j,\sim j} A_{\sim j}^{-1} A_{\sim j,j\langle} & A_{j\langle j\bullet} & 0 \\ A_{j\bullet} & A_{j\bullet} & A_{j\bullet j\rangle} \\ \hline 0 & 0 & I_j \end{array} \right] \left[ \begin{array}{c} \mathbf{u}_{j\langle}^{(\frac{1}{2})} \\ \mathbf{u}_{j\bullet}^{(\frac{1}{2})} \\ \hline \mathbf{u}_{j\rangle}^{(\frac{1}{2})} \end{array} \right] = \left[ \begin{array}{c} \mathbf{f}_{j\langle} - A_{j,j-1\overline{\bullet}} \mathbf{u}_{j-1\overline{\bullet}}^{(\frac{1}{2})} \\ \mathbf{f}_{j\bullet} \\ \hline 0 \end{array} \right].$$

By (48), we know that the upper-left 2-by-2 block matrix in (51) equals  $T_j$ . From the first equation of (50), we see that the first two rows of the r.h.s. of (51) equal  $\mathbf{f}_2 - L_1 \mathbf{v}_1$ . Given that  $T_j$  is invertible and that the decomposition is nonoverlapping, we have from (51) and Algorithm 7 that

$$(52) \quad \mathbf{v}_j = \left[ \mathbf{u}_{j\langle}^{(\frac{1}{2})}; \mathbf{u}_{j\overline{\bullet}}^{(\frac{1}{2})} \right], \quad \mathbf{u}_{j[\cdot]}^{(\frac{1}{2})} = 0.$$

Thus, by induction, (52) holds for all  $j = 1, \dots, J-1$  and

$$\mathbf{u}_J = \mathbf{v}_J = \left[ \mathbf{u}_{J\langle}^{(1)}; \mathbf{u}_{J\overline{\bullet}}^{(1)} \right].$$

In Algorithm 7 we substitute  $T_j \mathbf{v}_j$  from the forward sweep into the backward sweep and obtain the equivalent backward solve

$$T_j \mathbf{u}_j = \mathbf{f}_j - L_{j-1} \mathbf{v}_{j-1} - U_j \mathbf{u}_{j+1}.$$

First, we note that the coefficient matrix  $T_j$  is the same as in the forward solve. Second, compared to the forward solve, the present r.h.s. has an extra term  $-U_j \mathbf{u}_{j+1}$  which corresponds to using the new Dirichlet data taken from the neighboring subdomain on the right. So Algorithm 7 and the specified case of Algorithm 2 remain equivalent in their backward solves, and we have for  $j = J, \dots, 1$ <sup>18</sup>

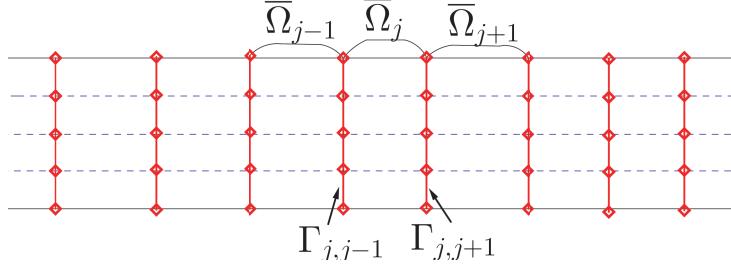
$$\mathbf{u}_j = \left[ \mathbf{u}_{j\langle}^{(1)}; \mathbf{u}_{j\overline{\bullet}}^{(1)} \right].$$

Thus, the equivalence of the two algorithms is proved.  $\square$

Based on Theorem 30, the PDE analogue of Algorithm 7 can be stated as Algorithm 1 with a nonoverlapping decomposition, zero initial guess, and  $\mathcal{Q}_{j\langle}^{\langle} = \mathcal{I}$ ,  $\mathcal{P}_{j\langle}^{\langle} = \text{DtN}_j^{\langle}$ ,  $\mathcal{Q}_{j\rangle}^{\rangle} = 0$ ,  $\mathcal{P}_{j\rangle}^{\rangle} = \mathcal{I}$ . Next, we revisit the AILU and the sweeping preconditioners. Based on Theorem 30, it is straightforward to get the following corollaries.

<sup>17</sup>When  $j = 2$ , we need to remove the nonexistent block.

<sup>18</sup>When  $j = 1$ , we need to remove the nonexistent block.



**Fig. 3** Nonoverlapping domain decomposition with empty interior,  $\diamond \in \Gamma_{*,\#}$ .

COROLLARY 31. *The AILU preconditioner in [78] is equivalent to one step of the DOSM with a nonoverlapping decomposition such that the subdomain interiors are empty (i.e.,  $\Theta_j = \emptyset$ ; see Figure 3), zero initial guess, and second-order absorbing transmission conditions on the left interfaces and Dirichlet transmission conditions on the right interfaces of subdomains.*

COROLLARY 32. *The sweeping preconditioners in [51, 52] are equivalent to one step of the DOSM with a nonoverlapping decomposition such that the subdomain interiors are empty (i.e.,  $\Theta_j = \emptyset$ ; see Figure 3), zero initial guess, and PML or  $\mathcal{H}$ -matrix transmission conditions on the left interfaces and Dirichlet transmission conditions on the right interfaces of subdomains.*

Here we finish our discussions of the algorithms. First we point out an analogy between the LU factorization of the matrix from the discretization of  $\partial_{xx} + \partial_{yy} + k^2$  and the formal analytic factorization of the differential operator,

$$(53) \quad \partial_{xx} + \partial_{yy} + k^2 = (\partial_x - i\sqrt{\partial_{yy} + k^2})(\partial_x + i\sqrt{\partial_{yy} + k^2}).$$

This analogy was first drawn in [77]. The factorization in (53) represents a reformulation of the two-way wave (Helmholtz) equation as two one-way wave equations. Hence, the original *boundary value problem* (BVP) given by the Helmholtz equation (11) can be solved in terms of certain *initial value problems* (IVPs) of the one-way wave equations. The forward substitution of the lower triangular system and the backward solution of the upper triangular system at the matrix level are related to solving these IVPs. Such analytic factorizations have been studied by many researchers; see, e.g., [100, 125]. Next, we give a derivation of the factorization based on a family of DtN operators and explain its relation to Algorithm 1. We will do so for the more general case with curved domains and curved interfaces.

We assume that the domain  $\Omega$  can be described by the curvilinear coordinates,

$$\Omega = \left\{ \mathbf{x} \in \mathbb{R}^d \mid \mathbf{x} = (x_l)_{l=1}^d, x_l = x_l(\xi_1, \dots, \xi_d), \xi_1 \in (a, b) \subset \mathbb{R}, (\xi_2, \dots, \xi_d) \in Y \subset \mathbb{R}^{d-1} \right\},$$

with  $(\frac{\partial x_j}{\partial \xi_i})$  nonsingular and  $x_j$  sufficiently smooth in  $\xi$ . We may view  $\Omega$  as a topological cylinder with the axial variable  $\xi_1$ . For  $s \in [a, b]$ , we denote

$$\Omega^s := \left\{ \mathbf{x} \in \Omega \mid x_l = x_l(\xi_1, \dots, \xi_d), \xi_1 \in (a, s), (\xi_2, \dots, \xi_d) \in Y \right\},$$

$$\Gamma^s := \left\{ \mathbf{x} \in \Omega \mid x_l = x_l(s, \xi_2, \dots, \xi_d), (\xi_2, \dots, \xi_d) \in Y \right\}.$$

Let  $d = 2$  for simplicity. In the curvilinear coordinates, the operator  $\mathcal{L}$  of (11) becomes

$$\mathcal{L}v = -\left(\frac{\partial \xi_1}{\partial x_1} \frac{\partial}{\partial \xi_1} + \frac{\partial \xi_2}{\partial x_1} \frac{\partial}{\partial \xi_2}\right)\left(\beta_1^1 \frac{\partial v}{\partial \xi_1} + \beta_2^1 \frac{\partial v}{\partial \xi_2}\right) - \left(\frac{\partial \xi_1}{\partial x_2} \frac{\partial}{\partial \xi_1} + \frac{\partial \xi_2}{\partial x_2} \frac{\partial}{\partial \xi_2}\right)\left(\beta_1^2 \frac{\partial v}{\partial \xi_1} + \beta_2^2 \frac{\partial v}{\partial \xi_2}\right) - \frac{\omega^2}{\kappa}v,$$

where  $\beta_l^j = \sum_{m=1}^d \alpha_m^j \frac{\partial \xi_l}{\partial x_m}$  and  $(\alpha_l^j)$  is the coefficient matrix  $\alpha$  in Cartesian coordinates. We assume that  $\mathcal{L}$  can be rewritten in the form

$$\mathcal{L}v = \gamma_3 \left\{ \frac{\partial}{\partial \xi_1} \left( \gamma_1 \frac{\partial v}{\partial \xi_1} + \gamma_2 \frac{\partial v}{\partial \xi_2} + \gamma_0 v \right) - \mathcal{L}_2 v \right\},$$

with  $\gamma_j = \gamma_j(\xi_1, \xi_2)$ ,  $j = 1, 2, 3$ ,  $\gamma_3$  and  $\gamma_1$  nowhere zero, and  $\mathcal{L}_2$  a partial differential operator w.r.t.  $\xi_2$  only. This assumption can be verified if  $\beta_1^1, \beta_1^2$  are sufficiently smooth or if  $\xi_1 = x_1, \xi_2 = x_2$  and  $\alpha_1^2$  is sufficiently smooth. We define the operator-valued function  $\mathcal{P}(s)$  for  $s \in [a, b]$  as the  $s$ -dependent generalized DtN operator (we assume the problem below is well-posed):

$$\begin{aligned} \mathcal{P}(s) : d \rightarrow & \left( \gamma_1 \frac{\partial v}{\partial \xi_1} + \gamma_2 \frac{\partial v}{\partial \xi_2} + \gamma_0 v \right) |_{\Gamma^s}, \text{ s.t.} & \mathcal{L}v = 0 & \text{in } \Omega^s, \\ & \mathcal{B}v = 0 & \text{on } \partial \Omega^s \cap \partial \Omega, \\ & v = d & \text{on } \Gamma^s. \end{aligned}$$

Let us consider how  $\mathcal{P}(s)$  changes with  $s$ . Let  $v$  be the solution in the definition of  $\mathcal{P}(s)$ . We have for  $\Delta s < 0$ ,

$$\begin{aligned} \gamma_1 \frac{\partial v}{\partial \xi_1}(s, \xi_2) + \gamma_2 \frac{\partial v}{\partial \xi_2}(s, \xi_2) + \gamma_0 v(s, \xi_2) &= \mathcal{P}(s)v(s, \xi_2), & \xi_2 \in Y, \\ \gamma_1 \frac{\partial v}{\partial \xi_1}(s + \Delta s, \xi_2) + \gamma_2 \frac{\partial v}{\partial \xi_2}(s + \Delta s, \xi_2) + \gamma_0 v(s + \Delta s, \xi_2) &= \mathcal{P}(s + \Delta s)v(s + \Delta s, \xi_2), & \xi_2 \in Y. \end{aligned}$$

Subtracting the two equations and dividing by  $\Delta s$ , we get

$$\begin{aligned} 1/\Delta s \cdot \{(\gamma_1 \partial_1 v + \gamma_2 \partial_2 v + \gamma_0 v)(s + \Delta s, \xi_2) - (\gamma_1 \partial_1 v + \gamma_2 \partial_2 v + \gamma_0 v)(s, \xi_2)\} \\ = 1/\Delta s \cdot \{\mathcal{P}(s + \Delta s) - \mathcal{P}(s)\}v(s + \Delta s, \xi_2) + \mathcal{P}(s)\{v(s + \Delta s, \xi_2) - v(s, \xi_2)\}/\Delta s. \end{aligned}$$

We assume that the difference quotients above converge as  $\Delta s \rightarrow 0$ , and we find

$$(54) \quad \frac{\partial}{\partial \xi_1} \left( \gamma_1 \frac{\partial v}{\partial \xi_1} + \gamma_2 \frac{\partial v}{\partial \xi_2} + \gamma_0 v \right) (s, \xi_2) = \mathcal{P}'(s)v(s, \xi_2) + \mathcal{P}(s) \frac{\partial v}{\partial \xi_1}(s, \xi_2).$$

Using  $\mathcal{L}v = 0$  and  $\gamma_3 \neq 0$ , we find that  $\mathcal{L}_2(s, \xi_2)v(s, \xi_2)$  is equal to the l.h.s. of (54) and thus to the r.h.s. too. We further replace  $\frac{\partial v}{\partial \xi_1}(s, \xi_2)$  with the definition of  $\mathcal{P}(s)$  to obtain

$$\mathcal{L}_2(s, \cdot)v(s, \cdot) = \mathcal{P}'(s)v(s, \cdot) + \mathcal{P}(s)\{\gamma_1^{-1}(s, \cdot)(\mathcal{P}(s) - \gamma_2(s, \cdot)\partial_2 - \gamma_0(s, \cdot))v(s, \cdot)\}.$$

Removing  $v(s, \cdot)$  from the above equation, we obtain the differential Riccati equation

$$(55) \quad \mathcal{P}'(s) = \mathcal{P}(s)\{\gamma_1^{-1}(s, \cdot)(-\mathcal{P}(s) + \gamma_2(s, \cdot)\partial_2 + \gamma_0(s, \cdot))\} + \mathcal{L}_2(s, \cdot).$$

As mentioned in [102], (55) can also be obtained from (4) when the width of the subdomain is equal to the mesh size and goes to zero. The initial value  $\mathcal{P}(a)$  for (55) can be obtained from the boundary condition  $\mathcal{B}v = 0$  on  $\Gamma^a$  if the condition is not of Dirichlet type (we assume this in the following derivation; otherwise, we should not

use the DtN operator but the NtD operator for  $\mathcal{P}$ ). In particular, if  $a = -\infty$  and there exists  $a' \in \mathbb{R}$  such that the problem in the definition of  $\mathcal{P}(s)$  is independent of  $s \leq a'$ , then by letting  $\mathcal{P}'(s) = 0$  we obtain from the differential Riccati equation the algebraic Riccati equation

$$\mathcal{P}(s) \{ \gamma_1^{-1}(s, \cdot) (-\mathcal{P}(s) + \gamma_2(s, \cdot) \partial_2 + \gamma_0(s, \cdot)) \} + \mathcal{L}_2(s, \cdot) = 0 \quad \forall s \leq a'.$$

The solution of the algebraic Riccati equation at  $s = a'$  gives us an initial value  $\mathcal{P}(a')$  for the differential Riccati equation. In what follows, we assume  $\mathcal{P}$  has been precomputed on  $[a, b]$ .

We introduce  $w := (\gamma_1 \frac{\partial u}{\partial \xi_1} + \gamma_2 \frac{\partial u}{\partial \xi_2} + \gamma_0 u) - \mathcal{P}u$  with  $u$  the solution of (11). Again, by the definition of  $\mathcal{P}$ , the initial value  $w(a, \cdot)$  can be acquired from  $\mathcal{B}u = g$  on  $\Gamma^a$ . For example, if  $\mathcal{B} = \tilde{\gamma}_1 \frac{\partial}{\partial \xi_1} + \tilde{\gamma}_2 \frac{\partial}{\partial \xi_2} + \tilde{\gamma}_0$  and  $v$  is from the definition of  $\mathcal{P}(a)$ , i.e.,  $v(a, \cdot) = u(a, \cdot)$ , we have  $\mathcal{B}(u - v) = \tilde{\gamma}_1 \frac{\partial(u - v)}{\partial \xi_1} = g$  on  $\Gamma^a$  and

$$w(a, \cdot) = \gamma_1 \frac{\partial(u - v)}{\partial \xi_1}(a, \cdot) + \gamma_2 \frac{\partial(u - v)}{\partial \xi_2}(a, \cdot) + \gamma_0(u - v)(a, \cdot) = \gamma_1 \frac{\partial(u - v)}{\partial \xi_1}(a, \cdot) = \gamma_1 \tilde{\gamma}_1^{-1} g.$$

We calculate the partial derivative of  $w$ ,

$$\begin{aligned} \frac{\partial w}{\partial \xi_1} &= \frac{\partial}{\partial \xi_1} \left( \gamma_1 \frac{\partial u}{\partial \xi_1} + \gamma_2 \frac{\partial u}{\partial \xi_2} + \gamma_0 u \right) - \mathcal{P}'u - \mathcal{P} \frac{\partial u}{\partial \xi_1} \\ &= \gamma_3^{-1} f + \mathcal{L}_2 u - \mathcal{P}'u - \mathcal{P} \frac{\partial u}{\partial \xi_1} \\ &= \gamma_3^{-1} f + \mathcal{P} \{ \gamma_1^{-1} (\mathcal{P}u - \gamma_2 \partial_2 u - \gamma_0 u) \} - \mathcal{P} \frac{\partial u}{\partial \xi_1} \\ (56) \quad &= \gamma_3^{-1} f - \mathcal{P} \{ \gamma_1^{-1} w \}, \end{aligned}$$

where we have successively used the PDE satisfied by  $u$ , the differential Riccati equation of  $\mathcal{P}$ , and the definition of  $w$ . Thus, we have obtained an IVP for  $w$  which is the analogue of the “L” system of the LU factorization. The analytic analogue of the “U” system from which to recover  $u$  is simply the definition of  $w$ ,

$$(57) \quad \gamma_1 \frac{\partial u}{\partial \xi_1} = w - \gamma_2 \frac{\partial u}{\partial \xi_2} - \gamma_0 u + \mathcal{P}u.$$

The initial value for this system is set on  $\Gamma^b$  and can be sought again from the boundary condition  $\mathcal{B}u = g$  and the one-way wave equation itself at  $\xi_1 = b$ . We thus have as the analytic analogue of the LU factorization

$$\frac{\partial}{\partial \xi_1} \left( \gamma_1 \frac{\partial}{\partial \xi_1} + \gamma_2 \frac{\partial}{\partial \xi_2} + \gamma_0 \right) - \mathcal{L}_2 = \left( \frac{\partial}{\partial \xi_1} + \mathcal{P} \{ \gamma_1^{-1} \cdot \} \right) \left( \gamma_1 \frac{\partial}{\partial \xi_1} + \gamma_2 \frac{\partial}{\partial \xi_2} + \gamma_0 - \mathcal{P} \right),$$

which can be verified for an arbitrary function  $v(\xi_1, \xi_2)$  as follows:

$$\begin{aligned} &\left( \frac{\partial}{\partial \xi_1} + \mathcal{P} \{ \gamma_1^{-1} \cdot \} \right) \left( \gamma_1 \frac{\partial}{\partial \xi_1} + \gamma_2 \frac{\partial}{\partial \xi_2} + \gamma_0 - \mathcal{P} \right) v \\ &= \left( \frac{\partial}{\partial \xi_1} + \mathcal{P} \{ \gamma_1^{-1} \cdot \} \right) \left( \gamma_1 \frac{\partial v}{\partial \xi_1} + \gamma_2 \frac{\partial v}{\partial \xi_2} + \gamma_0 v - \mathcal{P}v \right) \\ &= \frac{\partial}{\partial \xi_1} \left( \gamma_1 \frac{\partial v}{\partial \xi_1} + \gamma_2 \frac{\partial v}{\partial \xi_2} + \gamma_0 v \right) - \frac{\partial}{\partial \xi_1} (\mathcal{P}v) + \mathcal{P} \frac{\partial v}{\partial \xi_1} + \mathcal{P} \{ \gamma_1^{-1} (\gamma_2 \frac{\partial v}{\partial \xi_2} + \gamma_0 v - \mathcal{P}v) \} \\ &= \frac{\partial}{\partial \xi_1} \left( \gamma_1 \frac{\partial v}{\partial \xi_1} + \gamma_2 \frac{\partial v}{\partial \xi_2} + \gamma_0 v \right) - \mathcal{L}_2 v, \end{aligned}$$

where to obtain the last identity we substituted the differential Riccati equation (55). Note that all of the derivation above needs to be justified in appropriate function spaces, for which we refer to, e.g., [102].

Solving the IVP in (56) is not the only way to get  $w$ . We can also solve the original problem (11) restricted to  $\Omega^{s_1}$  ( $s_1 \leq b$ ) complemented with an arbitrary boundary condition on  $\Gamma^{s_1}$  that guarantees well-posedness, which results in  $\tilde{u}$ . From the proof of Theorem 17, we have  $w = (\gamma_1 \frac{\partial \tilde{u}}{\partial \xi_1} + \gamma_2 \frac{\partial \tilde{u}}{\partial \xi_2} + \gamma_0 \tilde{u}) - \mathcal{P}\tilde{u}$  on  $\Gamma^t$  for all  $t \in (a, s_1]$ . Supposing  $w$  is known in  $\Omega^{s_1}$ , to obtain  $w$  in  $\Omega^{s_2} - \Omega^{s_1}$  for  $s_2 > s_1$ , we only have to solve the original problem restricted to  $\Omega^{s_2} - \Omega^{s_1}$ , where  $\tilde{u}$  satisfies the boundary condition  $(\gamma_1 \frac{\partial \tilde{u}}{\partial \xi_1} + \gamma_2 \frac{\partial \tilde{u}}{\partial \xi_2} + \gamma_0 \tilde{u}) - \mathcal{P}\tilde{u} = w$  on  $\Gamma^{s_1}$  and an arbitrary boundary condition for well-posedness on  $\Gamma^{s_2}$ ; then, we have  $w = (\gamma_1 \frac{\partial \tilde{u}}{\partial \xi_1} + \gamma_2 \frac{\partial \tilde{u}}{\partial \xi_2} + \gamma_0 \tilde{u}) - \mathcal{P}\tilde{u}$  on  $\Gamma^t$  for all  $t \in (a, s_2]$ . This process continues forward until  $\Gamma^b$  whereupon  $w$  is obtained in  $\Omega$ . Then we solve (11) restricted to  $\Omega^b - \Omega^{s_{J-1}}$  for  $u$  with  $w$  providing interface data on  $\Gamma^{s_{J-1}}$ . To find  $u$  further backward in  $\Omega^{s_{J-1}} - \Omega^{s_{J-2}}$ , we again use  $w$  as interface data on  $\Gamma^{s_{J-2}}$ , while an arbitrary boundary condition on  $\Gamma^{s_{J-1}}$ , as long as the resulting problem is well-posed, can be extracted from already-known  $u$  in  $\Omega^b - \Omega^{s_{J-1}}$ . This process continues backward until  $\Gamma^a$ . The forward plus backward processes constitute exactly Algorithm 1. In other words, we may view Algorithm 1 as a way of solving the IVPs for  $w$  and  $u$  in (56) and (57).

**8. Methods Motivated by Physics.** We now present several algorithms motivated by various intuitions from physics and developed using Green's function techniques. We start with the special case considered in section 5, where the source term vanished outside a subdomain  $\Omega_j$ , in which we showed how to truncate the original problem to  $\Omega_j$  to avoid discretizing the big domain  $\Omega$ . To be able to use this as a building block for a more general solver, we need two further ingredients: first, since we are now not only interested in the near-field solution  $u$  in  $\Omega_j$ , but also the far-field  $u$  in  $\Omega - \Omega_j$ , we need to be able to map the near-field waves to the far-field. This is a classical engineering problem; see, e.g., [162, pp. 329–352]. Second, we may also have sources outside  $\Omega_j$  which stimulate waves that come into  $\Omega_j$ . The question is then how to incorporate the influence of these exterior sources on the local solution on the subdomain  $\Omega_j$ .

In the rest of this section we assume that  $g = 0$  in (11) to simplify our presentation. From the solution formula in (38), namely,

$$u(\mathbf{x}) = \int_{\Omega} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y},$$

we see that if we restrict to  $\mathbf{x}, \mathbf{y} \in \Omega_j$ , then the corresponding diagonal part of  $G(\mathbf{x}, \mathbf{y})$  can be well approximated by a good truncation of the corresponding BVP to  $\Omega_j$ . The second point raised in the last paragraph actually asks how to approximate the off-diagonal parts of  $G(\mathbf{x}, \mathbf{y})$  when  $\mathbf{x}, \mathbf{y}$  are in *different* subdomains. This is a core problem studied in  $\mathcal{H}$ -matrix and similar techniques (see the references mentioned in section 4), but a direct approximation of the off-diagonal parts of the Green's function is difficult for waves traveling long-distance in heterogeneous media. As an alternative, one can first solve for the diagonal parts, i.e., the near-field waves stimulated by the sources within each subdomain, and then propagate the waves gradually subdomain by subdomain from near to far. This is possible because of the so-called equivalence theorem in engineering, which states that if we enclose a source by a surface, referred to as a Huygens surface, then the stimulated waves in the exterior can be determined

from the waves on the Huygens surface, thought of as new equivalent sources that are called currents in engineering. For example, once we have  $u_{1,1} := u_{,1}|_{\Omega_1}$  with  $u_{,1}(\mathbf{x}) := \int_{\Omega_1} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}$ ,  $\mathbf{x} \in \Omega$ , we should also be able to find  $u_{2,1} := u_{,1}|_{\Omega_2}$ . In fact,  $u_{,1}$  solves the BVP

$$\mathcal{L}u_{,1} = f_1 \text{ in } \Omega, \quad \mathcal{B}u_{,1} = 0 \text{ on } \partial\Omega,$$

where  $f_1 := \mathcal{E}_1(f|_{\Omega_1})$ ; so we deduce that  $u_{2,1}$  can be obtained from

$$(58) \quad \begin{aligned} \mathcal{L}u_{2,1} &= 0 && \text{in } \Omega_2, \\ \mathcal{B}u_{2,1} &= 0 && \text{on } \partial\Omega \cap \partial\Omega_2, \\ \mathcal{B}_2^{\langle} u_{2,1} &= \mathcal{B}_2^{\langle} u_{1,1} && \text{on } \Gamma_{2,1}, \\ \mathbf{n}_2^T \alpha \nabla u_{2,1} + \text{DtN}_2 u_{2,1} &= 0 && \text{on } \Gamma_{2,3}, \end{aligned}$$

where  $\mathcal{B}_2^{\langle}$  is an arbitrary boundary operator so that the problem is well-posed, and we assume  $\text{DtN}_2$  is well-defined. We see that the influence of  $f_1$  on the waves in  $\Omega_2$  has been transformed to an equivalent surface current  $\mathcal{B}_2^{\langle} u_{1,1}$ . In summary, the near-field waves  $u_{1,1}$  generate a surface current  $\mathcal{B}_2^{\langle} u_{1,1}$  from which one can recover the far-field waves  $u_{2,1}$ , as the equivalence theorem says.

Since in  $\Omega_2$  we also want  $u_{2,2}(\mathbf{x}) = \int_{\Omega_2} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}$ ,  $\mathbf{x} \in \Omega_2$ , it is convenient to add the source  $f_2$  directly in (58) and to solve for  $(u_{2,1} + u_{2,2})(\mathbf{x}) = u_{2,1:2}(\mathbf{x}) := \int_{\Omega_1 \cup \Omega_2} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}$ ,  $\mathbf{x} \in \Omega_2$ , at once from

$$(59) \quad \begin{aligned} \mathcal{L}u_{2,1:2} &= f_2 && \text{in } \Omega_2, \\ \mathcal{B}u_{2,1:2} &= 0 && \text{on } \partial\Omega \cap \partial\Omega_2, \\ \mathbf{n}_2^T \alpha \nabla u_{2,1:2} + \text{DtN}_2 u_{2,1:2} &= \mathbf{n}_2^T \alpha \nabla u_{1,1} + \text{DtN}_2 u_{1,1} && \text{on } \Gamma_{2,1}, \\ \mathbf{n}_2^T \alpha \nabla u_{2,1:2} + \text{DtN}_2 u_{2,1:2} &= 0 && \text{on } \Gamma_{2,3}, \end{aligned}$$

where we specified  $\mathcal{B}_2^{\langle}$  of (58) as the transparent boundary operator to simulate the waves generated by  $f_2$  without spurious reflections. Using (37), the solution of (59) can be represented as

$$u_{2,1:2}(\mathbf{x}) = \int_{\Omega_2} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y} + \int_{\Gamma_{2,1}} G(\mathbf{x}, \mathbf{y}) \lambda_{2\langle}(\mathbf{y}) d\sigma(\mathbf{y}), \quad \mathbf{x} \in \Omega_2,$$

where  $\lambda_{2\langle} := \mathcal{B}_2^{\langle} u_{1,1} = \mathbf{n}_2^T \alpha \nabla u_{1,1} + \text{DtN}_2 u_{1,1}$ . Now that  $u_{2,1:2}$  contains the influence of both  $f_1$  and  $f_2$ , this influence can be passed on to  $\Omega_3$  through a transmission condition on  $\Gamma_{3,2}$ , and using a transparent transmission condition also then permits us to include the influence of  $f_3$  locally in  $\Omega_3$ . This process continues until we obtain  $u_{J,1:J}$ , which is the exact solution of (11) restricted to  $\Omega_J$ , i.e.,  $u_{J,1:J}(\mathbf{x}) = \int_{\Omega} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}$ ,  $\mathbf{x} \in \Omega_J$ . Now that we have  $u_{j,1:j}$ ,  $j = 1, \dots, J$ , and the interface data  $\lambda_{j+1\langle} := \mathcal{B}_{j+1}^{\langle} u_{j,1:j} = \mathbf{n}_{j+1}^T \alpha \nabla u_{j,1:j} + \text{DtN}_{j+1} u_{j,1:j}$ ,  $j = 1, \dots, J-1$ , we want to add the waves  $u_{j,j+1:J}$ , stimulated by the sources on the right of  $\Omega_j$ , to  $u_{j,1:j}$  to get  $u_{j,1:J} = u_{j,1:j} + u_{j,j+1:J}$ , the solution of the original BVP in (11) restricted to  $\Omega_j$ . We note that  $\mathcal{B}_{j+1}^{\langle} u_{j,1:j} = \mathcal{B}_{j+1}^{\langle} u_{j,1:j} = \lambda_{j+1\langle}$  because  $\mathcal{B}_{j+1}^{\langle} u_{j,j+1:J} = 0$  by Lemma 10. That is, the waves from  $\Omega_{j+1:J}$  pass through  $\Gamma_{j+1,j}$  transparently. For  $u_{J-1,1:J}$ , the other interface data  $\mathcal{B}_{J-1}^{\rangle} u_{J-1,1:J}$  on  $\Gamma_{J-1,J}$  is available from the known solution  $u_{J,1:J}$ .

Therefore,  $u_{J-1,1:J}$  satisfies the BVP

$$(60) \quad \begin{aligned} \mathcal{L}v_{J-1} &= f_{J-1} && \text{in } \Omega_{J-1}, \\ \mathcal{B}v_{J-1} &= 0 && \text{on } \partial\Omega \cap \partial\Omega_{J-1}, \\ \mathbf{n}_{J-1}^T \alpha \nabla v_{J-1} + \text{DtN}_{J-1} v_{J-1} &= \lambda_{J-1} \langle && \text{on } \Gamma_{J-1,J-2}, \\ \mathcal{B}_{J-1}^\rangle v_{J-1} &= \mathcal{B}_{J-1}^\rangle u_{J,1:J} && \text{on } \Gamma_{J-1,J}, \end{aligned}$$

where all the data is known,  $\mathcal{B}_{J-1}^\rangle$  is arbitrary as long as (60) is well-posed, and the first two equations are just taken from (11). In other words, (60) is set up according to what the solution  $u$  of (11) satisfies, and the unique solvability of (60) justifies that its solution can only be  $v_{J-1} = u_{J-1,1:J} = u|_{\Omega_{J-1}}$ . Having obtained  $u_{J-1,1:J}$ , the exact information can be passed backward further through  $\Gamma_{J-2,J-1}$ . This process continues until we obtain the exact solution in all the subdomains. We can also formulate this process using the representation formula in (37). For example, if  $\lambda_{J-1} := \mathcal{B}_{J-1}^\rangle u_{J,1:J} = \mathbf{n}_{J-1}^T \alpha \nabla u_{J,1:J} + \text{DtN}_{J-1} u_{J,1:J}$ , then solving (60) is equivalent to computing for  $\mathbf{x} \in \Omega_{J-1}$ ,

$$u_{J-1,1:J}(\mathbf{x}) = \int_{\Omega_{J-1}} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y} + \int_{\Gamma_{J-1,J-2}} G(\mathbf{x}, \mathbf{y}) \lambda_{J-1} \langle(\mathbf{y}) d\sigma(\mathbf{y}) + \int_{\Gamma_{J-1,J}} G(\mathbf{x}, \mathbf{y}) \lambda_{J-1} \rangle(\mathbf{y}) d\sigma(\mathbf{y}).$$

We have now presented the basic ideas digested from [28, 157, 179, 180], and have again derived Algorithm 1. To propagate the waves based on physical insight, we were forced here to use absorbing transmission conditions on  $\Gamma_{j,j+1}$  in the forward sweep. In the next subsections, we will explain in detail the different paths that led to the invention of the new methods in [28, 157, 179, 180]. We will see that these new methods were derived in quite different forms, but it will become clear how closely they are related to the algorithms discussed in sections 6 and 7.

**8.1. The Source Transfer Method Using Equivalent Volume Sources.** The source transfer method from [28] is based on a decomposition of  $\Omega$  into nonoverlapping and serially connected layers  $O_j$ ,  $j = 0, \dots, J$ , which are combined into subdomains  $\Omega_j := O_{j-1} \cup \Gamma_j \cup O_j$  with  $\Gamma_j := \partial O_{j-1} \cap \partial O_j$  for  $j = 1, \dots, J$ . We saw this decomposition in Remark 5, and we also assume here that the resulting system is block tridiagonal, as in Remark 5. The key idea of the source transfer method is the physical intuition that it is possible to transfer the sources before  $O_J$  into  $O_{J-1}$  without changing the wave field in  $O_J$ . This is done layer by layer. First, the source in  $O_0$  is transferred to  $O_1$  without changing the wave field to the right of  $O_1$ , i.e., in  $O_j$ ,  $j = 2, \dots, J$ . In terms of the Green's function, we need to find a map  $\Psi_1$  that transfers  $\tilde{f}_{1\emptyset} := f|_{O_0}$  to the source  $\Psi_1(\tilde{f}_{1\emptyset})$  defined in  $O_1$  such that

$$\int_{O_0} G(\mathbf{x}, \mathbf{y}) \tilde{f}_{1\emptyset}(\mathbf{y}) d\mathbf{y} = \int_{O_1} G(\mathbf{x}, \mathbf{y}) \Psi_1(\tilde{f}_{1\emptyset})(\mathbf{y}) d\mathbf{y} \quad \forall \mathbf{x} \in O_l, l = 2, \dots, J.$$

Then we define  $\tilde{f}_{2\emptyset} := f|_{O_1} + \Psi_1(\tilde{f}_{1\emptyset})$ . For  $j = 1, \dots, J-2$ , we try to find a map  $\Psi_{j+1}$  that transfers  $\tilde{f}_{j+1\emptyset}$  to the source  $\Psi_{j+1}(\tilde{f}_{j+1\emptyset})$  in  $O_{j+1}$  such that for  $l = j+2, \dots, J$ ,

$$(61) \quad \int_{O_j} G(\mathbf{x}, \mathbf{y}) \tilde{f}_{j+1\emptyset}(\mathbf{y}) d\mathbf{y} = \int_{O_{j+1}} G(\mathbf{x}, \mathbf{y}) \Psi_{j+1}(\tilde{f}_{j+1\emptyset})(\mathbf{y}) d\mathbf{y} \quad \forall \mathbf{x} \in O_l,$$

and define  $\tilde{f}_{j+2\ell} := f|_{O_{j+1}} + \Psi_{j+1}(\tilde{f}_{j+1\ell})$ . Eventually, we get  $\tilde{f}_{J\ell}$  and the wave field in  $O_J$  of the original problem in (11) is given by

$$u_{J\ell}(\mathbf{x}) = \int_{O_J} G(\mathbf{x}, \mathbf{y}) f_{J\ell}(\mathbf{y}) d\mathbf{y} + \int_{O_{J-1}} G(\mathbf{x}, \mathbf{y}) \tilde{f}_{J\ell}(\mathbf{y}) d\mathbf{y} \quad \forall \mathbf{x} \in O_J.$$

Once  $u_{J\ell}$  is known, it leaves a Dirichlet trace on  $\Gamma_J$  which, together with the transferred source  $\tilde{f}_{J-1\ell}$  and the source in  $O_{J-1}$ , results in the wave field in  $O_{J-1}$ ,

$$\begin{aligned} u_{J-1\ell}(\mathbf{x}) &= \int_{O_{J-1}} G_{J-1}(\mathbf{x}, \mathbf{y}) f_{J-1\ell}(\mathbf{y}) d\mathbf{y} + \int_{O_{J-2}} G_{J-1}(\mathbf{x}, \mathbf{y}) \tilde{f}_{J-1\ell}(\mathbf{y}) d\mathbf{y} \\ &\quad + \int_{\Gamma_J} [\mathbf{n}^T \alpha^T \nabla_{\mathbf{y}} G_{J-1}(\mathbf{x}, \mathbf{y})] u_{J\ell}(\mathbf{y}) d\sigma(\mathbf{y}) \quad \forall \mathbf{x} \in O_{J-1}, \end{aligned}$$

where  $G_{J-1}$  is the Green's function in  $\Omega_{J-1}$  satisfying a transparent boundary condition on  $\Gamma_{J-2}$  and a homogeneous Dirichlet condition on  $\Gamma_J$ . This amounts to solving a BVP in  $\Omega_{J-1}$  with Dirichlet boundary condition  $u_{J-1} = u_J$  on  $\Gamma_J$  and the transparent boundary condition on  $\Gamma_{J-2}$ . Afterwards, the wave field in  $O_{J-1}$  can be again extended backward to  $O_{J-2}$ . This process continues until we have obtained the wave field in all the layers.

The authors of [28] emphasize that “*the key step in the method is the source transfer algorithm*,” which results in (61). So how can one obtain the source transfer functions  $\Psi_{j+1}$ ? While the source transfer appeared very naturally in the block LU factorization in (7), it is a bit more involved to find  $\Psi_{j+1}$  in the present setting: the authors substitute the source  $\tilde{f}_{j+1\ell}$  in  $O_j$  with the generated wave field  $v_{j+1}$  in  $\Omega_{j+1}$  by using the PDE  $\mathcal{L}v_{j+1} = \tilde{f}_{j+1}$  in  $\Omega_{j+1}$  (let  $\tilde{f}_{j+1}$  be the zero extension of  $\tilde{f}_{j+1\ell}$  to  $\Omega_{j+1}$ ). Substituting this and  $-\frac{\omega^2}{\kappa}G(\mathbf{x}, \mathbf{y}) = \nabla_{\mathbf{y}}^T(\alpha^T \nabla_{\mathbf{y}} G(\mathbf{x}, \mathbf{y}))$  at  $\mathbf{x} \neq \mathbf{y}$  into the l.h.s. of (61), they obtain for  $\mathbf{x} \in O_l$ ,  $l = j+2, \dots, J$ ,

$$\begin{aligned} &\int_{O_j} G(\mathbf{x}, \mathbf{y}) \tilde{f}_{j+1\ell}(\mathbf{y}) d\mathbf{y} \\ &= \int_{O_j} [-\nabla^T(\alpha \nabla v_{j+1}(\mathbf{y}))] G(\mathbf{x}, \mathbf{y}) + [\nabla_{\mathbf{y}}^T(\alpha^T \nabla_{\mathbf{y}} G(\mathbf{x}, \mathbf{y}))] v_{j+1}(\mathbf{y}) d\mathbf{y}. \end{aligned}$$

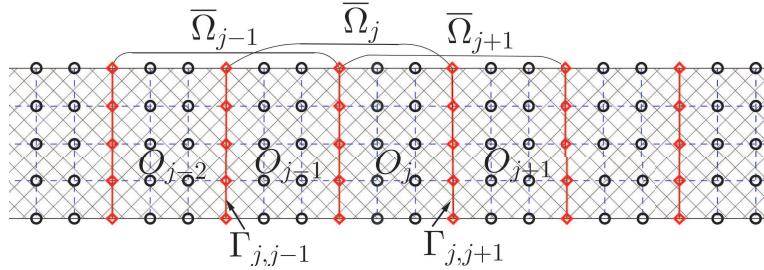
Integrating by parts and substituting the boundary conditions (transparent on  $\Gamma_j$  relative to  $O_j$  for both  $v_{j+1}$  and  $G(\mathbf{x}, \cdot)$  with  $\mathbf{x}$  to the right of  $O_{j+1}$ ) leads to

$$\begin{aligned} (62) \quad &\int_{O_j} G(\mathbf{x}, \mathbf{y}) \tilde{f}_{j+1\ell}(\mathbf{y}) d\mathbf{y} \\ &= \int_{\Gamma_{j+1}} -[\mathbf{n}_j^T \alpha \nabla v_{j+1}(\mathbf{y})] G(\mathbf{x}, \mathbf{y}) + [\mathbf{n}_j^T \alpha^T \nabla_{\mathbf{y}} G(\mathbf{x}, \mathbf{y})] v_{j+1}(\mathbf{y}) d\sigma(\mathbf{y}). \end{aligned}$$

The idea for transferring the source in  $O_j$  to  $O_{j+1}$  consists in a secondary integration by parts but from  $\Gamma_{j+1}$  to  $O_{j+1}$ . This will involve another surface integral,

$$(63) \quad \int_{\Gamma_{j+2}} [\mathbf{n}_{j+1}^T \alpha \nabla v_{j+1}(\mathbf{y})] G(\mathbf{x}, \mathbf{y}) - [\mathbf{n}_{j+1}^T \alpha^T \nabla_{\mathbf{y}} G(\mathbf{x}, \mathbf{y})] v_{j+1}(\mathbf{y}) d\sigma(\mathbf{y}).$$

Since  $\Gamma_{j+2}$  is *not* a transparent boundary for  $G(\mathbf{x}, \mathbf{y})$ ,  $\mathbf{y} \in O_{j+1}$ ,  $\mathbf{x} \in O_l$  ( $l > j+1$ ), the above surface integral in general does not vanish. Note that, however, the information



**Fig. 4** Overlapping domain decomposition with contacting overlaps,  $\circ \in O_*$ ,  $\diamond \in \Gamma_{*,\#}$ .

to be transferred is all from  $\Gamma_{j+1}$ , which is provided by the Dirichlet and Neumann traces of  $v_{j+1}$ ; see (62). So  $v_{j+1}$  can be modified in  $O_{j+1}$  without changing this information while letting the Dirichlet and Neumann traces on  $\Gamma_{j+2}$  vanish to get rid of (63). The authors use a function  $\beta_{j+1}$  for this purpose, which smoothly damps  $v_{j+1}$  from  $\Gamma_{j+1}$  to  $\Gamma_{j+2}$  such that

$$(64) \quad \begin{aligned} \beta_{j+1} &= 1, \quad (\alpha^T \mathbf{n}_j)^T \nabla \beta_{j+1} = 0 \text{ on } \Gamma_{j+1}, \quad \beta_{j+1} = 0, \quad (\alpha^T \mathbf{n}_j)^T \nabla \beta_{j+1} = 0 \text{ on } \Gamma_{j+2}, \\ &\mathcal{B}(\beta_{j+1} v_{j+1}) = 0 \text{ on } \partial O_{j+1} \cap \partial \Omega. \end{aligned}$$

Otherwise, the precise shape of the function  $\beta_{j+1}$  has no influence on the algorithm. Substituting  $\beta_{j+1} v_{j+1}$  for  $v_{j+1}$  in the r.h.s. of (62) and (63) and summing, we find

$$\begin{aligned} &\int_{O_j} G(\mathbf{x}, \mathbf{y}) \tilde{f}_{j+1\#}(\mathbf{y}) d\mathbf{y} \\ &= \int_{\partial O_{j+1}} [\mathbf{n}^T \alpha \nabla (\beta_{j+1} v_{j+1})(\mathbf{y})] G(\mathbf{x}, \mathbf{y}) - [\mathbf{n}^T \alpha^T \nabla_y G(\mathbf{x}, \mathbf{y})] (\beta_{j+1} v_{j+1})(\mathbf{y}) d\sigma(\mathbf{y}). \end{aligned}$$

Integrating by parts for the r.h.s. and using  $\mathcal{M}_y G(\mathbf{x}, \mathbf{y}) = 0$  in  $O_{j+1}$  for  $\mathbf{x} \notin O_{j+1}$  yields the identity

$$\int_{O_j} G(\mathbf{x}, \mathbf{y}) \tilde{f}_{j+1\#}(\mathbf{y}) d\mathbf{y} = \int_{O_{j+1}} G(\mathbf{x}, \mathbf{y}) \left\{ \nabla^T [\alpha \nabla (\beta_{j+1} v_{j+1})(\mathbf{y})] + \frac{\omega^2}{\kappa} \beta_{j+1} v_{j+1}(\mathbf{y}) \right\} d\mathbf{y}.$$

The sum inside the above curly braces is thus the source transfer function  $\Psi_{j+1}(\tilde{f}_{j+1\#})$  we were looking for; see (61). We can now define the source transfer method; see Algorithm 8 at the PDE level and Algorithm 9 at the matrix level. Despite the quite different motivating ideas, these algorithms look very similar to Algorithms 3 and 4. There is one difference though: in the forward sweep, the source transfer methods do not use the source in the right overlap  $O_j$  for the subproblem in  $\Omega_j$ . One can, however, regard  $O_{j-1}$  as the physical subdomain and consider  $O_j$  to already belong to the PML region so that  $O_j \cup \Omega_j^{pml}$  becomes the PML region for  $O_{j-1}$ . Then the source transfer methods can also be derived directly as DOSMs in the *local* deferred correction form, and we obtain the following equivalence results.

**THEOREM 33.** *Suppose the subproblems of the source transfer Algorithm 8 are well-posed. Then Algorithm 8 is equivalent to the DOSM preconditioner shown in Algorithm 1 in the specific case where each subdomain consists of two contacting overlaps (see Figure 4), and using PML transmission conditions on the interfaces in*

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**Algorithm 8. Source transfer preconditioner at the PDE level** ([28, Algorithm 3.1–3.2]).

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Input the source  $f$  and  $g$ . Let  $\tilde{f}_1 \leftarrow f$  in  $O_0$  and  $\tilde{f}_1 \leftarrow 0$ , otherwise. Solve successively for  $j = 1, \dots, J - 1$ ,

$$\begin{aligned} \mathcal{L} v_j &= \tilde{f}_j && \text{in } \Omega_j, \\ \mathcal{B} v_j &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathbf{n}_j^T \alpha \nabla v_j + \text{DtN}_j^{pml} v_j &= 0 && \text{on } \Gamma_{j,j-1}, \\ \mathbf{n}_j^T \alpha \nabla v_j + \text{DtN}_j^{pml} v_j &= 0 && \text{on } \Gamma_{j,j+1}, \end{aligned}$$

where  $\text{DtN}_j^{pml}$  is defined by the PML along  $\Gamma_{j,j-1}$  and  $\Gamma_{j,j+1}$  (see Remark 13 for practical implementation), and after each solve we let  $\tilde{f}_{j+1} \leftarrow f - \mathcal{L}(\beta_j v_j)$  in  $O_j$ , and  $\tilde{f}_{j+1} \leftarrow 0$  otherwise, and  $\beta_j$  satisfies (64).

Let  $\tilde{f}_j$  be unchanged in  $O_{j-1}$  but  $\tilde{f}_j \leftarrow f$  in  $O_j$ . Solve in order of  $j = J, \dots, 1$  the problem

$$\begin{aligned} \mathcal{L} \tilde{u}_j &= \tilde{f}_j && \text{in } \Omega_j, \\ \mathcal{B} \tilde{u}_j &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathbf{n}_j^T \alpha \nabla \tilde{u}_j + \text{DtN}_j^{pml} \tilde{u}_j &= 0 && \text{on } \Gamma_{j,j-1}, \\ \tilde{u}_j &= \tilde{u}_{j+1} && \text{on } \Gamma_{j,j+1}. \end{aligned}$$

Output the global approximation  $\tilde{u} \leftarrow \tilde{u}_j$  in  $O_j$ ,  $j = 1, \dots, J$ , and  $\tilde{u} \leftarrow \tilde{u}_1$  in  $O_0$ .

---

**Algorithm 9. Source transfer preconditioner at the matrix level.**

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Input the r.h.s.  $\mathbf{f}$ . Let  $\tilde{\mathbf{f}}_{1\langle} \leftarrow \mathbf{f}_{1\langle}$ . Solve successively for  $j = 1, \dots, J - 1$ ,

$$\begin{bmatrix} \tilde{S}_{j\langle}^{\langle} & A_{j\langle j-1\rangle} & & \\ A_{j-1\rangle j\langle} & A_{j-1\rangle} & A_{j-1\rangle j+1\langle} & \\ & A_{j+1\langle j-1\rangle} & A_{j+1\langle} & A_{j+1\langle j\rangle} \\ & & A_{j\rangle j+1\langle} & A_{j\rangle} & A_{j\rangle j\langle} \\ & & & A_{j\rangle j\rangle} & \tilde{S}_{j\rangle}^{\rangle} \end{bmatrix} \begin{bmatrix} \mathbf{v}_{j\langle} \\ \mathbf{v}_{j\langle} \\ \mathbf{v}_{j[} \\ \mathbf{v}_{j\rangle} \\ \mathbf{v}_{j\rangle} \end{bmatrix} = \begin{bmatrix} 0 \\ \tilde{\mathbf{f}}_{j\langle} \\ \mathbf{f}_{j+1\langle} \\ 0 \\ 0 \end{bmatrix},$$

where  $\tilde{S}_{j\langle}^{\langle}$  and  $\tilde{S}_{j\rangle}^{\rangle}$  are defined by the PML (see Remark 14 for practical implementation), and after each solve we let  $\tilde{\mathbf{f}}_{j+1\langle} \leftarrow \mathbf{f}_{j\rangle} - A_{j\rangle} I_{j\rangle}^j (D_j \mathbf{v}_j) - A_{j\rangle j+1\langle} I_{j+1\langle}^j (D_j \mathbf{v}_j)$ , where  $D_j$  satisfies

$$(65) \quad I_{j\rangle}^j D_j = 0, \quad A_{j\rangle j\langle} I_{j\rangle}^j D_j = 0, \quad I_{j+1\langle}^j (D_j - I_j) = 0, \quad A_{j+1\langle j\rangle} I_{j\rangle}^j (D_j - I_j) = 0.$$

Solve in order of  $j = J, \dots, 1$  the following problem:

$$\begin{bmatrix} \tilde{S}_{j\langle}^{\langle} & A_{j\langle j-1\rangle} & & \\ A_{j-1\rangle j\langle} & A_{j-1\rangle} & A_{j-1\rangle j+1\langle} & \\ & A_{j+1\langle j-1\rangle} & A_{j+1\langle} & A_{j+1\langle j\rangle} \\ & & A_{j\rangle j+1\langle} & A_{j\rangle} & A_{j\rangle j\langle} \\ & & & 0 & I_{j\rangle} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{u}}_{j\langle} \\ \tilde{\mathbf{u}}_{j\langle} \\ \tilde{\mathbf{u}}_{j[} \\ \tilde{\mathbf{u}}_{j\rangle} \\ \tilde{\mathbf{u}}_{j\rangle} \end{bmatrix} = \begin{bmatrix} 0 \\ \tilde{\mathbf{f}}_{j\langle} \\ \mathbf{f}_{j+1\langle} \\ \mathbf{f}_{j\rangle} \\ \tilde{\mathbf{u}}_{j+1\langle} \end{bmatrix}.$$

Output the global approximation  $\tilde{\mathbf{u}} \leftarrow \tilde{\mathbf{u}}_j$  in  $\overline{O}_j$ ,  $j = 1, \dots, J$ , and  $\tilde{\mathbf{u}} \leftarrow \tilde{\mathbf{u}}_1$  in  $O_0$ .

---

the forward sweep and Dirichlet instead of PML on the right interfaces in the backward sweep; moreover, in the forward sweep the source terms in the right overlap of each subdomain are put to zero, which turns the right overlap effectively into part of the PML on the right of the subdomain.

*Proof.* We will prove several identities between the iterates generated by the two algorithms. Since we are considering the algorithms as preconditioners, we use a zero initial guess for Algorithm 1. We start from the iterate of Algorithm 1 for the specific case stated in the theorem:

$$\begin{aligned}\mathcal{L} u_1^{(\frac{1}{2})} &= \hat{f}_1 && \text{in } \Omega_1, \\ \mathcal{B} u_1^{(\frac{1}{2})} &= g && \text{on } \partial\Omega \cap \partial\Omega_1, \\ \mathbf{n}_1^T \alpha \nabla u_1^{(\frac{1}{2})} + \text{DtN}_1^{pml} u_1^{(\frac{1}{2})} &= 0 && \text{on } \Gamma_{1,2},\end{aligned}$$

where  $\hat{f}_j = f$  in  $O_{j-1}$ , and  $\hat{f}_j = 0$  otherwise, for  $j = 1, \dots, J-1$ . This is exactly what we solve for  $v_1$  in Algorithm 8. By uniqueness of the solution, we see that  $u_1^{(\frac{1}{2})} = v_1$ . Assuming now that  $u_{j-1}^{(\frac{1}{2})} = v_{j-1}$  in  $O_{j-1}$ , we will show that this relation also holds for  $j$  replacing  $j-1$ . In the  $j$ th forward substep of Algorithm 1, we solve

$$(66) \quad \begin{aligned}\mathcal{L} u_j^{(\frac{1}{2})} &= \hat{f}_j && \text{in } \Omega_j, \\ \mathcal{B} u_j^{(\frac{1}{2})} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathbf{n}_j^T \alpha \nabla u_j^{(\frac{1}{2})} + \text{DtN}_j^{pml} u_j^{(\frac{1}{2})} &= \mathbf{n}_j^T \alpha \nabla u_{j-1}^{(\frac{1}{2})} + \text{DtN}_j^{pml} u_{j-1}^{(\frac{1}{2})} && \text{on } \Gamma_{j,j-1}, \\ \mathbf{n}_j^T \alpha \nabla u_j^{(\frac{1}{2})} + \text{DtN}_j^{pml} u_j^{(\frac{1}{2})} &= 0 && \text{on } \Gamma_{j,j+1}.\end{aligned}$$

We extend  $\beta_{j-1} u_{j-1}^{(\frac{1}{2})}$  by zero into  $O_j$  and substitute the correction  $u_j^{(\frac{1}{2})} - \beta_{j-1} u_{j-1}^{(\frac{1}{2})}$  for  $u_j^{(\frac{1}{2})}$  into (66). Using (64), we find that the BVP satisfied by the correction term is

$$\begin{aligned}\mathcal{L} \left( u_j^{(\frac{1}{2})} - \beta_{j-1} u_{j-1}^{(\frac{1}{2})} \right) &= \hat{f}_j - \mathcal{L}(\beta_{j-1} u_{j-1}^{(\frac{1}{2})}) && \text{in } \Omega_j, \\ \mathcal{B} \left( u_j^{(\frac{1}{2})} - \beta_{j-1} u_{j-1}^{(\frac{1}{2})} \right) &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \left( \mathbf{n}_j^T \alpha \nabla + \text{DtN}_j^{pml} \right) \left( u_j^{(\frac{1}{2})} - \beta_{j-1} u_{j-1}^{(\frac{1}{2})} \right) &= 0 && \text{on } \Gamma_{j,j-1}, \\ \left( \mathbf{n}_j^T \alpha \nabla + \text{DtN}_j^{pml} \right) \left( u_j^{(\frac{1}{2})} - \beta_{j-1} u_{j-1}^{(\frac{1}{2})} \right) &= 0 && \text{on } \Gamma_{j,j+1}.\end{aligned}$$

Since we assumed that  $u_{j-1}^{(\frac{1}{2})} = v_{j-1}$  in  $O_{j-1} = \Omega_j \cap \Omega_{j-1}$ , the above BVP is exactly the same as the BVP for  $v_j$  in Algorithm 8. By uniqueness of the solution, we thus deduce that  $v_j = u_j^{(\frac{1}{2})} - \beta_{j-1} u_{j-1}^{(\frac{1}{2})}$  in  $\Omega_j$  and, in particular,  $v_j = u_j^{(\frac{1}{2})}$  in  $O_j$ . By induction, this last relation then holds for all  $j = 1, \dots, J-1$ . In the backward sweep of Algorithm 1, we solve the subdomain problem

$$\begin{aligned}\mathcal{L} u_j^{(1)} &= f && \text{in } \Omega_j, \\ \mathcal{B} u_j^{(1)} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathbf{n}_j^T \alpha \nabla u_j^{(1)} + \text{DtN}_j^{pml} u_j^{(1)} &= \mathbf{n}_j^T \alpha \nabla u_{j-1}^{(\frac{1}{2})} + \text{DtN}_j^{pml} u_{j-1}^{(\frac{1}{2})} && \text{on } \Gamma_{j,j-1}, \\ u_j^{(1)} &= u_{j+1}^{(1)} && \text{on } \Gamma_{j,j+1}.\end{aligned}$$

By the same argument as before, we can show that  $\tilde{u}_j = u_j^{(1)}$  in  $O_j$  for  $j = J, \dots, 1$  and  $\tilde{u}_1 = u_1^{(1)}$  in  $O_0$ .  $\square$

**THEOREM 34.** *Assume that the subproblems of the discrete source transfer Algorithm 9 are well-posed. Then Algorithm 9 is equivalent to the discrete DOSM preconditioner shown in Algorithm 2, in the specific case at the discrete level corresponding to the case stated in Theorem 33 at the continuous level.*

*Proof.* In the specific case, and with zero initial guess for its use as a preconditioner, Algorithm 2 first solves

$$\begin{bmatrix} A_{1\langle} & A_{1\langle 2\langle} \\ A_{2\langle 1\langle} & A_{2\langle} & A_{2\langle 1\rangle} \\ & A_{1\rangle 2\langle} & A_{1\rangle} & A_{1\rangle 1\rangle} \\ & & A_{1\rangle 1\rangle} & \tilde{S}_1\rangle \end{bmatrix} \begin{bmatrix} \mathbf{u}_1^{(\frac{1}{2})} \\ \mathbf{u}_1^{(\frac{1}{2})} \\ \mathbf{u}_1^{(\frac{1}{2})} \\ \mathbf{u}_1^{(\frac{1}{2})} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{1\langle} \\ \mathbf{f}_{2\langle} \\ 0 \\ 0 \end{bmatrix},$$

which is exactly the same problem for  $\mathbf{v}_1$  in Algorithm 9; so  $\mathbf{u}_1^{(\frac{1}{2})} = \mathbf{v}_1$  by uniqueness of the solution. Now assuming that

$$(67) \quad \mathbf{u}_{j-1\rangle}^{(\frac{1}{2})} = \mathbf{v}_{j-1\rangle}, \quad \mathbf{u}_{j-1[}^{(\frac{1}{2})} = \mathbf{v}_{j-1[},$$

we will show these relations also hold for  $j+1$  replacing  $j$ . In the specific version of Algorithm 2,  $\mathbf{u}_j^{(\frac{1}{2})}$  solves

$$\begin{bmatrix} \tilde{S}_{j\langle} & A_{j\langle j-1\rangle} \\ A_{j-1\rangle j\langle} & A_{j-1\rangle} & A_{j-1\rangle j+1\langle} \\ & A_{j+1\langle j-1\rangle} & A_{j+1\langle} & A_{j+1\langle j\rangle} \\ & A_{j\rangle j+1\langle} & A_{j\rangle} & A_{j\rangle j\rangle} \\ & A_{j\rangle j\rangle} & \tilde{S}_j\rangle \end{bmatrix} \begin{bmatrix} \mathbf{u}_j^{(\frac{1}{2})} \\ \mathbf{u}_j^{(\frac{1}{2})} \\ \mathbf{u}_j^{(\frac{1}{2})} \\ \mathbf{u}_j^{(\frac{1}{2})} \\ \mathbf{u}_j^{(\frac{1}{2})} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{j\langle} + (\tilde{S}_{j\langle} - A_{j\langle}) \mathbf{u}_{j-1\langle}^{(\frac{1}{2})} - A_{j\langle j-2\rangle} \mathbf{u}_{j-1\rangle}^{(\frac{1}{2})} \\ \mathbf{f}_{j\langle} \\ \mathbf{f}_{j[} \\ 0 \\ 0 \end{bmatrix}.$$

We can further rewrite the above system into the equivalent system

$$\begin{aligned} & \begin{bmatrix} \tilde{S}_{j\langle} & A_{j\langle j-1\rangle} \\ A_{j-1\rangle j\langle} & A_{j-1\rangle} & A_{j-1\rangle j+1\langle} \\ & A_{j+1\langle j-1\rangle} & A_{j+1\langle} & A_{j+1\langle j\rangle} \\ & A_{j\rangle j+1\langle} & A_{j\rangle} & A_{j\rangle j\rangle} \\ & A_{j\rangle j\rangle} & \tilde{S}_j\rangle \end{bmatrix} \begin{bmatrix} \mathbf{u}_j^{(\frac{1}{2})} - I_{j\langle}^{j-1}(D_{j-1}\mathbf{u}_{j-1}^{(\frac{1}{2})}) \\ \mathbf{u}_{j\langle}^{(\frac{1}{2})} - I_{j-1\rangle}^{j-1}(D_{j-1}\mathbf{u}_{j-1}^{(\frac{1}{2})}) \\ \mathbf{u}_{j[}^{(\frac{1}{2})} \\ \mathbf{u}_{j\rangle}^{(\frac{1}{2})} \\ \mathbf{u}_{j\rangle}^{(\frac{1}{2})} \end{bmatrix} \\ &= \begin{bmatrix} 0 \\ \mathbf{f}_{j-1\rangle} - A_{j-1\rangle} I_{j-1\rangle}^{j-1}(D_{j-1}\mathbf{u}_{j-1}^{(\frac{1}{2})}) - A_{j-1\rangle j\langle} I_{j\langle}^{j-1}(D_{j-1}\mathbf{u}_{j-1}^{(\frac{1}{2})}) \\ \mathbf{f}_{j+1\langle} \\ 0 \\ 0 \end{bmatrix}, \end{aligned}$$

where for the first row we have used  $I_{j\langle}^{j-1}(D_{j-1}\mathbf{u}_{j-1}^{(\frac{1}{2})}) = \mathbf{u}_{j-1[}^{(\frac{1}{2})}$ ,  $A_{j\langle j-1\rangle} I_{j-1\rangle}^{j-1}(D_{j-1}\mathbf{u}_{j-1}^{(\frac{1}{2})}) = A_{j\langle j-1\rangle} \mathbf{u}_{j-1\rangle}^{(\frac{1}{2})}$  from (65), and  $A_{j\langle j-2\rangle} \mathbf{u}_{j-1\rangle}^{(\frac{1}{2})} + A_{j\langle} \mathbf{u}_{j-1[}^{(\frac{1}{2})} + A_{j\langle j-1\rangle} \mathbf{u}_{j-1\rangle}^{(\frac{1}{2})} = \mathbf{f}_{j\langle}$  from the system for  $\mathbf{u}_{j-1}^{(\frac{1}{2})}$ . By (67) this is exactly the same problem for  $\mathbf{v}_j$  in Algorithm 9. By induction, we have  $\mathbf{u}_{j\rangle}^{(\frac{1}{2})} = \mathbf{v}_{j\rangle}$  and  $\mathbf{u}_{j[}^{(\frac{1}{2})} = \mathbf{v}_{j[}$  for all  $j = 1, \dots, J-1$ .

By similar arguments, we can also show that in the backward sweep,  $\mathbf{u}_{j\top}^{(1)} = \tilde{\mathbf{u}}_{j\top}$  and  $\mathbf{u}_{j\|}^{(1)} = \tilde{\mathbf{u}}_{j\|}$  for all  $j = J, \dots, 2$ , and  $\mathbf{u}_1^{(1)} = \tilde{\mathbf{u}}_1$ .  $\square$

**8.2. The Method Using Single Layer Potentials.** Stolk summarizes in [157] the main ideas for the method based on single layer potentials as follows: “*A new domain decomposition method is introduced for the heterogeneous 2-D and 3-D Helmholtz equations. Transmission conditions based on the perfectly matched layer (PML) are derived that avoid artificial reflections and match incoming and outgoing waves at the subdomain interfaces.*”

To motivate the method based on single layer potentials, we consider the free space problem in a homogeneous medium. In this case, the source in each subdomain generates waves biased in two directions, forward and backward, which both are outgoing relative to the subdomain. In each subdomain, we are interested in the sum of the waves stimulated by *all* the sources, including the sources from the other subdomains. We must thus account for the waves incoming from all the other subdomains in each subdomain. The idea of the algorithm based on single layer potentials is forward propagation and accumulation of the waves from the first subdomain to the last one so that the waves in  $\Omega_j$ ,  $1 \leq j \leq J$ , have accounted for all the forward going waves generated from the sources in  $\Omega_l$  for all  $l < j$ . Then, a similar procedure can be carried out backward so that the waves in  $\Omega_j$  also contain the backward going waves generated from the sources in  $\Omega_m$  for all  $m > j$ . The actual backward sweep in [157], however, solves for the correction from the residual.

To transfer the waves, the author in [157] states, “*We have constructed new transmission conditions ... These are designed to ensure that:*

- (i) *the boundary conditions at the subdomain interfaces are non-reflecting;*
- (ii) *if  $\Omega_{j-1}$  and  $\Omega_j$  are neighboring subdomains, then the outgoing wave field from  $\Omega_{j-1}$  equals the incoming wave field in  $\Omega_j$  at the joint boundary and vice versa.*

*This is achieved in a simple and accurate way using a PML boundary layer added to the subdomains and single layer potentials.*” As noted in [157], a related approach has been studied in [148] that is also motivated by matching the incoming and outgoing waves. There is, however, a difference in the concrete forms used to achieve the matching; see Remark 26 for a brief review of the form used in [148].

The representation of incoming waves is a well-studied topic in computational electromagnetics; see [162, pp. 185–220]. The common idea is to represent the incoming wave  $v_{j-1}$  from  $\Omega_{j-1}$  to  $\Omega_j$  as an equivalent source term on the surface  $\Gamma_{j,j-1}$ . In [157], the proposed equivalent source is  $2\delta(s_{j-1})\mathbf{n}_j^T \alpha \nabla v_{j-1}$ ; here  $s_{j-1}$  is a local coordinate normal to  $\Gamma_{j,j-1}$  and  $s_{j-1} = 0$  corresponds to  $\Gamma_{j,j-1}$ , and  $\delta(s_{j-1})$  here represents a surface delta function. The author in [157] states:<sup>19</sup>

a short intuitive explanation goes as follows. The term  $v_{j-1}|_{\Gamma_{j,j-1}}$  exclusively contains forward going waves because of the presence of a PML non-reflecting layer immediately to its right.<sup>20</sup> The term  $2\delta(s_{j-1})\mathbf{n}_j^T \alpha \nabla v_{j-1}$  is meant to cause the same forward going wave field in the field  $v_j$  as in the field  $v_{j-1}$ . . . . the source generates waves propagating both forwardly and backwardly in a symmetric fashion. The factor 2 is introduced so that the forward propagating part equals  $v_{j-1}$  on  $\Gamma_{j,j-1}$ . The backward propagating part is absorbed in the neighboring PML layer [along  $\Gamma_{j,j-1}$  for  $\Omega_j$ ].

<sup>19</sup>We replaced the original notation in the quote by the notation used in this article.

<sup>20</sup>In fact, the PML is placed on the right of  $\Gamma_{j-1,j}$  for  $\Omega_{j-1}$ .

Let us take a closer look at the reasoning above: we want to extend the waves  $v_{j-1}$  from  $\Omega_{j-1}$  to  $\Omega_j$ . By (37), we have for  $\mathbf{x} \in \Omega_j$ ,

$$(68) \quad v_{j-1}(\mathbf{x}) = \int_{\Gamma_{j,j-1}} (\mathbf{n}_j^T \alpha \nabla v_{j-1})(\mathbf{y}) G(\mathbf{x}, \mathbf{y}) - \mathbf{n}_j^T(\mathbf{y}) (\alpha^T(\mathbf{y}) \nabla_{\mathbf{y}} G(\mathbf{x}, \mathbf{y})) v_{j-1}(\mathbf{y}) d\sigma(\mathbf{y}).$$

The Green's function  $G(\mathbf{x}, \mathbf{y})$  represents the wave field at  $\mathbf{y} \in \Gamma_{j,j-1}$  stimulated by a point source at  $\mathbf{x} \in \Omega_j$ . For the free space problem in a homogeneous medium, if two point sources at  $\mathbf{x}$  and  $\mathbf{x}'$  are symmetric w.r.t.  $\Gamma_{j,j-1}$ , then the stimulated waves generated by the individual point sources are also symmetric w.r.t.  $\Gamma_{j,j-1}$ .<sup>21</sup> Hence,

$$(69) \quad \begin{aligned} & \forall \mathbf{x} \in \Omega_j, \mathbf{x}' \text{ and } \mathbf{x} \text{ symmetric w.r.t. } \Gamma_{j,j-1}, \forall \mathbf{y} \in \Gamma_{j,j-1} : \\ & G(\mathbf{x}, \mathbf{y}) = G(\mathbf{x}', \mathbf{y}), \mathbf{n}_j^T(\mathbf{y}) (\alpha^T(\mathbf{y}) \nabla_{\mathbf{y}} (G(\mathbf{x}, \mathbf{y}) + G(\mathbf{x}', \mathbf{y}))) = 0. \end{aligned}$$

Since both  $v_{j-1}$  and  $G(\mathbf{x}', \cdot)$  satisfy homogeneous Helmholtz equations in  $\Omega_j$  and represent outgoing waves to the right of  $\Gamma_{j,j+1}$ , by using Green's identity we obtain

$$\int_{\Gamma_{j,j-1}} \mathbf{n}_j^T(\mathbf{y}) (\alpha^T(\mathbf{y}) \nabla_{\mathbf{y}} G(\mathbf{x}', \mathbf{y})) v_{j-1}(\mathbf{y}) d\sigma(\mathbf{y}) = \int_{\Gamma_{j,j-1}} \mathbf{n}_j^T(\mathbf{y}) (\alpha \nabla v_{j-1}(\mathbf{y})) G(\mathbf{x}', \mathbf{y}) d\sigma(\mathbf{y}).$$

Substituting this and (69) into (68), we find the single layer potential representation

$$v_{j-1}(\mathbf{x}) = \int_{\Gamma_{j,j-1}} 2 \mathbf{n}_j^T(\mathbf{y}) (\alpha \nabla v_{j-1}(\mathbf{y})) G(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}), \quad \mathbf{x} \in \Omega_j,$$

which is equivalent to being stimulated by the surface source

$$v_{j-1}(\mathbf{x}) = \int_{\Omega_j} 2\delta(s_{j-1}(\mathbf{y})) \mathbf{n}_j^T(\mathbf{y}) (\alpha \nabla v_{j-1}(\mathbf{y})) G(\mathbf{x}, \mathbf{y}) d\mathbf{y}, \quad \mathbf{x} \in \Omega_j.$$

This, under the symmetry assumption (69), justifies the equivalent source proposed in [157]. One can also calculate the representation in closed form; cf. [112].

The forward sweep in the method based on single layer potentials is performed up to the last subdomain  $\Omega_J$ . Then, a global approximation is defined by setting  $v := v_j$  in  $\Omega_j$ ,  $j = 1, \dots, J$  (the subdomains are nonoverlapping), and a deferred correction problem will then be solved in the backward sweep. Note that  $v$  has in general jumps across interfaces between subdomains, and the residual  $\tilde{f} := f - \mathcal{L}u$  involves a very singular distribution—the derivative of the surface delta function,  $\delta'(s_{j-1})$ . To avoid the potential obscurity of deciding to which subdomain such a singular distribution on an *interface* belongs, it is suggested in [157] to use for the backward sweep another set of nonoverlapping subdomains that contains these distribution residuals in the interior of the subdomains. These residuals are then taken as new sources which stimulate the correction wave field. A procedure similar to the forward sweep but from the last subdomain to the first one is carried out to find an approximation of the correction. Adding the correction to the wave field previously obtained with the forward sweep gives a global approximate solution of the original problem, which finalizes the definition of the preconditioner based on single layer potentials. Using two sets of subdomains could potentially double the cost of factorization. This situation can be avoided by the following trick from [157]: for the first set of subdomains the PML along  $\Gamma_{j,j+1}$  begins with using the original operator near  $\Gamma_{j,j+1}$ , and only after

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<sup>21</sup>This is like in the method of images for solving PDEs in a half space; cf. [177].

a certain distance, say, one mesh cell, does it change to the PML modified operator. The second set of subdomains is defined by moving  $\Gamma_{j,j+1}$  forward by one mesh cell, but keeping the PML augmented region  $\Omega_j \cup \Omega_j^{pml}$  the same as before (i.e., just moving outward the interfaces that separate  $\Omega_j$  and  $\Omega_j^{pml}$  so that  $\Omega_j$  gets bigger and  $\Omega_j^{pml}$  gets smaller). In this way, every subdomain matrix is unchanged from the forward sweep to the backward sweep and the same factorization can be used.

We summarize the preconditioner based on single layer potentials in Algorithm 10 at the PDE level and in Algorithm 11 at the matrix level. For the matrix version, we give two variants: the first one, originally presented in [157], is especially designed for the five point (or seven point in three dimensions) finite difference scheme with  $u$  discretized at integer grid points and the continuous interfaces located at half grid points. The second form is motivated by finite element methods with the discrete interfaces superposed on the continuous interfaces. While the first matrix form can be explained as a special discretization of the PDE Algorithm 10, the second matrix form is equivalent (under some assumptions) to the first matrix form, and unlike the PDE form the second matrix form uses the same partition for the forward and the backward sweeps. Both matrix forms do the extension and restriction like ASH does; see Remark 20.

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**Algorithm 10. Single layer potential** preconditioner at the **PDE** level.

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Input the source terms  $f$  and  $g$ . Suppose the decomposition is nonoverlapping. Solve successively for  $j = 1, \dots, J$ ,

$$\begin{aligned} \mathcal{L}v_j &= f + 2\delta(s_{j-1})\mathbf{n}_j^T \alpha \nabla v_{j-1} && \text{in } \Omega_j, \\ \mathcal{B}v_j &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathbf{n}_j^T \alpha \nabla v_j + \text{DtN}_j^{pml} v_j &= 0 && \text{on } \Gamma_{j,j-1}, \\ \mathbf{n}_j^T \alpha \nabla v_j + \text{DtN}_j^{pml} v_j &= 0 && \text{on } \Gamma_{j,j+1}, \end{aligned}$$

where  $\text{DtN}_j^{pml}$  is the PML-DtN operator along  $\Gamma_{j,j-1}$  and  $\Gamma_{j,j+1}$  (see Remark 13 for practical implementation),  $s_{j-1}$  is a local coordinate normal to  $\Gamma_{j,j-1}$  and  $s_{j-1} = 0$  corresponds to  $\Gamma_{j,j-1}$ , and  $\delta(s_{j-1})$  here represents a surface delta function. The PML for  $\Omega_j$  along  $\Gamma_{j,j+1}$  has a small starting zone between  $\Gamma_{j,j+1}$ , and  $\Gamma_{j,j+1}^h$  where the original operator  $\mathcal{L}$  is used.

Let  $v \leftarrow v_j$  in  $\Omega_j$ ,  $j = 1, \dots, J$ , and compute the residual  $\tilde{f} \leftarrow f - \mathcal{L}v$  in  $\Omega$ .

Denote by  $\tilde{\Omega}_j$  the resulting subdomain by moving forward the boundaries  $\Gamma_{j,j+1}$  to  $\Gamma_{j,j+1}^h$  and  $\Gamma_{j,j-1}$  to  $\Gamma_{j,j-1}^h$ . In order of  $j = J-1, \dots, 1$ , solve the problem

$$\begin{aligned} \mathcal{L}w_j &= \tilde{f} + 2\delta(s_j)\mathbf{n}_j^T \alpha \nabla w_{j+1} && \text{in } \tilde{\Omega}_j, \\ \mathcal{B}w_j &= g && \text{on } \partial\Omega \cap \partial\tilde{\Omega}_j, \\ \mathbf{n}_j^T \alpha \nabla w_j + \text{DtN}_j^{pml} w_j &= 0 && \text{on } \Gamma_{j,j-1}^h, \\ \mathbf{n}_j^T \alpha \nabla w_j + \text{DtN}_j^{pml} w_j &= 0 && \text{on } \Gamma_{j,j+1}^h, \end{aligned}$$

where the  $\text{DtN}_j^{pml}$  on  $\Gamma_{j,j+1}^h$  ( $\Gamma_{j,j-1}^h$ ) uses the PML as the subset (superset) of the PML for  $v_j$  on  $\Gamma_{j,j+1}$  ( $\Gamma_{j,j-1}$ ) that starts later (earlier using the original operator). Output  $\tilde{u} \leftarrow v + w_j$  in  $\tilde{\Omega}_j$ ,  $j = 1, \dots, J-1$ , and  $\tilde{u} \leftarrow v$  in  $\tilde{\Omega}_J$ .

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**THEOREM 35.** *Suppose the subproblems of Algorithm 10 are well-posed. If the PML-DtN operators on the two sides of each interface are equal, i.e.,  $\text{DtN}_j^{pml} = \text{DtN}_{j+1}^{pml}$  on  $\Gamma_{j,j+1}$  and on  $\Gamma_{j,j+1}^h$ , then the single layer potential preconditioner as shown in Algorithm 10 is equivalent to one iteration of Algorithm 1 with zero initial*

**Algorithm 11.** Single layer potential preconditioner at the **matrix** level.

Input the r.h.s.  $\mathbf{f}$ . Suppose the  $\Omega_j$ 's are nonoverlapping. Choose one of the following two forms (see Theorem 36 for their equivalence under certain conditions).

**Form 1.** Extend the nonoverlapping subdomains one layer beyond each interface. We indicate the extra d.o.f. beyond the left interfaces of the  $j$ th subdomain by the subscripts  $j\langle\langle$  or  $j-1\langle\langle$ , and similarly for  $j\rangle\rangle$  or  $j+1\rangle\rangle$ .

Solve successively for  $j = 1, \dots, J$ ,

$$\begin{bmatrix} \tilde{S}_{j\langle\langle}^{\langle} & A_{j\langle\langle j\langle} & & \\ A_{j\langle\langle j\langle} & A_{j\langle} & A_{j\langle j\bullet} & \\ & A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} \\ & & A_{j\rangle j\bullet} & A_{j\rangle} & A_{j\rangle j\rangle} \\ & & & A_{j\rangle j\rangle} & \tilde{S}_{j\rangle\rangle}^{\rangle} \end{bmatrix} \begin{bmatrix} \mathbf{v}_{j\langle\langle} \\ \mathbf{v}_{j\langle} \\ \mathbf{v}_{j\bullet} \\ \mathbf{v}_{j\rangle} \\ \mathbf{v}_{j\rangle\rangle} \end{bmatrix} = \begin{bmatrix} \mathbf{v}_{j-1\langle\langle} + A_{j\langle\langle j\langle} \mathbf{v}_{j-1\langle} \\ \mathbf{f}_{j\langle} - A_{j\langle\langle j\langle} \mathbf{v}_{j-1\langle} - \mathbf{v}_{j-1\langle} \\ \mathbf{f}_{j\bullet} \\ 0 \\ 0 \end{bmatrix},$$

where  $\tilde{S}_{j\langle\langle}^{\langle}$  and  $\tilde{S}_{j\rangle\rangle}^{\rangle}$  are the Schur complements from the PML (see Remark 14 for practical implementation).

Let  $\mathbf{v} \leftarrow \sum_{j=1}^J R_j^T (I_j^{j\langle} I_{j\langle}^j + I_j^{j\bullet} I_{j\bullet}^j) \mathbf{v}_j$  and compute  $\tilde{\mathbf{f}} \leftarrow \mathbf{f} - A\mathbf{v}$ . Let  $\mathbf{w}_J \leftarrow 0$ .

In order of  $j = J-1, \dots, 1$ , solve the correction problem

$$\begin{bmatrix} \tilde{S}_{j\langle\langle}^{\langle} & A_{j\langle\langle j\langle} & & \\ A_{j\langle\langle j\langle} & A_{j\langle} & A_{j\langle j\bullet} & \\ & A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} \\ & & A_{j\rangle j\bullet} & A_{j\rangle} & A_{j\rangle j\rangle} \\ & & & A_{j\rangle j\rangle} & \tilde{S}_{j\rangle\rangle}^{\rangle} \end{bmatrix} \begin{bmatrix} \mathbf{w}_{j\langle\langle} \\ \mathbf{w}_{j\langle} \\ \mathbf{w}_{j\bullet} \\ \mathbf{w}_{j\rangle} \\ \mathbf{w}_{j\rangle\rangle} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \tilde{\mathbf{f}}_{j\bullet} \\ \tilde{\mathbf{f}}_{j\rangle} - A_{j\rangle j\rangle} \mathbf{w}_{j+1\langle} - \mathbf{w}_{j+1\langle} \\ \mathbf{w}_{j+1\langle} + A_{j\rangle j\rangle} \mathbf{w}_{j+1\langle} \end{bmatrix}.$$

Compute the output  $\tilde{\mathbf{u}} \leftarrow \mathbf{v} + \sum_{j=1}^{J-1} R_j^T (I_j^{j\bullet} I_{j\bullet}^j + I_j^{j\rangle} I_{j\rangle}^j) \mathbf{w}_j$ .

**Form 2.** Solve successively for  $j = 1, \dots, J$ ,

$$\begin{bmatrix} \tilde{S}_{j\langle}^{\langle} & A_{j\langle j\bullet} & & \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} & \\ & A_{j\rangle j\bullet} & \tilde{S}_{j\rangle\rangle}^{\rangle} & \end{bmatrix} \begin{bmatrix} \mathbf{v}_{j\langle} \\ \mathbf{v}_{j\bullet} \\ \mathbf{v}_{j\rangle} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{j\langle} - 2A_{j\langle j-1\bullet} \mathbf{v}_{j-1\bullet} - A_{j\langle} \mathbf{v}_{j-1\langle} \\ \mathbf{f}_{j\bullet} \\ 0 \end{bmatrix},$$

where  $\tilde{S}_{j\langle}^{\langle}$  and  $\tilde{S}_{j\rangle\rangle}^{\rangle}$  are the Schur complements from the PML (see Remark 14 for practical implementation).

Let  $\mathbf{v} \leftarrow \sum_{j=1}^J R_j^T (I_j^{j\langle} I_{j\langle}^j + I_j^{j\bullet} I_{j\bullet}^j) \mathbf{v}_j$  and compute  $\tilde{\mathbf{f}} \leftarrow \mathbf{f} - A\mathbf{v}$ . Let  $\mathbf{w}_J \leftarrow 0$ .

In order of  $j = J-1, \dots, 1$ , solve the correction problem

$$\begin{bmatrix} \tilde{S}_{j\langle}^{\langle} & A_{j\langle j\bullet} & & \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\rangle} & \\ & A_{j\rangle j\bullet} & \tilde{S}_{j\rangle\rangle}^{\rangle} & \end{bmatrix} \begin{bmatrix} \mathbf{w}_{j\langle} \\ \mathbf{w}_{j\bullet} \\ \mathbf{w}_{j\rangle} \end{bmatrix} = \begin{bmatrix} 0 \\ \tilde{\mathbf{f}}_{j\bullet} \\ \tilde{\mathbf{f}}_{j\rangle} - 2A_{j\rangle j+1\bullet} \mathbf{w}_{j+1\bullet} - A_{j\rangle} \mathbf{w}_{j+1\langle} \end{bmatrix}.$$

Compute the output  $\tilde{\mathbf{u}} \leftarrow \mathbf{v} + \sum_{j=1}^{J-1} R_j^T (I_j^{j\bullet} I_{j\bullet}^j + I_j^{j\rangle} I_{j\rangle}^j) \mathbf{w}_j$ .

*guess*,  $\mathcal{Q}_j^{\langle} = \mathcal{I}$ ,  $\mathcal{P}_j^{\langle} = \text{DtN}_j^{pml}|_{\Gamma_{j,j-1}^h}$ ,  $\mathcal{Q}_j^{\rangle} = \mathcal{I}$ ,  $\mathcal{P}_j^{\rangle} = \text{DtN}_j^{pml}|_{\Gamma_{j,j+1}^h}$ , and using the two nonoverlapping partitions as in Algorithm 10, one partition for the forward sweep and the other for the backward sweep.

*Proof.* By the zero initial guess and the specific conditions for Algorithm 1 in the theorem, the  $(j-1)$ st subproblem of Algorithm 1 imposes the following condition on

$\Gamma_{j-1,j} = \Gamma_{j,j-1}$ , since the partition is nonoverlapping:

$$\mathbf{n}_{j-1}^T \alpha \nabla v_{j-1} + \text{DtN}_{j-1}^{pml} v_{j-1} = 0.$$

Note that  $\mathbf{n}_j = -\mathbf{n}_{j-1}$  on  $\Gamma_{j,j-1}$ . Substituting these conditions and the assumption  $\text{DtN}_j^{pml} = \text{DtN}_{j-1}^{pml}$  into the transmission condition on  $\Gamma_{j,j-1}$  of the  $j$ th subproblem, we find

$$\mathbf{n}_j^T \alpha \nabla v_j + \text{DtN}_j^{pml} v_j = 2\mathbf{n}_j^T \alpha \nabla v_{j-1},$$

which imposes a Neumann jump between  $\Omega_j$  and the PML on the other side of  $\Gamma_{j,j-1}$ . We recover the forward sweep of Algorithm 10 by moving the Neumann jump to the r.h.s. of the PDE as a surface source. Between the forward and the backward sweeps, Algorithm 10 takes the residual  $\tilde{f}$  and introduces overlaps of the old subdomains used in the forward sweep and the new subdomains used in the backward sweep. This gives the deferred correction form as in Algorithm 3 but mixed with the single layer potential on  $\Gamma_{j,j+1}^h$  too. Then we can conclude by adapting the proof of Theorem 21 and the same arguments as in the forward sweep.  $\square$

**THEOREM 36.** *Let Algorithm 4 use  $Q_{j\langle}^\langle = I_{j\langle}$ ,  $Q_{j\rangle}^\rangle = I_{j\rangle}$ ,  $P_{j\langle}^\langle = \tilde{S}_{j\langle}^\langle - A_{j\langle}^\langle$ ,  $P_{j\rangle}^\rangle = \tilde{S}_{j\rangle}^\rangle - A_{j\rangle}^\rangle$ , and let the initial guess be zero. The following statements about Algorithm 11 then hold:*

- 1° Suppose the subproblems of the first form of Algorithm 11 are well-posed and  $\tilde{S}_{j\langle}^\langle$ ,  $\tilde{S}_{j\rangle}^\rangle$  are invertible. Let  $\tilde{S}_{j\langle}^\langle := A_{j\langle} - A_{j\langle j\langle}(\tilde{S}_{j\langle}^\langle)^{-1}A_{j\langle j\langle}$ , and  $\tilde{S}_{j\rangle}^\rangle := A_{j\rangle} - A_{j\rangle j\rangle}(\tilde{S}_{j\rangle}^\rangle)^{-1}A_{j\rangle j\rangle}$ . If  $I_{j\langle\langle} = I_{j\langle} = -A_{j\langle j\langle}$ ,  $\tilde{S}_{j\langle}^\langle = \tilde{S}_{j-1\rangle}^\rangle$  for  $j = 2, \dots, J$ ,  $I_{j\rangle\rangle} = I_{j\rangle} = -A_{j\rangle j\rangle}$ ,  $\tilde{S}_{j\rangle}^\rangle = \tilde{S}_{j+1\langle}^\langle$  for  $j = 1, \dots, J-1$ , and  $A_{j\langle j-1\bullet} = [0, A_{j\langle j\langle}]$ , then the first form of Algorithm 11 is equivalent to the harmonic extension variant of Algorithm 4; see Remark 20.
- 2° Suppose the subproblems of the second form of Algorithm 11 are well-posed. If  $\tilde{S}_{j\langle}^\langle = \tilde{S}_{j-1\rangle}^\rangle$  for  $j = 2, \dots, J$  and  $\tilde{S}_{j\rangle}^\rangle = \tilde{S}_{j+1\langle}^\langle$  for  $j = 1, \dots, J-1$ , then the second form of Algorithm 11 is equivalent to the harmonic extension variant of Algorithm 4; see Remark 20.

*Proof.* We first prove claim 1°. We eliminate the first and the last rows of the  $j$ th forward subproblem and substitute with the assumptions of 1° to obtain

$$(70) \quad \begin{bmatrix} \tilde{S}_{j\langle}^\langle & A_{j\langle j\bullet} \\ A_{j\bullet j\langle} & A_{j\bullet} \\ A_{j\rangle j\bullet} & \tilde{S}_{j\rangle}^\rangle \end{bmatrix} \begin{bmatrix} \mathbf{v}_{j\langle} \\ \mathbf{v}_{j\bullet} \\ \mathbf{v}_{j\rangle} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{j\langle} - A_{j\langle j\langle}(\mathbf{v}_{j-1\langle} + (\tilde{S}_{j\langle}^\langle - A_{j\langle})\mathbf{v}_{j-1\rangle} + (\tilde{S}_{j\langle}^\langle)^{-1}\mathbf{v}_{j-1\langle} - \mathbf{v}_{j-1\rangle}) \\ \mathbf{f}_{j\bullet} \\ 0 \end{bmatrix}.$$

It can be shown that the underlined expression on the right above vanishes: in fact, the above subproblem is also used with  $j-1$  replacing  $j$ . In particular, the last row of the  $(j-1)$ st subproblem reads

$$(71) \quad A_{j-1\rangle j-1\bullet} \mathbf{v}_{j-1\bullet} + \tilde{S}_{j-1\rangle}^\rangle \mathbf{v}_{j-1\rangle} = 0.$$

Recalling that  $j-1\rangle$  and  $j\langle$  correspond to the same d.o.f., because the decomposition is nonoverlapping, and the assumptions that  $A_{j\langle j-1\bullet} = [0, A_{j\langle j\langle}]$ ,  $A_{j\langle j\langle} = -I_{j\langle\langle}$  and  $\tilde{S}_{j-1\rangle}^\rangle = \tilde{S}_{j\langle\langle}^\langle$ , we obtain from (71) that  $\tilde{S}_{j\langle\langle}^\langle \mathbf{v}_{j-1\langle} = \mathbf{v}_{j-1\langle}$ . This shows that

the underlined expression in (70) is zero. Similar to (26), (70) is almost the same subproblem used in Algorithm 1 but (70) puts zero on the last row of the r.h.s., which is a trait of the harmonic extension variant. By reusing some arguments from the proof of Theorem 23, we can show the equivalence to Algorithm 4 and conclude with claim 1°.

To prove claim 2°, the key is to show that the r.h.s. from the second form of Algorithm 11 is the same as the r.h.s. from Algorithm 2 except that the former puts zeros on the right interfaces in the forward sweep, and on the left interfaces in the backward sweep. Similar to (26), we may write the first row of the r.h.s. from the forward sweep of Algorithm 2 as

$$\mathbf{f}_{j\langle} - A_{j\langle j-1\bullet} \mathbf{u}_{j-1\bullet}^{(\frac{1}{2})} + (\tilde{S}_{j\langle}^{\langle} - A_{j\langle}) \mathbf{u}_{j-1\lceil}^{(\frac{1}{2})}.$$

Using the assumption that  $\tilde{S}_{j\langle}^{\langle} = \tilde{S}_{j-1\rangle}^{\rangle}$  and the last row (with zeroed r.h.s.) of the  $(j-1)$ st subproblem similar to (71), we see that the above expression is equal to

$$\mathbf{f}_{j\langle} - 2A_{j\langle j-1\bullet} \mathbf{u}_{j-1\bullet}^{(\frac{1}{2})} - A_{j\langle} \mathbf{u}_{j-1\lceil}^{(\frac{1}{2})}.$$

This is exactly the same as in the forward sweep of Algorithm 11. The remaining part of the proof of claim 2° can now be completed as in the proof of Theorem 23.  $\square$

There is a final ingredient used in [157] based on the idea of right preconditioning. A preconditioner  $M^{-1}$  such as the one defined by Algorithm 11 can be used on either the left or the right of the original operator  $A$ . For right preconditioning of (17), one first uses an iterative method like Krylov or Richardson to solve  $AM^{-1}\mathbf{r} = f$  for  $\mathbf{r}$ , and then obtains the solution  $\mathbf{u}$  of (17) by computing  $\mathbf{u} = M^{-1}\mathbf{r}$ . Let  $\mathbf{r}^{(n)}$  for  $n \geq 0$  be the iterates for  $\mathbf{r}$ . Denote  $\mathbf{v}^{(n+1)} := M^{-1}\mathbf{r}^{(n)}$ . It can be shown that if  $\mathbf{r}^{(0)} = \mathbf{f} - A\mathbf{u}^{(0)}$  and  $\mathbf{r}^{(n)}$  and  $\mathbf{u}^{(n)}$  are generated by the Richardson iterations

$$\mathbf{r}^{(n+1)} = \mathbf{r}^{(n)} + \mathbf{f} - AM^{-1}\mathbf{r}^{(n)}, \quad \mathbf{u}^{(n+1)} = \mathbf{u}^{(n)} + M^{-1}(\mathbf{f} - A\mathbf{u}^{(n)}),$$

then we have the relation  $\mathbf{u}^{(n)} = \mathbf{v}^{(n)} + (I - M^{-1}A)^{n-1}\mathbf{u}^{(0)}$  for  $n \geq 1$ . There is also a relation between the GMRES iterates for the left and the right preconditioned systems; see [146].

If one solves the restricted version of the original problem exactly in the interior of the subdomains using a direct solver, and then glues the resulting local approximations into a global approximation, then the global approximation mostly has a zero residual, except where the residual is influenced by values of the global approximation from different subdomains; see, e.g., [71]. This is why in Algorithm 10, the intermediate residual  $\tilde{f}$  is concentrated in the neighborhood of the interfaces  $\Gamma_{j,j-1}$ ,  $j \geq 2$ , and the output  $\tilde{u}$  leaves the residual  $f - \mathcal{L}\tilde{u}$  concentrated in the neighborhood of the shifted interfaces  $\Gamma_{j,j-1}^h$ ,  $j \geq 2$ . In Algorithm 11, a component of  $\tilde{\mathbf{f}}$  is nonzero only if the corresponding row in the matrix  $A$  has at least one nonzero entry belonging to a column associated with an interface d.o.f., and the residual left by the output  $\tilde{\mathbf{u}}$  also has a similar sparsity. The sparsity of the residuals can be leveraged in the right preconditioned system because the essential unknowns become the nonzero components of the residual. This was studied in detail in [107] and was also suggested by Stolk in [157] for the preconditioner based on single layer potentials. We summarize the sparse residual algorithm in Algorithm 12 and justify it in Theorem 37. Note that this substructured form can be adapted to all the preconditioners resulting in sparse resid-

uals, e.g., Algorithm 4. Compared to Algorithm 6, the reduced system in Algorithm 12 is typically of twice the size but free of the need to apply the PML-DtN operators.

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**Algorithm 12.** Residual substructuring when most rows of  $I - AM^{-1}$  vanish.

Construct the 0-1 matrix  $R_r$  such that  $(I - R_r^T R_r)(I - AM^{-1}) = 0$  and  $R_r R_r^T = I_r$ . Set an initial guess  $\mathbf{u}^{(0)}$  such that  $(I - R_r^T R_r)(\mathbf{f} - A\mathbf{u}^{(0)}) = 0$ , e.g.,  $\mathbf{u}^{(0)} \leftarrow M^{-1}\mathbf{f}$ . Let  $\mathbf{h}_r \leftarrow R_r(\mathbf{f} - A\mathbf{u}^{(0)})$ . Solve (approximately) the substructured system for  $\mathbf{r}_r$ :

$$(72) \quad (R_r A M^{-1} R_r^T) \mathbf{r}_r = \mathbf{h}_r.$$

Let  $\mathbf{u} \leftarrow M^{-1} R_r^T \mathbf{r}_r + \mathbf{u}^{(0)}$ , which is (approximately) the solution of (17).

---

**THEOREM 37.** *If  $A$  and  $M^{-1}$  are invertible, then the substructured system in (72) is well-posed, and if, in addition, (72) is solved exactly, then the output  $\mathbf{u}$  from Algorithm 12 is indeed the solution of (17).*

*Proof.* We first assume that (72) has at least one solution. Hence,

$$R_r^T R_r A M^{-1} R_r^T \mathbf{r}_r = R_r^T \mathbf{h}_r = R_r^T R_r (\mathbf{f} - A\mathbf{u}^{(0)}) = \mathbf{f} - A\mathbf{u}^{(0)},$$

where the last equality follows from the assumption on  $\mathbf{u}^{(0)}$ . By the assumptions on  $R_r$ , we also have

$$(I - R_r^T R_r) A M^{-1} R_r^T \mathbf{r}_r = (I - R_r^T R_r) R_r^T \mathbf{r}_r = 0.$$

Summing the two identities above, we obtain

$$A M^{-1} R_r^T \mathbf{r}_r = \mathbf{f} - A\mathbf{u}^{(0)},$$

or  $A\mathbf{u} = A(M^{-1} R_r^T \mathbf{r}_r + \mathbf{u}^{(0)}) = \mathbf{f}$ ; that is, the output of Algorithm 12 is indeed the solution of (17). Now if  $\mathbf{h}_r = 0$ , then by the assumption on  $\mathbf{u}^{(0)}$  we have  $A M^{-1} R_r^T \mathbf{r}_r = \mathbf{f} - A\mathbf{u}^{(0)} = 0$ , which, since  $A$  and  $M^{-1}$  are invertible, implies  $R_r^T \mathbf{r}_r = 0$  and further  $\mathbf{r}_r = 0$  using  $R_r R_r^T = I_r$ . Hence, (72) is well-posed.  $\square$

### 8.3. Method of Polarized Traces Using Single and Double Layer Potentials.

We have already seen that (68) can be used to propagate the wave field in  $\Omega_{j-1}$  to  $\Omega_j$ . The only data we take from the previous subdomain are the Neumann and Dirichlet traces on the interface  $\Gamma_{j,j-1}$ . The method of polarized traces introduced in [180] iterates the Neumann and Dirichlet traces from neighboring subdomains in the substeps of the forward and backward sweeps, and upon completion of a double sweep, a global approximation is constructed using the representation formula (37) in subdomains where the volume potentials have been precomputed before the sweeps.<sup>22</sup> We summarize the polarized traces preconditioner in Algorithm 13 at the PDE level. The relation to Algorithm 1 is shown in Theorem 38.

**THEOREM 38.** *Suppose the subproblems used for the  $v_j^0$  in Algorithm 13 are well-posed. Let  $\{u_j^{(\frac{1}{2})}\}_{j=1}^{J-1}$  and  $\{u_j^{(1)}\}_{j=1}^J$  be generated by Algorithm 1 with zero initial guess, with  $\mathcal{Q}$  being the identity and  $\mathcal{P}$  equal to the PML-DtN operators. Let  $u_J^{(\frac{1}{2})} := 0$*

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<sup>22</sup>In the full paper [179] that followed [180], a substructured system for the traces is first solved instead of the original system. For brevity, we will describe only the global form preconditioner, from which the corresponding substructured system is easy to derive.

---

**Algorithm 13.** Polarized traces preconditioner at the PDE level [180, Algorithm 1].

---

Input the source term  $f$  and assume for simplicity  $g = 0$  in (11).

Suppose  $\Omega$  is decomposed into nonoverlapping subdomains.

Independently for  $j = 1, \dots, J$  solve

$$\begin{aligned} \mathcal{L} v_j^0 &= f_j && \text{in } \Omega_j, \\ \mathcal{B} v_j^0 &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathbf{n}_j^T \alpha \nabla v_j^0 + \text{DtN}_j^{pml} v_j^0 &= 0 && \text{on } \Gamma_{j,j-1}, \\ \mathbf{n}_j^T \alpha \nabla v_j^0 + \text{DtN}_j^{pml} v_j^0 &= 0 && \text{on } \Gamma_{j,j+1}, \end{aligned}$$

where  $f_j := f|_{\Omega_j}$ ; see Remark 13 for a practical implementation of the PML-DtN operators. Denote by  $G_j(\mathbf{x}, \mathbf{y})$  the Green's function for the subproblem above. We have  $v_j^0(\mathbf{x}) = \int_{\Omega_j} G_j(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}$  for  $\mathbf{x} \in \Omega_j$ .

Let  $\lambda_{1\langle}^D \leftarrow 0$ ,  $\lambda_{1\langle}^N \leftarrow 0$ . Successively for  $j = 2, \dots, J$  compute for all  $\mathbf{x} \in \Gamma_{j,j-1}$ ,

$$\begin{aligned} \lambda_{j\langle}^D(\mathbf{x}) &\leftarrow (\mathcal{S}_{j\langle} \lambda_{j-1\langle}^N)(\mathbf{x}) - (\mathcal{D}_{j\langle} \lambda_{j-1\langle}^D)(\mathbf{x}) + v_{j-1}^0(\mathbf{x}), \\ \lambda_{j\langle}^N(\mathbf{x}) &\leftarrow (\mathcal{D}_{j\langle}^* \lambda_{j-1\langle}^N)(\mathbf{x}) - (\mathcal{N}_{j\langle} \lambda_{j-1\langle}^D)(\mathbf{x}) + (\mathbf{n}_j^T \alpha \nabla v_{j-1}^0)(\mathbf{x}), \end{aligned}$$

where the four surface potentials vanish for  $j = 2$  and are given for  $j \geq 3$  by

$$(73) \quad \begin{aligned} (\mathcal{S}_{j\langle} w)(\mathbf{x}) &:= \int_{\Gamma_{j-1,j-2}} w(\mathbf{y}) G_{j-1}(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}), \\ (\mathcal{D}_{j\langle} w)(\mathbf{x}) &:= \int_{\Gamma_{j-1,j-2}} w(\mathbf{y}) (\mathbf{n}_{j-1}^T \alpha^T)(\mathbf{y}) \nabla_{\mathbf{y}} G_{j-1}(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}), \\ (\mathcal{D}_{j\langle}^* w)(\mathbf{x}) &:= \int_{\Gamma_{j-1,j-2}} w(\mathbf{y}) (\mathbf{n}_j^T \alpha)(\mathbf{x}) \nabla_{\mathbf{x}} G_{j-1}(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}), \\ (\mathcal{N}_{j\langle} w)(\mathbf{x}) &:= \int_{\Gamma_{j-1,j-2}} w(\mathbf{y}) (\mathbf{n}_j^T \alpha)(\mathbf{x}) \nabla_{\mathbf{x}} \left\{ (\mathbf{n}_{j-1}^T \alpha^T)(\mathbf{y}) \nabla_{\mathbf{y}} G_{j-1}(\mathbf{x}, \mathbf{y}) \right\} d\sigma(\mathbf{y}). \end{aligned}$$

Let  $\lambda_{J\rangle}^D \leftarrow 0$ ,  $\lambda_{J\rangle}^N \leftarrow 0$ . Successively for  $j = J-1, \dots, 1$  compute for all  $\mathbf{x} \in \Gamma_{j,j+1}$ ,

$$\begin{aligned} \lambda_{j\rangle}^D(\mathbf{x}) &\leftarrow (\mathcal{S}_{j\rangle} \lambda_{j+1\rangle}^N)(\mathbf{x}) - (\mathcal{D}_{j\rangle} \lambda_{j+1\rangle}^D)(\mathbf{x}) + v_{j+1}^0(\mathbf{x}), \\ \lambda_{j\rangle}^N(\mathbf{x}) &\leftarrow (\mathcal{D}_{j\rangle}^* \lambda_{j+1\rangle}^N)(\mathbf{x}) - (\mathcal{N}_{j\rangle} \lambda_{j+1\rangle}^D)(\mathbf{x}) + (\mathbf{n}_j^T \alpha \nabla v_{j+1}^0)(\mathbf{x}), \end{aligned}$$

where the four surface potentials vanish for  $j = J-1$  and are given for  $j \leq J-2$  by

$$(74) \quad \begin{aligned} (\mathcal{S}_{j\rangle} w)(\mathbf{x}) &:= \int_{\Gamma_{j+1,j+2}} w(\mathbf{y}) G_{j+1}(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}), \\ (\mathcal{D}_{j\rangle} w)(\mathbf{x}) &:= \int_{\Gamma_{j+1,j+2}} w(\mathbf{y}) (\mathbf{n}_{j+1}^T \alpha^T)(\mathbf{y}) \nabla_{\mathbf{y}} G_{j+1}(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}), \\ (\mathcal{D}_{j\rangle}^* w)(\mathbf{x}) &:= \int_{\Gamma_{j+1,j+2}} w(\mathbf{y}) (\mathbf{n}_j^T \alpha)(\mathbf{x}) \nabla_{\mathbf{x}} G_{j+1}(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}), \\ (\mathcal{N}_{j\rangle} w)(\mathbf{x}) &:= \int_{\Gamma_{j+1,j+2}} w(\mathbf{y}) (\mathbf{n}_j^T \alpha)(\mathbf{x}) \nabla_{\mathbf{x}} \left\{ (\mathbf{n}_{j+1}^T \alpha^T)(\mathbf{y}) \nabla_{\mathbf{y}} G_{j+1}(\mathbf{x}, \mathbf{y}) \right\} d\sigma(\mathbf{y}). \end{aligned}$$

Recover independently the subdomain solutions for  $\mathbf{x} \in \Omega_j$ ,  $j = 1, \dots, J$ , by

$$(75) \quad \begin{aligned} v_j(\mathbf{x}) &\leftarrow v_j^0(\mathbf{x}) + \int_{\Gamma_{j,j-1}} \lambda_{j\langle}^N(\mathbf{y}) G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}) - \int_{\Gamma_{j,j-1}} \lambda_{j\langle}^D(\mathbf{y}) (\mathbf{n}_j^T \alpha^T)(\mathbf{y}) \nabla_{\mathbf{y}} G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}) \\ &\quad + \int_{\Gamma_{j,j+1}} \lambda_{j\rangle}^N(\mathbf{y}) G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}) - \int_{\Gamma_{j,j+1}} \lambda_{j\rangle}^D(\mathbf{y}) (\mathbf{n}_j^T \alpha^T)(\mathbf{y}) \nabla_{\mathbf{y}} G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}). \end{aligned}$$

Output the global approximation  $\tilde{u} \leftarrow v_j$  in  $\Omega_j$ ,  $j = 1, \dots, J$ .

---

be defined on  $\Omega_J$ . We have for Algorithm 13  $\lambda_{j\langle}^D = u_{j-1}^{(\frac{1}{2})}$ ,  $\lambda_{j\langle}^N = \mathbf{n}_j^T \alpha \nabla u_{j-1}^{(\frac{1}{2})}$  on  $\Gamma_{j,j-1}$ , and  $\lambda_{j\rangle}^D = u_{j+1}^{(1)} - u_{j+1}^{(\frac{1}{2})} + v_{j+1}^0$ ,  $\lambda_{j\rangle}^N = \mathbf{n}_j^T \alpha \nabla (u_{j+1}^{(1)} - u_{j+1}^{(\frac{1}{2})} + v_{j+1}^0)$  on  $\Gamma_{j,j+1}$ . Therefore,  $v_j = u_j^{(1)}$  in  $\Omega_j$ .

*Proof.* For simplicity, we consider only the case  $g = 0$  in (11). According to Algorithms 1 and 13,  $u_1^{(\frac{1}{2})} = v_1^0$  in  $\Omega_1$  and so

$$(76) \quad \lambda_{2\langle}^D = u_1^{(\frac{1}{2})}, \quad \lambda_{2\langle}^N = \mathbf{n}_2^T \alpha \nabla u_1^{(\frac{1}{2})} \quad \text{on } \Gamma_{2,1}.$$

From the algorithms, we also have for any fixed  $\mathbf{x} \in \Omega_j$ ,  $j = 2, \dots, J$ ,

$$\begin{aligned} (\mathbf{n}_j^T \alpha \nabla + \text{DtN}_j^{pml})(u_j^{(\frac{1}{2})} - u_{j-1}^{(\frac{1}{2})}) &= (\mathbf{n}_j^T \alpha^T \nabla + \text{DtN}_j^{pml*})G_j(\mathbf{x}, \cdot) = 0 \text{ on } \Gamma_{j,j-1}, \\ (\mathbf{n}_j^T \alpha \nabla + \text{DtN}_j^{pml})u_j^{(\frac{1}{2})} &= (\mathbf{n}_j^T \alpha^T \nabla + \text{DtN}_j^{pml*})G_j(\mathbf{x}, \cdot) = 0 \text{ on } \Gamma_{j,j+1}, \end{aligned}$$

where  $\text{DtN}_j^{pml*}$  is similar to  $\text{DtN}_j^{pml}$  but using  $\alpha^T$  instead of  $\alpha$ . By the representation formula in (37) on  $\bar{\Omega}_j \cup \bar{\Omega}_{j\rangle}^{pml}$ , where  $\Omega_{j\rangle}^{pml}$  is the PML region along  $\Gamma_{j,j+1}$ , we have

$$\begin{aligned} u_j^{(\frac{1}{2})}(\mathbf{x}) &= \int_{\Omega_j} f(\mathbf{y})G_j(\mathbf{x}, \mathbf{y}) d\mathbf{y} + \int_{\Gamma_{j,j-1}} \mathbf{n}_j^T \alpha \nabla u_j^{(\frac{1}{2})}(\mathbf{y})G_j(\mathbf{x}, \mathbf{y}) - \mathbf{n}_j^T \alpha^T \nabla_y G_j(\mathbf{x}, \mathbf{y})u_j^{(\frac{1}{2})}(\mathbf{y}) d\sigma(\mathbf{y}) \\ (77) \quad &= v_j^0(\mathbf{x}) + \int_{\Gamma_{j,j-1}} (\mathbf{n}_j^T \alpha \nabla + \text{DtN}_j^{pml})u_j^{(\frac{1}{2})}(\mathbf{y})G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}) \end{aligned}$$

$$(78) \quad = v_j^0(\mathbf{x}) + \int_{\Gamma_{j,j-1}} (\mathbf{n}_j^T \alpha \nabla + \text{DtN}_j^{pml})u_{j-1}^{(\frac{1}{2})}(\mathbf{y})G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y})$$

$$(79) \quad = v_j^0(\mathbf{x}) + \int_{\Gamma_{j,j-1}} G_j(\mathbf{x}, \mathbf{y})\mathbf{n}_j^T \alpha \nabla u_{j-1}^{(\frac{1}{2})}(\mathbf{y}) - u_{j-1}^{(\frac{1}{2})}(\mathbf{y})\mathbf{n}_j^T \alpha^T \nabla_y G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}),$$

where no integrals show up on the other boundaries of  $\bar{\Omega}_j \cup \bar{\Omega}_{j\rangle}^{pml}$  because the boundary conditions there are homogeneous. Equation (77) is obtained by substituting the PML condition for  $G_j(\mathbf{x}, \cdot)$  and using the following identity for any fixed  $\mathbf{x} \in \Omega_j$  and any trace  $v(\mathbf{y})$  (which can be proved by the definition of  $\text{DtN}_j^{pml}$ ):

$$(80) \quad \int_{\Gamma_{j,j-1}} v(\mathbf{y})\text{DtN}_j^{pml*}G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}) = \int_{\Gamma_{j,j-1}} G_j(\mathbf{x}, \mathbf{y})\text{DtN}_j^{pml}v(\mathbf{y}) d\sigma(\mathbf{y}).$$

Equation (78) follows from the transmission conditions, and (79) is obtained by applying (80) and again substituting the PML condition for  $G_j(\mathbf{x}, \cdot)$ . Assuming that

$$(81) \quad \lambda_{j\langle}^D = u_{j-1}^{(\frac{1}{2})}, \quad \lambda_{j\langle}^N = \mathbf{n}_j^T \alpha \nabla u_{j-1}^{(\frac{1}{2})} \quad \text{on } \Gamma_{j,j-1},$$

we substitute them into (79) and taking Dirichlet and Neumann traces of  $u_j^{(\frac{1}{2})}$  on  $\mathbf{x} \in \Gamma_{j+1,j}$ , we find (81) holds for  $j+1$  replacing  $j$ . By induction based on (76), we conclude that (81) holds for all  $j = 2, \dots, J$ . Inserting (81) into (77) yields (for  $j = J$  change the l.h.s. to  $u_J^{(1)}$ )

$$(82) \quad u_j^{(\frac{1}{2})}(\mathbf{x}) = v_j^0(\mathbf{x}) + \int_{\Gamma_{j,j-1}} G_j(\mathbf{x}, \mathbf{y})\lambda_{j\langle}^N(\mathbf{y}) - \lambda_{j\langle}^D(\mathbf{y})\mathbf{n}_j^T \alpha^T \nabla_y G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}).$$

In particular, we have  $u_J^{(1)} = v_J$  with  $v_J$  from Algorithm 13.

In the backward sweep of Algorithm 1, we denote  $w_j := u_j^{(1)} - u_j^{(\frac{1}{2})} + v_j^0$ ,  $j = J-1, \dots, 1$ , and  $w_J := u_J^{(1)}$ . We find  $w_j$  satisfies the PML conditions, homogeneous on  $\Gamma_{j,j-1}$  but inhomogeneous on  $\Gamma_{j,j+1}$ . By arguments similar to the last paragraph, we can show for all  $j = J-1, \dots, 1$  that

$$\lambda_{j\rangle}^D = w_{j+1}, \quad \lambda_{j\rangle}^N = \mathbf{n}_j^T \alpha \nabla w_{j+1} \quad \text{on } \Gamma_{j,j+1},$$

and further

$$(83) \quad w_j(\mathbf{x}) = v_j^0(\mathbf{x}) + \int_{\Gamma_{j,j+1}} G_j(\mathbf{x}, \mathbf{y}) \lambda_{j\rangle}^N(\mathbf{y}) - \lambda_{j\rangle}^D(\mathbf{y}) \mathbf{n}_j^T \alpha^T \nabla_{\mathbf{y}} G_j(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}).$$

Combining (82) and (83), we conclude that  $u_j^{(1)} = v_j$  with  $v_j$  from Algorithm 13.  $\square$

*Remark 39.* Algorithm 13 includes a new technique not present in Algorithm 1. First, note that the local solutions of the original problem can be represented as sums of the left-going and right-going waves. Furthermore, the two parts can be simulated independently of each other; that is, the backward sweep of Algorithm 13 can be performed in parallel with the forward sweep, whereas the backward sweep of Algorithm 1 aims to simulate the total waves and thus needs to wait for the forward sweep to finish. Algorithm 1 can be modified in the same spirit: just use the data from the original problem for an initial solve on the subdomains, zero the left interface data in the backward sweep, add the approximations from the forward/backward sweep, and subtract that from the initial solve to find the total waves. Alternatively, for the block 2-by-2 interface system in Remark 29 use block Jacobi instead of Gauss–Seidel. Similar techniques were proposed in [139, 158]. For Algorithm 13, the waves from the forward/backward sweep have different *polarized* directions and they are propagated through their Dirichlet and Neumann *traces*, which gives the name of the method.

*Remark 40.* In the preceding sections, we did not discuss in detail solvers for the subproblems. Typically, LU factorizations are precomputed before the iteration starts, and they are then reused for the different r.h.s. in the iterative procedure. Even for the substructured forms, the typical way is *not* to precompute the interface operators explicitly (see Remark 29), but only to implement them as matrix actions through the subdomain LU solves. The reason is two-fold: first, to build an interface operator in a naive way, we need to solve the subdomain problem as many times as the number of d.o.f. on the interface; second, the resulting matrix is dense and a naive multiplication with a vector is not cheap. However, developments of low rank formats of matrices such as  $\mathcal{H}$ -matrices have greatly improved the situation. For example, for the Laplace equation, the method in [88] reduces the building cost to  $\mathcal{O}(N^{2-(2/d)})$  and the application cost to  $\mathcal{O}(N^{1/2})$  in two dimensions and  $\mathcal{O}(N)$  in three dimensions, and some tests for the Helmholtz equation are also performed. In [179, 180], low rank techniques are used for building and applying the surface potentials in (73)–(75) for Algorithm 13.

To bring Algorithm 13 to the matrix level, we first translate the representation formula from (37) into matrix language. Suppose  $G$  is the matrix analogue of the Green's function, i.e.,

$$(84) \quad \begin{bmatrix} G_e & G_{eb} & G_{ei} \\ G_{be} & G_b & G_{bi} \\ G_{ie} & G_{ib} & G_i \end{bmatrix} \begin{bmatrix} A_e & A_{eb} & \\ A_{be} & A_b & A_{bi} \\ & A_{ib} & A_i \end{bmatrix} = \begin{bmatrix} I_e & & \\ & I_b & \\ & & I_i \end{bmatrix},$$

where the rows and columns with the subscripts containing  $e$  may all be empty. Let  $\mathbf{u}$  satisfy

$$(85) \quad \begin{bmatrix} \tilde{A}_b & A_{bi} \\ A_{ib} & A_i \end{bmatrix} \begin{bmatrix} \mathbf{u}_b \\ \mathbf{u}_i \end{bmatrix} = \begin{bmatrix} \mathbf{f}_b + \boldsymbol{\lambda}_b \\ \mathbf{f}_i \end{bmatrix}.$$

Then we have the following representation formula for  $\mathbf{u}_i$ .

PROPOSITION 41. *If (84) holds, then (85) implies*

$$(86) \quad \mathbf{u}_i = G_i \mathbf{f}_i + G_{ib} \mathbf{f}_b + G_{ib} \boldsymbol{\lambda}_b^N - \{G_{ib} A_b^{(i)} + G_i A_{ib}\} \mathbf{u}_b,$$

where  $\boldsymbol{\lambda}_b^N := A_b^{(i)} \mathbf{u}_b + A_{bi} \mathbf{u}_i - \mathbf{f}_b$  and  $A_b^{(i)}$  is an arbitrary matrix of appropriate size.

*Proof.* Inserting the definition of  $\boldsymbol{\lambda}_b^N$  and the last row of (85) into the r.h.s. of (86) we obtain

$$\text{r.h.s. of (86)} = (G_i A_i + G_{ib} A_{bi}) \mathbf{u}_i.$$

On the other hand, from Equation (84) we have  $G_i A_i + G_{ib} A_{bi} = I_i$ , which turns the above equation into (86).  $\square$

From (86), we can recognize  $[G_i, G_{ib}]$ ,  $G_{ib}$ , and  $G_{ib} A_b^{(i)} + G_i A_{ib}$  as the volume, single layer, and double layer potentials. We now give the matrix analogue<sup>23</sup> of Algorithm 13 in Algorithm 14 and prove its equivalence to Algorithm 2 in Theorem 42.

THEOREM 42. *Suppose the subproblems for the  $\mathbf{v}_j^0$  in Algorithm 14 are well-posed. Let  $\{\mathbf{u}_j^{(\frac{1}{2})}\}_{j=1}^{J-1}$  and  $\{\mathbf{u}_j^{(1)}\}_{j=1}^J$  be generated by Algorithm 2 with zero initial guess, with  $Q$  equal to the identity and with  $P$  equal to the PML-DtN operators. Let  $\mathbf{u}_j^{(\frac{1}{2})} := 0$ . We have for Algorithm 14  $\boldsymbol{\lambda}_{j\langle}^D = \mathbf{u}_{j-1\langle}^{(\frac{1}{2})}$ ,  $\boldsymbol{\lambda}_{j\langle}^N = -A_{j\langle}^{\langle} \mathbf{u}_{j-1\langle}^{(\frac{1}{2})} - A_{j\langle j-1\bullet} \mathbf{u}_{j-1\bullet}^{(\frac{1}{2})}$ , and  $\boldsymbol{\lambda}_{j\rangle}^D = \mathbf{u}_{j+1\rangle}^{(1)} - \mathbf{u}_{j+1\langle}^{(\frac{1}{2})} + \mathbf{v}_{j+1\langle}^0$ ,  $\boldsymbol{\lambda}_{j\rangle}^N = -A_{j\rangle}^{\langle} (\mathbf{u}_{j+1\rangle}^{(1)} - \mathbf{u}_{j+1\langle}^{(\frac{1}{2})} + \mathbf{v}_{j+1\langle}^0) - A_{j\rangle j+1\bullet} (\mathbf{u}_{j+1\bullet}^{(1)} - \mathbf{u}_{j+1\bullet}^{(\frac{1}{2})} + \mathbf{v}_{j+1\bullet}^0)$ . Therefore, we have  $\mathbf{v}_{j\bullet} = \mathbf{u}_{j\bullet}^{(1)}$ .*

*Proof.* From the algorithms, we have  $\mathbf{u}_1^{(\frac{1}{2})} = \mathbf{v}_1^0$  and so

$$(87) \quad \boldsymbol{\lambda}_{2\langle}^D = \mathbf{u}_{1\langle}^{(\frac{1}{2})}, \quad \boldsymbol{\lambda}_{2\langle}^N = -(A_{2\langle}^{\langle} \mathbf{u}_{1\langle}^{(\frac{1}{2})} + A_{2\langle 1\bullet} \mathbf{u}_{1\bullet}^{(\frac{1}{2})}).$$

Since  $G^{(j)}$  is the inverse of the coefficient matrix of the  $j$ th subproblem of Algorithm 2, the solution can be represented as

$$(88) \quad \begin{bmatrix} \mathbf{u}_{j\bullet}^{(\frac{1}{2})} \\ \mathbf{u}_{j\rangle}^{(\frac{1}{2})} \end{bmatrix} = \begin{bmatrix} G_{j\bullet j\langle}^{(j)} & G_{j\bullet}^{(j)} & G_{j\bullet j\rangle}^{(j)} \\ G_{j\rangle j\langle}^{(j)} & G_{j\rangle j\bullet}^{(j)} & G_{j\rangle}^{(j)} \end{bmatrix} \begin{bmatrix} \mathbf{f}_{j\langle} + (\tilde{S}_{j\langle}^{(j)} - A_{j\langle}) \mathbf{u}_{j-1\langle}^{(\frac{1}{2})} - A_{j\langle j-1\bullet} \mathbf{u}_{j-1\bullet}^{(\frac{1}{2})} \\ \mathbf{f}_{j\bullet} \\ \mathbf{f}_{j\rangle} \end{bmatrix}.$$

<sup>23</sup>In the full paper [179] that appeared after [180], the matrix form of Algorithm 13 is derived by a first-order finite difference discretization of the Neumann derivatives.  $\boldsymbol{\lambda}_{j*}^N$  is not introduced but is replaced with the d.o.f. immediately next to  $\boldsymbol{\lambda}_{j*}^D$  in  $\Omega_j$ . Since this difference is only minor, we will not study this variant further here. A referee pointed out to us that our presentation here is closer to [178, Appendix C].

**Algorithm 14.** Polarized traces preconditioner at the matrix level.

Input the r.h.s.  $\mathbf{f}$ . Suppose the decomposition is nonoverlapping.

Independently for  $j = 1, \dots, J$  solve

$$\begin{bmatrix} \tilde{S}_{j\langle}^{\langle} & A_{j\langle j\bullet} & A_{j\bullet j\langle} \\ A_{j\bullet j\langle} & A_{j\bullet} & A_{j\bullet j\bullet} \\ A_{j\rangle j\bullet} & A_{j\rangle} & \tilde{S}_{j\rangle}^{\rangle} \end{bmatrix} \begin{bmatrix} \mathbf{v}_{j\langle}^0 \\ \mathbf{v}_{j\bullet}^0 \\ \mathbf{v}_{j\rangle}^0 \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{j\langle} \\ \mathbf{f}_{j\bullet} \\ \mathbf{f}_{j\rangle} \end{bmatrix},$$

where  $\tilde{S}_{j\langle}^{\langle}$  and  $\tilde{S}_{j\rangle}^{\rangle}$  are defined by the Schur complements of the PML exterior to  $\Omega_j$  (see Remark 14 for practical implementation). Denote by  $G^{(j)}$  the inverse of the above coefficient matrix and let it be partitioned in the same way as the above coefficient matrix, e.g.,  $G_{j\bullet j\langle}^{(j)} := I_{j\bullet}^j G^{(j)} I_j^{j\langle}$ . We can represent  $\mathbf{v}_j^0 = G^{(j)}[\mathbf{f}_{j\langle}; \mathbf{f}_{j\bullet}; \mathbf{f}_{j\rangle}]$ .

Let  $\boldsymbol{\lambda}_{1\langle}^D \leftarrow 0$  and  $\boldsymbol{\lambda}_{1\langle}^N \leftarrow 0$ . Compute successively for  $j = 2, \dots, J$ ,

$$\begin{aligned} \boldsymbol{\lambda}_{j\langle}^D &\leftarrow S_{j\langle} \boldsymbol{\lambda}_{j-1\langle}^N - D_{j\langle} \boldsymbol{\lambda}_{j-1\langle}^D + \mathbf{v}_{j-1[}^0, \\ \boldsymbol{\lambda}_{j\langle}^N &\leftarrow D_{j\langle}^* \boldsymbol{\lambda}_{j-1\langle}^N - N_{j\langle} \boldsymbol{\lambda}_{j-1\langle}^D - (A_{j\langle}^{\langle} \mathbf{v}_{j-1[}^0 + A_{j\langle j-1\bullet} \mathbf{v}_{j-1\bullet}^0), \end{aligned}$$

where the matrix potentials vanish for  $j = 2$  and are given for  $j \geq 3$  by

$$\begin{aligned} S_{j\langle} &:= G_{j\langle j-1\langle}^{(j-1)}, \quad D_{j\langle} := G_{j\langle j-1\langle}^{(j-1)} A_{j-1\langle}^{\langle} + G_{j\langle j-1\bullet}^{(j-1)} A_{j-1\bullet j-1\langle}, \quad D_{j\langle}^* := -A_{j\langle}^{\langle} G_{j\langle j-1\langle}^{(j-1)} - A_{j\langle j-1\bullet} G_{j-1\bullet j-1\langle}^{(j-1)}, \\ N_{j\langle} &:= -A_{j\langle}^{\langle} (G_{j\langle j-1\langle}^{(j-1)} A_{j-1\langle}^{\langle} + G_{j\langle j-1\bullet}^{(j-1)} A_{j-1\bullet j-1\langle}) - A_{j\langle j-1\bullet} (G_{j-1\bullet j-1\langle}^{(j-1)} A_{j-1\langle}^{\langle} + G_{j-1\bullet}^{(j-1)} A_{j-1\bullet j-1\langle}). \end{aligned}$$

Let  $\boldsymbol{\lambda}_{J\rangle}^D \leftarrow 0$  and  $\boldsymbol{\lambda}_{J\rangle}^N \leftarrow 0$ . Compute successively for  $j = J-1, \dots, 1$ ,

$$\begin{aligned} \boldsymbol{\lambda}_{j\rangle}^D &\leftarrow S_{j\rangle} \boldsymbol{\lambda}_{j+1\rangle}^N - D_{j\rangle} \boldsymbol{\lambda}_{j+1\rangle}^D + \mathbf{v}_{j+1[}^0, \\ \boldsymbol{\lambda}_{j\rangle}^N &\leftarrow D_{j\rangle}^* \boldsymbol{\lambda}_{j+1\rangle}^N - N_{j\rangle} \boldsymbol{\lambda}_{j+1\rangle}^D - (A_{j\rangle}^{\rangle} \mathbf{v}_{j+1[}^0 + A_{j\rangle j+1\bullet} \mathbf{v}_{j+1\bullet}^0), \end{aligned}$$

where the matrix potentials vanish for  $j = J-1$  and are given for  $j \leq J-2$  by

$$\begin{aligned} S_{j\rangle} &:= G_{j\rangle j+1\rangle}^{(j+1)}, \quad D_{j\rangle} := G_{j\rangle j+1\rangle}^{(j+1)} A_{j+1\rangle}^{\rangle} + G_{j\rangle j+1\bullet}^{(j+1)} A_{j+1\bullet j+1\rangle}, \quad D_{j\rangle}^* := -A_{j\rangle}^{\rangle} G_{j\rangle j+1\rangle}^{(j+1)} - A_{j\rangle j+1\bullet} G_{j+1\bullet j+1\rangle}^{(j+1)}, \\ N_{j\rangle} &:= -A_{j\rangle}^{\rangle} (G_{j\rangle j+1\rangle}^{(j+1)} A_{j+1\rangle}^{\rangle} + G_{j\rangle j+1\bullet}^{(j+1)} A_{j+1\bullet j+1\rangle}) - A_{j\rangle j+1\bullet} (G_{j+1\bullet j+1\rangle}^{(j+1)} A_{j+1\rangle}^{\rangle} + G_{j+1\bullet}^{(j+1)} A_{j+1\bullet j+1\rangle}). \end{aligned}$$

Recover the subdomain solutions independently for  $j = 1, \dots, J$ ,

$$\mathbf{v}_{j\bullet} \leftarrow G_{j\bullet j\langle}^{(j)} \boldsymbol{\lambda}_{j\langle}^N - (G_{j\bullet j\langle}^{(j)} A_{j\langle}^{\langle} + G_{j\bullet j\bullet}^{(j)} A_{j\bullet j\langle}) \boldsymbol{\lambda}_{j\langle}^D + G_{j\bullet j\rangle}^{(j)} \boldsymbol{\lambda}_{j\rangle}^N - (G_{j\bullet j\rangle}^{(j)} A_{j\rangle}^{\rangle} + G_{j\bullet j\bullet}^{(j)} A_{j\bullet j\rangle}) \boldsymbol{\lambda}_{j\rangle}^D + \mathbf{v}_{j\bullet}^0.$$

Output  $\tilde{\mathbf{u}} \leftarrow \sum_{j=1}^J R_j^T (I_j^{j\langle} \boldsymbol{\lambda}_{j\langle}^D + I_j^{j\bullet} \mathbf{v}_{j\bullet})$ .

We claim that the following identity holds:

$$(89) \quad \begin{bmatrix} \mathbf{u}_{j\bullet}^{(\frac{1}{2})} \\ \mathbf{u}_{j\rangle}^{(\frac{1}{2})} \end{bmatrix} = \begin{bmatrix} G_{j\bullet j\langle}^{(j)} & G_{j\bullet}^{(j)} & G_{j\bullet j\rangle}^{(j)} \\ G_{j\rangle j\langle}^{(j)} & G_{j\rangle}^{(j)} & G_{j\rangle j\bullet}^{(j)} \\ G_{j\rangle j\bullet}^{(j)} & G_{j\rangle}^{(j)} & G_{j\rangle}^{(j)} \end{bmatrix} \begin{bmatrix} \mathbf{f}_{j\langle} \\ \mathbf{f}_{j\bullet} \\ \mathbf{f}_{j\rangle} \end{bmatrix} - \begin{bmatrix} G_{j\bullet j\langle}^{(j)} \\ G_{j\rangle j\langle}^{(j)} \\ G_{j\rangle j\bullet}^{(j)} \end{bmatrix} (A_{j\langle}^{\langle} \mathbf{u}_{j-1[}^{(\frac{1}{2})} + A_{j\langle j-1\bullet} \mathbf{u}_{j-1\bullet}^{(\frac{1}{2})}) \\ - \left\{ \begin{bmatrix} G_{j\bullet j\langle}^{(j)} \\ G_{j\rangle j\langle}^{(j)} \end{bmatrix} A_{j\langle}^{\langle} + \begin{bmatrix} G_{j\bullet}^{(j)} & G_{j\bullet j\rangle}^{(j)} \\ G_{j\rangle j\bullet}^{(j)} & G_{j\rangle}^{(j)} \end{bmatrix} \begin{bmatrix} A_{j\bullet j\langle} \\ 0 \end{bmatrix} \right\} \mathbf{u}_{j-1[}^{(\frac{1}{2})}.$$

In fact, the difference in the r.h.s. between (88) and (89) is

$$\left\{ \begin{bmatrix} G_{j\bullet j\langle}^{(j)} & G_{j\bullet}^{(j)} \\ G_{j\rangle j\langle}^{(j)} & G_{j\rangle j\bullet}^{(j)} \end{bmatrix} \begin{bmatrix} \tilde{S}_{j\langle}^{(\frac{1}{2})} \\ A_{j\bullet j\langle} \end{bmatrix} \right\} \mathbf{u}_{j-1[}^{(\frac{1}{2})},$$

and the matrix in the braces vanishes because  $G^{(j)}$  is the inverse of the coefficient matrix of the subproblem for  $\mathbf{v}_j^0$  of Algorithm 14. Assuming that

$$(90) \quad \boldsymbol{\lambda}_{j\langle}^D = \mathbf{u}_{j-1[}^{(\frac{1}{2})}, \quad \boldsymbol{\lambda}_{j\langle}^N = -A_{j\langle}^{\rangle} \mathbf{u}_{j-1[}^{(\frac{1}{2})} - A_{j\rangle j-1\bullet} \mathbf{u}_{j-1\bullet}^{(\frac{1}{2})},$$

we substitute (90) into (89), take the Dirichlet and Neumann traces on  $\Gamma_{j+1,j}$ , and compare the results with the updating rules in Algorithm 14 to see that (90) also holds for  $j+1$  replacing  $j$ . By induction based on (87), we conclude that (90) holds for all  $j = 2, \dots, J$ . Substituting (90) and  $\mathbf{v}_j^0$  into (89) yields (for  $j = J$  change the l.h.s. to  $\mathbf{u}_J^{(1)}$ )

$$(91) \quad \mathbf{u}_{j\bullet}^{(\frac{1}{2})} = \mathbf{v}_{j\bullet}^0 + G_{j\bullet j\langle}^{(j)} \boldsymbol{\lambda}_{j\langle}^N - \left( G_{j\bullet j\langle}^{(j)} A_{j\langle}^{\rangle} + G_{j\bullet}^{(j)} A_{j\bullet j\langle} \right) \boldsymbol{\lambda}_{j\langle}^D.$$

In particular, we have  $\mathbf{u}_{J\bullet}^{(1)} = \mathbf{v}_{J\bullet}$  with  $\mathbf{v}_J$  from Algorithm 14.

In the backward sweep of Algorithm 2, we denote  $\mathbf{w}_j := \mathbf{u}_j^{(1)} - \mathbf{u}_j^{(\frac{1}{2})} + \mathbf{v}_j^0$ ,  $j = J-1, \dots, 1$ , and  $\mathbf{w}_J := \mathbf{u}_J^{(1)}$ . By arguments similar to the last paragraph we can show for all  $j = J-1, \dots, 1$  that

$$\boldsymbol{\lambda}_{j\rangle}^D = \mathbf{w}_{j+1]}, \quad \boldsymbol{\lambda}_{j\rangle}^N = -A_{j\rangle}^{\rangle} \mathbf{w}_{j+1]} - A_{j\rangle j+1\bullet} \mathbf{w}_{j+1\bullet},$$

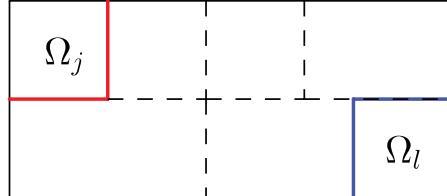
and further

$$(92) \quad \mathbf{w}_{j\bullet} = \mathbf{v}_{j\bullet}^0 + G_{j\bullet j\rangle}^{(j)} \boldsymbol{\lambda}_{j\rangle}^N - \left( G_{j\bullet j\rangle}^{(j)} A_{j\rangle}^{\rangle} + G_{j\bullet}^{(j)} A_{j\bullet j\rangle} \right) \boldsymbol{\lambda}_{j\rangle}^D.$$

Combining (91) and (92), we conclude that  $\mathbf{u}_{j\bullet}^{(1)} = \mathbf{v}_{j\bullet}$ .  $\square$

*Remark 43.* In Algorithm 14, the global approximation  $\tilde{\mathbf{u}}$  is different from  $\mathbf{u}^{(1)}$  of Algorithm 4. In Algorithm 14,  $R_{j\rangle} \tilde{\mathbf{u}} = \mathbf{u}_{j\rangle}^{(\frac{1}{2})}$  with  $\mathbf{u}_{j\rangle}^{(\frac{1}{2})}$  from Algorithm 2, while Algorithm 4 takes  $R_{j\rangle} \mathbf{u}^{(1)} = \mathbf{u}_{j+1]}^{(1)}$  with  $\mathbf{u}_{j+1]}^{(1)}$  from Algorithm 2.

**9. Optimal Parallel Schwarz Methods for Arbitrary Decompositions.** All the methods discussed so far only apply for a domain decomposition into a sequence of subdomains, and the information is passed gradually from one subdomain to its neighbor through the linear adjacency of the decomposition. The methods converge after one double sweep if the appropriate DtN operators are used in the transmission conditions between the subdomains. If the subdomain solves are performed in parallel, then the methods converge in a number of iterations that equals the number of subdomains, as was first pointed out in [133] (see also [131]), and this result was generalized



**Fig. 5** Two subdomains in an arbitrary decomposition.

in [135] to domain decompositions whose connectivity graph has no cycles. Whether an optimal Schwarz method exists for an *arbitrary* decomposition was a question until the method was first created in [72]. The method converges in two iterations and thus the iteration matrix is nilpotent of degree two; each iteration exposes parallelism *between* the subdomains in solving the subproblems and after the first iteration an all-to-all communication is invoked to transmit the interface data between every pair of subdomains (even if they are not adjacent). Note that the communication happens on the whole interfaces of the subdomains, e.g.,  $\Omega_j$  will map the data on the entirety of  $\partial\Omega_j \cap \Omega$  to the data on the entirety of  $\partial\Omega_l \cap \Omega$  and send them to  $\Omega_l$ ; see Figure 5.

The optimal algorithm in [72] was derived at the discrete level using linear algebra techniques, and is thus valid for various types of discretized PDEs. We give here an equivalent formulation at the continuous level, to complete the pair of discrete and continuous algorithms as was done for all the other methods in this review. In the optimal algorithm from [72],  $\Omega_l$  needs to take into account all the exterior sources as well as the interior source. Taking into account the interior source requires putting a transparent boundary condition on  $\partial\Omega_l \cap \Omega$ , while the exterior sources have to be taken into account with the data  $\lambda_{l,j} := \sum_{j \neq l} \lambda_{l,j}$  in the transmission condition on  $\partial\Omega_l \cap \Omega$ . Here,  $\lambda_{l,j}$  and  $\lambda_{j,j}$  are certain types of traces on  $\partial\Omega_l \cap \Omega$  and  $\partial\Omega_j \cap \Omega$  of the wave field generated by the source in  $\Omega_j$ . The map that turns  $\lambda_{j,j}$  into  $\lambda_{l,j}$  is

$$(93) \quad \begin{aligned} \mathcal{F}_{l,j} : \lambda_{j,j} &\rightarrow \lambda_{l,j} = (\mathcal{B}_l v)|_{\partial\Omega_l \cap \Omega}, \text{ s.t.} \\ &\quad \mathcal{L} v = 0 \quad \text{in } \Omega - \Omega_j, \\ &\quad \mathcal{B} v = 0 \quad \text{on } \partial\Omega - \partial\Omega_j, \\ &\quad \mathcal{C}_j v = \lambda_{j,j} \quad \text{on } \partial\Omega_j \cap \Omega, \end{aligned}$$

where  $\mathcal{C}_j$  is the trace operator corresponding to  $\lambda_{j,j}$ , and  $\mathcal{B}_l$  is the trace operator corresponding to  $\lambda_{l,j}$ . For convenience, we can take  $\mathcal{B}_l := \mathcal{T}_l$ , where  $\mathcal{T}_l$  is a transparent boundary operator for the truncation of  $\Omega$  to  $\Omega_l$ , which allows us to simulate the waves generated by  $\lambda_l$  and the interior source together by the subproblem in  $\Omega_l$ . We may use some approximation  $\tilde{\mathcal{F}}_{l,j}$  of the operator in (93) to define a preconditioner, which leads to the algorithm given in Algorithm 15.

**THEOREM 44.** *If in Algorithm 15  $\tilde{\mathcal{F}}_{l,j} = \mathcal{F}_{l,j}$  is uniquely defined as in (93) and  $\mathcal{B}_j$  is an exact transparent boundary operator, then the preconditioner given by Algorithm 15 is exact, i.e., the output  $\tilde{u}$  is the solution of (11). This means the iteration operator is nilpotent of degree two.*

*Proof.* The proof is straightforward by well-posedness and linearity.  $\square$

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**Algorithm 15.** Optimized Schwarz preconditioner using **global transmission** conditions at the **PDE** level.

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Input the source terms  $f$  and  $g$ .

Suppose the decomposition is arbitrary such that  $\cup_{j=1}^J \bar{\Omega}_j = \bar{\Omega}$ .

Solve the following subproblems independently for  $j = 1, \dots, J$ :

$$\begin{aligned}\mathcal{L} v_j^{(\frac{1}{2})} &= f && \text{in } \Omega_j, \\ \mathcal{B} v_j^{(\frac{1}{2})} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathcal{B}_j v_j^{(\frac{1}{2})} &= 0 && \text{on } \partial\Omega_j - \partial\Omega,\end{aligned}$$

where  $\mathcal{B}_j$  is an approximation of a transparent boundary operator for truncation of  $\Omega$  to  $\Omega_j$ . Take the trace  $\lambda_{j,j} \leftarrow \mathcal{C}_j v_j^{(\frac{1}{2})}$  on  $\partial\Omega_j - \partial\Omega$  and map it to  $\lambda_{l,j} \leftarrow \tilde{\mathcal{F}}_{l,j} \lambda_{j,j}$  on  $\partial\Omega_l - \partial\Omega$  for all  $l \neq j$ . Here,  $\tilde{\mathcal{F}}_{l,j}$  is an approximation of  $\mathcal{F}_{l,j}$  in (93).

Solve the following subproblems independently for  $j = 1, \dots, J$ :

$$\begin{aligned}\mathcal{L} v_j^{(1)} &= f && \text{in } \Omega_j, \\ \mathcal{B} v_j^{(1)} &= g && \text{on } \partial\Omega \cap \partial\Omega_j, \\ \mathcal{B}_j v_j^{(1)} &= \sum_{l \neq j} \lambda_{j,l} && \text{on } \partial\Omega_j - \partial\Omega.\end{aligned}$$

---

Output  $\tilde{u} \leftarrow \sum_{j=1}^J \mathcal{E}_j (\phi_j v_j^{(1)})$  with  $\mathcal{E}_j$  the extension by zero to  $\Omega$ , and  $\sum_{j=1}^J \mathcal{E}_j \phi_j = 1$ .

---

As seen from Theorem 44, approximating (93) is crucial for Algorithm 15. Essentially, this consists in approximating the off-diagonal part of the Green's function corresponding to the two interfaces. However, at the time of writing this article, no effort has been made toward a practical realization of Algorithm 15.

**10. Numerical Experiments.** The main goal of our article is both theoretical and formal, namely, to show that there is a common principle behind the new Helmholtz preconditioners based on sequential domain decomposition. Numerically, impressive results have been shown for these algorithms in the literature; see, for example, [29, 52, 111, 139, 157, 179]. Nevertheless, it is interesting and right that the readers of this review should also see when these new algorithms get into difficulty, which motivated us to add this section. Some of the results here have appeared in [85].

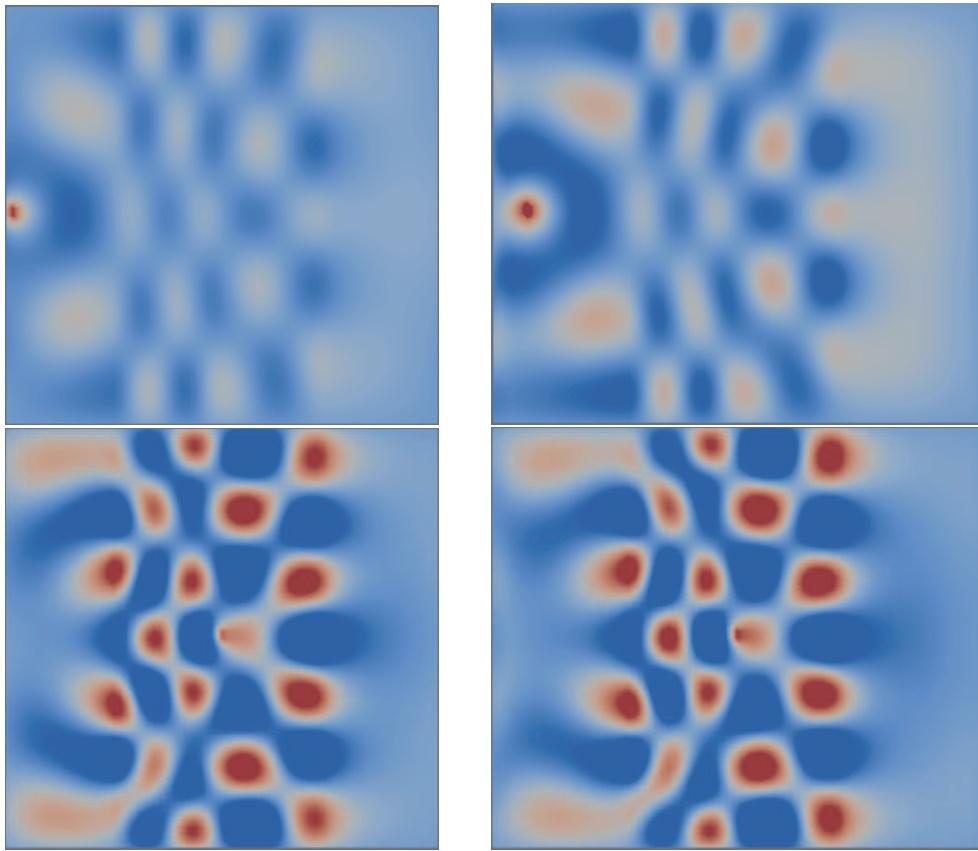
We consider the Helmholtz equation on the unit square

$$(94) \quad (\Delta + k(x)^2)u = f \quad \text{in } \Omega := (0, 1)^2,$$

with suitable boundary conditions for well-posedness. We discretize (94) by the classical five point finite difference method. We split the square sequentially in the  $x$  direction into  $p = 4, 8, 16$  equal strips representing the subdomains with vertical interfaces. Each subdomain has its own constant wavenumber. For the case of four subdomains, we use the wavenumbers

$$(95) \quad k = [20 \ 20 \ 20 \ 20] + \alpha[0 \ 20 \ 10 \ -10],$$

where  $\alpha$  is a contrast parameter, and for larger  $p$  we just repeat this structure. The



**Fig. 6** Guided waves from a point source near the left boundary (first row) or near the center (second row), with homogeneous Dirichlet conditions on the top and bottom and Robin conditions (first column) or PMLs (second column) on the left and right boundaries. The media have four layers separated by vertical interfaces as in (95) with  $\alpha = 1$ .

mesh resolution we choose guarantees at least ten points per wavelength for this experiment. We start with the case of a wave guide in the  $x$  direction, where we use Robin or PML radiation conditions on the left and right, and homogeneous Dirichlet conditions on top and bottom. We show in Figure 6 the real part of the solution<sup>24</sup> we obtain in the four-layered medium with  $\alpha = 1$  stimulated by a point source at  $x = 2h$ ,  $y = \frac{1-h}{2}$  in the top row, and for the point source at  $x = \frac{1}{2}$ ,  $y = \frac{1-h}{2}$  in the bottom row.

We are going to test the two fundamental algorithms mentioned in section 2: one based on the factorization and the other based on the nonoverlapping Schwarz method. As stated in Theorem 30, the factorization method has (approximate) DtN or Schur complement derived transmission conditions on the *left* interfaces of subdomains, and Dirichlet conditions on the right. For the nonoverlapping DOSM (see Algorithms 3 and 4), we use the version with (approximate) DtN derived transmission conditions on *both* interfaces of each subdomain. For the case of a constant medium, i.e.,  $\alpha = 0$  in

<sup>24</sup>The Dirichlet boundary points are not plotted, but the PMLs are plotted.

**Table 2** LU iteration numbers in the wave guide setting.

$\alpha$	$p = 4$			$p = 8$			$p = 16$		
	Iterative	GMRES	Iterative	GMRES	Iterative	GMRES	Iterative	GMRES	Iterative
0	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1
0.001	4 3 3	3 3 3	5 3 3	4 3 3	6 3 3	4 3 3	6 3 3	4 3 3	4 3 3
0.005	6 4 4	5 3 4	12 5 5	7 4 4	13 5 4	8 5 5	11 6 6	8 5 5	8 5 5
0.01	8 5 4	5 4 4	16 6 5	8 5 5	38 7 7	38 7 7	11 6 6	11 6 6	11 6 6
0.05	- 8 6	8 6 5	- 17 12	16 7 8	- 12 26	22 9 10	- 12 26	22 9 10	- 12 26
0.1	32 10 11	10 7 6	- - -	18 11 11	- - -	26 14 15	- - -	26 14 15	- - -
1	- - -	20 19 19	- - -	45 38 38	- - -	86 63 62	- - -	86 63 62	- - -
0	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1
0.001	4 2 3	3 3 3	5 3 3	4 3 3	7 4 4	4 3 3	6 4 4	6 4 4	6 4 4
0.005	7 3 3	5 3 3	- 5 4	- 4 4	30 6 6	30 6 6	12 6 5	12 6 5	12 6 5
0.01	11 4 4	6 4 4	- 6 5	11 5 5	- 10 10	19 7 6	- 10 10	19 7 6	- 10 10
0.05	- - -	13 7 6	- - -	23 12 11	- - -	47 17 16	- - -	47 17 16	- - -
0.1	- 22 31	14 9 9	- - -	23 12 11	- - -	50 24 23	- - -	50 24 23	- - -
1	- - -	36 21 19	- - -	70 64 64	- - -	95 90	- - -	95 90	- - -

(95), we use the exact DtN for (94). That is, we calculate the exact Schur complement for the discretized problem. For  $\alpha > 0$ , we approximate the DtN for (94) by the exact DtN for the Helmholtz equation in a modified medium: when calculating the exterior DtN on the *left* interface of a subdomain, all the medium to the *left* of the subdomain is assumed to be the identity extension of the medium in the *left* neighborhood of the subdomain.<sup>25</sup> On the right interface of a subdomain we do the same. Of course, this approximation has errors for heterogeneous media, and we will see that these errors have a dramatic impact on the convergence of the algorithms, something which is not yet well documented in the literature on these methods.

We test the two algorithms both as iterative solvers and as preconditioners for GMRES for varying contrast parameter  $\alpha$  and subdomain numbers. We do this for mesh size  $h = 1/64$  and the contrast profile in (95), and on a refined mesh with  $h = 1/128$ , but also for a profile with twice the size for the wavenumber, i.e.,

$$(96) \quad k = [40 \ 40 \ 40 \ 40] + \alpha[0 \ 40 \ 20 \ -20],$$

so that we still have at least ten points per wavelength resolution. We show in Tables 2 and 3 the number of iterations the methods took, where we stopped the iterative version of the algorithms and GMRES when the residual was reduced by  $1e-6$ , and we started with a zero initial guess of the solution  $u$  for a random source term  $f$  in the physical domain  $\Omega$  of (94). In the PMLs outside  $\Omega$ , both the initial guess and the source term are set to zero. The three columns within each “Iterative” or “GMRES” column correspond to Robin conditions, PMLs of thickness five times the mesh size, and PMLs of thickness ten times the mesh size on the left and right of the original domain. The top parts are for the smaller wavenumber experiment in (95), and the bottom parts are for the larger wavenumber experiment in (96). We first see that for  $\alpha = 0$ , i.e., in the constant wavenumber case, the factorization is exact, and both the iterative version and GMRES converge in one iteration step. As soon as we have a nonconstant wavenumber, however, already for  $\alpha = 0.001$ , the factorization is not exact any more. Nevertheless the algorithms still converge well, up to  $\alpha = 0.01$  in the

<sup>25</sup>This is a common assumption upon which most of the ABC and PML techniques are based.

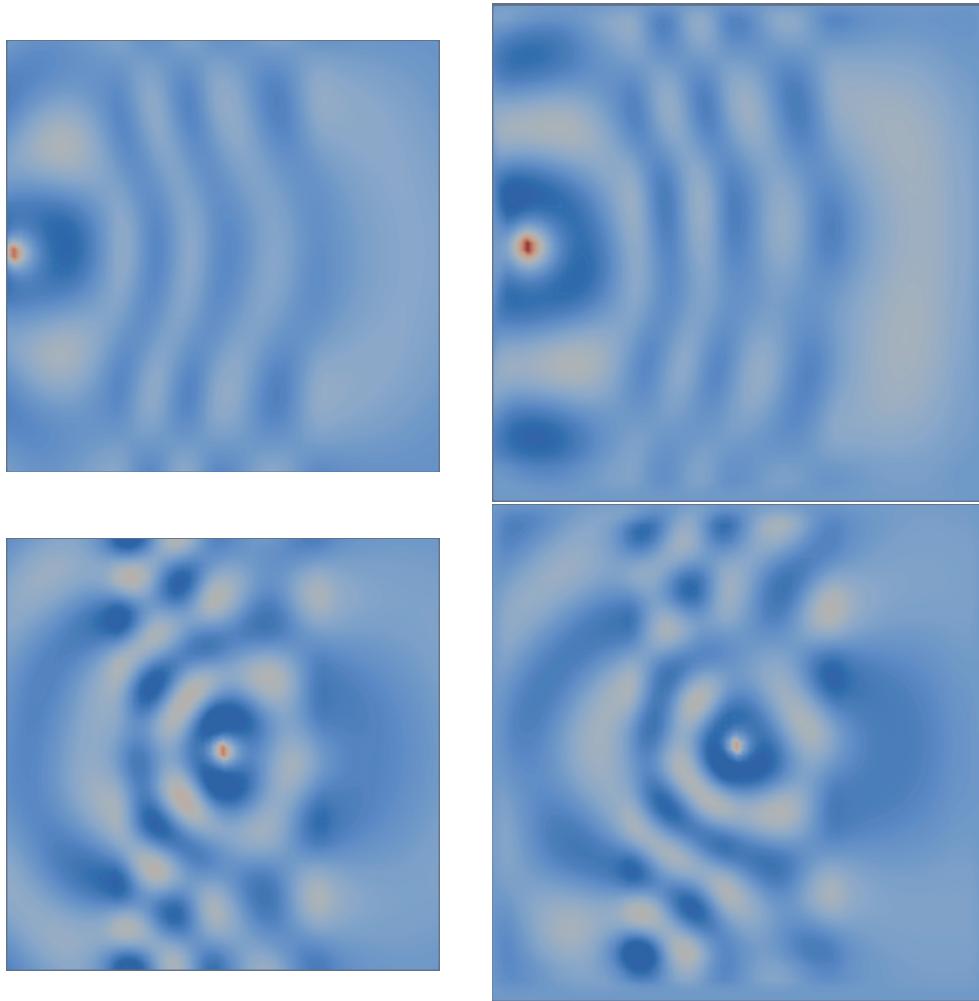
**Table 3** Schwarz iteration numbers in the wave guide setting.

$\alpha$	$p = 4$			$p = 8$			$p = 16$		
	Iterative	GMRES	Iterative	GMRES	Iterative	GMRES	Iterative	GMRES	Iterative
0	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1
0.001	3 2 2	3 2 2	3 2 2	3 2 2	3 2 2	3 2 2	3 2 2	3 2 2	3 2 2
0.005	5 3 3	4 3 3	5 3 3	4 3 3	5 3 3	4 3 3	5 3 3	4 3 3	5 3 3
0.01	7 4 3	4 3 3	7 4 4	5 3 3	7 4 4	5 3 3	7 4 4	5 4 3	5 4 3
0.05	42 12 7	7 5 4	- 16 12	9 5 5	- 21 17	13 7 6	- - -	- - -	- - -
0.1	- - -	9 7 6	- - -	14 12 11	- - -	20 17 17	- - -	- - -	- - -
1	- - -	26 23 24	- - -	48 47 47	- - -	59 68 65	- - -	- - -	- - -
0	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1	1 1 1
0.001	3 2 3	3 2 2	3 2 3	3 2 3	3 2 2	3 2 3	3 2 3	3 2 2	3 2 2
0.005	5 3 4	4 3 3	6 3 4	5 3 3	7 3 4	5 4 3	- - -	- - -	- - -
0.01	8 4 6	5 4 4	12 4 6	6 4 4	30 5 6	7 5 4	- - -	- - -	- - -
0.05	- - -	10 7 6	- - -	16 11 10	- - -	22 16 16	- - -	- - -	- - -
0.1	- - -	13 11 9	- - -	19 14 13	- - -	32 22 22	- - -	- - -	- - -
1	- - -	43 40 38	- - -	79 77 77	- - -	- - -	- - -	- - -	- - -

smaller wavenumber case in the top parts of the tables, i.e., a one percent variation in the wavenumber  $k$ . For larger contrast, the iterative version of the algorithms cannot be used any more, and GMRES now deteriorates rapidly, for example, if the contrast is at a factor of two, i.e.,  $\alpha = 1$ , GMRES iteration numbers double when  $p$  goes from 4 to 8, and the two algorithms are not robust any more. In the higher wavenumber case in the bottom parts of the tables, they deteriorate even more rapidly for higher contrast. We can also see by comparing the last lines in the top and bottom parts of the tables that doubling the wavenumber leads to a remarkable growth of the iteration numbers with GMRES as soon as the contrast is large enough, and that GMRES fails to converge in less than hundred iterations at the bottom right.

We next perform the same set of experiments, but now using Robin or PML conditions all around the original domain; see Figure 7, Table 4, and Table 5. We see that the outer radiation conditions are better than the wave guide setting for the two algorithms, and they now work in the iterative version up to about a 10 percent variation of the wavenumber in this specific experiment. As soon as there is a variation as large as a factor of two, however, the algorithms are not effective solvers any more, the iterative versions diverge, and GMRES iteration numbers deteriorate when the number of subdomains increases and also when the wavenumber is doubled. One thus has to be careful when claiming optimality of algorithms in this class of Helmholtz preconditioners.

**11. Conclusions.** We have seen that for a large class of new Helmholtz solvers the underlying mathematical technique is the same: the solvers are based on a nilpotent iteration given by a double sweep in a sequential domain decomposition that uses the exact Dirichlet-to-Neumann operators for transmission conditions at the interfaces. At the linear algebra level, the corresponding algorithm is based on an exact block LU factorization of the matrix. From domain decomposition, it is known that when the solves are performed in parallel, instead of in a sweeping fashion, the method is still nilpotent, but convergence is then achieved in a number of iterations corresponding to the number of subdomains [131, 133]. If the domain decomposition is more general, such that the connectivity graph includes cycles and thus cross points between subdomains are present, we have given an algorithm at the continuous level based on the discrete algorithm in [72] that is still nilpotent. This algorithm requires



**Fig. 7** Scattered waves from a point source near the left boundary (first row) or near the center (second row), with Robin conditions (first column) or PMLs (second column, bigger since the plot includes the PML region) all around the square domain. The media have four layers separated by vertical interfaces as in (95) with  $\alpha = 1$ .

communication of each subdomain with every other one, and convergence is achieved in two iterations. While there is currently no practical realization of this algorithm, the fact that the algorithm converges in two iterations, independent of the number of subdomains, suggests that a coarse space component is active in this optimal algorithm. Coarse spaces leading to nilpotent iterations were first described in the lecture notes [68], and then in [70, 71], with successful approximations in [74, 75]. The property that domain decomposition methods in general are nilpotent has only very recently been investigated in more detail; see [23]. None of the Helmholtz solvers we described in this article use coarse space techniques at the time of writing, which leads us to expect that this area of research will remain very active over the coming years.

**Table 4** LU iteration numbers for a domain with Robin or PMLs all around.

$\alpha$	$p = 4$			$p = 8$			$p = 16$		
	Iterative	GMRES		Iterative	GMRES		Iterative	GMRES	
0	1 1 1	1 1 1		1 1 1	1 1 1		1 1 1	1 1 1	
0.001	2 2 2	2 2 2		3 3 2	3 2 2		3 3 3	3 3 3	
0.005	3 3 3	3 3 3		4 3 3	4 3 3		4 3 3	4 3 3	
0.01	3 3 3	3 3 3		4 4 3	4 3 3		5 4 4	5 4 3	
0.05	5 5 5	5 4 4		7 5 5	6 5 5		8 6 5	8 5 5	
0.1	7 6 5	6 5 5		9 6 6	8 6 6		12 7 7	10 7 6	
1	- 31 27	15 12 12		- - -	32 25 22		- - -	58 34 29	
0	1 1 1	1 1 1		1 1 1	1 1 1		1 1 1	1 1 1	
0.001	3 2 2	3 2 2		3 2 2	3 2 2		3 3 3	3 3 3	
0.005	3 3 3	3 3 3		4 3 3	4 3 3		5 3 3	5 3 3	
0.01	4 3 3	4 3 3		5 3 3	5 3 3		6 4 4	6 4 4	
0.05	6 4 4	6 4 4		10 5 5	8 5 5		14 6 6	11 6 6	
0.1	8 5 5	7 5 5		13 6 6	10 6 6		14 8 7	12 8 7	
1	- - -	52 23 13	12	- - -	39 24 22		- - -	99 61 48	

**Table 5** Schwarz iteration numbers for a domain with Robin conditions or PMLs all around.

$\alpha$	$p = 4$			$p = 8$			$p = 16$		
	Iterative	GMRES		Iterative	GMRES		Iterative	GMRES	
0	1 1 1	1 1 1		1 1 1	1 1 1		1 1 1	1 1 1	
0.001	3 2 2	2 2 2		2 2 2	2 2 2		2 2 2	2 2 2	
0.005	3 3 3	3 3 3		3 3 3	3 3 3		3 3 3	3 3 3	
0.01	3 3 3	3 3 3		3 3 3	3 3 3		3 3 3	3 3 3	
0.05	5 4 4	4 4 4		5 5 4	4 4 4		5 5 4	4 4 4	
0.1	6 5 5	5 5 4		6 6 5	5 5 5		7 6 5	6 5 5	
1	- - -	23 33 37		- - -	35 44 44		- - -	41 43 48	
0	1 1 1	1 1 1		1 1 1	1 1 1		1 1 1	1 1 1	
0.001	3 2 2	2 2 2		3 3 2	2 2 2		3 3 2	2 2 2	
0.005	3 3 3	3 3 3		3 3 3	3 3 3		3 3 3	3 3 3	
0.01	4 3 3	3 3 3		3 3 3	3 3 3		3 3 3	3 3 3	
0.05	5 5 5	5 4 4		5 5 5	5 4 4		5 5 5	5 5 4	
0.1	7 7 6	6 6 5		9 7 6	7 6 5		9 7 7	7 6 6	
1	- - -	32 43 45		- - -	49 54 61		- - -	79 94 75	

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