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Domain Decomposition for Boundary Integral Equations via Local Multi-Trace Formulations

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Abstract We review the ideas behind and the construction of so-called local multi-trace boundary integral equations for second-order boundary value problems with piecewise constant coefficients. These formulations have received considerable attention recently as a promising domain-decomposition approach to boundary element methods.

Key words: Boundary integral equations (BIE), Calderón projectors, local multi-trace BIE, optimized transmission conditions, Schwarz method

1 Introduction

This article is devoted to a formal derivation and discussion of a class of boundary integral equation (BIE) formulations that have recently been introduced for second-order transmission problems. We chose to dub this class “local multi-trace BIE formulations” (MTF), which is inspired by two key features of its members:

- (i) The methods rely on at least two pairs of trace data as unknowns on interfaces. The accounts for the attribute “multi-trace”.
- (ii) Formally, they are constructed by taking into account transmission conditions pointwise or, at least, on parts of sub-domain boundaries, which is indicated by the “local” attribute.

Initially, the development of these new methods was pursued independently by numerical analysts and in computational electrical engineering, driven by different objectives. In numerical analysis, the focus was on composite structures, that is, partial differential equations with piecewise constant coefficients. There, the main motivation was to find first-kind boundary integral formulations that, after Galerkin boundary element discretization, are amenable to operator preconditioning, a possibility not offered by classical approaches, see [3, Section 4]. In engineering, researchers were guided by a domain decomposition paradigm, aiming to localize

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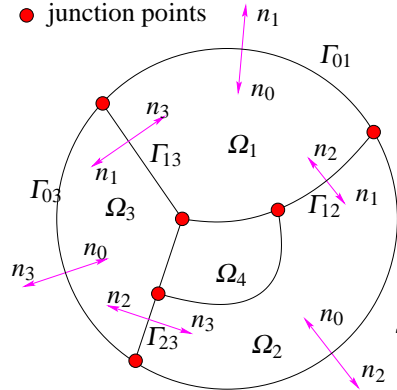
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boundary integral equations for electromagnetic wave propagation at artificial interfaces for the sake of parallelization and block-preconditioning.

Both research efforts have been fairly successful: on the one hand, a comprehensive theoretical understanding of the simplest representative of a local multi-trace BIE formulations for Helmholtz transmission problem could be achieved in [8]. In a wider context the method is also covered in [3]. On the other hand, a host of impressive applications of multi-trace methods is documented in computational electromagnetism. A surface integral equation domain decomposition method based on multi-trace formulation is presented in [15, 14] for time-harmonic electromagnetic wave scatterings from homogeneous targets. The treatment of general bounded composite targets is discussed in [13].

This article looks at MTF from a mathematical point of view, but, inspired by the developments in the engineering community, adopts a different and more general perspective compared to [8]. This work is mainly conceptual and does not aim to pursue any comprehensive analysis. Rather it is meant to chart new ideas and directions of research. We have not included any numerical results nor are we going to discuss details of Galerkin discretization by means of boundary elements. Detailed studies of convergence of multi-trace BIE for 2D acoustic scattering discretized by means of low-order boundary elements (BEM) are reported in [8, Sect. 5]. Concerning the application of multi-trace methods for solving electromagnetic scattering problems, convergence studies can be found in [13] for scattering at both single homogeneous objects and composite penetrable objects. Several complex large-scale simulations are covered in [14] and demonstrate the capability of these methods to model multi-scale electrically large targets.

2 Transmission Problems



Let $\Omega_i \subset \mathbb{R}^d$, $d = 2, 3$, $i = 0, \dots, N$, be disjoint open connected Lipschitz “material sub-domains” that form a partition in the sense that $\mathbb{R}^3 = \overline{\Omega}_0 \cup \dots \cup \overline{\Omega}_N$. Among them only Ω_0 is unbounded. Two adjacent sub-domains Ω_i and Ω_j are separated by their common interface Γ_{ij} , whose union forms the skeleton Σ . For $N > 1$ the skeleton Σ will usually not be orientable, nor be a manifold.

Given diffusion coefficients $\mu_i > 0$, $i = 0, \dots, N$, we focus on the model transmission problem that seeks $U_i \in H_{\text{loc}}^1(\Omega_i)$, $i = 0, \dots, N$, solving

$$\mathbf{L}_i U_i := -\operatorname{div}(\mu_i \mathbf{grad} U_i) + U_i = 0 \quad \text{in } \Omega_i, \quad (1a)$$

$$U_i|_{\Gamma_{ij}} - U_j|_{\Gamma_{ij}} = 0, \quad \mu_i \frac{\partial U_i}{\partial n_i} \Big|_{\Gamma_{ij}} + \mu_j \frac{\partial U_j}{\partial n_j} \Big|_{\Gamma_{ij}} = 0 \quad \text{on } \Gamma_{ij}, \quad (1b)$$

plus suitable decay conditions at infinity for $U - U_{\text{inc}}$, where the “incident field” U_{inc} is an entire solution of $\mathbf{L}_0 U_{\text{inc}} = 0$ on Ω_0 [11, Ch. 8]. The weak formulation of (1) is posed on the Sobolev space $H^1(\mathbb{R}^3)$.

The transmission conditions (1b) connect two kinds of canonical traces on both sides of interfaces. These traces are the Dirichlet trace $\mathbb{T}_{D,i}$, and Neumann trace $\mathbb{T}_{N,i}$, defined for smooth functions on $\overline{\Omega}_i$ through

$$\mathbb{T}_{D,i} U_i := U_i|_{\partial\Omega_i}, \quad \mathbb{T}_{N,i} U_i := \mu_i \mathbf{grad} U_i \cdot \mathbf{n}_i|_{\partial\Omega_i}. \quad (2)$$

They can be extended to continuous operators [16, Sect. 2.6 & 2.7] ¹

$$\mathbb{T}_{D,i} : H^1(\Omega_i) \rightarrow H^{\frac{1}{2}}(\partial\Omega_i), \quad \mathbb{T}_{N,i} : H(\Delta, \Omega_i) \rightarrow H^{-\frac{1}{2}}(\partial\Omega_i). \quad (3)$$

Then, (1b) can be recast as

$$\begin{pmatrix} \mathbb{T}_{D,i} \\ \mathbb{T}_{N,i} \end{pmatrix} U_i = \begin{pmatrix} \text{Id} & 0 \\ 0 & -\text{Id} \end{pmatrix} \begin{pmatrix} \mathbb{T}_{D,j} \\ \mathbb{T}_{N,j} \end{pmatrix} U_j \quad \text{on } \Gamma_{ij}, \quad (4)$$

for which we embrace the compact notation $\mathbb{T}_i U_i = \mathbb{X} \mathbb{T}_j U_j$ with obvious meanings of the operators \mathbb{T}_i and \mathbb{X} .

Remark 1. In fact, multi-trace boundary integral equations were first developed for acoustic and electromagnetic scattering problems and we emphasize that the ideas of this article will naturally apply to them, see [3].

3 Basic Multi-Trace Formulation

For the sake of lucidity, in this section we largely restrict ourselves to the situation $N = 2$, as sketched in Figure 1 for $d = 2$. For the purpose of presenting the local multi-trace formulation this case is generic and completely captures the ideas and essence of the methods.

3.1 Preliminaries

The starting point for deriving multi-trace boundary integral equations is the characterization of traces of local solutions of (1) as the range of a (compound) boundary integral operator known as *Calderón projector*, see [3, Sect. 2.3], [16, Sect. 3.6],

¹ As usual, $H(\Delta, \Omega) := \{U \in H^1(\Omega) : \Delta U \in L^2(\Omega)\}$.

and [9, Sect. 5.6]. For the Calderón projector associated with the PDE $L_i U_i = 0$ on Ω_i we write

$$\mathbb{P}_i : H^{\frac{1}{2}}(\partial\Omega_i) \times H^{-\frac{1}{2}}(\partial\Omega_i) \rightarrow H^{\frac{1}{2}}(\partial\Omega_i) \times H^{-\frac{1}{2}}(\partial\Omega_i), \quad (5)$$

and recall that \mathbb{P}_i is connected to the four key boundary integral operators for 2nd-order scalar PDEs according to

$$\mathbb{P}_i = \mathbb{A}_i + \frac{1}{2}\text{Id} \quad , \quad \mathbb{A}_i = \begin{pmatrix} -K_i & V_i \\ W_i & K'_i \end{pmatrix}, \quad (6)$$

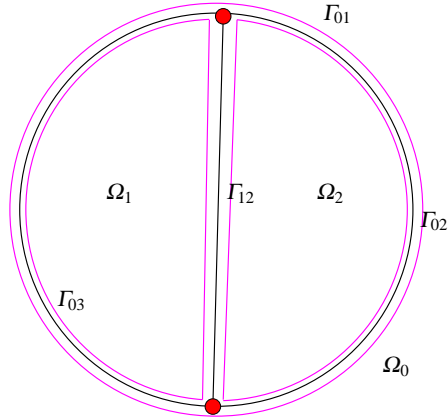
where we have adopted the notations K_i, V_i, W_i, K'_i from [16, Sect. 3.1] for the double layer, single layer, hypersingular, and adjoint double layer boundary integral operators on $\partial\Omega_i$, respectively. The Calderón projectors owe their importance to the following fundamental theorem [3, Thm. 2.6].

Theorem 1. *If and only if U_i solves $L_i U_i = 0$ in Ω_i (and satisfies exponential decay conditions at ∞ for $i = 0$), then $(\text{Id} - \mathbb{P}_i)\mathbb{T}_i U_i = 0$.*

Here, in the interest of compact notation, we relied on the total trace operator $\mathbb{T}_i := \begin{pmatrix} T_{D,i} \\ T_{N,i} \end{pmatrix}$. Thus, if U is a solution of (1), we conclude from Theorem 1

$$\begin{aligned} (-\mathbb{A}_i + \frac{1}{2}\text{Id}) \mathbb{T}_i U &= 0, \quad i = 1, 2, \\ (-\mathbb{A}_0 + \frac{1}{2}\text{Id}) \mathbb{T}_0(U - U_{\text{inc}}) &= 0. \end{aligned} \quad (7)$$

Fig. 1 Geometric situation “ $N = 2$ ” in 2D for derivation of multi-trace boundary integral formulations. Black lines indicate the sub-domain boundaries, magenta lines stand for Cauchy traces, of which there are two on each interface in the multi-trace setting. Red dots mark junction points.



3.2 Derivation

The derivation of the basic MTF casts both (7) and the transmission conditions (4) into weak form. To do so, we need bilinear pairings²

$$[u_i, v_i]_{\partial\Omega_i} := \langle u, v \rangle_{\partial\Omega_i} + \langle v, \mu \rangle_{\partial\Omega_i}, \quad u_i := \begin{pmatrix} u \\ \mu \end{pmatrix}, \quad v_i := \begin{pmatrix} v \\ \nu \end{pmatrix} \in \mathcal{T}(\partial\Omega_i), \quad (8)$$

on the *local Cauchy trace spaces*³

$$\mathcal{T}(\partial\Omega_i) := H^{\frac{1}{2}}(\partial\Omega_i) \times H^{-\frac{1}{2}}(\partial\Omega_i). \quad (9)$$

In (8), angle brackets designated the bi-linear duality product between $H^{\frac{1}{2}}(\partial\Omega_i)$ and $H^{-\frac{1}{2}}(\partial\Omega_i)$, which reduces to an L^2 -pairing for sufficiently regular functions. Then (7) is equivalent to

$$\left[\left(-\mathbb{A}_i + \frac{1}{2}\text{Id} \right) \mathbb{T}_i U, v_i \right]_{\partial\Omega_i} = \text{r.h.s.} \quad \forall v_i \in \mathcal{T}(\partial\Omega_i), \quad i = 0, 1, 2, \quad (10)$$

with “r.h.s.”, here and below, representing a linear form on the trial space that provides the excitation.

A possible weak form the transmission conditions (4) can sloppily be stated as

$$\left[\mathbb{T}_i U - \mathbb{X} \mathbb{T}_j U, v_i|_{\Gamma_{ij}} \right]_{\Gamma_{ij}} = 0 \quad \forall “v_i \in \mathcal{T}(\partial\Omega_i)” \quad (11)$$

The attribute “sloppy” and the quotation marks hint at fundamental problems haunting (11) and those lurk in the failure of the bi-linear pairing $[\cdot, \cdot]_{\Gamma_{ij}}$ to be well defined for restrictions of generic traces to Γ_{ij} .

Temporarily sweeping these difficulties under the rug (and restricting ourselves to the situation $N = 2$ illustrated in Figure 1), we now combine (10) and (11) into

$$\begin{aligned} & \left[\left(\mathbb{A}_0 - \frac{1}{2}\text{Id} \right) \mathbb{T}_0 U, v_0 \right]_{\partial\Omega_0} - \sigma_{01} \left[\mathbb{T}_0 U - \mathbb{X} \mathbb{T}_1 U, v_0|_{\Gamma_{01}} \right]_{\Gamma_{01}} \\ & - \sigma_{02} \left[\mathbb{T}_0 U - \mathbb{X} \mathbb{T}_2 U, v_0|_{\Gamma_{02}} \right]_{\Gamma_{02}} = \text{r.h.s.} \quad \forall “v_0 \in \mathcal{T}(\partial\Omega_0)” , \\ & \left[\left(\mathbb{A}_1 - \frac{1}{2}\text{Id} \right) \mathbb{T}_1 U, v_1 \right]_{\partial\Omega_1} - \sigma_{10} \left[\mathbb{T}_1 U - \mathbb{X} \mathbb{T}_0 U, v_1|_{\Gamma_{10}} \right]_{\Gamma_{10}} \\ & - \sigma_{12} \left[\mathbb{T}_1 U - \mathbb{X} \mathbb{T}_2 U, v_1|_{\Gamma_{12}} \right]_{\Gamma_{12}} = \text{r.h.s.} \quad \forall “v_1 \in \mathcal{T}(\partial\Omega_1)” , \\ & \left[\left(\mathbb{A}_2 - \frac{1}{2}\text{Id} \right) \mathbb{T}_2 U, v_2 \right]_{\partial\Omega_2} - \sigma_{21} \left[\mathbb{T}_2 U - \mathbb{X} \mathbb{T}_1 U, v_2|_{\Gamma_{21}} \right]_{\Gamma_{21}} \\ & - \sigma_{20} \left[\mathbb{T}_2 U - \mathbb{X} \mathbb{T}_0 U, v_2|_{\Gamma_{20}} \right]_{\Gamma_{20}} = \text{r.h.s.} \quad \forall “v_2 \in \mathcal{T}(\partial\Omega_2)” , \end{aligned} \quad (12)$$

² Fraktur font is used to designate functions in the Cauchy trace space, whereas Roman typeface is reserved for Dirichlet traces, and Greek symbols for Neumann traces.

³ By Cauchy trace spaces we mean combined Dirichlet and Neumann traces.

where the σ_{ij} are non-zero weights. These are equations satisfied by the local Cauchy traces $\mathbb{T}_i U$, $i = 0, 1, 2$. Next, we treat these traces as unknowns and call them u_1 , u_2 , and u_3 which converts (12) into a system of (variational) boundary integral equations. It deserves the label “multi-trace”, because the unknowns are separate Cauchy traces for each sub-domain, which yields two pairs of unknown traces on each interface, twice the number used in most other boundary integral formulations, see Figure 1. Adopting a compact notation, (for $N = 2$) the problem is posed on the *multi-trace space*

$$\mathcal{MT}(\Sigma) := \mathcal{T}(\partial\Omega_0) \times \mathcal{T}(\partial\Omega_1) \times \mathcal{T}(\partial\Omega_2). \quad (13)$$

The special variant of (12) proposed in [8] is recovered by setting $\sigma_{ij} = -\frac{1}{2}$. To see, why this is a special choice, note that, for instance,

$$\left[u_0, v_0|_{\Gamma_{01}} \right]_{\Gamma_{01}} + \left[u_0, v_0|_{\Gamma_{02}} \right]_{\Gamma_{02}} = [u_0, v_0]_{\partial\Omega_0}, \quad u, v \in \mathcal{T}(\partial\Omega_0).$$

Thus, we achieve a massive cancellation of terms and arrive at the *basic multi-trace formulation*: seek $(u_0, u_1, u_2) \in \mathcal{MT}(\Sigma)$ such that

$$\begin{aligned} [\mathbb{A}_0 u_0, v_0]_{\partial\Omega_0} - \frac{1}{2} \left[\mathbb{X} u_1|_{\Gamma_{01}}, v_0|_{\Gamma_{01}} \right]_{\Gamma_{01}} - \frac{1}{2} \left[\mathbb{X} u_2|_{\Gamma_{02}}, v_0|_{\Gamma_{02}} \right]_{\Gamma_{02}} &= \text{r.h.s.} \\ &\quad \forall “v_0 \in \mathcal{T}(\partial\Omega_0)” , \\ [\mathbb{A}_1 u_1, v_1]_{\partial\Omega_1} - \frac{1}{2} \left[\mathbb{X} u_0|_{\Gamma_{10}}, v_1|_{\Gamma_{10}} \right]_{\Gamma_{10}} - \frac{1}{2} \left[\mathbb{X} u_2|_{\Gamma_{12}}, v_1|_{\Gamma_{12}} \right]_{\Gamma_{12}} &= \text{r.h.s.} \\ &\quad \forall “v_1 \in \mathcal{T}(\partial\Omega_1)” , \\ [\mathbb{A}_2 u_2, v_2]_{\partial\Omega_2} - \frac{1}{2} \left[\mathbb{X} u_1|_{\Gamma_{21}}, v_2|_{\Gamma_{21}} \right]_{\Gamma_{21}} - \frac{1}{2} \left[\mathbb{X} u_0|_{\Gamma_{20}}, v_2|_{\Gamma_{20}} \right]_{\Gamma_{20}} &= \text{r.h.s.} \\ &\quad \forall “v_2 \in \mathcal{T}(\partial\Omega_2)” , \end{aligned} \quad (14)$$

where, again, the quotation marks acknowledge difficulties besetting the use of generic traces as trial and test functions. The variational formulations for general N can be found in [3, Sect. 6] and [8, Sect. 3.2.3].

3.3 Analysis

Let us take a closer look at the coupling terms in (14). For $u_i \in \mathcal{T}(\partial\Omega_i)$ and $v_j \in \mathcal{T}(\partial\Omega_j)$ we find

$$\mathbb{X} u_i|_{\Gamma_{ij}}, v_j|_{\Gamma_{ij}} \in H^{\frac{1}{2}}(\Gamma_{ij}) \times H^{-\frac{1}{2}}(\Gamma_{ij}).$$

Unfortunately, $H^{\frac{1}{2}}(\Gamma_{ij})$ and $H^{-\frac{1}{2}}(\Gamma_{ij})$ are not in duality with pivot space $L^2(\Gamma_{ij})$. More precisely, $(u_i, v_j) \mapsto [\mathbb{X} u_i|_{\Gamma_{ij}}, v_j|_{\Gamma_{ij}}]_{\Gamma_{ij}}$ is not bounded on $\mathcal{T}(\partial\Omega_i) \times \mathcal{T}(\partial\Omega_j)$, which renders (14) meaningless without the quotation marks.

As a remedy, more regular test functions have to be used, namely functions whose restrictions to Γ_{ij} belong to the $L^2(\Gamma_{ij})$ -dual of $H^{\frac{1}{2}}(\Gamma_{ij}) \times H^{-\frac{1}{2}}(\Gamma_{ij})$, which is known to coincide with $\tilde{H}^{\frac{1}{2}}(\Gamma_{ij}) \times \tilde{H}^{-\frac{1}{2}}(\Gamma_{ij})$, where the latter spaces are spaces of functions, whose extensions by zero from Γ_{ij} to $\partial\Omega_j$ are still valid functions in $H^{\frac{1}{2}}(\partial\Omega_j) \times H^{-\frac{1}{2}}(\partial\Omega_j)$. We remind that $\tilde{H}^{\frac{1}{2}}(\Gamma_{ij}) \times \tilde{H}^{-\frac{1}{2}}(\Gamma_{ij})$ is a *dense* subspace of $H^{\frac{1}{2}}(\Gamma_{ij}) \times H^{-\frac{1}{2}}(\Gamma_{ij})$ with *strictly stronger norm*, see [11, Ch. 3] and [8, Sect. 2]. Thus, proper test spaces in (14) are

$$\widetilde{\mathcal{T}}(\partial\Omega_j) = \bigotimes_{i \neq j} \tilde{H}^{\frac{1}{2}}(\Gamma_{ij}) \times \tilde{H}^{-\frac{1}{2}}(\Gamma_{ij}), \quad j = 0, 1, 2, \quad (15)$$

since the bilinear form m associated with (14) turns out to be bounded as a mapping

$$m : \mathcal{MT}(\Sigma) \times \widetilde{\mathcal{MT}}(\Sigma) \rightarrow \mathbb{R},$$

where $\widetilde{\mathcal{MT}}(\Sigma)$ is defined in analogy to (13) this time based on $\widetilde{\mathcal{T}}(\partial\Omega_j)$.

A key observation concerns the *block skew-symmetric* structure of (14) due to

$$[\mathbb{X} u_i|_{\Gamma_{ij}}, v_j|_{\Gamma_{ij}}]_{\Gamma_{ij}} = - [\mathbb{X} v_j|_{\Gamma_{ij}}, u_i|_{\Gamma_{ij}}]_{\Gamma_{ij}}, \quad \begin{array}{l} u_i \in \widetilde{\mathcal{T}}(\partial\Omega_i), \\ v_j \in \widetilde{\mathcal{T}}(\partial\Omega_j). \end{array} \quad (16)$$

In light of the well known ellipticity of the boundary integral operators [16, Sect. 3.5.1]

$$\exists C > 0 : \quad |[\mathbb{A}_j v_j, v_j]_{\partial\Omega_j}| \geq C \|v_j\|_{\mathcal{T}(\partial\Omega_j)}^2 \quad \forall v_j \in \mathcal{T}(\partial\Omega_j), \quad (17)$$

(16) immediately implies the $\mathcal{MT}(\Sigma)$ -ellipticity of m :

$$\exists C > 0 : \quad |m(\vec{v}, \vec{v})| \geq C \|\vec{v}\|_{\mathcal{MT}(\Sigma)}^2 \quad \forall \vec{v} \in \widetilde{\mathcal{MT}}(\Sigma). \quad (18)$$

From (18) we conclude existence and uniqueness of solutions of (14) with trial space $\widetilde{\mathcal{MT}}(\Sigma)$. Not straightforwardly, however, because the lack of continuity of m on $\mathcal{MT}(\Sigma) \times \mathcal{MT}(\Sigma)$ bars us from appealing to the Riesz representation theorem. Fortunately, as elaborated in [8, Sect. 3.2.8], we can rely a result by J.L. Lions [10, Ch. III, Thm. 1.1] along with the density of $\widetilde{\mathcal{MT}}(\Sigma)$ in $\mathcal{MT}(\Sigma)$:

Theorem 2. *The variational problem (14) on $\mathcal{MT}(\Sigma) \times \widetilde{\mathcal{MT}}(\Sigma)$ possesses a unique solution in $\mathcal{MT}(\Sigma)$ that depends continuously on the right hand side.*

Remark 2. The result of Theorem 2 crucially hinges on the ellipticity (18), which can be taken for granted only for the choice $\sigma_{ij} = -\frac{1}{2}$. For general weights σ_{ij} existence and uniqueness of solutions of (12) is an open problem.

Remark 3. For scattering problems the sesqui-linear form of (14) will be merely coercive. In this case uniqueness of solutions has to be established by other arguments, see [8, Sect. 3.2.6], and existence follows from Fredholm theory.

4 Transformed Multi-Trace Formulations

4.1 Optimal transmission conditions

An important motivation for the development of multi-trace BIE was the desire to obtain linear systems of equations that readily lend themselves to additive Schwarz (“block Jacobi”) preconditioning. On the level of the transmission problem (1), this amounts to solving local boundary value problems on Ω_i using Dirichlet or Neumann boundary data from the previous iterates on the adjacent sub-domains. However, the transmission conditions (1b) may not lead to satisfactory convergence.

To understand how alternative transmission conditions can boost an additive Schwarz iteration, let us examine the very simple situation with $N = 1$, $\Sigma = \Gamma := \partial\Omega_0 = \partial\Omega_1$. There is a special transmission condition that effects convergence in one step! To state it, we introduce the Dirichlet-to-Neumann (DtN) operators

$$\text{DtN}_0, \text{DtN}_1 : H^{\frac{1}{2}}(\Gamma) \rightarrow H^{-\frac{1}{2}}(\Gamma) \quad (19)$$

and their inverses, the Neumann-to-Dirichlet (NtD) operators

$$\text{NtD}_0, \text{NtD}_1 : H^{-\frac{1}{2}}(\Gamma) \rightarrow H^{\frac{1}{2}}(\Gamma) \quad , \quad \text{NtD}_i = \text{DtN}_i^{-1} . \quad (20)$$

The subscript indicates whether they are associated with a boundary value problem $L_i U = 0$ on Ω_0 or Ω_1 , respectively. Recall that DtN operators, sometimes called Steklov-Poincaré operators, return the Neumann trace of a solution of a boundary value problem for prescribed Dirichlet data [11, Ch. 4]. The DtN operators associated with bounded subdomains are linear, but DtN_0 is merely affine due to the “nonzero boundary condition at infinity” imposed through U_{inc} . In any case, the linear parts of the operators DtN_i and NtD_i are symmetric and positive.

Based on these operators, we introduce modified transmission conditions across Γ :

$$\mathcal{T}_{D,1} U - \text{NtD}_1(\mathcal{T}_{N,1} U) = \mathcal{T}_{D,0} U + \text{NtD}_1(\mathcal{T}_{N,0} U) , \quad (21a)$$

$$\text{DtN}_0(\mathcal{T}_{D,1} U) + \mathcal{T}_{N,1} U = \text{DtN}_0(\mathcal{T}_{D,0} U) - \mathcal{T}_{N,0} U . \quad (21b)$$

These transmission conditions are perfectly symmetric with respect to Ω_0 and Ω_1 , since, thanks to $\text{NtD}_i = \text{DtN}_i^{-1}$, we can rewrite (21) in the equivalent form

$$\text{DtN}_1(\mathcal{T}_{D,1} U) - \mathcal{T}_{N,1} U = \text{DtN}_1(\mathcal{T}_{D,0} U) + \mathcal{T}_{N,0} U , \quad (22a)$$

$$\mathcal{T}_{D,1} U + \text{NtD}_0(\mathcal{T}_{N,1} U) = \mathcal{T}_{D,0} U - \text{NtD}_0(\mathcal{T}_{N,0} U) . \quad (22b)$$

Invertibility of the involved operators yields another equivalence

$$(21) \Leftrightarrow (22) \Leftrightarrow \begin{cases} \mathbb{T}_{D,1} U = \mathbb{T}_{D,0} U, \\ \mathbb{T}_{N,1} U = -\mathbb{T}_{N,0} U, \end{cases} \quad (23)$$

which confirms that the original transmission conditions (4) are implied by our modified versions.

Following the policy of Section 3.2, we aim for an MTF based on (21) and first cast the transmission conditions into weak form

$$[(\text{Id} + \mathbb{M}) \mathbb{T}_1 U - (\text{Id} + \mathbb{M}) \mathbb{X}(\mathbb{T}_0 U), \mathbf{v}]_\Gamma = 0 \quad \forall \mathbf{v} \in \mathcal{T}(\Gamma), \quad (24)$$

$$\Updownarrow$$

$$[(\text{Id} - \mathbb{M}) \mathbb{T}_0 U - (\text{Id} - \mathbb{M}) \mathbb{X}(\mathbb{T}_1 U), \mathbf{v}]_\Gamma = 0 \quad \forall \mathbf{v} \in \mathcal{T}(\Gamma), \quad (25)$$

with an affine linear operator

$$\mathbb{M} := \begin{pmatrix} 0 & -\text{NtD}_1 \\ \text{DtN}_0 & 0 \end{pmatrix} : \mathcal{T}(\Gamma) \rightarrow \mathcal{T}(\Gamma). \quad (26)$$

Note that in the above manipulations, we have used $\mathbb{X}\mathbb{M} = -\mathbb{M}\mathbb{X}$. This yields the generalized multi-trace formulation: seek $u_0, u_1 \in \mathcal{T}(\Gamma)$ such that

$$[(-\mathbb{A}_0 + \frac{1}{2}\text{Id}) u_0, \mathbf{v}]_\Gamma + \sigma_{01} [(\text{Id} - \mathbb{M}) u_0 - (\text{Id} - \mathbb{M}) \mathbb{X} u_1, \mathbf{v}]_\Gamma = 0, \quad (27a)$$

$$\sigma_{10} [(\text{Id} + \mathbb{M}) u_1 - (\text{Id} + \mathbb{M}) \mathbb{X} u_0, \mathbf{v}]_\Gamma + [(-\mathbb{A}_1 + \frac{1}{2}\text{Id}) u_1, \mathbf{v}]_\Gamma = 0, \quad (27b)$$

for all $\mathbf{v} \in \mathcal{T}(\Gamma)$. Again, we may go after cancellation by setting $\sigma_{01} = \sigma_{10} = -\frac{1}{2}$, so that (27a) is simplified to: seek $u_0, u_1 \in \mathcal{T}(\Gamma)$ such that

$$-[(\mathbb{A}_0 - \frac{1}{2}\mathbb{M}) u_0, \mathbf{v}]_\Gamma + \frac{1}{2} [(\text{Id} - \mathbb{M}) \mathbb{X} u_1, \mathbf{v}]_\Gamma = 0, \quad (28a)$$

$$\frac{1}{2} [(\text{Id} + \mathbb{M}) \mathbb{X} u_0, \mathbf{v}]_\Gamma - [(\mathbb{A}_1 + \frac{1}{2}\mathbb{M}) u_1, \mathbf{v}]_\Gamma = 0, \quad (28b)$$

for all $\mathbf{v} \in \mathcal{T}(\Gamma)$. This linear variational problem may be solved by means of the following (undamped) additive Schwarz method: given approximations $u_0^{(k)}, u_1^{(k)} \in \mathcal{T}(\Gamma)$, $k = 0, 1, \dots$, compute $u_0^{(k+1)}, u_1^{(k+1)} \in \mathcal{T}(\Gamma)$ as solutions of

$$-[(\mathbb{A}_0 - \frac{1}{2}\mathbb{M}) u_0^{(k+1)}, \mathbf{v}]_\Gamma + \frac{1}{2} [(\text{Id} - \mathbb{M}) \mathbb{X} u_1^{(k)}, \mathbf{v}]_\Gamma = 0, \quad \forall \mathbf{v} \in \mathcal{T}(\Gamma) \quad (29a)$$

$$\frac{1}{2} [(\text{Id} + \mathbb{M}) \mathbb{X} u_0^{(k)}, \mathbf{v}]_\Gamma - [(\mathbb{A}_1 + \frac{1}{2}\mathbb{M}) u_1^{(k+1)}, \mathbf{v}]_\Gamma = 0. \quad (29b)$$

Lemma 1. *Assuming unique solvability of the linear variational problem (29), and $u_0^{(0)} = u_1^{(0)} = 0$, the iteration will become stationary after one step, with $\mathbb{T}_0 U = u_0^{(1)}$ and $\mathbb{T}_1 U = u_1^{(1)}$, where U is the solution of the transmission problem (1).*

Proof. Consider the boundary value problem posed on Ω_0 :

$$-\operatorname{div}(\mu_0 \mathbf{grad} U^{(k+1)}) + U^{(k+1)} = 0 \quad \text{in } \Omega_0, \quad (30a)$$

$$\operatorname{DtN}_1(\mathbb{T}_{D,0} U^{(k+1)}) + \mathbb{T}_{N,0} U^{(k+1)} = \operatorname{DtN}_1(\mathbb{T}_{D,1} U^{(k)}) - \mathbb{T}_{N,1} U^{(k)} \quad \text{on } \Gamma, \quad (30b)$$

$$\operatorname{DtN}_0(\mathbb{T}_{D,0} U^{(k+1)}) - \mathbb{T}_{N,0} U^{(k+1)} = \operatorname{DtN}_0(\mathbb{T}_{D,1} U^{(k)}) + \mathbb{T}_{N,1} U^{(k)} \quad \text{on } \Gamma, \quad (30c)$$

$$U^{(k+1)} - U_{\text{inc}} \quad \text{satisfies decay conditions at } \infty, \quad (30d)$$

and assume that it has a solution. Then, recalling Theorem 1 and the definition of \mathbb{M} , we find that with $u_1^{(k)} := \mathbb{T}_1 U^{(k)}$ the Cauchy traces $u_0^{(k+1)} := \mathbb{T}_0 U^{(k+1)}$ provide a solution of (29a). However, in general (30) will fail to be a meaningful boundary value problem, because too many boundary conditions are imposed on Γ . Yet, if $U^{(k)} = 0$, then the boundary conditions (30b) and (30c) become

$$\operatorname{DtN}_1(\mathbb{T}_{D,0} U^{(1)}) + \mathbb{T}_{N,0} U^{(1)} = 0 \quad \text{on } \Gamma, \quad (31a)$$

$$\operatorname{DtN}_0(\mathbb{T}_{D,0} U^{(1)}) - \mathbb{T}_{N,0} U^{(1)} = \operatorname{DtN}_0(0) \quad \text{on } \Gamma. \quad (31b)$$

Notice that (31b) is redundant, satisfied by *any* solution of (30a) complying with (30d). What remains in terms of effective boundary conditions on Γ is (31a), which represents a well-posed impedance boundary condition and guarantees the existence of a unique solution $U^{(k+1)}$. The Cauchy trace $u_0^{(1)} := \mathbb{T}_0 U^{(k)}$ of that solution will satisfy

$$-\left[\left(\mathbb{A}_0 - \frac{1}{2}\mathbb{M}\right)u_0^{(1)}, \mathbf{v}\right]_\Gamma = \frac{1}{2} \left[\begin{pmatrix} 0 \\ \operatorname{DtN}_0(0) \end{pmatrix}, \mathbf{v} \right]_\Gamma, \quad (32)$$

which agrees with the variational problem (29a) to be solved in the first step of the Schwarz iteration with initial guess $u_1^{(0)} = 0$.

Similar considerations apply to (29b). Here we start from the boundary value problem with redundant boundary conditions

$$-\operatorname{div}(\mu_1 \mathbf{grad} U^{(k+1)}) + U^{(k+1)} = 0 \quad \text{in } \Omega_1, \quad (33a)$$

$$\operatorname{DtN}_0(\mathbb{T}_{D,1} U^{(k+1)}) + \mathbb{T}_{N,1} U^{(k+1)} = \operatorname{DtN}_0(\mathbb{T}_{D,0} U^{(k)}) - \mathbb{T}_{N,0} U^{(k)} \quad \text{on } \Gamma, \quad (33b)$$

$$\operatorname{DtN}_1(\mathbb{T}_{D,1} U^{(k+1)}) - \mathbb{T}_{N,1} U^{(k+1)} = \operatorname{DtN}_1(\mathbb{T}_{D,0} U^{(k)}) + \mathbb{T}_{N,0} U^{(k)} \quad \text{on } \Gamma. \quad (33c)$$

If this has a solution $u^{(k+1)}$, its Cauchy trace $u_1^{(k+1)} := \mathbb{T}_1 U^{(k+1)}$ will solve (29b) provided that $u_0^{(k)} := \mathbb{T}_0 U^{(k)}$. Again, if $U^{(k)} = 0$, the boundary conditions on Γ are converted into

$$\operatorname{DtN}_0(\mathbb{T}_{D,1} U^{(1)}) + \mathbb{T}_{N,1} U^{(1)} = \operatorname{DtN}_0(0) \quad \text{on } \Gamma, \quad (34a)$$

$$\operatorname{DtN}_1(\mathbb{T}_{D,1} U^{(1)}) - \mathbb{T}_{N,1} U^{(1)} = 0 \quad \text{on } \Gamma, \quad (34b)$$

and the second is always fulfilled and can be dropped. This results in a well posed elliptic boundary value problem and the Cauchy trace $u_1^{(1)} := \mathbb{T}_1 U^{(k+1)}$ solves

$$\left[(\mathbb{A}_1 + \frac{1}{2}\mathbb{M})\mathbf{u}_1^{(1)}, \mathbf{v} \right]_\Gamma = \frac{1}{2} \left[\begin{pmatrix} 0 \\ \text{DtN}_0(0) \end{pmatrix}, \mathbf{v} \right]_\Gamma, \quad (35)$$

which amounts to the second linear problem faced in the first step of the Schwarz method (29) starting from zero.

By the definition of the Dirichlet-to-Neumann operators, the combined solutions of the boundary value problems (30a), (31a), (30d) and (33a), (34a) provide a solution of the transmission problem (1). Thus $\mathbf{u}_0^{(1)}$ and $\mathbf{u}_1^{(1)}$ from (32) and (35) are the Cauchy traces of that solution. Here we rely on the assumption of the Lemma that ensures uniqueness of $\mathbf{u}_0^{(1)}$ and $\mathbf{u}_1^{(1)}$. Thus they are the desired final solutions and the Schwarz iteration will become stationary after one step. \square

As a consequence of this Lemma, the additive Schwarz iteration (29) converges after two steps, thanks to the transmission conditions (21)/(22), which we call “optimal” for this reason. Unfortunately, the “optimal transmission conditions” destroy positivity of the resulting multi-trace operator, which turned out a key property in Section 3.3, see (18). We still find

$$[(\text{Id} - \mathbb{M}) \mathbb{X} \mathbf{v}_1, \mathbf{v}_0]_\Gamma = -[(\text{Id} + \mathbb{M}) \mathbb{X} \mathbf{v}_0, \mathbf{v}_1]_\Gamma \quad \forall \mathbf{v}_0, \mathbf{v}_1 \in \mathcal{T}(\partial\Omega),$$

but the ellipticity of the diagonal operators, e.g.,

$$\mathbb{A}_0 - \frac{1}{2}\mathbb{M} = \begin{pmatrix} -\mathbf{K}_0 & \mathbf{V}_0 + \frac{1}{2}\text{NtD}_1 \\ \mathbf{W}_0 - \frac{1}{2}\text{DtN}_0 & \mathbf{K}'_0 \end{pmatrix}, \quad (36)$$

is lost. Hence, rigorous results about existence and uniqueness of solutions of (28) are still missing even in the case $N = 1$. This is an open problem for future research.

Moreover, the optimal transmission conditions (21) require the realization of DtN and NtD operators. Their exact implementation is not an option for practical schemes. Thus, in the next section we consider local approximations for the optimal transmission conditions.

4.2 Local impedance transmission conditions

The considerations of the previous section suggest that for $N > 1$ we use transmission conditions similar to (21) *locally* on the interface Γ_{ij} , where $\text{DtN}_j, \text{DtN}_i$ etc. are replaced by suitable approximations. The resulting so-called local impedance transmission conditions across the interface Γ_{ij} can be written in the form

$$\mathbf{B}_{ij}(\mathbf{T}_{D,i}U) + \mathbf{T}_{N,i}U = \mathbf{B}_{ij}(\mathbf{T}_{D,j}U) - \mathbf{T}_{N,j}U, \quad (37a)$$

$$\mathbf{B}_{ji}(\mathbf{T}_{D,i}U) - \mathbf{T}_{N,i}U = \mathbf{B}_{ji}(\mathbf{T}_{D,j}U) + \mathbf{T}_{N,j}U. \quad (37b)$$

where \mathbf{B}_{ij} and \mathbf{B}_{ji} are invertible (affine) linear operators of “DtN-type” mapping $H^{\frac{1}{2}}(\Gamma_{ij})$ onto $H^{-\frac{1}{2}}(\Gamma_{ij})$. Parallel to the switch from (21) to (22), invertibility of the

involved operators yields another equivalence

$$\mathbb{T}_{D,i}U + \mathbb{C}_{ij}(\mathbb{T}_{N,i}U) = \mathbb{T}_{D,j}U - \mathbb{C}_{ij}(\mathbb{T}_{N,j}U), \quad (38a)$$

$$\mathbb{T}_{D,i}U - \mathbb{C}_{ji}(\mathbb{T}_{N,i}U) = \mathbb{T}_{D,j}U + \mathbb{C}_{ji}(\mathbb{T}_{N,j}U). \quad (38b)$$

where $\mathbb{C}_{ij} = \mathbb{B}_{ij}^{-1} : H^{-\frac{1}{2}}(\Gamma_{ij}) \rightarrow H^{\frac{1}{2}}(\Gamma_{ij})$ and $\mathbb{C}_{ji} = \mathbb{B}_{ji}^{-1} : H^{-\frac{1}{2}}(\Gamma_{ij}) \rightarrow H^{\frac{1}{2}}(\Gamma_{ij})$. We can then write the weak form of the local impedance transmission conditions as:

$$[(\text{Id} + \mathbb{S}_{ij})\mathbb{T}_jU - (\text{Id} + \mathbb{S}_{ij})\mathbb{X}(\mathbb{T}_iU), \mathbf{v}]_{\Gamma_{ij}} = 0 \quad \forall \mathbf{v} \in \widetilde{\mathcal{T}}(\Gamma_{ij}), \quad (39)$$

$$\Updownarrow$$

$$[(\text{Id} - \mathbb{S}_{ij})\mathbb{T}_iU - (\text{Id} - \mathbb{S}_{ij})\mathbb{X}(\mathbb{T}_jU), \mathbf{v}]_{\Gamma_{ij}} = 0 \quad \forall \mathbf{v} \in \widetilde{\mathcal{T}}(\Gamma_{ij}), \quad (40)$$

with an affine linear operator

$$\mathbb{S}_{ij} := \begin{pmatrix} 0 & \mathbb{C}_{ij} \\ -\mathbb{B}_{ji} & 0 \end{pmatrix} : \mathcal{T}(\Gamma_{ij}) \rightarrow \mathcal{T}(\Gamma_{ij}). \quad (41)$$

Retracing the steps detailed in Section 3.2 based on (39), we end up with the *local multi-trace variational problem*, here stated for $N = 2$: seek $(u_0, u_1, u_2) \in \mathcal{MT}(\Sigma)$ such that

$$\begin{aligned} & [\mathbb{A}_0 u_0, \mathbf{v}_0]_{\partial\Omega_0} + \frac{1}{2} [\mathbb{S}_{01} u_0, \mathbf{v}_0]_{\Gamma_{01}} + \frac{1}{2} [\mathbb{S}_{02} u_0, \mathbf{v}_0]_{\Gamma_{02}} - \\ & \quad \frac{1}{2} [(\text{Id} + \mathbb{S}_{01})\mathbb{X} u_1, \mathbf{v}_0]_{\Gamma_{01}} - \frac{1}{2} [(\text{Id} + \mathbb{S}_{02})\mathbb{X} u_2, \mathbf{v}_0]_{\Gamma_{02}} = 0, \\ & [\mathbb{A}_1 u_1, \mathbf{v}_1]_{\partial\Omega_1} + \frac{1}{2} [\mathbb{S}_{10} u_1, \mathbf{v}_1]_{\Gamma_{01}} + \frac{1}{2} [\mathbb{S}_{12} u_1, \mathbf{v}_1]_{\Gamma_{12}} - \\ & \quad \frac{1}{2} [(\text{Id} + \mathbb{S}_{10})\mathbb{X} u_0, \mathbf{v}_1]_{\Gamma_{01}} - \frac{1}{2} [(\text{Id} + \mathbb{S}_{12})\mathbb{X} u_2, \mathbf{v}_1]_{\Gamma_{12}} = 0, \\ & [\mathbb{A}_2 u_2, \mathbf{v}_2]_{\partial\Omega_2} + \frac{1}{2} [\mathbb{S}_{20} u_2, \mathbf{v}_2]_{\Gamma_{02}} + \frac{1}{2} [\mathbb{S}_{21} u_2, \mathbf{v}_2]_{\Gamma_{12}} - \\ & \quad \frac{1}{2} [(\text{Id} + \mathbb{S}_{20})\mathbb{X} u_0, \mathbf{v}_2]_{\Gamma_{02}} - \frac{1}{2} [(\text{Id} + \mathbb{S}_{21})\mathbb{X} u_1, \mathbf{v}_2]_{\Gamma_{12}} = 0, \end{aligned} \quad (42)$$

for all $(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) \in \widetilde{\mathcal{MT}}(\Sigma)$. Of course, local pairings on interfaces involve restrictions onto those interfaces even if not apparent from the notation. As explained in Section 3.3, this entails using the more regular test space $\widetilde{\mathcal{MT}}(\Sigma)$.

An additive Schwarz method analogous to (29) may be applied to (42) as an iterative solver or preconditioner. The corresponding undamped iteration seeks $(u_0^{(k+1)}, u_1^{(k+1)}, u_2^{(k+1)}) \in \mathcal{MT}(\Sigma)$ such that

$$\begin{aligned}
& \left[\mathbb{A}_0 \mathbf{u}_0^{(k+1)}, \mathbf{v}_0 \right]_{\partial \Omega_0} + \frac{1}{2} \left[\mathbb{S}_{01} \mathbf{u}_0^{(k+1)}, \mathbf{v}_0 \right]_{\Gamma_{01}} + \frac{1}{2} \left[\mathbb{S}_{02} \mathbf{u}_0^{(k+1)}, \mathbf{v}_0 \right]_{\Gamma_{02}} - \\
& \quad \frac{1}{2} \left[(\text{Id} + \mathbb{S}_{01}) \mathbb{X} \mathbf{u}_1^{(k)}, \mathbf{v}_0 \right]_{\Gamma_{01}} - \frac{1}{2} \left[(\text{Id} + \mathbb{S}_{02}) \mathbb{X} \mathbf{u}_2^{(k)}, \mathbf{v}_0 \right]_{\Gamma_{02}} = 0, \\
& \left[\mathbb{A}_1 \mathbf{u}_1^{(k+1)}, \mathbf{v}_1 \right]_{\partial \Omega_1} + \frac{1}{2} \left[\mathbb{S}_{10} \mathbf{u}_1^{(k+1)}, \mathbf{v}_1 \right]_{\Gamma_{01}} + \frac{1}{2} \left[\mathbb{S}_{12} \mathbf{u}_1^{(k+1)}, \mathbf{v}_1 \right]_{\Gamma_{12}} - \\
& \quad \frac{1}{2} \left[(\text{Id} + \mathbb{S}_{10}) \mathbb{X} \mathbf{u}_0^{(k)}, \mathbf{v}_1 \right]_{\Gamma_{01}} - \frac{1}{2} \left[(\text{Id} + \mathbb{S}_{12}) \mathbb{X} \mathbf{u}_2^{(k+1)}, \mathbf{v}_1 \right]_{\Gamma_{12}} = 0, \\
& \left[\mathbb{A}_2 \mathbf{u}_2^{(k+1)}, \mathbf{v}_2 \right]_{\partial \Omega_2} + \frac{1}{2} \left[\mathbb{S}_{20} \mathbf{u}_2^{(k+1)}, \mathbf{v}_2 \right]_{\Gamma_{02}} + \frac{1}{2} \left[\mathbb{S}_{21} \mathbf{u}_2^{(k+1)}, \mathbf{v}_2 \right]_{\Gamma_{12}} - \\
& \quad \frac{1}{2} \left[(\text{Id} + \mathbb{S}_{20}) \mathbb{X} \mathbf{u}_0^{(k)}, \mathbf{v}_2 \right]_{\Gamma_{02}} - \frac{1}{2} \left[(\text{Id} + \mathbb{S}_{21}) \mathbb{X} \mathbf{u}_1^{(k)}, \mathbf{v}_2 \right]_{\Gamma_{12}} = 0,
\end{aligned} \tag{43}$$

for all $(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) \in \widetilde{\mathcal{MT}}(\Sigma)$, where a superscript (k) indicates the use of approximations from the previous iteration. As is clear from the considerations of Section 4.1 the choice of B_i, B_j will directly affect the convergence of the Schwarz iteration applied to the multi-trace variational problem. A systematic study still has to be conducted.

Remark 4. So far, the development and analysis of multi-trace methods have focused on acoustic and electromagnetic *wave propagation problems*, see [3, Sect. 1.2]. There the simplest choice for approximate local Dirichlet-to-Neumann operators seems to be a first order complex Robin transmission condition (TC), introduced in [4], where the operators are chosen in the form

$$B_{ij} = B_{ji} = -\eta_{ij} \iota \kappa, \quad \eta_{ij} \in \mathbb{R}. \tag{44}$$

This choice makes the Schwarz iteration converge quickly for propagating eigenmodes, though the evanescent modes fail to converge. Further work has sought to improve the Robin TCs to ensure convergence of both propagating and evanescent modes [2, 1]. Of particular interest are the so-called optimized Schwarz methods, where the coefficients used in the transmission conditions are obtained by solving min-max optimization problems for half-space model problems. These include the optimized Schwarz method with two-sided Robin TCs [7] and optimized second order transmission conditions [6]. Schwarz methods with high order transmission conditions have also been developed for high frequency time-harmonic Maxwell's Equations. We mention recent works [5] and [12]. The former one is based on the optimized Schwarz methods. The latter develops a true second order TC together with a global plane wave deflation technique to further improve the convergence for electrically large problems.

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