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Convergence of an ADI splitting for Maxwell's equations

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Abstract The convergence of an alternating direction implicit method for Maxwell's equations on product domains is investigated. Unlike the classical Yee scheme and most other integrators proposed in the literature, this method is both unconditionally stable and computationally cheap. We prove second-order convergence of the time-discretization in the framework of operator semigroup theory. In contrast to formal considerations based on Taylor expansions, our convergence analysis respects the unboundedness of the involved differential operators. The proofs are based on results concerning the regularity of the Cauchy problems, which then allow to apply an abstract convergence proof by Hansen and Ostermann [13].

Keywords Maxwell's equations, alternating direction implicit method, Peaceman-Rachford splitting, well-posedness, regularity, error analysis, time integration, semigroups

Mathematics Subject Classification (2000) Primary: 65M12. Secondary: 35Q61, 47D03, 65J10.

1 Introduction

Maxwell's equations provide the foundation for the modern theory of electromagnetism, and solving these equations numerically is a crucial task in the analysis and design of antennas, photonic cristals, waveguides, and mobile communication devices. In the majority of simulations, the solution of Maxwell's equations is approximated with finite-difference time-domain methods (cf. [22]). Within this class, the Yee scheme [27] is particularly popular,

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but since this method is explicit, instability can only be avoided if a sufficiently small step size is chosen. This can seriously affect the efficiency of the method; cf. [22]. On the other hand, using an implicit and unconditionally stable Runge-Kutta method for the time integration may decrease the necessary number of time-steps, but the price to pay is a large linear system which has to be solved in each step. Thus, the total numerical costs of such an implicit method is often not significantly smaller than the computational work of the Yee scheme.

A major breakthrough for the simulation of Maxwell equations posed on a cuboid or on the whole of $\mathbb{R}^3$ was achieved around 2000 in [17; 18; 28], where an unconditionally stable and computationally efficient alternating direction implicit (ADI) method was proposed. The main idea is, roughly speaking, to decompose the Maxwell operator into two parts and to propagate the associated sub-flows in such a way that the implicitness is reduced to one-dimensional problems. Hence, instead of the large linear systems with large bandwidth arising in the discretization of the full 3d problem, only small linear systems with tridiagonal matrices have to be solved in each time-step. This invention raised a lot of interest, and a large number of follow-up papers can be found in the literature, see, e.g., [7; 10; 9; 11] and references therein. Moreover, the operator splitting approach was modified and extended for the construction of new methods by composition; cf. [2; 8; 14; 15; 24; 25; 26] and Chapter 18 in [22]. Splitting and composition methods for ordinary differential equations are discussed in Section II.4-II.5 in [12].

It is well known that the method proposed in [17; 28] is formally of second order in time and space. Most of the convergence results found in the literature use Taylor expansion of the exact solution to prove second order error bounds. Ultimately, this leads to bounds where the leading error term depends on the norm of the finite difference matrices used in the spatial discretization. However, since these matrices approximate unbounded differential operators, their norm tends to infinity when the spatial mesh width tends to zero. Hence, such an analysis only proves that the method converges with order two in time if a *fixed* spatial mesh is considered. The argument does not reveal whether or not the accuracy of the time integration is reduced when the spatial approximation is refined.

The main goal of this paper is to prove that under suitable regularity conditions the second-order convergence in time is indeed not affected by the spatial discretization. To this end, we prove an error bound for the semi-discretization in a framework of operator semigroup theory which takes into account that all operators involving spatial derivatives are unbounded. Our error analysis is based on an explicit formula for the global error, which was already used in [13] in a different setting. To estimate the terms in our error formula, we need the skew-adjointness both of the operator governing the Maxwell equation and of the operators arising in the splitting. Here, it is crucial to choose the correct boundary conditions for the splitted problems. It remains one core term, which has to be treated by means of a detailed regularity analysis given in Lemmas 3.6 and 3.7.

In Section 2 we introduce Maxwell's equations on $\mathbb{R}^3$ and on a cuboid, and we formulate the method from [28] as a Peaceman-Rachford splitting method. The computational advantage of this approach is explained in Section 2.3. Section 3 is devoted to the analysis of Maxwell's equations. We describe and investigate in detail the analytical setting and establish the necessary regularity results. Based on this analytical background, we present our error analysis of the semi-discretization on $\mathbb{R}^3$ and on a cuboid in Section 4 (cf. Theorems 4.2 and 4.5). The convergence results are confirmed by numerical examples which illustrate how the accuracy is affected if the regularity of the initial data or of the coefficients is low. Finally, we present the proofs of two technical lemmas in the appendix.

Notation. Throughout the article, the Euclidean scalar product on $\mathbb{R}^3$ is denoted by $x \cdot y$. We write $Y \hookrightarrow Z$ if a Banach space Y is continuously embedded into a Banach space Z. The domain $D(A)$ of a linear operator A is endowed with the graph norm $\|x\| + \|Ax\|$. The domain of a product of linear operators is defined by

$$D(AB) = \{x \in D(B) \mid Bx \in D(A)\}$$

and recursively for more factors such as A^n. We use real valued function spaces. All constants that only depend on the coefficients ε and μ are denoted by c.

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2 The ADI splitting for Maxwell's equations

2.1 Maxwell's equations

We consider linear Maxwell's equations without sources on $\mathbb{R}^3$

$$\begin{aligned} \partial_t \mathbf{E}(t) &= \tfrac{1}{\varepsilon} \operatorname{rot} \mathbf{H}(t), && t \in \mathbb{R},\ x \in \mathbb{R}^3, \\ \partial_t \mathbf{H}(t) &= -\tfrac{1}{\mu} \operatorname{rot} \mathbf{E}(t), && t \in \mathbb{R},\ x \in \mathbb{R}^3, \\ \operatorname{div} \varepsilon \mathbf{E}(t) = 0,& \quad \operatorname{div} \mu \mathbf{H}(t) = 0, && t \in \mathbb{R},\ x \in \mathbb{R}^3, \\ \mathbf{E}(0) = \mathbf{E}^0,& \quad \mathbf{H}(0) = \mathbf{H}^0, && x \in \mathbb{R}^3, \end{aligned} \tag{1}$$

and on the cuboid $Q = (a_1^-, a_1^+) \times (a_2^-, a_2^+) \times (a_3^-, a_3^+) \subseteq \mathbb{R}^3$

$$\begin{aligned} \partial_t \mathbf{E}(t) &= \tfrac{1}{\varepsilon} \operatorname{rot} \mathbf{H}(t), && t \in \mathbb{R},\ x \in Q, \\ \partial_t \mathbf{H}(t) &= -\tfrac{1}{\mu} \operatorname{rot} \mathbf{E}(t), && t \in \mathbb{R},\ x \in Q, \\ \operatorname{div} \varepsilon \mathbf{E}(t) = 0,& \quad \operatorname{div} \mu \mathbf{H}(t) = 0, && t \in \mathbb{R},\ x \in Q, \\ \mathbf{E}(t) \times \nu = 0,& \quad \mu \mathbf{H}(t) \cdot \nu = 0, && t \in \mathbb{R},\ x \in \partial Q, \\ \mathbf{E}(0) = \mathbf{E}^0,& \quad \mathbf{H}(0) = \mathbf{H}^0, && x \in Q, \end{aligned} \tag{2}$$

with a perfectly conducting boundary. The electric field $\mathbf{E} = \mathbf{E}(t, x)$ and the magnetic field $\mathbf{H} = \mathbf{H}(t, x)$ vary in time and space, but the spatial variable

x will usually be omitted. The corresponding initial fields are $\mathbf{E}^0 \in L^2(\Omega)^3$ and $\mathbf{H}^0 \in L^2(\Omega)^3$, where $\Omega \in \{\mathbb{R}^3, Q\}$. We assume that the permittivity $\varepsilon \in L^\infty(\Omega)$ and the permeability $\mu \in L^\infty(\Omega)$ are given functions which satisfy $\varepsilon(x), \mu(x) \geq \delta > 0$ for a constant $\delta > 0$. In the boundary conditions of (2), ν is the outer unit normal on the boundary ∂Q (defined outside the edges). The differential operators and boundary conditions are understood in the sense of distributions and traces, respectively. It is known that these equations are well-posed in $L^2(\Omega)^6$, see, e.g., Theorem 8.5 in [16] or Section XVII.B.4.4 in [5]. More precisely, the *Maxwell operator*

$$M = \begin{pmatrix} 0 & \frac{1}{\varepsilon}\operatorname{rot} \\ -\frac{1}{\mu}\operatorname{rot} & 0 \end{pmatrix} \tag{3}$$

is skew-adjoint on a certain subspace of $L^2(\Omega)^6$ if we include the divergence and boundary conditions in a suitable way in this subspace and in the domain of M, and if we equip $L^2(\Omega)^6$ with the scalar product corresponding to the energy of the fields. Moreover, the divergence conditions for $\varepsilon\mathbf{E}$ and for $\mu\mathbf{H}$ and the boundary condition for $\mu\mathbf{H}$ follow from the other equations in (1) or (2) if the initial fields satisfy these conditions, see Propositions 3.1 and 3.5.

However, it is hard to find a detailed proof for these results in the present generality. Moreover, the framework of the well-posedness results is needed for our error analysis. We have thus included the arguments in Section 3, which focuses on additional regularity properties of M. The proofs are postponed to the appendix.

2.2 ADI splitting scheme

The time discretization proposed in [28] is based on the idea to split the differential operator rot into

$$\operatorname{rot} = C_1 - C_2 \quad \text{with} \quad C_1 = \begin{pmatrix} 0 & 0 & \partial_2 \\ \partial_3 & 0 & 0 \\ 0 & \partial_1 & 0 \end{pmatrix}, \qquad C_2 = \begin{pmatrix} 0 & \partial_3 & 0 \\ 0 & 0 & \partial_1 \\ \partial_2 & 0 & 0 \end{pmatrix}$$

and to define

$$A = \begin{pmatrix} 0 & \frac{1}{\varepsilon} C_1 \\ \frac{1}{\mu} C_2 & 0 \end{pmatrix} \qquad \text{and} \qquad B = \begin{pmatrix} 0 & -\frac{1}{\varepsilon} C_2 \\ -\frac{1}{\mu} C_1 & 0 \end{pmatrix}.$$

The operators A and B act on $L^2(\Omega)^6$. They are endowed with the “maximal” domains

$$\begin{aligned} D_{\mathbb{R}^3}(A) &= \{(u,v) \in L^2(\mathbb{R}^3)^6 \mid (C_1 v, C_2 u) \in L^2(\mathbb{R}^3)^6\}, \\ D_{\mathbb{R}^3}(B) &= \{(u,v) \in L^2(\mathbb{R}^3)^6 \mid (C_2 v, C_1 u) \in L^2(\mathbb{R}^3)^6\} \end{aligned}$$

on the full space $\mathbb{R}^3$ and with “partial” Dirichlet boundary conditions

$$
\begin{aligned}
D_Q(A) = \{(u,v) \in L^2(Q)^6 \mid (C_1 v, C_2 u) \in L^2(Q)^6,& \\
u_1 = 0 \text{ on } \Gamma_2^{\pm},\ u_2 = 0 \text{ on } \Gamma_3^{\pm},\ u_3 = 0 \text{ on } \Gamma_1^{\pm}\},& \\
D_Q(B) = \{(u,v) \in L^2(Q)^6 \mid (C_2 v, C_1 u) \in L^2(Q)^6,& \\
u_1 = 0 \text{ on } \Gamma_3^{\pm},\ u_2 = 0 \text{ on } \Gamma_1^{\pm}, u_3 = 0 \text{ on } \Gamma_2^{\pm}\}&
\end{aligned}
$$

on Q. Often we will omit the subscript indicating the spatial domain. Here and below Γ_j^- and Γ_j^+ are the open faces of Q given by $x_j = a_j^-$ and $x_j = a_j^+$, respectively, for $j = 1,2,3$. Note that the boundary conditions in $D_Q(A)$ and $D_Q(B)$ are well defined since the corresponding partial derivatives are square integrable. The domains of A and B are chosen such that $D(A) \cap D(B) \subseteq D(M)$ and $Aw + Bw = Mw$ for $w \in D(A) \cap D(B)$ and for both $\Omega = \mathbb{R}^3$ and $\Omega = Q$. For each of the two cases, the domain of M will be defined in the next section. We remark that A and B do neither respect the divergence condition nor the magnetic boundary condition of Maxwell's equations.

For a step size $\tau > 0$ and $w \in D(B)$, the ADI splitting method proposed in [28] can now be formulated as

$$
S_\tau w = (I - \tfrac{\tau}{2} B)^{-1}(I + \tfrac{\tau}{2} A)(I - \tfrac{\tau}{2} A)^{-1}(I + \tfrac{\tau}{2} B)w. \tag{4}
$$

Hence, this scheme is a special case of the Peaceman-Rachford method, cf. [13]. We will show in Section 4 that A and B are skew-adjoint (cf. Lemmas 4.1 and 4.3) and thus the above inverses exist. Moreover, this implies $\|(I + \frac{\tau}{2} A)(I - \frac{\tau}{2} A)^{-1}\| = \|(I + \frac{\tau}{2} B)(I - \frac{\tau}{2} B)^{-1}\| = 1$ in a suitable norm, and since the approximation w_n obtained after n steps is given by

$$
\begin{aligned}
S_\tau^n w &= (I - \tfrac{\tau}{2} B)^{-1} P_\tau^{n-1} (I + \tfrac{\tau}{2} A)(I - \tfrac{\tau}{2} A)^{-1}(I + \tfrac{\tau}{2} B)w \\
\text{with } P_\tau &= (I + \tfrac{\tau}{2} A)(I - \tfrac{\tau}{2} A)^{-1}(I + \tfrac{\tau}{2} B)(I - \tfrac{\tau}{2} B)^{-1},
\end{aligned}
$$

it follows that

$$
\|S_\tau^n w\| \le \|(I - \tfrac{\tau}{2} B)^{-1}\| \cdot \|(I + \tfrac{\tau}{2} B)w\|.
$$

Since the right-hand side is independent of n, the method is unconditionally stable. This was proved in a similar way in [7] for matrices instead of operators. Alternative proofs of the unconditional stability can be found, e.g., in [15].

Our main Theorems 4.2 and 4.5 say that

the ADI splitting scheme $S_\tau^n(\mathbf{E}^0, \mathbf{H}^0)$ converges quadratically in $L^2(\Omega)^6$ to the solutions of (1), resp. (2), if $\mathbf{E}^0$, $\mathbf{H}^0$, ε and μ are sufficiently regular.

2.3 Efficient formulation of the ADI splitting scheme on $\mathbb{R}^3$

As the definition (4) indicates, each time step of the ADI splitting method involves two implicit substeps corresponding to the two inverses. In [28], the approximations

$$
\begin{aligned}
(\mathbf{E}^n, \mathbf{H}^n) &= S_\tau^n(\mathbf{E}^0, \mathbf{H}^0) \in D(B) \qquad \text{and} \\
(\mathbf{E}^{n+\frac12}, \mathbf{H}^{n+\frac12}) &= (I - \tfrac{\tau}{2} A)^{-1}(I + \tfrac{\tau}{2} B)(\mathbf{E}^n, \mathbf{H}^n) \in D(A), \qquad n \in \mathbb{N},
\end{aligned} \tag{5}
$$

were replaced by equivalent ones in such a way that the linear systems arising from the implicit parts can be solved in a very efficient way. This idea is the main advantage of the method over most other implicit methods.

We first derive the equivalent scheme in $\mathbb{R}^3$. The first half step given by (5) can be written as

$$\begin{aligned}
\mathbf{E}^{n+\frac{1}{2}} &= \mathbf{E}^n - \tfrac{\tau}{2\varepsilon}C_2\mathbf{H}^n + \tfrac{\tau}{2\varepsilon}C_1\mathbf{H}^{n+\frac{1}{2}},\\
\mathbf{H}^{n+\frac{1}{2}} &= \mathbf{H}^n - \tfrac{\tau}{2\mu}C_1\mathbf{E}^n + \tfrac{\tau}{2\mu}C_2\mathbf{E}^{n+\frac{1}{2}}.
\end{aligned}$$

We eliminate $\mathbf{H}^{n+\frac{1}{2}}$ by inserting the second equality into the first to deduce

$$\begin{aligned}
\mathbf{E}^{n+\frac{1}{2}} &= \mathbf{E}^n - \tfrac{\tau}{2\varepsilon}C_2\mathbf{H}^n + \tfrac{\tau}{2\varepsilon}C_1\big(\mathbf{H}^n - \tfrac{\tau}{2\mu}C_1\mathbf{E}^n + \tfrac{\tau}{2\mu}C_2\mathbf{E}^{n+\frac{1}{2}}\big)\\
&= \mathbf{E}^n + \tfrac{\tau}{2\varepsilon}(C_1 - C_2)\mathbf{H}^n - \tfrac{\tau^2}{4\varepsilon}C_1\mu^{-1}C_1\mathbf{E}^n + \tfrac{\tau^2}{4\varepsilon}C_1\mu^{-1}C_2\mathbf{E}^{n+\frac{1}{2}}.
\end{aligned}$$

Here one applies partial derivatives to functions in $L^2(\mathbb{R}^3)$ so that from now on the equations for $\mathbf{E}^{n+\frac{1}{2}}$ and $\mathbf{E}^{n+1}$ hold in $H^{-1}(\mathbb{R}^3)^3$. This leads to the equivalent scheme

$$\begin{aligned}
\big(I - \tfrac{\tau^2}{4\varepsilon}C_1\mu^{-1}C_2\big)\mathbf{E}^{n+\frac{1}{2}} &= \mathbf{E}^n + \tfrac{\tau}{2\varepsilon}(C_1 - C_2)\mathbf{H}^n - \tfrac{\tau^2}{4\varepsilon}C_1\mu^{-1}C_1\mathbf{E}^n,\\
\mathbf{H}^{n+\frac{1}{2}} &= \mathbf{H}^n - \tfrac{\tau}{2\mu}C_1\mathbf{E}^n + \tfrac{\tau}{2\mu}C_2\mathbf{E}^{n+\frac{1}{2}}.
\end{aligned} \tag{6}$$

Similarly, the second half step can be transformed into

$$\begin{aligned}
\big(I - \tfrac{\tau^2}{4\varepsilon}C_2\mu^{-1}C_1\big)\mathbf{E}^{n+1} &= \mathbf{E}^{n+\frac{1}{2}} + \tfrac{\tau}{2\varepsilon}(C_1 - C_2)\mathbf{H}^{n+\frac{1}{2}} - \tfrac{\tau^2}{4\varepsilon}C_2\mu^{-1}C_2\mathbf{E}^{n+\frac{1}{2}},\\
\mathbf{H}^{n+1} &= \mathbf{H}^{n+\frac{1}{2}} + \tfrac{\tau}{2\mu}C_2\mathbf{E}^{n+\frac{1}{2}} - \tfrac{\tau}{2\mu}C_1\mathbf{E}^{n+1}.
\end{aligned} \tag{7}$$

The implicit parts are thus reduced to the products

$$\begin{aligned}
C_1\mu^{-1}C_2 &= \begin{pmatrix} \partial_2\mu^{-1}\partial_2 & 0 & 0\\ 0 & \partial_3\mu^{-1}\partial_3 & 0\\ 0 & 0 & \partial_1\mu^{-1}\partial_1 \end{pmatrix},\\
C_2\mu^{-1}C_1 &= \begin{pmatrix} \partial_3\mu^{-1}\partial_3 & 0 & 0\\ 0 & \partial_1\mu^{-1}\partial_1 & 0\\ 0 & 0 & \partial_2\mu^{-1}\partial_2 \end{pmatrix},
\end{aligned} \tag{8}$$

which are diagonal, such that the implicit steps are fully decoupled. Since each of the differential operators on the diagonal acts only on *one* of the spatial directions, the spatial discretization of (6) and (7) involves linear systems which are considerably smaller than the corresponding systems in the direct formulation (5). In Section 4.3 we extend this derivation to the case of the cuboid Q which is more involved due to the boundary conditions. We will see that the approximations given by (5) satisfy (6) and (7) in a weak sense.

3 Analysis of Maxwell's equations

In this section we show the well-posedness of the Maxwell systems (1) and (2) and establish certain additional regularity properties. Throughout, Ω denotes an open set in $\mathbb{R}^3$. We are given $\varepsilon, \mu \in L^\infty(\Omega)$ with $\varepsilon, \mu \geq \delta > 0$ for a constant $\delta > 0$. The state space $X = L^2(\Omega)^6$ is endowed with the weighted scalar product given by

$$((\mathbf{E}, \mathbf{H})|(u, v))_X = (\mathbf{E}|u)_\varepsilon + (\mathbf{H}|v)_\mu = \int_\Omega \varepsilon \mathbf{E} \cdot u \, \mathrm{d}x + \int_\Omega \mu \mathbf{H} \cdot v \, \mathrm{d}x \qquad (9)$$

which is equivalent to the standard scalar product in $L^2(\Omega)^6$ by our assumptions on ε and μ. We will further need the spaces

$$\begin{aligned} H(\mathrm{rot}) &= H(\mathrm{rot}, \Omega) = \{u \in L^2(\Omega)^3 \mid \mathrm{rot}\, u \in L^2(\Omega)^3\}, \\ H(\mathrm{div}) &= H(\mathrm{div}, \Omega) = \{u \in L^2(\Omega)^3 \mid \mathrm{div}\, u \in L^2(\Omega)\}. \end{aligned}$$

Since the differential operators are defined in distributional sense, it is straightforward to verify that rot and div are closed in $L^2(\Omega)^3$ if endowed with their "maximal" domains $H(\mathrm{rot}, \Omega)$ and $H(\mathrm{div}, \Omega)$, respectively. These spaces are thus complete if equipped with the graph norm of the respective operators. Often we will omit the spatial domain in the notation. We point out that $u \in H(\mathrm{rot})$ means that, e.g., $\partial_2 u_3 - \partial_3 u_2$ belongs to $L^2(\Omega)$ though the partial derivatives $\partial_2 u_3$ and $\partial_3 u_2$ do not need to be functions.

3.1 Well-posedness and regularity on the full space $\mathbb{R}^3$

We will first treat the full space setting ($\Omega = \mathbb{R}^3$) separately since this case is less technical and here the line of arguments is quite transparent. We first note that the space of test functions $C_c^\infty(\mathbb{R}^3)^3$ is dense in $H(\mathrm{rot}, \mathbb{R}^3)$ and $H(\mathrm{div}, \mathbb{R}^3)$, which can be seen by standard (scalar) cutoff functions and mollifiers. The equations

$$\begin{aligned} \int_{\mathbb{R}^3} \mathrm{rot}\, u \cdot \varphi \, \mathrm{d}x &= \int_{\mathbb{R}^3} u \cdot \mathrm{rot}\, \varphi \, \mathrm{d}x, \\ \int_{\mathbb{R}^3} \psi \, \mathrm{div}\, v \, \mathrm{d}x &= -\int_{\mathbb{R}^3} v \cdot \nabla \psi \, \mathrm{d}x \end{aligned} \qquad (10)$$

hold for test functions and hence for all $u, \varphi \in H(\mathrm{rot}, \mathbb{R}^3)$, $v \in H(\mathrm{div}, \mathbb{R}^3)$, and $\psi \in H^1(\mathbb{R}^3)$. To treat the Maxwell system, we further need the closed subspace

$$X_0 = \{(\mathbf{E}, \mathbf{H}) \in L^2(\mathbb{R}^3)^6 \mid \mathrm{div}(\varepsilon \mathbf{E}) = \mathrm{div}(\mu \mathbf{H}) = 0\}$$

of X. Recall the expression of the Maxwell operator M from (3). We endow this operator on X and its restriction M_0 to X_0 with the domains

$$D(M) = D_{\mathbb{R}^3}(M) = H(\mathrm{rot}, \mathbb{R}^3)^2, \qquad D(M_0) = D_{\mathbb{R}^3}(M_0) = D_{\mathbb{R}^3}(M) \cap X_0.$$

Here and below we usually omit the subscript indicating the spatial domain. Actually, only the operator M_0 is physically relevant, but sometimes also M is useful in the analysis. We next show the well-posedness of (1).

Proposition 3.1. *Let $\Omega = \mathbb{R}^3$ and $\varepsilon, \mu \in L^\infty(\mathbb{R}^3)$ satisfy $\varepsilon, \mu \geq \delta > 0$ for a constant $\delta > 0$. Then the Maxwell operators M and M_0 are skew-adjoint on X and X_0, and thus generate unitary C_0–groups $T(t) = e^{tM}$ on X and $T_0(t) = e^{tM_0}$ on X_0 for $t \in \mathbb{R}$, respectively. Therefore, for each $(\mathbf{E}^0, \mathbf{H}^0) \in D(M_0)$ we have a unique solution $(\mathbf{E}, \mathbf{H}) \in C^1(\mathbb{R}; L^2(\mathbb{R}^3)^6) \cap C(\mathbb{R}; D(M_0))$ of (1).*

Moreover, M maps $D(M)$ into X_0. Hence, $D(M_0^j) = D(M^j) \cap X_0$ and the operators $T_0(t)$ and $(\lambda I - M_0)^{-1}$ are the restrictions of $T(t)$ and $(\lambda I - M)^{-1}$ to X_0, for all $j \in \mathbb{N}$, $t \in \mathbb{R}$, and $\lambda \in \mathbb{R} \setminus \{0\}$.

Proof. We first note that M and M_0 are closed because of the closedness of rot and div. To show the skew-symmetry of M, we take $w = (\mathbf{E}, \mathbf{H})$ and $w' = (\mathbf{E}', \mathbf{H}')$ in $D(M)$. The integration by parts formula (10) then implies

$$\begin{aligned}
(Mw|w')_X &= (\tfrac{1}{\varepsilon} \operatorname{rot} \mathbf{H} | \mathbf{E}')_\varepsilon - (\tfrac{1}{\mu} \operatorname{rot} \mathbf{E} | \mathbf{H}')_\mu \\
&= \int_{\mathbb{R}^3} \operatorname{rot} \mathbf{H} \cdot \mathbf{E}' \, \mathrm{d}x - \int_{\mathbb{R}^3} \operatorname{rot} \mathbf{E} \cdot \mathbf{H}' \, \mathrm{d}x \\
&= \int_{\mathbb{R}^3} \mathbf{H} \cdot \operatorname{rot} \mathbf{E}' \, \mathrm{d}x - \int_{\mathbb{R}^3} \mathbf{E} \cdot \operatorname{rot} \mathbf{H}' \, \mathrm{d}x \\
&= -(\mathbf{H} | -\tfrac{1}{\mu} \operatorname{rot} \mathbf{E}')_\mu - (\mathbf{E} | \tfrac{1}{\varepsilon} \operatorname{rot} \mathbf{H}')_\varepsilon \\
&= -(w|Mw')_X,
\end{aligned}$$

and analogously for M_0.

By standard spectral theory, e.g., [20, Corollary to Theorem VIII.3], the operator M is skew-adjoint if $I \pm M$ has dense range. Skew-adjointness then implies the assertions about generation and well-posedness in view of Stone's theorem [20, Theorem VIII.8]. For given $(f, g) \in X$ we have to solve the equations

$$\mathbf{E} \pm \tfrac{1}{\varepsilon} \mathrm{rot} \mathbf{H} = f, \qquad \mathbf{H} \mp \tfrac{1}{\mu} \mathrm{rot} \mathbf{E} = g \tag{11}$$

with unknowns $\mathbf{E}, \mathbf{H} \in H(\mathrm{rot})$. It can be assumed that $g \in H(\mathrm{rot})$ because $H(\mathrm{rot})$ is dense in X. Formally inserting the second equation of (11) into the first one, we obtain the problem

$$\varepsilon \mathbf{E} + \mathrm{rot}(\tfrac{1}{\mu} \mathrm{rot} \mathbf{E}) = \varepsilon f \mp \mathrm{rot} g =: h \in L^2(\mathbb{R}^3)^3. \tag{12}$$

To solve this problem, we consider the symmetric bilinear form

$$a(u, v) = \int_{\mathbb{R}^3} (\varepsilon u \cdot v + \tfrac{1}{\mu} \operatorname{rot} u \cdot \operatorname{rot} v) \, \mathrm{d}x \tag{13}$$

on $H(\mathrm{rot})$. Observe that a is continuous and coercive. The Lax–Milgram lemma thus yields the existence of a field $\mathbf{E} \in H(\mathrm{rot})$ such that

$$\int_{\mathbb{R}^3} (\varepsilon \mathbf{E} \cdot v + \tfrac{1}{\mu} \operatorname{rot} \mathbf{E} \cdot \operatorname{rot} v) \, \mathrm{d}x = \int_{\mathbb{R}^3} h \cdot v \, \mathrm{d}x$$

holds for all $v \in H(\mathrm{rot})$. Since $h - \varepsilon \mathbf{E} \in L^2(\mathbb{R}^3)^3$, this fact implies that $\mathrm{rot}(\frac{1}{\mu}\,\mathrm{rot}\,\mathbf{E}) \in L^2(\mathbb{R}^3)^3$ and that $\mathbf{E}$ satisfies (12). If we now define $\mathbf{H} \in H(\mathrm{rot})$ by the second equation in (11), we obtain a solution $(\mathbf{E}, \mathbf{H}) \in D(M)$ of (11), as asserted.

Observe that $\mathrm{div}\,\mathrm{rot} = 0$ holds also in a distributional sense. If (f, g) in (11) belongs to X_0, we thus infer $(\mathbf{E}, \mathbf{H}) \in D(M) \cap X_0 = D(M_0)$. Hence, M_0 is skew-adjoint in X_0. We further have $MD(M) \subseteq X_0$, which in turn yields the assertions about the powers and the resolvent. The identity $T_0(t) = T(t)|_{X_0}$ then follows from the resolvent approximation of the semigroups, see Corollary III.5.5 in [6]. $\square$

Our approach relies on additional regularity properties of $D(M_0^2)$, proved in the following lemma. In principle this result is known, cf. Corollary IX.1.8 in [4], but we give the short and instructive proof for completeness. We write $f \in L^p(\mathbb{R}^3) + L^q(\mathbb{R}^3)$ if $f = f_1 + f_2$ with $f_1 \in L^p(\mathbb{R}^3)$ and $f_2 \in L^q(\mathbb{R}^3)$.

Lemma 3.2. *Let $\Omega = \mathbb{R}^3$ and $\varepsilon, \mu \in W^{1,\infty}(\mathbb{R}^3)$ with $\varepsilon, \mu \geq \delta > 0$ and $\partial_i \partial_j \varphi \in L^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for $\varphi \in \{\varepsilon, \mu\}$ and all $i, j \in \{1, 2, 3\}$. Then, it holds that $D(M_0^2) \hookrightarrow H^2(\mathbb{R}^3)^6$.*

Proof. Let $w = (\mathbf{E}, \mathbf{H}) \in D(M_0^2)$. Since ε and μ are Lipschitz and $\mathrm{div}(\varepsilon \mathbf{E}) = 0$, the function

$$\mathrm{div}\,\mathbf{E} = \mathrm{div}(\varepsilon^{-1}\varepsilon \mathbf{E}) = \varepsilon^{-1}\,\mathrm{div}(\varepsilon \mathbf{E}) + \nabla \varepsilon^{-1} \cdot \varepsilon \mathbf{E} = -\varepsilon^{-1} \nabla \varepsilon \cdot \mathbf{E} \tag{14}$$

is contained in $L^2(\mathbb{R}^3)$, and analogously for $\mathbf{H}$. We compute

$$\begin{aligned} \mathrm{rot}(\tfrac{1}{\mu}\,\mathrm{rot}\,\mathbf{E}) &= \nabla \mu^{-1} \times \mathrm{rot}\,\mathbf{E} + \mu^{-1}\,\mathrm{rot}\,\mathrm{rot}\,\mathbf{E} \qquad (15)\\ &= \nabla \mu^{-1} \times \mathrm{rot}\,\mathbf{E} + \mu^{-1}(-\Delta \mathbf{E} + \nabla\,\mathrm{div}\,\mathbf{E}) \\ &= -\mu^{-1} \Delta \mathbf{E} - \mu^{-2}\,\nabla \mu \times \mathrm{rot}\,\mathbf{E} - \mu^{-1}\,\nabla(\varepsilon^{-1} \nabla \varepsilon \cdot \mathbf{E}). \qquad (16) \end{aligned}$$

Note that the left hand side is equal to the first component of $-\varepsilon M^2 w$ and thus its norm in $L^2(\mathbb{R}^3)^3$ is bounded by $c\,\|M^2 w\|_X$. Moreover, $\|\mathrm{rot}\,\mathbf{E}\|_{L^2} \leq c\,\|Mw\|_X \leq c\,(\|w\|_X + \|M^2 w\|_X)$. Hence, $\Delta \mathbf{E}$ belongs to $H^{-1}(\mathbb{R}^3)^3 \supseteq \nabla L^2(\mathbb{R}^3)$. Standard elliptic regularity results [19, Proposition 5.9.1] now imply that $\mathbf{E} \in H^1(\mathbb{R}^3)^3$ and $\|\mathbf{E}\|_{H^1} \leq c\,(\|w\|_X + \|M^2 w\|_X)$. Sobolev's embedding theorem further yields $\mathbf{E} \in L^6(\mathbb{R}^3)^3$ so that the term $\nabla(\varepsilon^{-1} \nabla \varepsilon \cdot \mathbf{E})$ is contained in $L^2(\mathbb{R}^3)^3$ by the assumptions on ε. From (16) we then infer that $\Delta \mathbf{E} \in L^2(\mathbb{R}^3)$ and $\|\Delta \mathbf{E}\|_{L^2} \leq c\,(\|w\|_X + \|M^2 w\|_X)$. Again by elliptic regularity results [19, Proposition 5.9.1] it follows that $\mathbf{E} \in H^2(\mathbb{R}^3)^3$ and $\|\mathbf{E}\|_{H^2} \leq c\,(\|w\|_X + \|M^2 w\|_X)$. $\mathbf{H}$ can be treated in the same way. $\square$

3.2 Well-posedness and regularity on a Lipschitz domain

We state and prove the basic facts for a general open set $\Omega \subset \mathbb{R}^3$ with a bounded Lipschitz boundary $\partial\Omega \neq \emptyset$ (and specialize to $\Omega = Q$ later). In this case the set $C^\infty(\overline{\Omega})^3$ is dense in $H(\mathrm{rot}, \Omega)$ and $H(\mathrm{div}, \Omega)$, see Theorems IX.1.1

and IX.1.2 in [4]. We further need to explain the boundary conditions in (2). Let R be the restriction map to $\partial\Omega$. Due to Theorem IX.1.2 of [4], the tangential trace $u \mapsto Ru \times \nu$ (initially defined on $C^\infty(\overline{\Omega})^3$) extends to a bounded linear map from $H(\mathrm{rot})$ to $H^{-1/2}(\partial\Omega)^3$, which we still denote by $u \times \nu$ for simplicity. Moreover, we have the integration by parts formula

$$\int_\Omega u \cdot \operatorname{rot} \varphi \,\mathrm{d}x = \int_\Omega \varphi \cdot \operatorname{rot} u \,\mathrm{d}x + \langle u \times \nu, \varphi \rangle_{\partial\Omega} \quad \forall u \in H(\mathrm{rot}),\ \varphi \in H^1(\Omega)^3, \tag{17}$$

see (1.17) in Section IX.1 of [4]. Here the brackets designate the duality pairing between $H^{-1/2}(\partial\Omega)^3$ and $H^{1/2}(\partial\Omega)^3$ (and also between $H^{-1/2}(\partial\Omega)$ and $H^{1/2}(\partial\Omega)$). We remark that the trace operator γ maps $H^1(\Omega)$ onto $H^{1/2}(\partial\Omega)$ and that we usually write φ instead of $\gamma\varphi$.

Similarly, the normal trace $v \mapsto Rv \cdot \nu$ (defined on $C^\infty(\overline{\Omega})^3$) extends to a bounded linear map from $H(\mathrm{div})$ to $H^{-1/2}(\partial\Omega)$, denoted by $v \mapsto v \cdot \nu$. It also holds

$$\int_\Omega v \cdot \nabla\psi \,\mathrm{d}x = -\int_\Omega \psi \operatorname{div} v \,\mathrm{d}x + \langle v \cdot \nu, \psi \rangle_{\partial\Omega} \quad v \in H(\mathrm{div}),\ \psi \in H^1(\Omega), \tag{18}$$

see Theorem IX.1.1 in [4]. We further need the closed subspace

$$H_0(\mathrm{rot}) = H_0(\mathrm{rot}, \Omega) = \{u \in H(\mathrm{rot}, \Omega) \,|\, u \times \nu = 0 \ \text{ on } \partial\Omega\}$$

of $H(\mathrm{rot}, \Omega)$. By approximation, one can extend (17) to

$$\int_\Omega u \cdot \operatorname{rot} \varphi \,\mathrm{d}x = \int_\Omega \varphi \cdot \operatorname{rot} u \,\mathrm{d}x \quad \forall \varphi \in H(\mathrm{rot}),\ u \in H_0(\mathrm{rot}). \tag{19}$$

Test functions are dense in $H_0(\mathrm{rot})$ with respect to the norm in $H(\mathrm{rot})$, see Theorem IX.1.2 of [4]. The above traces of functions in $H(\mathrm{rot})$ and $H(\mathrm{div})$ are only distributions, in general, and thus a bit tricky. We add two technical remarks in this context which are needed below.

Remark 3.3. *Traces like $\mu\mathbf{H} \cdot \nu = 0$ as in (2) are defined for the product $\mu\mathbf{H} \in H(\mathrm{div})$. The product could be misleading here, as we do not claim that μ or $\mathbf{H}$ have a trace without further assumptions. However, if $\mu \in W^{1,\infty}(\Omega)$, $\mathbf{H} \in L^2(\Omega)^3$ and $\operatorname{div}(\mu\mathbf{H}) = 0$, then we derive $\mathbf{H} \in H(\mathrm{div})$ as in (14) so that the trace $\nu \cdot \mathbf{H}$ exists in $H^{-1/2}(\partial\Omega)$. To determine the trace, we take $\varphi \in H^1(\Omega)$ and set $\psi := \mu^{-1}\varphi \in H^1(\Omega)$. Formula (18) yields*

$$\begin{aligned}\langle \mathbf{H} \cdot \nu, \varphi \rangle_{\partial\Omega} = \langle \mathbf{H} \cdot \nu, \mu\psi \rangle_{\partial\Omega} &= \int_\Omega \big(\mu\psi \operatorname{div} \mathbf{H} + \nabla(\mu\psi) \cdot \mathbf{H}\big) \,\mathrm{d}x \\ &= \int_\Omega \big(\psi \operatorname{div}(\mu\mathbf{H}) + \nabla\psi \cdot \mu\mathbf{H}\big) \,\mathrm{d}x = \langle \mu\mathbf{H} \cdot \nu, \psi \rangle_{\partial\Omega}.\end{aligned}$$

For $\mu \in W^{1,\infty}(\Omega)$, the boundary condition $\mu\mathbf{H} \cdot \nu = 0$ is thus equivalent to $\mathbf{H} \cdot \nu = 0$. In a similar way, for $\mathbf{H} \in H^1(\Omega)^3$ and $\mu \in W^{1,\infty}(\Omega)$ one shows that the trace of $\mu\mathbf{H}$ is the product of the traces of μ and $\mathbf{H}$, where all traces are functions.

Remark 3.4. *One can restrict the traces in $H(\mathrm{rot})$ and $H(\mathrm{div})$ to relatively open subsets Γ_0 of $\partial\Omega$. To this aim, let $\Gamma_0, \Gamma_1 \subset \partial\Omega$ be disjoint and relatively open with $\overline{\Gamma_0} \cup \overline{\Gamma_1} = \partial\Omega$ such that $\partial\Gamma_0$ and $\partial\Gamma_1$ have surface measure 0 in $\partial\Omega$. Let $H^1_{\Gamma_1}(\Omega)^3$ be the subspace of functions $\varphi \in H^1(\Omega)^3$ whose traces vanish on Γ_1 (as an element of $L^2(\partial\Omega)^3$). The restriction $\phi_{|\Gamma_0}$ of a functional $\phi \in H^{-\frac{1}{2}}(\partial\Omega)^3$ to Γ_0 is defined as the restriction of ϕ to $H^1_{\Gamma_1}(\Omega)^3$. We also note that if $\phi_{|\Gamma_0}$ has a continuous extension to $L^2(\Gamma_0)^3$, then this extension is uniquely determined since $\gamma H^1_{\Gamma_1}(\Omega)^3$ is dense in $L^2(\Gamma_0)^3$ (and a subspace of $H^{\frac{1}{2}}(\Gamma_0)^3$), see Remarks 13.6.13 and 13.6.14 in [23].*

For the investigation of (2), we use the state spaces $X = L^2(\Omega)^6$ and

$$X_0 = \{(\mathbf{E},\mathbf{H}) \in L^2(\Omega)^6 \mid \operatorname{div}(\varepsilon\mathbf{E}) = \operatorname{div}(\mu\mathbf{H}) = 0,\ \mu\mathbf{H}\cdot\nu = 0 \text{ on } \partial\Omega\}$$

with the scalar product given by (9). The subspace X_0 is closed in X due to the closedness of div and the continuity of the normal trace. The *Maxwell operator* is now defined by

$$M = \begin{pmatrix} 0 & \frac{1}{\varepsilon}\mathrm{rot} \\ -\frac{1}{\mu}\mathrm{rot} & 0 \end{pmatrix}, \qquad D(M) = D_\Omega(M) = H_0(\mathrm{rot},\Omega) \times H(\mathrm{rot},\Omega) \quad (20)$$

in X. In view of (2), we mainly work with the restriction M_0 of M to the domain

$$D(M_0) = D_\Omega(M_0) = D_\Omega(M) \cap X_0.$$

We see in the next result that M maps $D(M)$ into X_0 and will thus consider M_0 as an operator in X_0.

Proposition 3.5. *Let $\Omega \subset \mathbb{R}^3$ be open with a bounded Lipschitz boundary $\partial\Omega \neq \emptyset$ and let $\varepsilon, \mu \in L^\infty(\Omega)$ satisfy $\varepsilon, \mu \geq \delta > 0$ for a constant $\delta > 0$. Then the Maxwell operators M and M_0 are skew-adjoint on X and X_0, and thus generate unitary C_0–groups $T(t) = e^{tM}$ on X and $T_0(t) = e^{tM_0}$ on X_0 for $t \in \mathbb{R}$, respectively. Therefore, for each $(\mathbf{E}^0, \mathbf{H}^0) \in D(M_0)$ we have a unique solution $(\mathbf{E},\mathbf{H}) \in C^1(\mathbb{R}; X_0) \cap C(\mathbb{R}; D(M_0))$ of (2).*

Moreover, M maps $D(M)$ into X_0. Hence, $D(M_0^j) = D(M^j) \cap X_0$ and the operators $T_0(t)$ and $(\lambda I - M_0)^{-1}$ are the restrictions of $T(t)$ and $(\lambda I - M)^{-1}$ to X_0, for all $j \in \mathbb{N}$, $t \in \mathbb{R}$, and $\lambda \in \mathbb{R} \setminus \{0\}$.

Proof. We first show that M maps $D(M)$ into X_0. In fact, the divergence conditions follow from $\operatorname{div}\mathrm{rot} = 0$. Moreover, $\mathrm{rot}\,\mathbf{E}$ thus possesses a normal trace if $(\mathbf{E},\mathbf{H}) \in D(M)$. Let $\varphi \in H^2(\Omega)$. The equations (18) and (17) then yield

$$\begin{aligned}\langle \nu\cdot\mathrm{rot}\,\mathbf{E}, \varphi\rangle_{\partial\Omega} &= -\int_\Omega \varphi \operatorname{div}\mathrm{rot}\,\mathbf{E}\,\mathrm{d}x + \langle \nu\cdot\mathrm{rot}\,\mathbf{E}, \varphi\rangle_{\partial\Omega} = \int_\Omega \mathrm{rot}\,\mathbf{E}\cdot\nabla\varphi\,\mathrm{d}x \\ &= \int_\Omega \mathbf{E}\cdot\mathrm{rot}\,\nabla\varphi\,\mathrm{d}x - \langle \mathbf{E}\times\nu, \nabla\varphi\rangle_{\partial\Omega} = 0,\end{aligned}$$

since $\operatorname{rot}\nabla = 0$ and $\mathbf{E} \in H_0(\operatorname{rot})$. By approximation, we deduce that $\langle \nu \cdot \operatorname{rot}\mathbf{E}, \varphi\rangle_{\partial\Omega} = 0$ for all $\varphi \in H^1(\Omega)$, and hence $\nu \cdot \mu\frac{1}{\mu}\operatorname{rot}\mathbf{E} = \nu \cdot \operatorname{rot}\mathbf{E} = 0$ as asserted.

The operators M and M_0 are closed in X and X_0, respectively, because of the closedness of X_0 and rot in X and the continuity of the tangential trace.

As in the proof of Proposition 3.1, one derives the skew-symmetry of M and M_0 now using (19). To show the range condition, one again employs the symmetric form $a(\cdot,\cdot)$ from (13) (with Ω instead of $\mathbb{R}^3$) which is defined on $H_0(\operatorname{rot},\Omega)$ this time. The remaining assertions then follow as in the proof of Proposition 3.1. □

We now come back to the special case $Q = (a_1^-, a_1^+) \times (a_2^-, a_2^+) \times (a_3^-, a_3^+)$. To transfer Lemma 3.2 to the present setting, we have to work much harder because of the boundary conditions. We need an auxiliary result ensuring H^2 regularity of the Laplacian on Q with mixed boundary conditions. It is surely known to experts, but since we could not detect a proof in the literature we present it in the appendix.

We employ the isometric isomorphisms

$$\begin{aligned} D_1 = \{v \in L^2(Q) \,|\, \partial_1 v \in L^2(Q)\} &\cong L^2((a_2^-, a_2^+) \times (a_3^-, a_3^+); H^1(a_1^-, a_1^+)) \\ &\cong H^1((a_1^-, a_1^+); L^2((a_2^-, a_2^+) \times (a_3^-, a_3^+))), \end{aligned}$$

and their analogues for ∂_2 and ∂_3 which follow easily from the corresponding isomorphisms with H^1 replaced by L^2. As a result, a function in D_1 has traces to $\Gamma_1^\pm$ that belong to $L^2((a_2^-, a_2^+) \times (a_3^-, a_3^+))$. The space $H^1_\Gamma(Q)$ is defined as in Remark 3.4.

Lemma 3.6. *Let Γ be a union of some of the six open faces of Q, Γ' be the union of the remaining open faces. Let $f \in L^2(Q)$. Then there is a unique function $v \in H^1_\Gamma(Q)$ such that*

$$\int_Q v\varphi \,\mathrm{d}x + \int_Q \nabla v \cdot \nabla\varphi \,\mathrm{d}x = \int_Q f\varphi \,\mathrm{d}x \qquad \text{for all} \quad \varphi \in H^1_\Gamma(Q). \tag{21}$$

Morever, the function v belongs to $D := \{v \in H^2(Q) \cap H^1_\Gamma(Q) \,|\, \partial_\nu v = 0 \text{ on } \Gamma'\}$ and $v - \Delta v = f$. Finally, the H^2–norm and the graph norm of Δ are equivalent on D.

The following results about regularity and boundary traces for $(\mathbf{E},\mathbf{H}) \in D(M_0^2)$ are crucial for our error analysis. As in Lemma 3.2 we need some smoothness of the coefficients. The regularity of the fields seem also to follow if one applies Theorem 4.8 of [3] to $\varepsilon\mathbf{E}$ and $\mu\mathbf{H}$ (cf. Paragraph 4.4.2 in [3]). However, the results in [3] are obtained in a framework of an elaborate study of singularities of time harmonic Maxwell equations in general polyhedral domains. In our opinion it is very useful to include a rather short, direct proof for the non-singular situation of a cuboid, which is given in the appendix.

Lemma 3.7. *Let $\varepsilon, \mu \in W^{1,\infty}(Q)$ with $\varepsilon, \mu \geq \delta > 0$ and $\partial_i \partial_j \varphi \in L^3(Q)$ for $\varphi \in \{\varepsilon, \mu\}$ and for all $i, j \in \{1, 2, 3\}$. It then holds $D(M_0^2) \hookrightarrow H^2(Q)^6$ and $(\mathbf{E}, \mathbf{H}) \in D(M_0^2)$ has the traces*

$$
\begin{aligned}
&\text{on } \Gamma_1^{\pm}: \quad E_2 = E_3 = 0, \quad \partial_2 E_2 = \partial_3 E_2 = \partial_2 E_3 = \partial_3 E_3 = 0,\\
&\text{on } \Gamma_2^{\pm}: \quad E_1 = E_3 = 0, \quad \partial_1 E_1 = \partial_3 E_1 = \partial_1 E_3 = \partial_3 E_3 = 0,\\
&\text{on } \Gamma_3^{\pm}: \quad E_1 = E_2 = 0, \quad \partial_1 E_1 = \partial_2 E_1 = \partial_1 E_2 = \partial_2 E_2 = 0,\\
&\text{on } \Gamma_1^{\pm}: \quad H_1 = 0, \quad \partial_2 H_1 = \partial_3 H_1 = 0,\\
&\text{on } \Gamma_2^{\pm}: \quad H_2 = 0, \quad \partial_1 H_2 = \partial_3 H_2 = 0,\\
&\text{on } \Gamma_3^{\pm}: \quad H_3 = 0, \quad \partial_1 H_3 = \partial_2 H_3 = 0.
\end{aligned}
$$

4 Error analysis

For the analysis of the splitting scheme (4), we define the operators

$$\Lambda_j(\tau) w = \frac{1}{\tau^j \, (j-1)!} \int_0^\tau (\tau - s)^{j-1} T_0(s) w \, \mathrm{d}s \tag{22}$$

for $j \in \mathbb{N}$, $\tau > 0$ and $w \in X_0$; cf. [13]. It can be checked that $\|\Lambda_j(\tau)\|_{X_0} \leq 1/(j!) \leq 1$. Setting $\Lambda_0(\tau) = T_0(\tau)$, one easily shows that

$$\tau M_0 \Lambda_{j+1}(\tau) w = \Lambda_j(\tau) w - \tfrac{1}{j!}\, w$$

for all $w \in D(M_0)$, $\tau > 0$ and $j \in \mathbb{N}_0$. In particular,

$$\Lambda_0 = I + \tau M_0 \Lambda_1 = I + \tau M_0 + \tau^2 M_0^2 \Lambda_2 = I + \tau M_0 + \tfrac{1}{2} \tau^2 M_0^2 + \tau^3 M_0^3 \Lambda_3 \tag{23}$$

on $D(M_0^3)$, with $\Lambda_j := \Lambda_j(\tau)$.

4.1 Splitting for Maxwell's equations on $\mathbb{R}^3$

The Peaceman–Rachford scheme (4) involves resolvents and Cayley transforms of τA and τB. For the stability of the scheme, these operators should be contractive which requires the dissipativity of A and B. Actually, we can prove even their skew-adjointness without assuming extra regularity for ε and μ. We point out that A and B act on X and not on X_0.

Lemma 4.1. *Let $\varepsilon, \mu \in L^\infty(\mathbb{R}^3)$ with $\varepsilon, \mu \geq \delta > 0$. Then A and B are skew-adjoint in X, and hence the operators $(I - \tau A)^{-1}$, $(I - \tau B)^{-1}$, $(I + \tau A)(I - \tau A)^{-1}$ and $(I + \tau B)(I - \tau B)^{-1}$ are contractive in X for each $\tau > 0$.*

Proof. We only consider A since the proof for B is analogous. We will show that A is skew-symmetric and that $I \pm A$ has dense range. Clearly, A is closed. The skew-adjointness of A then follows, which implies the other properties. Let $(u, v), (\varphi, \psi) \in D(A)$. Integrating by parts, we deduce

$$(A(u, v) | (\varphi, \psi))_X = (\varepsilon^{-1} C_1 v | \varphi)_\varepsilon + (\mu^{-1} C_2 u | \psi)_\mu \tag{24}$$

$$= \int_{\mathbb{R}^3} \Big((\partial_2 v_3\, \varphi_1 + \partial_3 v_1\, \varphi_2 + \partial_1 v_2\, \varphi_3) + (\partial_3 u_2\, \psi_1 + \partial_1 u_3\, \psi_2 + \partial_2 u_1\, \psi_3) \Big) \mathrm{d}x$$
$$= -\int_{\mathbb{R}^3} \big(v_3\, \partial_2 \varphi_1 + v_1\, \partial_3 \varphi_2 + v_2\, \partial_1 \varphi_3 + u_2\, \partial_3 \psi_1 + u_3\, \partial_1 \psi_2 + u_1\, \partial_2 \psi_3 \big)\, \mathrm{d}x$$
$$= -\int_{\mathbb{R}^3} (\varepsilon u \cdot \tfrac{1}{\varepsilon} C_1 \psi + \mu v \cdot \tfrac{1}{\mu} C_2 \varphi)\, \mathrm{d}x = -((u,v) | A(\varphi,\psi))_X.$$

To check the range condition, we take $(\varphi,\psi) \in X$ such that $\partial_2\psi_3$, $\partial_3\psi_1$ and $\partial_1\psi_2$ belong to $L^2(Q)^3$. We then look for $(\mathbf{E},\mathbf{H}) \in D(A)$ such that $(\mathbf{E},\mathbf{H}) \pm A(\mathbf{E},\mathbf{H}) = (\varphi,\psi)$. Reordering the lines, we write these equations as

$$\begin{aligned} E_1 \pm \tfrac{1}{\varepsilon}\, \partial_2 H_3 &= \varphi_1, \qquad & H_3 \pm \tfrac{1}{\mu}\, \partial_2 E_1 &= \psi_3, \\ E_2 \pm \tfrac{1}{\varepsilon}\, \partial_3 H_1 &= \varphi_2, \qquad & H_1 \pm \tfrac{1}{\mu}\, \partial_3 E_2 &= \psi_1, \\ E_3 \pm \tfrac{1}{\varepsilon}\, \partial_1 H_2 &= \varphi_3, \qquad & H_2 \pm \tfrac{1}{\mu}\, \partial_1 E_3 &= \psi_2. \end{aligned}$$

Formally, we insert the equations in the second column in the corresponding ones in the first column and multiply by ε, arriving at

$$\begin{aligned} \varepsilon E_1 - \partial_2(\tfrac{1}{\mu}\, \partial_2 E_1) &= \varepsilon\varphi_1 \mp \partial_2\psi_3 =: f_1 \in L^2(Q), \\ \varepsilon E_2 - \partial_3(\tfrac{1}{\mu}\, \partial_3 E_2) &= \varepsilon\varphi_2 \mp \partial_3\psi_1 =: f_2 \in L^2(Q), \\ \varepsilon E_3 - \partial_1(\tfrac{1}{\mu}\, \partial_1 E_3) &= \varepsilon\varphi_3 \mp \partial_1\psi_2 =: f_3 \in L^2(Q). \end{aligned}$$

We now start to solve these equations. To this aim, we introduce the operator $D_j = \partial_j \frac{1}{\mu}\, \partial_j$ with domain

$$D(D_j) = \{ u \in L^2(\mathbb{R}^3)^3 \,|\, \partial_j u, D_j u \in L^2(\mathbb{R}^3)^3 \}$$

with $j = 1,2,3$. Using Lax–Milgram, one obtains functions $E_{k(j)} \in D(D_j)$ such that $\varepsilon E_{k(j)} - D_{k(j)} E_{k(j)} = f_{k(j)}$, with $k(1) = 3$, $k(2) = 1$ and $k(3) = 2$. We then define

$$H_1 = \mp \tfrac{1}{\mu}\, \partial_3 E_2 + \psi_1, \qquad H_2 = \mp \tfrac{1}{\mu}\, \partial_1 E_3 + \psi_2, \qquad H_3 = \mp \tfrac{1}{\mu}\, \partial_2 E_1 + \psi_3.$$

Hence, $(\mathbf{E},\mathbf{H})$ belongs to $D(A)$ and satisfies $(\mathbf{E},\mathbf{H}) \pm A(\mathbf{E},\mathbf{H}) = (\varphi,\psi)$. □

We now state our convergence result for the full space. We point out that the convergence estimate is of second order and that it is proportional to a 'third order norm' (the graph norm of M_0^3) of the initial value, cf. Section 4.4.

Theorem 4.2. *Let $\varepsilon,\mu \in W^{1,\infty}(\mathbb{R}^3)$ with $\varepsilon,\mu \geq \delta > 0$ and $\partial_i\partial_j\varepsilon, \partial_i\partial_j\mu \in L^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for all $i,j \in \{1,2,3\}$. Then there is a constant $c > 0$ such that the splitting operator S_τ defined in (4) satisfies*

$$\|S_\tau^n w - T_0(n\tau) w\|_{L^2} \leq c t_{\mathrm{end}} \tau^2 (\|w\|_{L^2} + \|M_0^3 w\|_{L^2})$$

for all $w = (\mathbf{E},\mathbf{H}) \in D(M^3) \cap X_0 = D(M_0^3)$, $n \in \mathbb{N}$, $\tau > 0$ and $t_{\mathrm{end}} > 0$ with $n\tau \leq t_{\mathrm{end}}$.

Proof. Our proof is based on a formula for the difference $S_\tau^n - T_0(\tau n)$ which was established in the proof of Theorem 3.2 of [13] for the case that A, B and M_0 act on the same spaces. We fix $\tau > 0$ and $w \in D(M^3) \cap X_0$. Then $M_0^k \Lambda_j(\tau)w$ belongs to $D(M_0^{3-k}) \subset D(AB) \cap D(A)$ for $k = 0, 1$ and $j \in \mathbb{N}_0$ by Lemma 3.2 and the definition (22) of $\Lambda_j(\tau)$. We set $R_A = (I - \frac{\tau}{2}A)^{-1}$ and $R_B = (I - \frac{\tau}{2}B)^{-1}$. Recall that $Aw + Bw = M_0 w$. Using the formulas (23) for $\Lambda_0(\tau) = T_0(\tau)$, we compute

$$\begin{aligned}
S_\tau w - T_0(\tau)w &= R_B R_A \Big[(I + \tfrac{\tau}{2}A)(I + \tfrac{\tau}{2}B) - (I - \tfrac{\tau}{2}A)(I - \tfrac{\tau}{2}B)T_0(\tau)\Big]w \\
&= R_B R_A \Big[I + \tfrac{\tau}{2}M_0 + \tfrac{\tau^2}{4}AB - (I - \tfrac{\tau}{2}M_0 + \tfrac{\tau^2}{4}AB)\Lambda_0(\tau)\Big]w \\
&= R_B R_A \Big[I - \Lambda_0(\tau) + \tfrac{\tau}{2}M_0(I + \Lambda_0(\tau)) + \tfrac{\tau^2}{4}AB(I - \Lambda_0(\tau))\Big]w \\
&= R_B R_A \Big[-\tau M_0 - \tfrac{\tau^2}{2}M_0^2 - \tau^3 M_0^3 \Lambda_3(\tau) + \tfrac{\tau}{2}M_0(2 + \tau M_0 \\
&\qquad + \tau^2 M_0^2 \Lambda_2(\tau)) - \tfrac{\tau^3}{4}ABM_0\Lambda_1(\tau)\Big]w \\
&= \tau^3 R_B R_A \big[(\tfrac{1}{2}\Lambda_2(\tau) - \Lambda_3(\tau))M_0^3 - \tfrac{1}{4}ABM_0\Lambda_1(\tau)\big]w.
\end{aligned}$$

A telescoping sum then leads to

$$\begin{aligned}
S_\tau^n w - T_0(n\tau)w &= \sum_{j=0}^{n-1} S_\tau^{n-j-1}(S_\tau - T_0(\tau))T_0(j\tau)w \qquad (25)\\
&= \tau^3 \sum_{j=0}^{n-1} S_\tau^{n-j-1}(I - \tfrac{\tau}{2}B)^{-1}(I - \tfrac{\tau}{2}A)^{-1}[\tfrac{1}{2}\Lambda_2(\tau) - \Lambda_3(\tau)]T_0(j\tau)M_0^3 w \\
&\quad - \frac{\tau^3}{4}\sum_{j=0}^{n-1} S_\tau^{n-j-1}(I - \tfrac{\tau}{2}B)^{-1}(I - \tfrac{\tau}{2}A)^{-1}AB(I - M_0)^{-2}\Lambda_1(\tau)T_0(j\tau)w'
\end{aligned}$$

with $w' = (I - M_0)^2 M_0 w$. Lemmas 3.2 and 4.1 and the contractivity of $\Lambda_j(\tau)$ and $T_0(t)$ now imply the assertion. □

4.2 Splitting for Maxwell's equations on the cuboid Q

We first note that the boundary conditions in $D_Q(A)$ and $D_Q(B)$ are well defined in view of the discussion before Lemma 3.6. Moreover, the traces appearing in the definition of $D_Q(A)$ and $D_Q(B)$ are continuous from the respective domain into the L^2 space on the relevant face due to this discussion. As a result, A and B are closed in X. Again we can show their skew–adjointness.

Lemma 4.3. *Let $\varepsilon, \mu \in L^\infty(Q)$ with $\varepsilon, \mu \geq \delta > 0$. Then A and B are skew-adjoint in X, and hence the operators $(I - \tau A)^{-1}$, $(I - \tau B)^{-1}$, $(I + \tau A)(I - \tau A)^{-1}$ and $(I + \tau B)(I - \tau B)^{-1}$ are contractive in X for each $\tau > 0$.*

Proof. The proof is almost identical to that of Lemma 4.1. One can repeat the calculations in (24) on the spatial domain Q since all boundary terms in the integration by parts vanish thanks to the boundary conditions in $D_Q(A)$. Hence, A is skew-symmetric. In the proof of the range condition we only have to change the domain of D_j into

$$D(D_j) = \{u \in L^2(Q)^3 \,|\, \partial_j u, D_j u \in L^2(Q)^3,\ u = 0 \text{ on } \Gamma_j^\pm\}.$$

One then finishes the proof as in Lemma 4.1 □

Since both AB and M_0 are of second order, one may expect that $AB(I - M_0)^{-2}$ is bounded. This crucial fact directly follows from Lemma 3.7 which gives the needed H^2 regularity and boundary conditions for $w \in D(M_0^2)$.

Proposition 4.4. *Let $\varepsilon, \mu \in W^{1,\infty}(Q)$ with $\varepsilon, \mu \geq \delta > 0$ and $\partial_i \partial_j \varphi \in L^3(Q)$ for $\varphi \in \{\varepsilon, \mu\}$ and all $i, j \in \{1, 2, 3\}$. Then $D(M_0^2) = D(M^2) \cap X_0 \hookrightarrow H^2(Q)^6 \cap D(AB) \cap D(A)$ and $AB(I - M_0)^{-2} : X_0 \to X$ is bounded.*

Using the above proposition and $D(A) \cap D(B) \subseteq D(M)$, one can now establish our main convergence result on Q exactly as for $\mathbb{R}^3$.

Theorem 4.5. *Let $\varepsilon, \mu \in W^{1,\infty}(Q)$ with $\varepsilon, \mu \geq \delta > 0$ and $\partial_i \partial_j \varepsilon, \partial_i \partial_j \mu \in L^3(Q)$ for all $i, j \in \{1, 2, 3\}$. Then there is a constant $c > 0$ such that the splitting operator S_τ defined in (4) satisfies*

$$\|S_\tau^n w - T_0(n\tau) w\|_{L^2} \leq c t_{\text{end}} \tau^2 (\|w\|_{L^2} + \|M_0^3 w\|_{L^2}$$

for all $w = (\mathbf{E}, \mathbf{H}) \in D(M^3) \cap X_0 = D(M_0^3)$, $n \in \mathbb{N}$, $\tau > 0$ and $t_{\text{end}} > 0$ with $n\tau \leq t_{\text{end}}$.

4.3 Equivalence of the efficient reformulation of the method on the cuboid Q

In order to extend the efficient scheme from Section 2.3 to the case with boundary conditions, we use weak formulations of (6) and (7). We introduce the relevant test function spaces

$$\begin{aligned} Y_1 = \{u \in L^2(Q)^3 \,|\, &\partial_3 u_1, \partial_1 u_2, \partial_2 u_3 \in L^2(Q)^3; \\ &u_1 = 0 \text{ on } \Gamma_3^\pm,\quad u_2 = 0 \ \text{ on } \Gamma_1^\pm, u_3 = 0 \ \text{ on } \Gamma_2^\pm\}, \\ Y_2 = \{u \in L^2(Q)^3 \,|\, &\partial_2 u_1, \partial_3 u_2, \partial_1 u_3 \in L^2(Q)^3; \\ &u_1 = 0 \ \text{ on } \Gamma_2^\pm,\quad u_2 = 0 \ \text{ on } \Gamma_3^\pm, u_3 = 0 \ \text{ on } \Gamma_1^\pm\}. \end{aligned}$$

Observe that for $(u, \tilde{u}) \in D(A)$, $(v, \tilde{v}) \in D(B)$ and $\varphi \in Y_j$, we have $u \in Y_2$, $v \in Y_1$ and $C_j \varphi \in L^2(Q)^3$. Integration by parts shows that

$$\int_Q C_2 u \cdot \psi \,\mathrm{d}x = -\int_Q u \cdot C_1 \psi \,\mathrm{d}x, \qquad \int_Q C_1 v \cdot \varphi \,\mathrm{d}x = -\int_Q v \cdot C_2 \varphi \,\mathrm{d}x \quad (26)$$

for all $u \in Y_2$, $v \in Y_1$ and $\varphi, \psi \in L^2(Q)^3$ with $C_1 \psi, C_2 \varphi \in L^2(Q)^3$. In the next result, we use the weak versions of the differential operators in (8).

Proposition 4.6. *Let $\varepsilon, \mu \in W^{1,\infty}(Q)$ with $\varepsilon, \mu \geq \delta > 0$ and $\partial_i\partial_j\varepsilon, \partial_i\partial_j\mu \in L^3(Q)$ for all $i, j \in \{1, 2, 3\}$, and let $(\mathbf{E}^0, \mathbf{H}^0) \in D(M^3) \cap X_0$. We consider the approximations given by (5). Then, $(u, v) = (\mathbf{E}^{n+\frac{1}{2}}, \mathbf{H}^{n+\frac{1}{2}})$ is the unique solution in $D(A)$ of the decoupled system*

$$\begin{aligned}(u|\varphi)_\varepsilon + \tfrac{\tau^2}{4}\,(\tfrac{1}{\mu}C_2u|\tfrac{1}{\varepsilon}C_2\varphi)_\varepsilon &= (\mathbf{E}^n|\varphi)_\varepsilon - \tfrac{\tau}{2}\,(\mathbf{H}^n|\tfrac{1}{\varepsilon}C_2\varphi)_\varepsilon - \tfrac{\tau}{2}\,(\tfrac{1}{\mu}C_2\mathbf{H}^n|\varphi)_\mu \\ &\quad + \tfrac{\tau^2}{4}\,(\tfrac{1}{\mu}C_1\mathbf{E}^n|\tfrac{1}{\varepsilon}C_2\varphi)_\varepsilon \qquad \forall\ \varphi \in Y_2, \qquad (27)\\ v &= H^n - \tfrac{\tau}{2\mu}C_1\mathbf{E}^n + \tfrac{\tau}{2\mu}C_2u. \qquad (28)\end{aligned}$$

Moreover, $(u, v) = (\mathbf{E}^{n+1}, \mathbf{H}^{n+1})$ is the unique solution in $D(B)$ of the decoupled system

$$\begin{aligned}(u|\psi)_\varepsilon + \tfrac{\tau^2}{4}(\tfrac{1}{\mu}C_1u|\tfrac{1}{\varepsilon}C_1\psi)_\varepsilon &= (\mathbf{E}^{n+\frac{1}{2}}|\psi)_\varepsilon + \tfrac{\tau}{2}(\mathbf{H}^{n+\frac{1}{2}}|\tfrac{1}{\varepsilon}C_1\psi)_\varepsilon + \tfrac{\tau}{2}(\tfrac{1}{\mu}C_1\mathbf{H}^{n+\frac{1}{2}}|\psi)_\mu \\ &\quad + \tfrac{\tau^2}{4}\,(\tfrac{1}{\mu}C_2\mathbf{E}^{n+\frac{1}{2}}|\tfrac{1}{\varepsilon}C_1\psi)_\varepsilon \qquad \forall\ \psi \in Y_1, \qquad (29)\\ v &= \mathbf{H}^{n+\frac{1}{2}} + \tfrac{\tau}{2\mu}C_2\mathbf{E}^{n+\frac{1}{2}} - \tfrac{\tau}{2\mu}C_1u. \qquad (30)\end{aligned}$$

Proof. We focus on the first halfstep (27) since the second one can be treated in the same way. Let $(\varphi, \psi) \in D(A)$, i.e., $\varphi \in Y_2$ and $C_1\psi \in L^2(Q)^3$. First, a standard application of Lax–Milgram gives a solution $u \in Y_2$ of (27) for each $(\mathbf{E}^n, \mathbf{H}^n) \in D(B)$. We then define $v \in L^2(Q)^3$ by (28). Taking the ε–scalar product of (28) with $\frac{\tau}{2\varepsilon}C_2\varphi$ and adding it to the equation for u, we deduce

$$(u|\varphi)_\varepsilon + \tfrac{\tau}{2}\,(v|\tfrac{1}{\varepsilon}C_2\varphi)_\varepsilon = (\mathbf{E}^n|\varphi)_\varepsilon - \tfrac{\tau}{2}\,(\tfrac{1}{\mu}C_2\mathbf{H}^n|\varphi)_\mu,$$

which yields

$$(u|\varphi)_\varepsilon + \tfrac{\tau}{2}\,(v|\tfrac{1}{\mu}C_2\varphi)_\mu = (\mathbf{E}^n|\varphi)_\varepsilon - \tfrac{\tau}{2}\,(\tfrac{1}{\varepsilon}C_2\mathbf{H}^n|\varphi)_\varepsilon. \qquad (31)$$

We further take the μ–scalar product of (28) with ψ and obtain

$$\begin{aligned}(v|\psi)_\mu - \tfrac{\tau}{2}\,(C_2u|\psi) &= (\mathbf{H}^n|\psi)_\mu - \tfrac{\tau}{2}\,(\tfrac{1}{\mu}C_1\mathbf{E}^n|\psi)_\mu,\\ (v|\psi)_\mu + \tfrac{\tau}{2}\,(u|\tfrac{1}{\varepsilon}C_1\psi)_\varepsilon &= (\mathbf{H}^n|\psi)_\mu - \tfrac{\tau}{2}\,(\tfrac{1}{\mu}C_1\mathbf{E}^n|\psi)_\mu, \qquad (32)\end{aligned}$$

where we use (26). The sum of (31) and (32) can be written as

$$\big((u, v)|(I + \tfrac{\tau}{2}A)(\varphi, \psi)\big)_X = \big((I + \tfrac{\tau}{2}B)(\mathbf{E}^n, \mathbf{H}^n)|(\varphi, \psi)\big)_X$$

for all $(\varphi, \psi) \in D(A)$. On the other hand, (5) and Lemma 4.3 imply that

$$\big((\mathbf{E}^{n+\frac{1}{2}}, \mathbf{H}^{n+\frac{1}{2}})|(I + \tfrac{\tau}{2}A)(\varphi, \psi)\big)_X = \big((I + \tfrac{\tau}{2}B)(\mathbf{E}^n, \mathbf{H}^n)|(\varphi, \psi)\big)_X$$

holds for all $(\varphi, \psi) \in D(A)$. The difference $(\mathbf{E}^{n+\frac{1}{2}} - u, \mathbf{H}^{n+\frac{1}{2}} - v) \in X$ thus belongs to the kernel of $(I + \frac{\tau}{2}A)^* = (I - \frac{\tau}{2}A)$ which is trivial. Consequently, $(\mathbf{E}^{n+\frac{1}{2}}, \mathbf{H}^{n+\frac{1}{2}}) \in D(A)$ satisfies (27). $\square$

4.4 Numerical examples

In order to illustrate Theorem 4.5 we apply the numerical method (6)–(7) to two model problems. In both cases, we consider Maxwell's equations (2) on the unit cube $(0,1)\times(0,1)\times(0,1)$. For the spatial discretization the classical Yee grid (cf. [27] or Section 3.6 in [22]) with mesh width $h = 1/m$ is used ($m \in \mathbb{N}$). Hence, numerical approximations

$$\begin{aligned}
E_1^n(i+\tfrac12,j,k) &\approx \mathbf{E}_1\left(t_n,(i+\tfrac12)h,jh,kh\right),\\
E_2^n(i,j+\tfrac12,k) &\approx \mathbf{E}_2\left(t_n,ih,(j+\tfrac12)h,kh\right),\\
E_3^n(i,j,k+\tfrac12) &\approx \mathbf{E}_3\left(t_n,ih,jh,(k+\tfrac12)h\right),\\
H_1^n(i,j+\tfrac12,k+\tfrac12) &\approx \mathbf{H}_1\left(t_n,ih,(j+\tfrac12)h,(k+\tfrac12)h\right),\\
H_2^n(i+\tfrac12,j,k+\tfrac12) &\approx \mathbf{H}_2\left(t_n,(i+\tfrac12)h,jh,(k+\tfrac12)h\right),\\
H_3^n(i+\tfrac12,j+\tfrac12,k) &\approx \mathbf{H}_3\left(t_n,(i+\tfrac12)h,(j+\tfrac12)h,kh\right),
\end{aligned}$$

are computed on six different staggered grids, and all partial derivatives are approximated by central finite differences, for example

$$\begin{aligned}
\partial_2\mathbf{H}_3\left(t_n,(i+\tfrac12)h,jh,kh\right) &\approx \frac{H_3^n\left(i+\tfrac12,j+\tfrac12,k\right)-H_3^n\left(i+\tfrac12,j-\tfrac12,k\right)}{h}\\
\partial_3\mathbf{H}_2\left(t_n,(i+\tfrac12)h,jh,kh\right) &\approx \frac{H_2^n\left(i+\tfrac12,j,k+\tfrac12\right)-H_2^n\left(i+\tfrac12,j,k-\tfrac12\right)}{h}
\end{aligned}$$

and so on. Note that $\partial_3\mathbf{H}_2$ and $\partial_2\mathbf{H}_3$ are not approximated on the same grid as $\mathbf{H}_2$ and $\mathbf{H}_3$, respectively, but on the same grid as $\mathbf{E}_1$. This makes sense because (1) or (2) imply that

$$\partial_t\mathbf{E}_1 = \varepsilon^{-1}(\partial_2\mathbf{H}_3-\partial_3\mathbf{H}_2).$$

The other field components $\mathbf{E}_2$, $\mathbf{E}_3$, $\mathbf{H}_1$, $\mathbf{H}_2$, and $\mathbf{H}_3$ are treated similarly. The boundary conditions are implemented in a straightforward way: we simply let

$$\begin{aligned}
E_2^n(i,j+\tfrac12,k) = E_3^n(i,j,k+\tfrac12) &= 0 &&\text{for } i\in\{0,m\},\\
E_1^n(i+\tfrac12,j,k) = E_3^n(i,j,k+\tfrac12) &= 0 &&\text{for } j\in\{0,m\},\\
E_1^n(i+\tfrac12,j,k) = E_2^n(i,j+\tfrac12,k) &= 0 &&\text{for } k\in\{0,m\}
\end{aligned}$$

and

$$\begin{aligned}
H_1^n(i,j+\tfrac12,k+\tfrac12) &= 0 &&\text{for } i\in\{0,m\},\\
H_2^n(i+\tfrac12,j,k+\tfrac12) &= 0 &&\text{for } j\in\{0,m\},\\
H_3^n(i+\tfrac12,j+\tfrac12,k) &= 0 &&\text{for } k\in\{0,m\}.
\end{aligned}$$

This choice fits to the boundary conditions in (2), see Lemma 3.7.

Example 1: Impact of the regularity of the initial data on the accuracy

In the first example we let $\varepsilon \equiv 1$ and $\mu \equiv 1$. It can be verified by straightforward calculations that each of the functions

$$u^1_{\kappa\lambda}(t,x) = \begin{pmatrix} \sin(\kappa\pi x_2)\sin(\lambda\pi x_3)\cos(\sqrt{\kappa^2+\lambda^2}\pi t) \\ 0 \\ 0 \\ 0 \\ -\frac{\lambda}{\sqrt{\kappa^2+\lambda^2}}\sin(\kappa\pi x_2)\cos(\lambda\pi x_3)\sin(\sqrt{\kappa^2+\lambda^2}\pi t) \\ \frac{\kappa}{\sqrt{\kappa^2+\lambda^2}}\cos(\kappa\pi x_2)\sin(\lambda\pi x_3)\sin(\sqrt{\kappa^2+\lambda^2}\pi t) \end{pmatrix},$$

$$u^2_{\kappa\lambda}(t,x) = \begin{pmatrix} 0 \\ \sin(\kappa\pi x_1)\sin(\lambda\pi x_3)\cos(\sqrt{\kappa^2+\lambda^2}\pi t) \\ 0 \\ \frac{\lambda}{\sqrt{\kappa^2+\lambda^2}}\sin(\kappa\pi x_1)\cos(\lambda\pi x_3)\sin(\sqrt{\kappa^2+\lambda^2}\pi t) \\ 0 \\ -\frac{\kappa}{\sqrt{\kappa^2+\lambda^2}}\cos(\kappa\pi x_1)\sin(\lambda\pi x_3)\sin(\sqrt{\kappa^2+\lambda^2}\pi t) \end{pmatrix},$$

$$u^3_{\kappa\lambda}(t,x) = \begin{pmatrix} 0 \\ 0 \\ \sin(\kappa\pi x_1)\sin(\lambda\pi x_2)\cos(\sqrt{\kappa^2+\lambda^2}\pi t) \\ -\frac{\lambda}{\sqrt{\kappa^2+\lambda^2}}\sin(\kappa\pi x_1)\cos(\lambda\pi x_2)\sin(\sqrt{\kappa^2+\lambda^2}\pi t) \\ \frac{\kappa}{\sqrt{\kappa^2+\lambda^2}}\cos(\kappa\pi x_1)\sin(\lambda\pi x_2)\sin(\sqrt{\kappa^2+\lambda^2}\pi t) \\ 0 \end{pmatrix},$$

with $(\kappa,\lambda) \in \mathbb{Z}^2 \setminus \{(0,0)\}$ solves Maxwell's equations (2) including boundary and divergence conditions. More general solutions can be constructed by superposition

$$u(t,x) = \sum_{\kappa=0}^{\kappa_{\max}} \sum_{\lambda=0}^{\lambda_{\max}} \big(a^1_{\kappa\lambda}u^1_{\kappa\lambda}(t,x) + a^2_{\kappa\lambda}u^2_{\kappa\lambda}(t,x) + a^3_{\kappa\lambda}u^3_{\kappa\lambda}(t,x)\big) \tag{33}$$

with coefficients $a^\ell_{\kappa\lambda} \in \mathbb{R}$ and $a^\ell_{00} = 0$ for $\ell \in \{1,2,3\}$. The initial conditions are obtained by simply evaluating (33) for $t = 0$.

Numerical approximations were computed on the time-interval $[0,5]$ with different values of τ and h. For each combination, the spatial error at a fixed time is measured by the discrete counterpart of the norm $\|\cdot\|_{L^2}$, and for the global error we consider the maximum L^2-error over all time steps. In the first example, we let

$$a^1_{11} = \gamma, \qquad a^2_{11} = 2\gamma, \qquad a^3_{11} = 3\gamma, \qquad a^\ell_{\kappa\lambda} = 0 \text{ for all } (\kappa,\lambda) \neq (1,1) \tag{34}$$

with a constant γ chosen in such a way that $\|u(0,\cdot)\|_{L^2} = 1$. The result is shown in the left picture of Figure 1. For $\tau \geq 5 \cdot 2^{-9} \approx 0.0098$, the global error is dominated by the error of the time discretization. In perfect agreement with Theorem 4.5, we observe second-order convergence in time independently of

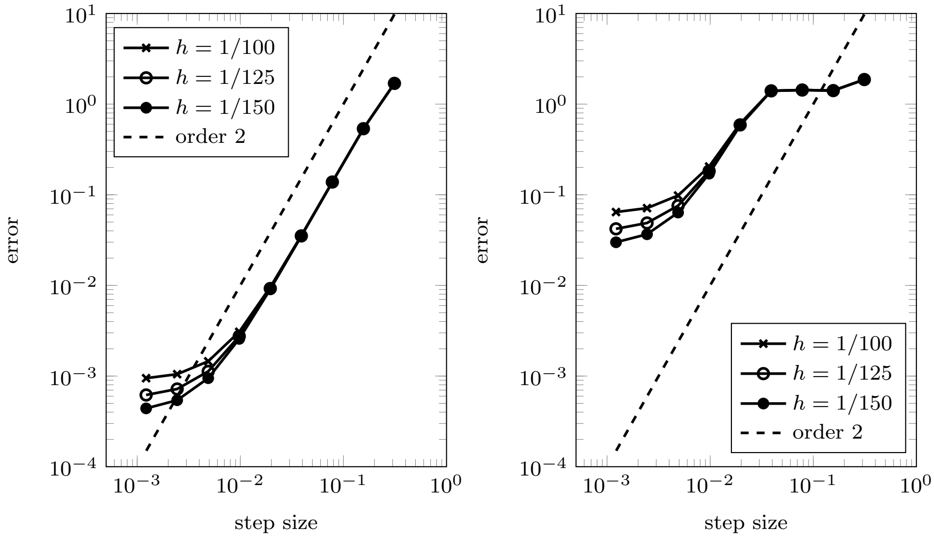

Fig. 1 Global error of the full discretization with step size $\tau = 5 \cdot 2^{-k}$ in time ($k = 4, 5, \ldots, 12$) and spatial mesh width $h = 1/100, 1/125, 1/150$. The dashed line shows the function $\tau \to 100 \cdot \tau^2$ for the sake of comparison. For the coefficients in the exact solution (33) we have chosen (34) in the left panel and (35) in the right panel. In both cases, γ was chosen in such a way that $\|u(0, \cdot)\|_{L^2} = 1$.

the mesh width, i.e. independently of the norms of the discretization matrices. For $\tau < 5 \cdot 2^{-9}$, the error of the space discretization starts to dominate the total error. As expected smaller values of h yield higher accuracy.

According to Theorem 4.5, the error of the ADI method depends on the smoothness of the initial data. In order to illustrate this, the same numerical experiment is repeated with

$$\begin{aligned} a^1_{11} &= \gamma, & a^2_{11} &= 2\gamma, & a^3_{11} &= 3\gamma, \\ a^1_{54} &= 3\gamma, & a^2_{35} &= 2\gamma, & a^3_{55} &= \gamma \end{aligned} \tag{35}$$

and $a^\ell_{\kappa\lambda} = 0$ for all other coefficients, where γ is again chosen in such a way that $\|u(0, \cdot)\|_{L^2} = 1$. In this example, the solution oscillates rapidly in space due to the terms corresponding to a^1_{54}, a^2_{35}, and a^3_{55}. The right picture in Figure 1 shows that the error does not explode, but that the convergence only starts for much smaller step sizes than before. The reason is that the term $\|M_0^3 w\|_{L^2}$ with $w = u(0, \cdot)$ in Theorem 4.5 is now much larger due to the lower regularity of the initial data. The error plot also indicates that the step size where convergence starts ($\tau < 5 \cdot 2^{-7} \approx 0.039$) does not depend on the mesh width h. The reason is that the term $\|M_0^3 w\|_{L^2}$ is independent of h.

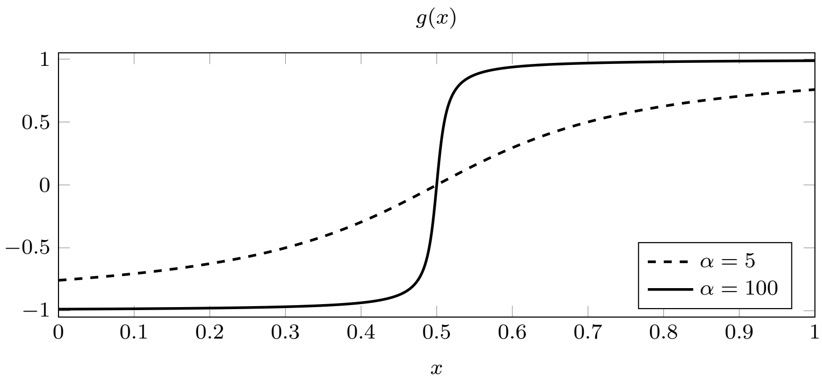

Fig. 2 Function $g(x_i)$ defined in (37).

Example 2: Impact of the regularity of the coefficients on the accuracy

In the second model problem we test how the accuracy is affected by the smoothness of the coefficient functions ε and μ. We let

$$\varepsilon(x) = \mu(x) = 2 + g(x_1)g(x_2)g(x_3), \tag{36}$$

$$g(x_i) = \frac{2}{\pi}\arctan\big(\alpha(x_i - 0.5)\big), \qquad i \in \{1,2,3\}, \tag{37}$$

and either $\alpha = 5$ or $\alpha = 100$. The function g is depicted in Figure 2. For $\alpha = 5$ both $\varepsilon(x)$ and $\mu(x)$ are so smooth that the convergence order two in time is not affected, which can be seen in Figure 3. For $\alpha = 100$, the function $g(x_i)$ rapidly changes its value from -1 to 1 when $x_i \approx 0.5$, and Figure 3 shows that in this case the low regularity of ε and μ spoils the order of convergence as expected. In this case, convergence of order two could only be observed for considerably smaller step sizes τ and a much smaller mesh width h. Since no explicit formula for the exact solution is available for our choice of $\varepsilon(x)$ and $\mu(x)$, the error of the time discretization was estimated by means of a reference solution which was computed with $\tau = 5 \cdot 2^{-11}$ and $h = 0.01$. For both values of α, we have used the initial data

$$\mathbf{E}(0,x) = \frac{\widetilde{\mathbf{E}}(0,x)}{\varepsilon(x)}, \qquad \mathbf{H}(0,x) = \frac{\widetilde{\mathbf{H}}(0,x)}{\mu(x)}, \qquad \begin{pmatrix}\tilde{\mathbf{E}}(0,x)\\ \tilde{\mathbf{H}}(0,x)\end{pmatrix} = u(0,x)$$

with u defined in (33) and parameters

$$a_{11}^1 = a_{11}^2 = a_{11}^3 = 1, \qquad\qquad a_{\kappa\lambda}^\ell = 0 \text{ for all } (\kappa,\lambda) \neq (1,1).$$

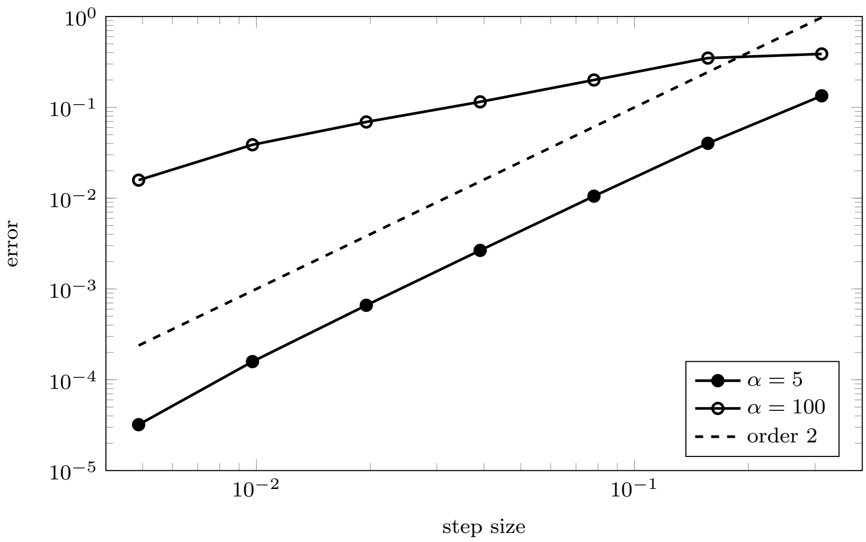

Fig. 3 Global error of the time discretization for non-constant coefficients (36), (37) with $\alpha = 5$ (dots) and $\alpha = 100$ (circles). Approximations were computed on the interval $[0, 5]$ with step size $\tau = 5 \cdot 2^{-k}$ $(k = 4, 5, \dots, 10)$ and spatial mesh width $h = 1/100$. The dashed line shows the function $\tau \to 10 \cdot \tau^2$ for the sake of comparison.

5 Appendix

We now present two proofs of Lemmas 3.6 and 3.7 we omitted in Section 3.

Proof of Lemma 3.6. Lax–Milgram provides us with a unique $v \in H^1_\Gamma(Q)$ satisfying (21). To show the asserted regularity of v, we consider the operators $A_j = -\partial_j^2$ on $L^2(Q)$ whose domain consists of those $w \in L^2(Q)$ such that $\partial_j^2 w \in L^2(Q)$, $w = 0$ on Γ_j^+ or on Γ_j^- if $\Gamma_j^+ \subseteq \Gamma$ or if $\Gamma_j^- \subseteq \Gamma$, respectively, and $\partial_j w = 0$ on Γ_j^+ or on Γ_j^- if $\Gamma_j^+ \subseteq \Gamma'$ or if $\Gamma_j^- \subseteq \Gamma'$, respectively. Here and below we have $j = 1, 2, 3$. For $u \in D(A_j)$ and $v \in D_j$, an integration by parts shows

$$\int_Q (uv + A_j u\, v)\, \mathrm{d}x = \int_Q (uv + \partial_j u\, \partial_j v)\, \mathrm{d}x =: a(u, v),$$

where a is a symmetric, continuous and coercive bilinear form. It is routine to check that A_j is the self adjoint operator induced by a. It is clear that A_j is positive. In particular, D_j is the domain of $A_j^{\frac{1}{2}}$ and hence $\partial_j A_j^{-\frac{1}{2}}$ is bounded on $L^2(Q)$.

To see that the resolvents of A_i and A_j commute, we observe that the resolvent of, say, A_1 is given by $((\lambda I + A_1)^{-1} f)(x, y, z) = (R_1(\lambda) f(\cdot, y, z))(x)$ for $\lambda > 0$, for almost every $(x, y, z) \in Q$ and the resolvent $R_1(\lambda)$ of the negative second derivative on $L^2(a_1^-, a_1^+)$ with the boundary conditions of A_1. Analogous facts hold for A_2 and A_3. If f is the product of $f_k \in L^2(a_k^-, a_k^+)$ for $k = 1, 2, 3$, then $(\lambda I + A_i)^{-1}(\lambda I + A_j)^{-1} f = (\lambda I + A_j)^{-1}(\lambda I + A_i)^{-1} f$. Since the span of such functions is dense in $L^2(Q)$, the resolvents commute.

As explained in Sections III.4, VII.2 and X.1 of [21], we thus have a joint functional calculus with respect to A_1, A_2 and A_3 for Borel measurable functions $\phi : \mathbb{R}_+^3 \to \mathbb{R}$. The operator $\phi(A_1, A_2, A_3)$ is bounded if ϕ is bounded, and for $h(\lambda) = 1 + \lambda_1 + \lambda_2 + \lambda_3$ we have $h(A_1, A_2, A_3) = I + A_1 + A_2 + A_3 =: I + A$ on the domain $D(A) := D(A_1) \cap D(A_2) \cap D(A_3)$. Set $\rho = 1/h$. Then $\rho(A_1, A_2, A_3)$ is bounded and it is the inverse of $I + A$, so that A is closed. Using the bounded functions $h_{i,j}(\lambda) = \lambda_i^{\frac{1}{2}} \lambda_j^{\frac{1}{2}} \rho(\lambda)$, we see that the operator $h_{ij}(A_1, A_2, A_3) = A_i^{\frac{1}{2}} A_j^{\frac{1}{2}} (I + A)^{-1}$ is bounded for all $i, j \in \{1, 2, 3\}$. This means that $D(A) \hookrightarrow H^2(Q)$ implying $D(A) = D$ and the equivalence of graph norm of Δ and the H^2–norm on D. It is then clear that $v = (I + A)^{-1} f$ is the required weak solution. □

Proof of Lemma 3.7. 1) Throughout, let $(\mathbf{E}, \mathbf{H}) \in D(M_0^2)$. It is known that a map $u \in H(\mathrm{rot}) \cap H(\mathrm{div})$ belongs to $H^1(Q)^3$ if $u \times \nu = 0$ or $u \cdot \nu = 0$ holds on ∂Q. Moreover, the H^1 norm of u is then dominated by $\|u\|_{L^2} + \|\operatorname{div} u\|_{L^2} + \|\operatorname{rot} u\|_{L^2}$, see, e.g., Theorem 2.17 in [1]. Note that the equations (14) and (16) still hold on Q. In particular $\operatorname{div} \mathbf{E}$ and $\operatorname{div} \mathbf{H}$ belong to $L^2(Q)^3$. We thus have $\mathbf{E}, \mathbf{H} \in H^1(Q)^3$ and $\|(\mathbf{E}, \mathbf{H})\|_{H^1} \le c\,(\|(\mathbf{E}, \mathbf{H})\|_X + \|M_0(\mathbf{E}, \mathbf{H})\|_X)$. The asserted zero–order traces for $\mathbf{E}$ and $\mathbf{H}$ now are a direct consequence of the boundary conditions $\mathbf{E} \times \nu = 0$ and $\mathbf{H} \cdot \nu = 0$, respectively.

Since $\mathbf{E}, \mathbf{H} \in H^1(Q)^3 \hookrightarrow L^6(Q)^3$ and $M^2(\mathbf{E}, \mathbf{H}) \in X$, equation (16) and the assumptions on ε and μ imply that $\Delta E_j, \Delta H_j \in L^2(Q)$. A standard localization argument then yields $E_j, H_j \in H^2_{\mathrm{loc}}(Q)^3$ for $j = 1, 2, 3$. In addition, the X–norm of $(\Delta \mathbf{E}, \Delta \mathbf{H})$ is bounded by that of $M_0^2(\mathbf{E}, \mathbf{H})$ and $(\mathbf{E}, \mathbf{H})$. We next establish the properties of the traces of $\mathbf{E}$ and $\mathbf{H}$ needed to derive $\mathbf{E}, \mathbf{H} \in H^2(Q)^3$ from Lemma 3.6.

2) We first consider E_1. We will actually show that εE_1 belongs to $H^2(Q)$ by applying Lemma 3.6 to εE_1. Because of

$$\partial_{kl} E_1 = \frac{1}{\varepsilon}\,\partial_{kl}(\varepsilon E_1) - \frac{\partial_k \varepsilon}{\varepsilon}\,\partial_l E_1 - \frac{\partial_l \varepsilon}{\varepsilon}\,\partial_k E_1 - \frac{\partial_{kl}\varepsilon}{\varepsilon}\,E_1, \tag{38}$$

it will then follow that $E_1 \in H^2(Q)$ employing $E_1 \in H^1(Q)$ and the assumed regularity of ε. At the present stage, from (38), $\Delta E_1 \in L^2(Q)$ and $E_1 \in H^2_{\mathrm{loc}}(Q)^3$ we can already infer that $f := (I - \Delta)(\varepsilon E_1) \in L^2(Q)$ and $\varepsilon E_1 \in H^2_{\mathrm{loc}}(Q)$. Part 1) shows that $\varepsilon E_1 = 0$ on the faces $\Gamma := \Gamma_2^- \cup \Gamma_2^+ \cup \Gamma_3^- \cup \Gamma_3^+$. Fix a function $\psi \in H^1(Q)$ with $\partial_2\psi, \partial_3\psi \in H^1(Q)$ and having support in $[a_1^-, a_1^+] \times [a_2^- + \eta, a_2^+ - \eta] \times [a_3^- + \eta, a_3^+ - \eta]$ for some small $\eta = \eta(\psi) > 0$. A given $\varphi \in H^1_\Gamma(Q)$ can be approximated in $H^1(Q)$ by such ψ employing cutoff and mollification in the (x_2, x_3) directions. For each sufficiently small $\kappa > 0$, we set

$$Q_\kappa = (a_1^- + \kappa, a_1^+ - \kappa) \times (a_2^- + \kappa, a_2^+ - \kappa) \times (a_3^- + \kappa, a_3^+ - \kappa).$$

We take $\kappa \in (0, \eta(\psi))$ and denote by $\Gamma_1^\pm(\kappa)$ the open faces of Q_κ containing points of the form $(a_1^\pm \pm \kappa, x_2, x_3)$. Integrating by parts and using $\operatorname{div}(\varepsilon \mathbf{E}) = 0$ as well as $\partial_j(\varepsilon E_j) \in H^1_{\mathrm{loc}}(Q)$ for $j = 1, 2, 3$, we conclude that

$$\begin{aligned}
\int_Q \nabla(\varepsilon E_1) \cdot \nabla \psi \, \mathrm{d}x + \int_Q \varepsilon E_1 \psi \, \mathrm{d}x &= \lim_{\kappa \to 0} \int_{Q_\kappa} \big(\varepsilon E_1 \psi + \nabla(\varepsilon E_1) \cdot \nabla \psi\big) \, \mathrm{d}x \\
&= \lim_{\kappa \to 0} \Big[\int_{Q_\kappa} (I - \Delta)(\varepsilon E_1) \psi \, \mathrm{d}x + \int_{\partial Q_\kappa} \psi \, \nabla(\varepsilon E_1) \cdot \nu \, \mathrm{d}\sigma \Big] \\
&= \int_Q f \psi \, \mathrm{d}x \pm \lim_{\kappa \to 0} \int_{\Gamma_1^\pm(\kappa)} \psi \, \partial_1(\varepsilon E_1) \, \mathrm{d}(x_2, x_3) \\
&= \int_Q f \psi \, \mathrm{d}x \mp \lim_{\kappa \to 0} \int_{\Gamma_1^\pm(\kappa)} \psi(\partial_2(\varepsilon E_2) + \partial_3(\varepsilon E_3)) \, \mathrm{d}(x_2, x_3) \\
&= \int_Q f \psi \, \mathrm{d}x \pm \lim_{\kappa \to 0} \int_{\Gamma_1^\pm(\kappa)} \big(\varepsilon E_2 \partial_2 \psi + \varepsilon E_3 \partial_3 \psi\big) \, \mathrm{d}(x_2, x_3) \\
&= \int_Q f \psi \, \mathrm{d}x. \qquad (39)
\end{aligned}$$

We have used that ψ vanishes near Γ for the penultimate equation and that $\varepsilon E_j, \partial_j \psi \in H^1(Q)^3$ and $\varepsilon E_j = 0$ on $\Gamma_1^\pm$ for $j = 2, 3$ in the last identity, see part 1). By approximation, equation (39) then holds for all $\psi \in H^1_\Gamma(Q)$, and hence Lemma 3.6 yields $\varepsilon E_1 \in H^2(Q)$ so that $E_1 \in H^2(Q)$ as explained above. In the same way, one sees that $E_2, E_3 \in H^2(Q)$. Moreover, $\|E_j\|_{H^2}$ is bounded by $c\,(\|E_j\|_{L^2} + \|\Delta E_j\|_{L^2})$ due to Lemma 3.6 and hence by $c\,(\|(\mathbf{E}, \mathbf{H})\|_X + \|M_0^2(\mathbf{E}, \mathbf{H})\|_X)$ in view of step 1).

We denote by γ_i the trace operator to $\Gamma_i^\pm$, where $i, j, k \in \{1, 2, 3\}$. Since $E_k \in H^2(Q)$, one can approximate E_k in $H^2(Q)$ by $v_n \in C^2(\overline{Q})$. Clearly, $\gamma_i \partial_j v_n = \partial_j \gamma_i v_n$ and thus $\gamma_i \partial_j E_k = \partial_j \gamma_i E_k$. As a result, the asserted first order boundary conditions of $\mathbf{E}$ follow from the already established 0–order boundary conditions of $\mathbf{E}$.

3) Next, we consider H_1 and set $g := (I - \Delta) H_1 \in L^2(Q)$. Here we have less Dirichlet boundary conditions, namely $H_j = 0$ on $\Gamma_j^\pm$ for $j = 1, 2, 3$. To deal with the Neumann conditions, we first note that

$$\begin{aligned}
&\operatorname{rot}(\varepsilon^{-1} \operatorname{rot} \mathbf{H}) \in L^2(Q)^3, \qquad \varepsilon^{-1} \operatorname{rot} \mathbf{H} \times \nu = 0 \text{ on } \partial Q, \\
&\operatorname{div}(\varepsilon^{-1} \operatorname{rot} \mathbf{H}) = \nabla \varepsilon^{-1} \cdot \operatorname{rot} \mathbf{H} \in L^2(Q).
\end{aligned}$$

Hence, $\varepsilon^{-1} \operatorname{rot} \mathbf{H}$ belongs to $H^1(Q)^3$ which yields $\operatorname{rot} \mathbf{H} \in H^1(Q)^3$. It also follows that $\operatorname{rot} \mathbf{H} \times \nu = 0$ on ∂Q. In particular, the first component of $\operatorname{rot} \mathbf{H}$ vanishes on $\Gamma_2^\pm \cup \Gamma_3^\pm$.

We set $\tilde{\Gamma} = \Gamma_1^- \cup \Gamma_1^+$ and define the faces $\Gamma_j^\pm(\kappa)$ of Q_κ in the jth direction for $j = 2, 3$, cf. step 2). We take functions $\psi \in H^1(Q)$ with $\partial_1 \psi \in H^1(Q)$ and having support in $[a_1^- + \eta, a_1^+ - \eta] \times [a_2^-, a_2^+] \times [a_3^-, a_3^+]$ for some $\eta > 0$. We choose $\kappa \in (0, \eta)$ so that ψ vanishes around $\Gamma_1^\pm(\kappa)$. As above, we deduce

$$\int_Q \nabla H_1 \cdot \nabla \psi \, \mathrm{d}x + \int_Q H_1 \psi \, \mathrm{d}x = \lim_{\kappa \to 0} \int_{Q_\kappa} \big(H_1 \psi + \nabla H_1 \cdot \nabla \psi\big) \, \mathrm{d}x$$

$$
\begin{aligned}
&= \lim_{\kappa\to 0} \Big[\int_{Q_\kappa} \psi\,(I-\Delta)H_1 \,\mathrm{d}x + \int_{\partial Q_\kappa} \psi\,\nu\cdot\nabla H_1 \,\mathrm{d}\sigma \Big] \\
&= \int_Q \psi\,(I-\Delta)H_1 \,\mathrm{d}x + \lim_{\kappa\to 0} \int_{\partial Q_\kappa} \big[\psi\,\nu\cdot\nabla H_1 - (\operatorname{rot}\mathbf{H}\times\nu)\cdot(\psi,0,0) \big] \,\mathrm{d}\sigma \\
&= \int_Q g\psi \,\mathrm{d}x + \lim_{\kappa\to 0} \int_{\partial Q_\kappa} \psi\,\nu\cdot\partial_1\mathbf{H} \,\mathrm{d}\sigma \\
&= \int_Q g\psi \,\mathrm{d}x \pm \lim_{\kappa\to 0} \Big[\int_{\Gamma_2^\pm(\kappa)} \psi\,\partial_1 H_2 \,\mathrm{d}\sigma + \int_{\Gamma_3^\pm(\kappa)} \psi\,\partial_1 H_3 \,\mathrm{d}\sigma \Big] \\
&= \int_Q g\psi \,\mathrm{d}x \mp \lim_{\kappa\to 0} \Big[\int_{\Gamma_2^\pm(\kappa)} H_2\,\partial_1\psi \,\mathrm{d}\sigma + \int_{\Gamma_3^\pm(\kappa)} H_3\,\partial_1\psi \,\mathrm{d}\sigma \Big] \\
&= \int_Q g\psi \,\mathrm{d}x.
\end{aligned}
$$

The remaining assertions now follow as in step 2). □

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