

# Parallel Domain Decomposition Solvers for the Time Harmonic Maxwell Equations

Sven Beuchler, Sebastian Kinnewig, and Thomas Wick

## 1 Introduction

The time harmonic Maxwell (THM) equations are of great interest in applied mathematics [12, 15, 11, 5, 6, 14] and current physics applications, e.g., the excellence cluster PhoenixD.<sup>1</sup> However, the numerical solution is challenging. This is specifically true for high wave numbers. Various solvers and preconditioners have been proposed, while the most promising are based on domain decomposition methods (DDM) [16]. In [5], a quasi-optimal domain decomposition (DD) algorithm was proposed, mathematically analyzed and demonstrated to perform well for several numerical examples.

The goal of this work is to employ the domain decomposition method from [5] and to re-implement the algorithm in the modern finite element library deal.II [2]. Therein, the construction of the subdomain interface conditions is a crucial aspect for which we use Impedance Boundary Conditions. Instead of handling the resulting linear system with a direct solver, which is typically done for the THM, we apply a well chosen block preconditioner to the linear system so we can solve it with an iterative solver like GMRES (generalized minimal residuals). Additionally high polynomial Nédélec elements are used in the implementation of the DDM, see [17].

This implementation is computationally compared to several other (classical) preconditioners such as incomplete LU, additive Schwarz, Schur complement. These comparisons are done for different wave numbers. Higher wave numbers are well-known to cause challenges for the numerical solution.

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Sven Beuchler, Sebastian Kinnewig, Thomas Wick  
Leibniz University Hannover, Institute of Applied Mathematics, Welfengarten 1, 30167 Hannover, Germany {beuchler,kinnewig,wick}@ifam.uni-hannover.de

and Cluster of Excellence PhoenixD (Photonics, Optics, and Engineering - Innovation Across Disciplines), Leibniz Universität Hannover, Germany

<sup>1</sup> <https://www.phoenixd.uni-hannover.de/en/>

The outline of this work is as follows: In the section 2 we introduce some notation. In section 3 we introduce the domain decomposition method (DDM) for the THM, furthermore we introduce a block preconditioner which will allow us to solve the THM with iterative solves instead of direct solvers inside of DDM. In the section 4 we will compare the results of the block preconditioner with the performance of different preconditioners. Moreover we will present some results of the combination of the preconditioner and the DDM for two benchmark problems.

## 2 Equations and finite element discretization

Let  $\Omega \subset \mathbb{R}^d$ ,  $d \in \{2, 3\}$  be a bounded domain with sufficiently smooth boundary  $\Gamma$ . The latter is partitioned into  $\Gamma = \Gamma^\infty \cup \Gamma^{\text{inc}}$ . Furthermore, the time harmonic Maxwell equations are then defined as follows: Find the electric field  $\mathbf{E} \in \mathbf{H}(\text{curl}, \Omega) := \{v \in \mathcal{L}^2(\Omega), \text{curl}(v) \in \mathcal{L}^2(\Omega)\}$  such that

$$\begin{cases} \text{curl}(\mu^{-1} \text{curl} \mathbf{E}) - \omega^2 \mathbf{E} & = \mathbf{0} & \text{in } \Omega \\ \mu^{-1} \gamma^t(\text{curl}(\mathbf{E})) - i\kappa\omega \gamma^T(\mathbf{E}) & = \mathbf{0} & \text{on } \Gamma^\infty \\ \gamma^T(\mathbf{E}) & = -\gamma^T(\mathbf{E}^{\text{inc}}) & \text{on } \Gamma^{\text{inc}} \end{cases}, \quad (1)$$

where  $\mathbf{E}^{\text{inc}} : \mathbb{R}^d \rightarrow \mathbb{C}^d$ ,  $d \in \{2, 3\}$  is some given incident electric field,  $\omega > 0$  is the wave number which is defined by  $\omega := \frac{2\pi}{\lambda}$ , where  $\lambda > 0$  is the wave length,  $\mu > 0$  is the relative permeability and  $\kappa > 0$  is the relative permittivity. Let  $\Omega$  be a domain with smooth interface. Following [9, 15], we define traces  $\gamma^t : \mathbf{H}(\text{curl}, \Omega) \rightarrow \mathbf{H}_\times^{-1/2}(\text{div}, \Gamma)$  and  $\gamma^T : \mathbf{H}(\text{curl}, \Omega) \rightarrow \mathbf{H}_\times^{-1/2}(\text{curl}, \Gamma)$  by

$$\gamma^t(\mathbf{v}) = \mathbf{n} \times \mathbf{v} \text{ and } \gamma^T(\mathbf{v}) = \mathbf{n} \times (\mathbf{v} \times \mathbf{n})$$

where the vector  $\mathbf{n}$  is the normal to  $\Omega$ ,  $\mathbf{H}_\times^{-1/2}(\text{div}, \Gamma) := \{\mathbf{v} \in \mathbf{H}^{-1/2}(\Gamma) : \mathbf{v} \cdot \mathbf{n} = 0, \text{div}_\Gamma \mathbf{v} \in \mathbf{H}^{-1/2}(\Gamma)\}$  is the space of well-defined surface divergence fields,  $\mathbf{H}_\times^{-1/2}(\text{curl}, \Gamma) := \{\mathbf{v} \in \mathbf{H}^{-1/2} : \mathbf{v} \cdot \mathbf{n} = 0, \text{curl}_\Gamma \mathbf{v} \in \mathbf{H}^{-1/2}(\Gamma)\}$  is the space of well-defined surface curls.

System (1) is called time harmonic, because the time dependence can be expressed by  $e^{i\omega\tau}$ , where  $\tau \geq 0$  denotes the time. For the implementation with the help of a Galerkin finite element method, we need the discrete weak form. Let  $\mathcal{N}_h^p := \{v_h \in X : v_h|_K(x) = a_K(x) + (x \times b_K(x)), a_K, b_K \in [P^p(K)]^3 \forall K \in \tau_h(\Omega)\}$  be the Nédélec space [15], where  $X = \{v \in \mathbf{H}(\text{curl}, \Omega) : v \times \mathbf{n}|_{\Gamma^{\text{inc}}} = v \times \mathbf{n}|_{\Gamma^\infty} \in L^2(\Gamma^\infty)\}$ . Based on the de-Rham cohomology, basis functions can be developed, [17]. Find  $\mathbf{E}_h \in \mathcal{N}_h^p(\Omega)$  such that

$$\begin{aligned} & \int_\Omega \left( \mu^{-1} \text{curl}(\mathbf{E}_h) \text{curl}(\boldsymbol{\varphi}_h) - \omega^2 \mathbf{E}_h \boldsymbol{\varphi}_h \right) dx \\ & + \int_{\Gamma^\infty} i\kappa\omega \gamma^T(\mathbf{E}_h) \gamma^T(\boldsymbol{\varphi}_h) ds = \int_{\Gamma^{\text{inc}}} \gamma^T(\mathbf{E}_h^{\text{inc}}) \gamma^T(\boldsymbol{\varphi}_h) ds \quad \forall \boldsymbol{\varphi}_h \in \mathcal{N}_h^p(\Omega). \end{aligned} \quad (2)$$

In order to obtain a block system for the numerical solution process, we define the following elementary integrals

$$\begin{aligned} (A)_{u,v} &= \int_{\Omega} \mu^{-1} \operatorname{curl}(\boldsymbol{\varphi}_u) \operatorname{curl}(\boldsymbol{\varphi}_v), & (M)_{u,v} &= \int_{\Omega} \boldsymbol{\varphi}_u \boldsymbol{\varphi}_v \\ (B)_{u,v} &= \int_{\Gamma^{\infty}} i\kappa\omega \boldsymbol{\gamma}^T(\boldsymbol{\varphi}_u) \boldsymbol{\gamma}^T(\boldsymbol{\varphi}_v), & (s)_u &= \int_{\Gamma^{\text{inc}}} \boldsymbol{\gamma}^T(\mathbf{E}^{\text{inc}}) \boldsymbol{\gamma}^T(\boldsymbol{\varphi}_u), \end{aligned} \quad (3)$$

where  $\boldsymbol{\varphi}_u, \boldsymbol{\varphi}_v \in \mathcal{N}_h^P(\Omega)$ . To this end, System (1) can be written in the form

$$\begin{pmatrix} A - \omega^2 M & -B \\ B & A - \omega^2 M \end{pmatrix} \begin{pmatrix} \mathbf{E}_{RE} \\ \mathbf{E}_{IM} \end{pmatrix} = \begin{pmatrix} \mathbf{s}_{RE} \\ \mathbf{s}_{IM} \end{pmatrix}, \quad (4)$$

where  $\mathbf{E} = \mathbf{E}_{RE} + i\mathbf{E}_{IM}$  and  $\mathbf{s} = \mathbf{s}_{RE} + i\mathbf{s}_{IM}$ , where  $i$  denotes the imaginary number.

### 3 Numerical solution with domain decomposition and preconditioners

#### 3.1 Domain decomposition

Due to the difficult structure of the time harmonic Maxwell equations, a successful approach to solve the THM is based on the DDM [16]. As the name suggests, the domain is divided into smaller subdomains. As these subdomains become small enough they can be handled by a direct solver. To this end, we divide the domain as follows:  $\Omega = \bigcup_{i=0}^{N_{\text{dom}}} \Omega_i$  where  $N_{\text{dom}}$  is the number of domains, since we consider a non-overlapping DDM  $\Omega_i \cap \Omega_j = \emptyset$ , if  $i \neq j \forall i, j \in \{1, \dots, N_{\text{dom}}\}$  and we denote the interface from two neighbouring cells by  $\partial\Omega_i \cap \partial\Omega_j = \Sigma_{ij} = \Sigma_{ji}$ ,  $\forall i, j \in \{1, \dots, N_{\text{dom}}\}$ .

The second step of the DD is an iterative method, indexed by  $k$ , to compute the overall electric field  $\mathbf{E}$ . Therefore we begin by solving System (1) on each subdomain  $\Omega_i$ , we denote the solution of every subsystem by  $\mathbf{E}_i^{k=0}$ . From this we can compute the first interface condition by

$$\mathbf{g}_{ji}^{k=0} := -\mu^{-1} \boldsymbol{\gamma}_i^t \left( \operatorname{curl} \left( \mathbf{E}_i^{k=0} \right) \right) - ikS \left( \boldsymbol{\gamma}_i^T \left( \mathbf{E}_i^{k=0} \right) \right), \quad (5)$$

where  $S$  describes some boundary operator, which we will discuss in more detail below. Afterward, we obtain the next iteration step  $\mathbf{E}_i^{k+1}$  via:

$$\begin{cases} \operatorname{curl}(\mu^{-1} \operatorname{curl}(\mathbf{E}_i^{k+1})) - \omega^2 \mathbf{E}_i^{k+1} & = \mathbf{0} & \text{in } \Omega_i \\ \mu^{-1} \gamma_i^t(\operatorname{curl}(\mathbf{E}_i^{k+1})) - i\kappa\omega \gamma_i^T(\mathbf{E}_i^{k+1}) & = 0 & \text{on } \Gamma_i^\infty \\ \gamma_i^T(\mathbf{E}_i^{k+1}) & = -\gamma_i^T(\mathbf{E}_i^{\text{inc}}) & \text{on } \Gamma_i^{\text{inc}} \\ \mu^{-1} S(\gamma_i^t(\operatorname{curl}(\mathbf{E}_i^{k+1}))) - i\kappa\omega \gamma_i^T(\mathbf{E}_i^{k+1}) & = g_{ji}^k & \text{on } \Sigma_{i,j} \end{cases} \quad (6)$$

Once  $\mathbf{E}_i^{k+1}$  is computed, the interface is updated by

$$g_{ji}^{k+1} = -\mu^{-1} \gamma_i^t(\operatorname{curl}(\mathbf{E}_i^{k+1})) - i\kappa S(\gamma_i^T(\mathbf{E}_i^{k+1})) = -g_{ij}^k - 2i\kappa S(\gamma_i^T(\mathbf{E}_i^{k+1})) \quad (7)$$

where  $\mathbf{E}_i^k \rightarrow \mathbf{E}|_{\Omega_i}$  as  $k \rightarrow \infty$ . This convergence depends strongly on the chosen surface operator  $S$ . For a convergence analysis when the IBC are considered, see [7]

This iteration above can be interpreted as one step of the Jacobi fixed point method for the linear system

$$(\mathbb{1} - \mathcal{A})\mathbf{g} = \mathbf{b} \quad (8)$$

where  $\mathbb{1}$  is the identity operator,  $\mathbf{b}$  is the vector of the incident electric field,  $\mathcal{A}$  is defined by  $\mathcal{A}\mathbf{g}^k = \mathbf{g}^{k+1}$  and Equations (6), (7). Convergence is achieved for  $\|(1 - \mathcal{A})\mathbf{g}^k - \mathbf{b}\| < TOL$  with some small tolerance  $TOL > 0$ . Often,  $TOL = 10^{-6}, \dots, 10^{-8}$ . Instead of a Jacobi fixed point method one can also use a GMRES method to solve (8) more efficiently.

The crucial point of the DD is the choice of the interface conditions between the subdomains. The easiest choice is a non-overlapping Schwarz decomposition, where Dirichlet like interface conditions are used. For large wave numbers, e.g. the parameter  $\omega$  becomes large, the system is highly indefinite. Consequently, a convergence of this algorithm for the time harmonic Maxwell equations for all  $\omega$  cannot be expected; see [8, 10]. An analysis for an overlapping additive Schwarz method is given in [4].

Rather, we need more sophisticated tools in which the easiest choice are Impedance Boundary Conditions (IBC), which can be classified as Robin like interface conditions

$$S = \mathbb{1}. \quad (9)$$

### 3.2 Preconditioner

As it is clear, the DDM is an iterative method, where we have to solve system (6) on each subdomain in each iteration step  $k$ . Usually, this is done by a direct solver, but instead, we can use a GMRES solver, which is preconditioned by an approximation of the block system

$$\begin{pmatrix} A - \omega^2 M & 0 \\ 0 & A - \omega^2 M \end{pmatrix}^{-1}. \quad (10)$$

Therefore we need to compute an approximation of  $(A - \omega^2 M)^{-1}$ , and we obtain this approximation by applying the AMG preconditioner provided by MueLu [3], where for the level transitions a direct solver is used. The latter is necessary, since otherwise the AMG preconditioner does not perform well for the THM. On the one hand, this procedure is cost expensive. On the other hand, we can reuse the preconditioner each time we solve system (6).

An other possible choice is to use the AMG preconditioner to compute directly an approximation of

$$\begin{pmatrix} A - \omega^2 M & -B \\ -B & A - \omega^2 M \end{pmatrix}^{-1}.$$

With this preconditioner only a few GMRES iterations are needed to solve the system (6). Since we computing an approximation of the complete inverse this comes with much higher memory consumption, than using (10) as preconditioner. Actually the memory consumption while using an iterative solver with (10) as an preconditioner is even lower, than the memory consumption from a direct solver, which we show numerically in the next chapter. Therefore the block diagonal preconditioner is used in the following.

## 4 Numerical tests

In this section, we compare the performance of different preconditioners for two numerical examples. We choose a simple wave guide as our benchmark problem, moreover we test the performance of our method on a Y beam splitter. Our implementation is based on the open-source finite element library deal.II [2] with Trilinos [13] and MueLu [3]. As a direct solver, MUMPS (Multifrontal Massively Parallel Sparse Direct Solver) [1] is used. We perform an additive domain decomposition and compute each step in parallel with MPI. For the computations an Intel Xeon Platinum 8268 CPU was used with up to 32 cores.

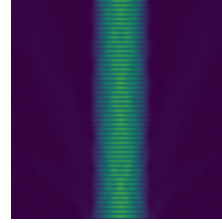
### 4.1 Example 1: Block benchmark

Before we test the domain decomposition method, we want to compare the performance of different preconditioners on a single domain. Therefore we consider a simple 2D squared domain decomposed of a material with a higher refractive index in the center a carrier material with a lower refractive index beside it, see Figure 1.

Table 1 displays the GMRES iterations with a relative accuracy of  $\epsilon = 10^{-8}$  for different preconditioners:

- ILU, incomplete LU decomposed of (4),

**Fig. 1:** As a benchmark problem, we consider a  $1 \times 1$  square with different wave numbers (here  $\lambda = 50$ ). In the center is a material with the refractive index  $n_{\text{center}} = 1.516$  and as cladding the refractive index of air was used  $n_{\text{air}} = 1.0$ . For the discretization Nédélec elements with the polynomial degree  $p = 1$  are used.

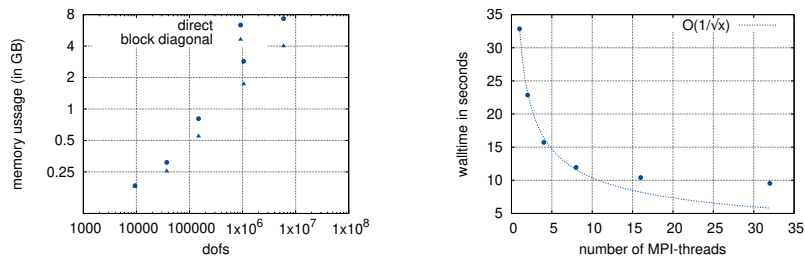


- the implemented additive Schwarz preconditioner of [2, 13]<sup>2</sup>,
- a Schur complement preconditioner based on<sup>3</sup>,
- the block preconditioner (10).

Overall, the GMRES iteration numbers grow for large  $\omega$ . In the case of the block preconditioner the GMRES iteration number first decreases and then increases for higher wave numbers.

**Table 1:** Example 1: GMRES iterations with different preconditioners.

wave number $\omega$	GMRES iterations with the preconditioner			
	ILU	additive Schwarz	Schur complement	block preconditioner
5.0	165	515	156	75
10.0	349	750	161	52
20.0	833	>2000	172	26
40.0	>2000	-	diverged	25
60.0	-	-	diverged	38
80.0	-	-	diverged	49

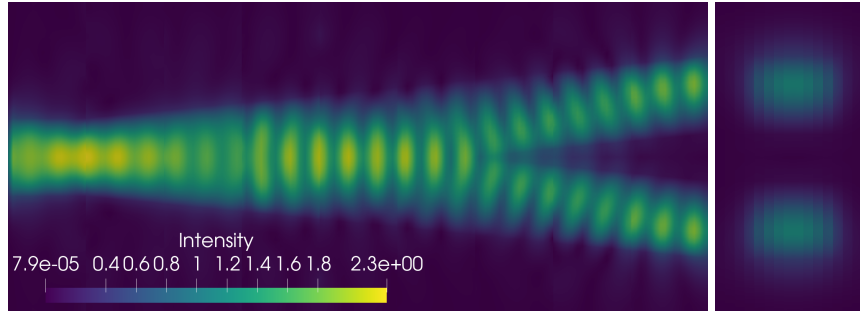


**Fig. 2:** On the left side: memory usage in dependence of the number of dofs. On the right side: walltime in dependence of the number of MPI-threads.

<sup>2</sup> [https://www.dealii.org/current/doxygen/deal.II/classTrilinosWrappers\\_1\\_1PreconditionSSOR.html](https://www.dealii.org/current/doxygen/deal.II/classTrilinosWrappers_1_1PreconditionSSOR.html)

<sup>3</sup> [https://www.dealii.org/current/doxygen/deal.II/step\\_22.html](https://www.dealii.org/current/doxygen/deal.II/step_22.html)

## 4.2 Example 2: Y beam splitter



**Fig. 3:** Intensity plot of the y beam splitter, on the left side is the intensity on the x-y plane and on the right side is the intensity at the output.

Similar as in the simple wave guide, we consider for the Y beam splitter an material with a higher refractive index placed inside of an carrier material with a lower refractive index. Here we consider a 3D model of a Y beam splitter. The mesh was divided into 9 subdomains, and the average number of GMRES iterations to solve the subdomains are given in table 2, are for the wave number  $\lambda = 20$ . For the discretization Nédélec elements with the polynomial degree  $p = 3$  are used.

**Table 2:** Example 2: GMRES iterations on each domain for the block preconditioner

subdomain id	1	2	3	4	5	6	7	8	9
average number of GMRES iterations	34	40	41	31	35	39	37	33	32

## 5 Conclusion

In this contribution, we implemented a domain decomposition method with a block preconditioner for the time harmonic Maxwell equations. Therein, a crucial aspect is the construction of the subdomain interface conditions. Our algorithmic developments are demonstrated for two configurations of practical relevance, namely a block benchmark and a Y beam splitter.

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