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An Open Source Domain Decomposition Solver for Time-Harmonic Electromagnetic Wave Problems

C. Geuzaine*, B. Thierry*, N. Marsic*, D. Colignon*, A. Vion*, S. Tournier*,
Y. Boubendir†, M. El Bouajaji‡, and X. Antoine‡

*Dept. of Electrical Engineering and Computer Science, Université de Liège, Institut Montefiore,
B-4000 Liège, Belgium
cgeuzaine@ulg.ac.be

† Department of Mathematical Sciences and Center for Applied Mathematics and Statistics, NJIT,
Univ. Heights. 323 Dr. M. L. King Jr. Blvd, Newark, NJ 07102, USA
yassine.boubendir@njit.edu

‡Institut Elie Cartan de Lorraine (IECL), Université de Lorraine, CNRS, INRIA Alice Team,
F-54506 Vandoeuvre-lès-Nancy Cedex, France
xavier.antoine@univ-lorraine.fr

Abstract—We present a flexible finite element solver for testing optimized Schwarz domain decomposition techniques for the time-harmonic Maxwell equations. After a review of non-overlapping Schwarz domain decomposition methods and associated transmission conditions, we discuss the implementation, based on the open source software GetDP and Gmsh. The solver, along with ready-to-use examples, is available online for further testing.

I. INTRODUCTION

In terms of computational methods, solving three-dimensional time-harmonic electromagnetic wave problems is known to be a challenging topic, especially in the high frequency regime. Among the various approaches that can be used to solve such problems, the finite element method (FEM) with an Absorbing Boundary Condition (ABC) or a Perfectly Matched Layer (PML) is widely used for its ability to handle complex geometrical configurations and materials with non-homogeneous electromagnetic properties [1]. However, the brute-force application of the FEM in the high-frequency regime leads to the solution of very large, complex and possibly indefinite linear systems. Direct sparse solvers do not scale well for such problems, and Krylov subspace iterative solvers can exhibit slow convergence, or even diverge [2]. Domain decomposition methods provide an alternative, iterating between subproblems of smaller sizes, amenable to sparse direct solvers.

Improving the convergence properties of the iterative process constitutes the key in designing an effective algorithm, in particular in the high frequency regime. The optimal convergence is obtained by using as transmission condition on each interface between subdomains the so-called Magnetic-to-Electric (MtE) map [3] linking the magnetic and the electric surface currents on the interface. This however leads to a very expensive procedure in practice, as the MtE operator is non-local. A great variety of techniques based on *local* transmission conditions have therefore been proposed to build practical

algorithms [4], [5], [6], [7], [8], [9], [10], [11], [12]. The aim of this paper is to review the most common ones and to present a flexible finite element framework to test and compare them, based on the open source software GetDP [13], [14], [15] and Gmsh [16], [17].

II. PROBLEM SETTING

For simplicity let us consider the problem of the scattering of electromagnetic waves by a bounded, perfectly conducting obstacle K in $\mathbb{R}^3$ with boundary Γ . In order to solve this problem with a volume discretization method, we truncate the exterior domain of propagation by using a fictitious boundary Γ^∞ , on which we use a Silver-Müller radiation condition. (All what follows holds in a more general setting, e.g., with non-homogeneous materials or different boundary conditions.) This leads to the following scattering problem in the bounded domain Ω , with boundaries Γ and Γ_∞ :

$$\begin{cases} \mathbf{curl} \mathbf{curl} \mathbf{E} - k^2 \mathbf{E} = \mathbf{0}, & \text{in } \Omega, \\ \gamma_T(\mathbf{E}) = -\gamma_T(\mathbf{E}^{\text{inc}}), & \text{on } \Gamma, \\ \gamma_T(\mathbf{E}) - \frac{\imath}{k} \gamma_t(\mathbf{curl} \mathbf{E}) = 0, & \text{on } \Gamma^\infty, \end{cases} \quad (1)$$

where $\mathbf{E}$ and $\mathbf{E}^{\text{inc}}$ respectively denote the scattered and the incident electric field, $k := 2\pi/\lambda$ denotes the wavenumber (λ is the wavelength), $\imath = \sqrt{-1}$ denotes the unit imaginary number, and γ_t and γ_T are the tangential trace and tangential component trace operators given by

$$\gamma_t : \mathbf{v} \mapsto \mathbf{n} \times \mathbf{v} \text{ and } \gamma_T : \mathbf{v} \mapsto \mathbf{n} \times (\mathbf{v} \times \mathbf{n}), \quad (2)$$

with $\mathbf{n}$ the unit outwardly directed normal to Ω .

III. NON-OVERLAPPING OPTIMIZED SCHWARZ DOMAIN DECOMPOSITION METHODS

Let us now focus on the construction of optimized non-overlapping Schwarz domain decomposition methods for the boundary-value problem (1). The first step of the method [4],

[18] consists in splitting Ω into several subdomains Ω_i , $i = 1, \dots, N_{\text{dom}}$, in such a way that

- $\bar{\Omega} = \bigcup_{i=1}^{N_{\text{dom}}} \bar{\Omega}_i$ ($i = 1, \dots, N_{\text{dom}}$),
- $\Omega_i \cap \Omega_j = \emptyset$, if $i \neq j$, ($i, j = 1, \dots, N_{\text{dom}}$),
- $\partial\Omega_i \cap \partial\Omega_j = \bar{\Sigma}_{ij} = \bar{\Sigma}_{ji}$ ($i, j = 1, \dots, N_{\text{dom}}$) is the fictitious interface separating Ω_i and Ω_j as long as its interior Σ_{ij} is not empty.

In a second step, we solve smaller size problems on each subdomain Ω_i by an iterative process (indexed by p) and using transmission boundary conditions defined by an operator $\mathcal{S}$: we compute $\mathbf{E}_i^{p+1}$, $1 \leq i \leq N_{\text{dom}}$, from $\mathbf{E}_j^p$, $1 \leq j \neq i \leq N_{\text{dom}}$, by

$$\begin{cases} \mathbf{curl} \mathbf{curl} \mathbf{E}_i^{p+1} - k^2 \mathbf{E}_i^{p+1} = \mathbf{0}, & \text{in } \Omega_i, \\ \gamma_T(\mathbf{E}_i^{p+1}) = -\gamma_T(\mathbf{E}_i^{\text{inc}}), & \text{on } \Gamma_i, \\ \gamma_T(\mathbf{E}_i^{p+1}) - \frac{\gamma}{k} \gamma_t(\mathbf{curl} \mathbf{E}_i^{p+1}) = \mathbf{0}, & \text{on } \Gamma_i^\infty, \\ \mathcal{S}(\gamma_T(\mathbf{E}_i^{p+1})) - \frac{\gamma}{k} \gamma_t(\mathbf{curl} \mathbf{E}_i^{p+1}) = \\ \mathcal{S}(\gamma_T(\mathbf{E}_j^p)) + \frac{\gamma}{k} \gamma_t(\mathbf{curl} \mathbf{E}_j^p) := \mathbf{g}_{ij}^p, & \text{on } \Sigma_{ij}, \end{cases} \quad (3)$$

and then form the quantities $\mathbf{g}_{ij}^p$ through

$$\begin{aligned} \mathbf{g}_{ij}^{p+1} &= \mathcal{S}(\gamma_T(\mathbf{E}_j^{p+1})) + \frac{\gamma}{k} \gamma_t(\mathbf{curl} \mathbf{E}_j^{p+1}) \\ &= -\mathbf{g}_{ij}^p + 2\mathcal{S}(\gamma_T(\mathbf{E}_j^{p+1})), & \text{on } \Sigma_{ij}, \end{aligned} \quad (4)$$

where $\mathbf{E}_i = \mathbf{E}|_{\Omega_i}$, $\mathbf{n}_i$ (resp. $\mathbf{n}_j$) is the outward unit normal to Ω_i (resp. Ω_j), $i, j = 1, \dots, N_{\text{dom}}$, $\Gamma_i = \partial\Omega_i \cap \Gamma$ and $\Gamma_i^\infty = \partial\Omega_i \cap \Gamma^\infty$.

Solving at each step all the local transmission problems through (3)-(4) may be rewritten as one application of the iteration operator $\mathcal{A} : \times_{i,j=1}^{N_{\text{dom}}} (L^2(\Sigma_{ij}))^3 \mapsto \times_{i,j=1}^{N_{\text{dom}}} (L^2(\Sigma_{ij}))^3$ defined by

$$\mathbf{g}^{p+1} = \mathcal{A}\mathbf{g}^p + \mathbf{b}, \quad (5)$$

where $\mathbf{g}^p$ is the set of boundary data $(\mathbf{g}_{ij}^p)_{1 \leq i, j \leq N_{\text{dom}}}$, and $\mathbf{b}$ is given by the incident wave field boundary data. Therefore, (3)-(4) can be interpreted as an iteration step of the Jacobi fixed point iteration method applied to the linear system

$$(\mathcal{I}_{N_{\text{dom}}^2} - \mathcal{A})\mathbf{g} = \mathbf{b}, \quad (6)$$

where $\mathcal{I}_{N_{\text{dom}}^2}$ is the identity matrix of size $N_{\text{dom}}^2 \times N_{\text{dom}}^2$. A consequence is that any Krylov subspace iterative solver could be used for solving this equation. This can significantly improve the convergence rate of the method most particularly if $\mathcal{S}$ is well-chosen.

IV. TRANSMISSION BOUNDARY CONDITIONS

The convergence of the domain decomposition algorithm is fundamentally related to the choice of the operator $\mathcal{S}$. The first converging iterative algorithm proposed by Després in [4] used a simple impedance boundary operator:

$$\mathcal{S}^0 = \mathcal{I}. \quad (7)$$

We will refer to the corresponding zeroth-order impedance boundary condition as IBC(0). A convergence analysis of the

DDM with IBC(0) and for two half-spaces of $\mathbb{R}^3$ has been developed in [6], [7]. The approach, based on Fourier transforms, shows that the algorithm converges only for the propagating modes. For the evanescent modes, the corresponding radius of convergence is equal to 1, which makes the method stagnate or diverge. To improve the convergence factor for these special modes, Alonso *et al.* [5] derived an optimized impedance boundary condition by using a Fourier frequency decomposition. They adapted the technique developed by Gander in [19] for the Helmholtz equation to get a zero order optimized “generalized” impedance boundary condition, hereafter called GIBC(α):

$$\mathcal{S}^\alpha = \alpha(\mathbf{I} - \frac{1}{k^2} \mathbf{curl}_{\Sigma_{ij}} \mathbf{curl}_{\Sigma_{ij}}), \quad (8)$$

where α is judiciously chosen thanks to an optimization process. The same condition is proposed in [6] for the first-order system of Maxwell’s equations. In [8], Peng *et al.* show that the DDM converges for a well-chosen complex-valued number α and a decomposition into two half-spaces but by considering both the TE (Transverse Electric) and TM (Transverse Magnetic) modes. The improvement of the rate of convergence for the evanescent modes is obtained at the price of the deterioration of the rate of convergence for the propagative modes. To improve this last transmission boundary condition for the two families of modes, Rawat and Lee [10] introduce the following optimized transmission boundary condition by using two second-order operators

$$\mathcal{S}^{\alpha, \beta} = (\mathbf{I} + \frac{\alpha}{k^2} \nabla_{\Sigma_{ij}} \text{div}_{\Sigma_{ij}})^{-1} (\mathbf{I} - \frac{\beta}{k^2} \mathbf{curl}_{\Sigma_{ij}} \mathbf{curl}_{\Sigma_{ij}}), \quad (9)$$

where α and β are chosen so that an optimal convergence rate is obtained for the (TE) and (TM) modes. We denote this boundary condition by GIBC(α, β). Similar boundary conditions are derived in [6] for the first-order Maxwell’s equations. Recently, in [11], the authors proved that the convergence rates and the optimization processes for the first- and second-order formulations are the same.

When developing optimized DDMs in [20], the authors used highly accurate square-root/Padé-type On-Surface Radiation Conditions (OSRCs) [21], [22], [23], [24], [12] as transmission boundary conditions, which are also GIBCs. While being easy-to-use and direct to implement in a finite element environment, these GIBCs lead to the construction of fast converging non-overlapping DDMs, most particularly when computing the solution to high-frequency three-dimensional acoustics scattering problems. In [12], the extension of this high-order OSRC has been developed for the three-dimensional first-order system of Maxwell’s equations. When coming back to the second-order formulation, the corresponding square-root GIBC (that we denote by GIBC(sq, ε)) for the DDM can be written as

$$\mathcal{S}^{\text{sq}, \varepsilon} = \mathbf{\Lambda}_{1, \varepsilon}^{-1} \mathbf{\Lambda}_{2, \varepsilon}, \quad (10)$$

with

$$\Lambda_{1,\varepsilon} = (\mathbf{I} + \nabla_{\Sigma_{ij}} \frac{1}{k_\varepsilon^2} \text{div}_{\Sigma_{ij}} - \text{curl}_{\Sigma_{ij}} \frac{1}{k_\varepsilon^2} \text{curl}_{\Sigma_{ij}})^{1/2},$$

$$\Lambda_{2,\varepsilon} = \mathbf{I} - \text{curl}_{\Sigma_{ij}} \frac{1}{k_\varepsilon^2} \text{curl}_{\Sigma_{ij}},$$

where the complex wavenumber k_ε is defined by: $k_\varepsilon = k + i\varepsilon$, with the optimal parameter $\varepsilon = 0.39k^{1/3}\mathcal{H}^{2/3}$. In the previous expression, $\mathcal{H}$ is the local mean curvature at the surface. Finally, $A^{1/2}$ stands for the square-root of the operator A , where the square-root of a complex-valued number z is taken with branch-cut along the negative real axis. The convergence analysis of (10) is presented in [25]. An equivalent form of this condition, more adapted for finite element discretization is given by

$$\Lambda_{2,\varepsilon}(\gamma_T(\mathbf{E}_i^{p+1})) - \frac{i}{k} \Lambda_{1,\varepsilon} \gamma_t(\text{curl } \mathbf{E}_i^{p+1}) =$$

$$\Lambda_{2,\varepsilon}(\gamma_T(\mathbf{E}_j^p)) + \frac{i}{k} \Lambda_{1,\varepsilon} \gamma_t(\text{curl } \mathbf{E}_j^p), \quad \text{on } \Gamma = \Sigma_{ij}. \quad (11)$$

The IBC (7) and the GIBCs (8)-(9) are defined by local surface operators. In contrast, the GIBC given by (10)-(11) is nonlocal because of the presence of the square-root operator. However, exactly as proposed in [20] for the Helmholtz equation, it can be efficiently and accurately localized thanks to a complex Padé approximation.

V. FINITE ELEMENT IMPLEMENTATION

The finite element implementation of the DDM with transmission conditions (7), (8)-(9) and (10)-(11) is carried out with the open source finite element solver GetDP [13], [14], [15]. GetDP uses mixed finite elements to discretize de Rham-type complexes in one, two and three dimensions. Its main feature is the closeness between the input data defining discrete problems (written by the user in ASCII data files) and the symbolic mathematical expressions of these problems. This allows us to write weak forms of (3) together with either (7), (8)-(9) or (10)-(11) directly in the input data file, and use the natural mixed finite element spaces suitable for discretization [26], [12].

For example, the relevant terms of the finite element formulation in the DDM using IBC(0) as transmission condition are directly written as follows in the input data file:

```
Galerkin { [ Dof{Curl E~{i}}, {Curl E~{i}} ];
  In Omega~{i}; Integration I; Jacobian V; }
Galerkin { [ -k[]^2 * Dof{E~{i}}, {E~{i}} ];
  In Omega~{i}; Integration I; Jacobian V; }
Galerkin { [ I[] * k[] * N[] /\ (N[] /\ Dof{E~{i}}), {E~{i}} ];
  In GammaInf~{i}; Integration I; Jacobian S; }
Galerkin { [ g~{i}[], {E~{i}} ];
  In Sigma~{i}; Integration I; Jacobian S; }
Galerkin { [ I[] * k[] * N[] /\ (N[] /\ Dof{E~{i}}), {E~{i}} ];
  In Sigma~{i}; Integration I; Jacobian S; }
```

where $[\dots]$ denotes an inner product. Other transmission conditions are implemented in a similar way, as is the update relation (4). The complete implementation is available online on the web site of the ONELAB project [27], [28]: http://onelab.info/wiki/DDM_for_Waves.

The parallel implementation of the iterative algorithm uses the built-in GetDP function `IterativeLinearSolver`, which takes as argument the GetDP operations that implement the matrix-vector product required by Krylov subspace solvers, and is based on PETSc [29] and MUMPS [30] for the parallel (MPI-based) implementation of the linear algebra routines:

```
IterativeLinearSolver["I-A", "gmres", tol, maxit, (...) ]
{
  // Enter sequential mode
  SetCommSelf;
  // Get subproblem(s) owned by the current CPU
  For k In {0: #ListOfSubdomains()-1}
    i = ListOfSubdomains(k);
    // Generate new RHS and solve linear system of subdomain i
    GenerateRHSGroup[Maxwell~{i}, Sigma~{i}];
    SolveAgain[Maxwell~{i}];
    // Compute boundary data
    GenerateRHSGroup[ComputeG~{i}, Sigma~{i}];
    SolveAgain[ComputeG~{idom}~{iSide}];
  EndFor
  (...)
  // Go back to parallel mode for outside GMRES iteration
  SetCommWorld;
}
```

As a byproduct all classical iterative schemes are readily available: GMRES, Deflated GMRES, BiCGSTAB, etc. This general implementation allows the solving of a wide variety of problems, with classical or mixed formulations, and scalar, vector or tensor unknowns. For wave propagation problems in particular, this means that acoustic, electromagnetic and elastodynamic problems can be solved with the same software, simply by changing the input data files. Moreover, the software is designed to work both on small scale problems (on a laptop, a tablet or even a mobile phone) and on large scale problems on clusters without changing the input files. For example, the exact same 3D waveguide model available online at http://onelab.info/wiki/DDM_for_Waves was tested with a few thousands unknowns on an iPhone, and with half a billion degrees of freedom, with 3,500 subdomains on a 3,500 cores Tier-1 supercomputer. A typical comparison of the convergence of the DDM using different transmission conditions is presented in Figure 1. In all cases, the mesh was generated with the open source mesh generator Gmsh [16], [17], which also allows to generate the meshes for all subdomains in parallel using MPI.

VI. CONCLUSION

We have briefly presented a flexible domain decomposition solver for time-harmonic electromagnetic wave problems, which can be used to test various transmission conditions in the framework of optimized Schwarz methods. The solver is available online as open source software, and can be used to solve a large range of problems, from small scale academic examples to large-scale industrial cases on distributed memory computer clusters.

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Fig. 1. Residual history of GMRES vs. number of iterations for the various transmission conditions, on a simple three-dimensional example (concentric spheres with 2 subdomains).

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