Application of operator splitting to the Maxwell equations including a source term [1]

M.A. Botchev [a,2,*], I. Faragó [b,3], R. Horváth [c,3]

[a] *Department of Applied Mathematics, University of Twente, P.O. Box 217, 7500 AE, Enschede, The Netherlands,* mbotchev@na-net.ornl.gov, *fax: +31 53 489 4833.*

[b] *Department of Applied Analysis, Eötvös Loránd University, Pázmány P. sétány 1/C, H-1117 Budapest, Hungary,* faragois@cs.elte.hu.

[c] *University of West-Hungary, Institute of Mathematics and Statistics, Erzsébet u. 9, H-9400 Sopron, Hungary,* rhorvath@ktk.nyme.hu.

Abstract

Motivated by numerical solution of the time-dependent Maxwell equations, we consider splitting methods for a linear system of differential equations $w'(t) = Aw(t) + f(t)$, $A \in \mathbb{R}^{n\times n}$ split into two subproblems $w_1'(t) = A_1 w_1(t) + f_1(t)$ and $w_2'(t) = A_2 w_2(t) + f_2(t)$, $A = A_1 + A_2$, $f = f_1 + f_2$. First, expressions for the leading term of the local error are derived for the Strang-Marchuk and the symmetrically weighted sequential splitting methods. The analysis, done in assumption that the subproblems are solved exactly, confirms the expected second order global accuracy of both schemes.

Second, several relevant numerical tests are performed for the Maxwell equations discretized in space either by finite differences or by finite elements. An interesting case is the splitting into the subproblems $w_1' = Aw_1$ and $w_2' = f$ (with the split-off source term f). For the central finite difference staggered discretization, we consider second order splitting schemes and compare them to the classical Yee scheme on a test problem with loss and source terms. For the vector Nédélec finite element discretizations, we test the Gautschi-Krylov time integration scheme. Applied in combination with the split-off source term, it leads to splitting schemes that are exact per split step. Thus, the time integration error of the schemes consists solely of the splitting error.

Mathematics Subject Classification: 65M12, 35Q60, 65M20, 65M06, 65M60, 78M10, 78M20.

Key words: splitting methods, Strang splitting, Maxwell equations, Yee method, staggered finite differences, Whitney finite elements, Gautschi cosine scheme, Krylov subspace methods

1 Introduction

In this paper we deal with time integration schemes for the time-dependent Maxwell equations discretized in space by finite differences or finite elements. A variety of these methods is often referred to as Finite Difference Time Domain (FDTD) or Finite Element Time Domain (FETD) methods [36]. Usually one expects that the time integration schemes in these methods
(i) are adequate to the spatial discretization used, lead to a small dispersion error and respect relevant discrete conservation laws,
(ii) are accurate enough, in particular have an appropriate time consistency order, and
(iii) are stable, allowing a sufficiently large time step size.

Within the FDTD framework, several schemes have been proposed [23,24,5,3] that increase the second order of the time and space discretization of the classical Yee method [41] and enhance its stability. In particular, methods developed in [23,24,5] are unconditionally stable due to the use of special structure (skew symmetry) of the matrices involved. As shown in [18,19], most of these methods can be seen as special cases of the time splitting methods [34,40,35,27,20] where the original time evolution problem is split in a number of subproblems. Recently, the so-called symplectic methods [14], satisfying some conservation laws of the original partial differential equations, have received attention in connection to the FDTD framework (see e.g. [33,21]).

The trends similar to ones observed in the FDTD methods can also be seen within the FETD approach. In particular, the well-known scheme of Rodrigue and White [31] is a straightforward generalization of the explicit leap-frog time stepping mechanism of the classical Yee scheme. Here only the damping conductivity terms are treated implicitly by the trapezoidal rule. The scheme is based on the edge and face Nédélec finite elements and reduces to the time-space discretization of the Yee scheme when applied on a uniform Cartesian grid with the mass lumping [31]. A class of popular FETD methods is formed by the Newmark β-schemes derived for the second order Maxwell equations [12,25]. For a usual choice of the involved parameters, the Newmark β-scheme is equivalent to the trapezoidal rule applied to the corresponding system of two first order equations. Symplectic higher order FETD schemes are considered

* Corresponding author
[1] An initial part of this work was supported by the Netherlands organization for Scientific Research NWO and the Hungarian Scientific Research Fund OTKA through research project NWO-048.011.041.
[2] Supported by the Dutch government through the national program BSIK: knowledge and research capacity, in the ICT project BRICKS (`http://www.bsik-bricks.nl`), theme MSV1.
[3] Supported by the Hungarian Scientific Research Fund OTKA grant No. 43765.

in [30].

In this paper, we consider operator splitting methods for numerical solution of the time-dependent Maxwell equations. Spatial discretization of the Maxwell equations usually leads to a linear system of differential equations

$$\boldsymbol{w}'(t) = A\boldsymbol{w}(t) + \boldsymbol{f}(t),$$

where $\boldsymbol{w}(t)$ is unknown vector function typically related to the electric and magnetic fields. Assuming that the system is split into two subproblems (see (3.11)), we provide an analysis of the leading term of the local error for two popular splitting methods: the Strang-Marchuk [27,35] splitting and the symmetrically weighted sequential (SWS) splitting [34]. The analysis, done in assumption that the subproblems are solved exactly, confirms the expected second order global accuracy of both splitting schemes.

Based on the obtained theoretical results, we consider several specific splitting schemes for the Maxwell equations discretized in space either by finite differences or finite elements. An interesting case is the splitting into the subproblems $\boldsymbol{w}_1' = A\boldsymbol{w}_1$ and $\boldsymbol{w}_2' = \boldsymbol{f}$ (with the split-off source term $\boldsymbol{f}$). For the central finite difference staggered discretization, we consider second order splitting schemes and compare them to the classical Yee scheme on a test problem with loss and source terms. Results of the numerical tests demonstrate efficiency of the splitting schemes.

For the vector Nédélec finite element discretizations, we test the Gautschi-Krylov time integration scheme [11,1]. This scheme was shown to be an efficient tool for solving the time-dependent Maxwell equations [1]. Applied in combination with the split-off source term, it leads to splitting schemes that are exact per split step. Thus, the time integration error of the schemes consists solely of the splitting error. An interesting question arises, whether such splitting schemes are more efficient, in terms of achieved accuracy and required computational work, than the unsplit Gautschi-Krylov scheme. Numerical experiments are performed that should provide an answer to this question.

We comment that a statement on the second order accuracy of the Stang-Marchuk splitting for the general nonlinear problems is given, without proof, in [20]. The local error of the Strang-Marchuk splitting for problems with bounded operators without the source term is analyzed in many books and papers, e.g. in [27,35]. The consistency of Strang/Marchuk splitting in general case (for not necessarily bounded operators) but, again, without the source term is studied in [10]. To our knowledge, the local error of the SWS splitting for problems with the source term has not been analyzed yet. For homogeneous problems with bounded operators, the SWS splitting was analyzed in [34,4] and, for unbounded operators without the source term, in [10].

The structure of the paper is as follows. In Section 2, the Maxwell equations and spatial finite difference and finite element discretizations are described. The local errors of the Strang-Marchuk and the SWS splitting schemes are analyzed in Section 3. Section 4 presents numerical experiments and the conclusions are made in Section 5.

2 The equations and spatial discretizations

2.1 Maxwell equations

The time-dependent Maxwell equations on a bounded domain $\Omega \in \mathbb{R}^3$ filled with lossy media can be written as

$$\begin{aligned} \partial_t \boldsymbol{D}_s &= \nabla \times \boldsymbol{H}_s - \sigma \boldsymbol{E}_s - \boldsymbol{J}_s, \\ \partial_t \boldsymbol{B}_s &= -\nabla \times \boldsymbol{E}_s, \\ \nabla \cdot \boldsymbol{D}_s &= \rho_s, \\ \nabla \cdot \boldsymbol{B}_s &= 0, \end{aligned} \tag{2.1}$$

with $\boldsymbol{E}_s$ and $\boldsymbol{H}_s$ ($\boldsymbol{D}_s$ and $\boldsymbol{B}_s$) being electric and magnetic fields (respectively, the electric and the magnetic flux densities), $\boldsymbol{J}_s$, ρ_s and σ being the electric current, charge density and conductivity, respectively. The used SI units are indicated by the subscript s. We assume the following given boundary and initial conditions:

$$\begin{aligned} &(\boldsymbol{n} \times \boldsymbol{E}_s)|_\Gamma = 0, \\ &\boldsymbol{E}_s|_{t_s=0} = \bar{\boldsymbol{E}}_0, \qquad \boldsymbol{H}_s|_{t_s=0} = \bar{\boldsymbol{H}}_0, \end{aligned} \tag{2.2}$$

where $\boldsymbol{n}$ is the outward normal vector to the domain boundary $\Gamma = \partial\Omega$. In addition to (2.1),(2.2), the following constitutive relations hold:

$$\boldsymbol{D}_s = \varepsilon \boldsymbol{E}_s, \quad \boldsymbol{B}_s = \mu \boldsymbol{H}_s, \tag{2.3}$$

where the dielectric permittivity $\varepsilon\,(=\varepsilon_0\varepsilon_r)$ and the magnetic permeability $\mu\,(=\mu_0\mu_r)$ are assumed to be space dependent tensors. Here, ε_0 and μ_0 are the free space dielectric permittivity and magnetic permeability, respectively, and ε_r and μ_r are material dependent dimensionless tensors called relative permittivity and relative permeability, respectively.

2.2 Dimensionless Maxwell equations

One often solves the Maxwell equations in a dimensionless form, thus avoiding working with very large numbers. To bring the equations to a dimensionless

form, we apply the following space and time scaling (see e.g. [1]):

$$x = \frac{x_s}{L} \quad \text{(similarly for } y,\ z\text{)}, \qquad t = \frac{c_0}{L} t_s, \tag{2.4}$$

with L being a reference length (in meters), and $c_0 = (\varepsilon_0 \mu_0)^{-1/2} \approx 3 \cdot 10^8$ m/s the speed of light in vacuum. The fields involved are also scaled as

$$\boldsymbol{E}_s(\mathbf{x}_s, t_s) = \tilde{H}_0 Z_0 \boldsymbol{E}(\mathbf{x}, t), \quad \boldsymbol{H}_s(\mathbf{x}_s, t_s) = \tilde{H}_0 \boldsymbol{H}(\mathbf{x}, t), \quad \boldsymbol{J}_s(\mathbf{x}_s, t_s) = \frac{\tilde{H}_0}{L} \boldsymbol{J}(\mathbf{x}, t), \tag{2.5}$$

where $\mathbf{x}_s = (x_s, y_s, z_s)$, $\mathbf{x} = (x, y, z)$, $Z_0 = \sqrt{\mu_0/\varepsilon_0}$ [Ohm] is the free space intrinsic impedance, and $\tilde{H}_0$ is a reference magnetic field strength [A/m]. Substituting the scaled quantities in (2.1) and using (2.3), we obtain:

$$\begin{aligned} \varepsilon_r \partial_t \boldsymbol{E} &= \nabla \times \boldsymbol{H} - \sigma_r \boldsymbol{E} - \boldsymbol{J}, \\ \mu_r \partial_t \boldsymbol{H} &= -\nabla \times \boldsymbol{E}, \end{aligned} \tag{2.6}$$

where $\sigma_r = L Z_0 \tilde{H}_0 \sigma$ [2]. System (2.6) can be written in the matrix form

$$\frac{\partial}{\partial t} \begin{bmatrix} \varepsilon_r \boldsymbol{E} \\ \mu_r \boldsymbol{H} \end{bmatrix} = \begin{bmatrix} -\sigma_r & \nabla\times \\ -\nabla\times & 0 \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix} - \begin{bmatrix} \boldsymbol{J} \\ 0 \end{bmatrix}. \tag{2.7}$$

Boundary and initial conditions (2.2) are scaled accordingly.

2.3 Finite difference space discretization

We introduce the notation $\mathcal{E} := \sqrt{\varepsilon_r}\boldsymbol{E}$, $\mathcal{H} := \sqrt{\mu_r}\boldsymbol{H}$, $\mathcal{J} := (1/\sqrt{\varepsilon_r})\boldsymbol{J}$ and rewrite (2.7) in the from

$$\frac{\partial}{\partial t} \begin{bmatrix} \mathcal{E} \\ \mathcal{H} \end{bmatrix} = \mathcal{A} \cdot \begin{bmatrix} \mathcal{E} \\ \mathcal{H} \end{bmatrix} - \begin{bmatrix} \mathcal{J} \\ 0 \end{bmatrix}, \tag{2.8}$$

where

$$\mathcal{A} = \begin{bmatrix} 0 & (1/\sqrt{\varepsilon_r})\nabla \times (1/\sqrt{\mu_r}) \\ -(1/\sqrt{\mu_r})\nabla \times (1/\sqrt{\varepsilon_r}) & 0 \end{bmatrix} + \begin{bmatrix} -\sigma_r/\sqrt{\varepsilon_r} & 0 \\ 0 & 0 \end{bmatrix}.$$

Note that the first operator here is skew-symmetric and the second one multiplies the $\mathcal{E}$ vector by $-\sigma_r/\sqrt{\varepsilon_r}$. The discretization of the Maxwell equations on non-colocated staggered grids combining with the structure (2.8) results in a semi-discrete system that has convenient properties. In this subsection, this discretization is briefly described.

Comparisons of the non-staggered, the colocated staggered and the non-colocated staggered grids (see, e.g., [26]) show that the last one has the most favorable properties for the spatial finite difference discretization of the Maxwell equations. The basic idea (known in the computational fluid dynamics already since the fifties through the Hansen scheme [39]) is to define two separate grids: one for the components of the electric field and one for the components of the magnetic field. These grids are shifted with a half mesh-size with respect to each other. In each grid point only one of the components is approximated. The building block of the discretization is the so-called Yee cell (Figure 1). In the sequel, we suppose that the number of Yee cells in the computational

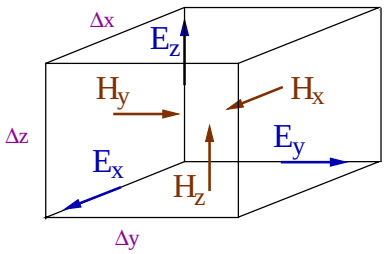

Fig. 1. The Yee cell with positions of the unknowns in the non-colocated staggered grid

space is N. In order to get a semi-discrete system we define the function $\mathcal{E}_x|_{i,j,k} : \mathbb{R} \to \mathbb{R}$ as $\mathcal{E}_x|_{i,j,k}(t) = \mathcal{E}(i\Delta x/2, j\Delta y/2, k\Delta z/2, t)$ for all odd integers i and even integers j, k such that the point $(i\Delta x/2, j\Delta y/2, k\Delta z/2)$ falls inside the computational domain. The functions $\mathcal{E}_y|_{i,j,k}$, $\mathcal{E}_z|_{i,j,k}$, $\mathcal{H}_\alpha|_{i,j,k}$ and $\mathcal{J}_\alpha|_{i,j,k}$ ($\alpha = x, y$ or z) can be defined similarly taking the positions of the field components into consideration. The above defined functions approximate the field components in the middle points of the faces and edges of the Yee cells.

Discretizing (2.7) on this grid by central differences, we obtain the following finite difference equation for $\mathcal{E}_x|_{i,j,k}$ (and, similarly, for the other unknowns):

$$\begin{aligned}\frac{\mathrm{d}\mathcal{E}_x|_{i,j,k}}{\mathrm{d}t} &= \frac{1}{\Delta y\sqrt{\varepsilon_{i,j,k}\mu_{i,j+1,k}}}\mathcal{H}_z|_{i,j+1,k} - \frac{1}{\Delta y\sqrt{\varepsilon_{i,j,k}\mu_{i,j-1,k}}}\mathcal{H}_z|_{i,j-1,k} \\ &+ \frac{1}{\Delta z\sqrt{\varepsilon_{i,j,k}\mu_{i,j,k-1}}}\mathcal{H}_y|_{i,j,k-1} - \frac{1}{\Delta z\sqrt{\varepsilon_{i,j,k}\mu_{i,j,k+1}}}\mathcal{H}_y|_{i,j,k+1} \\ &- \frac{\sigma_{i,j,k}}{\sqrt{\varepsilon_{i,j,k}}}\mathcal{E}_x|_{i,j,k} - \mathcal{J}_x|_{i,j,k}.\end{aligned} \tag{2.9}$$

where $\varepsilon_{i,j,k}$, $\mu_{i,j,k}$ and $\sigma_{i,j,k}$ denote ε_r, μ_r and σ_r at the point $(i\Delta x/2, j\Delta y/2, k\Delta z/2)$, respectively. Listing all the equations for all discretization points, we arrive at the Cauchy problem

$$\boldsymbol{w}'(t) = A\boldsymbol{w}(t) + \boldsymbol{f}(t), \ \boldsymbol{w}(0) \text{ is given}, \tag{2.10}$$

where the vector-scalar function $\boldsymbol{w} : \mathbb{R} \to \mathbb{R}^{6N}$ consists an arbitrary ordering of the functions $\mathcal{E}_x|_{i,j,k}$, $\mathcal{E}_y|_{i,j,k}$, $\mathcal{E}_z|_{i,j,k}$, $\mathcal{H}_x|_{i,j,k}$,$\mathcal{H}_y|_{i,j,k}$ and $\mathcal{H}_z|_{i,j,k}$ for all possible

integers i, j, k taken in an arbitrary order. The matrix $A \in \mathbb{R}^{6N\times 6N}$ is a sparse matrix that can be written as a sum of a skew-symmetric matrix and a diagonal matrix. Thus, the coefficient matrix in the semi-discretized equation inherits properties of the operator in (2.8). The rows of the skew-symmetric matrix accommodate the coefficients of the first four field components on the right-hand side of (2.9), the diagonal matrix contains the coefficient of the fifth term, and the vector $\boldsymbol{f}(t)$ contains the last term.

2.4 Finite element space discretization

In this finite element formulation we reduce Maxwell system (2.6) to a second order partial differential equation in the electric field and employ Nédélec's edge finite elements [29,28]. We apply the finite element discretization to the problems in lossless media, in other words in Sections 2.4 and 4.2 $\sigma_r \equiv 0$ (cf. (2.6)).

More specifically, by taking the time derivative of the first equation and the curl of the second equation in (2.6) one can obtain (recall $\sigma_r \equiv 0$)

$$\varepsilon_r \partial_{tt} \boldsymbol{E} + \nabla \times (\mu_r^{-1} \nabla \times \boldsymbol{E}) = -\partial_t \boldsymbol{J}. \tag{2.11}$$

This equation should be considered together with the dimensionless version of the boundary and initial conditions (2.2). In addition, initial condition for the first time derivative of $\boldsymbol{E}$ is delivered by writing down the first equation in (2.6) for the time $t = 0$.

Next, we consider a Galerkin weak formulation of (2.11) with respect to the space

$$H_0(\mathsf{curl}, \Omega) = \{\boldsymbol{u} \in L_2(\Omega)^3 |\ \nabla \times \boldsymbol{u} \in L_2(\Omega)^3,\ (\boldsymbol{n} \times \boldsymbol{u})|_\Gamma = 0\},$$

namely:

Find $\boldsymbol{E} \in H_0(\mathsf{curl}, \Omega)$ *such that* $\forall\, \boldsymbol{W} \in H_0(\mathsf{curl}, \Omega)$

$$\partial_{tt}(\varepsilon_r \boldsymbol{E}, \boldsymbol{W}) + (\mu_r^{-1} \nabla \times \boldsymbol{E}, \nabla \times \boldsymbol{W}) = -(\partial_t \boldsymbol{J}, \boldsymbol{W}). \tag{2.12}$$

We discretize (2.12) on a tetrahedral or hexahedral partition of Ω by means of Nédélec's first order edge basis functions $\boldsymbol{W}_j$ [29,28]

$$W_h = \operatorname{span}\{\boldsymbol{W}_j(x) \mid \text{all internal edges } j = 1, \ldots, N_{\mathsf{edge}}\},$$
$$\boldsymbol{W}_j \text{ is a linear function such that } \int_{\text{edge } i} \boldsymbol{W}_j \cdot \boldsymbol{t}_i = \delta_{ij},$$

where N_{edge} is the total number of the internal edges in the partition, $\boldsymbol{t}_j$ is the unit tangent vector along edge j and δ_{ij} is Kronecker's delta. We are thus searching for the numerical solution $\boldsymbol{E}_h$ in the form

$$\boldsymbol{E} \approx \boldsymbol{E}_h = \sum_{j=1}^{N} e_j(t)\boldsymbol{W}_j.$$

The discrete weak formulation reads:

Find $\boldsymbol{E}_h \in W_h$*, such that* $\forall\, \boldsymbol{W} \in W_h$

$$\partial_{tt}(\varepsilon_r \boldsymbol{E}_h, \boldsymbol{W}) + (\mu_r^{-1}\nabla \times \boldsymbol{E}_h, \nabla \times \boldsymbol{W}) = -(\partial_t \boldsymbol{J}, \boldsymbol{W}). \tag{2.13}$$

This discrete formulation can be written as a linear system of differential equations

$$M_\varepsilon \boldsymbol{e}'' + A_\mu \boldsymbol{e} = \boldsymbol{j}(t), \qquad M_\varepsilon, A_\mu \in \mathbb{R}^{N_{\mathsf{edge}} \times N_{\mathsf{edge}}}, \tag{2.14}$$

where

$$\begin{aligned} (M_\varepsilon)_{ij} &= (\varepsilon_r \boldsymbol{W}_i, \boldsymbol{W}_j), & (\boldsymbol{e}(t))_i &= e_i(t), \\ (A_\mu)_{ij} &= (\mu_r^{-1}\nabla \times \boldsymbol{W}_i, \nabla \times \boldsymbol{W}_j), & (\boldsymbol{j}(t))_i &= -(\partial_t \boldsymbol{J}, \boldsymbol{W}_i). \end{aligned} \tag{2.15}$$

When solving (2.14) numerically, we need to solve linear systems with the mass matrix M_ε. This matrix is often symmetric positive definite provided that ε is a symmetric positive definite tensor. Linear systems with M_ε can be solved with the help a direct sparse LU (or Cholesky) factorization or, when direct solvers are too expensive, by a preconditioned iterative method. It is then also convenient to rewrite (2.14) in the form

$$\begin{gathered} \boldsymbol{y}'' + \tilde{A}_{\varepsilon,\mu}\boldsymbol{y} = \tilde{\boldsymbol{j}}(t), \\ \boldsymbol{y} = U_\varepsilon \boldsymbol{e}, \quad \tilde{A}_{\varepsilon,\mu} = L_\varepsilon^{-1} A_\mu U_\varepsilon^{-1}, \quad \tilde{\boldsymbol{j}} = L_\varepsilon^{-1}\boldsymbol{j}, \quad L_\varepsilon U_\varepsilon = M_\varepsilon. \end{gathered} \tag{2.16}$$

Please note that the inverses of L_ε and U_ε are normally never computed explicitly, instead, to compute the action of the inverses on a vector, a linear system with L_ε or U_ε is solved.

We solve (2.16) by introducing an auxiliary variable

$$\boldsymbol{v}(t) \equiv \boldsymbol{y}'(t)$$

and writing (2.16) as a linear system of first order differential equations

$$\begin{gathered} \boldsymbol{w}'(t) = A\boldsymbol{w}(t) + \boldsymbol{f}(t), \qquad A \in \mathbb{R}^{2N_{\mathsf{edge}} \times 2N_{\mathsf{edge}}}, \\ \boldsymbol{w}(t) = \begin{bmatrix} \boldsymbol{v} \\ \boldsymbol{y} \end{bmatrix}, \quad A = \begin{bmatrix} 0 & -\tilde{A}_{\varepsilon,\mu} \\ I & 0 \end{bmatrix}, \quad \boldsymbol{f}(t) = \begin{bmatrix} \tilde{\boldsymbol{j}}(t) \\ 0 \end{bmatrix}, \end{gathered} \tag{2.17}$$

where I is the $N_{\mathsf{edge}} \times N_{\mathsf{edge}}$ identity matrix. Note that initial condition for the $\boldsymbol{y}$ part of the unknown vector function $\boldsymbol{w}(t)$ is delivered by dimensionless version of initial conditions (2.2) for the electric field, whereas the initial conditions for the $\boldsymbol{v}$ part of $\boldsymbol{w}(t)$ are obtained through the first equation in (2.6).

3 Splitting methods

3.1 Some mathematical preliminaries

Let $\boldsymbol{g}_\tau$ be a vector function defined on an interval $\mathcal{I} \subset \mathbb{R}$, $\boldsymbol{g}_\tau : \mathcal{I} \to \mathbb{R}^n$, with τ being a scalar parameter. We write $\boldsymbol{g}_\tau(t) = O(\tau^p)$ if there exists a constant $C_0 > 0$ such that for sufficiently small values of $|\tau|$

$$\|\boldsymbol{g}_\tau(t)\| \leqslant C_0|\tau|^p \tag{3.1}$$

holds uniformly with respect to $t \in \mathcal{I}$ and $\|\cdot\|$ is any vector norm on $\mathbb{R}^n$. For simplicity, we also write $O((\tau - s)^k)$ as $O(\tau - s)^k$. Similar notations are applied to scalar functions and vector functions of one variable.

For a function $\boldsymbol{v} : \mathcal{I} \to \mathbb{R}^n$ with integrable coordinate functions $v_i : \mathcal{I} \to \mathbb{R}$, the integral $\int_{\mathcal{I}} \boldsymbol{v}(t)dt$ is defined elementwise, i.e.,

$$\int_{\mathcal{I}} \boldsymbol{v}(t)dt \equiv [\int_{\mathcal{I}} v_i(t)dt\,]_{i=1}^n \in \mathbb{R}^n.$$

We will need the following result:

Lemma 3.1.1 *Assume that the interval $\mathcal{I}$ is of the length $|\mathcal{I}| = O(\tau^m)$, that is, there exists a constant $C_1 > 0$ such that for sufficiently small values $|\tau|$ it holds: $|\mathcal{I}| \leqslant C_1|\tau|^m$. Assume also that $\tau > 0$ and $\tau \in \mathcal{I}$ and that $\boldsymbol{f}_\tau(t) = O(\tau^p)$ and $\boldsymbol{g}_{\tau-s}(t) = O(\tau - s)^p$. Then*

$$\int_{\mathcal{I}} \boldsymbol{f}_\tau(s)ds = O(\tau^{p+m}), \qquad \int_{\mathcal{I}} \boldsymbol{g}_{\tau-s}(s)ds = O(\tau^{m+mp}). \tag{3.2}$$

Proof There exist constants $C_2 > 0$ and $C_3 > 0$ such that

$$\|\boldsymbol{f}_\tau(t)\| \leqslant C_2\tau^p, \qquad \|\boldsymbol{g}_{\tau-s}(t)\| \leqslant C_3|\tau - s|^p,$$

uniformly for all $t \in \mathcal{I}$. Hence, the coordinate functions $f_{\tau,i}(t)$, $g_{\tau-s,i}(t)$, $i = 1, \ldots, n$, are also bounded as $|f_{\tau,i}(t)| \leqslant C_2\tau^p$, $|g_{\tau-s,i}(t)| \leqslant C_3|\tau - s|^p$. Thus we

have

$$\left|\int_{\mathcal{I}} f_{\tau,i}(s)ds\right| \leqslant \int_{\mathcal{I}} |f_{\tau,i}(s)|ds \leqslant C_2\tau^p \int_{\mathcal{I}} ds \leqslant C_1C_2\tau^{p+m},$$
$$\left|\int_{\mathcal{I}} g_{\tau-s,i}(s)ds\right| \leqslant \int_{\mathcal{I}} |g_{\tau-s,i}(s)|ds \leqslant C_3 \int_{\mathcal{I}} \underbrace{|\tau-s|^p}_{\leqslant |\mathcal{I}|^p \leqslant C_1\tau^{mp}} ds \leqslant C_1C_3\tau^{mp} \int_{\mathcal{I}} ds \leqslant C_1^2C_3\tau^{mp+m}.$$

□

The commutator of the matrices $A \in \mathbb{R}^{n\times n}$ and $B \in \mathbb{R}^{n\times n}$ is denoted by $[A, B]$ and defined as

$$[A, B] \equiv AB - BA. \tag{3.3}$$

For any matrix $A \in \mathbb{R}^{n\times n}$ its matrix exponential is defined as

$$e^A \equiv \sum_{j=0}^{\infty} \frac{1}{j!} A^j.$$

Let $\boldsymbol{v} : \mathcal{I} \to \mathbb{R}^n$ be a given vector function such that $\|v(t)\|$ is bounded uniformly for all $t \in \mathcal{I}$. Using (3.1), we have

$$e^{\tau A}\boldsymbol{v}(t) = \sum_{j=0}^{m} \frac{1}{j!} A^j \boldsymbol{v}(t) + O(\tau^{m+1}), \qquad \forall t \in \mathcal{I},\ \forall m \in \mathbb{N}, \tag{3.4}$$

$$e^{\tau A} \cdot e^{\tau B}\boldsymbol{v}(t) = (I + \tau(A + B) + \frac{\tau^2}{2}(A^2 + B^2 + 2AB))\boldsymbol{v}(t) + O(\tau^3), \tag{3.5}$$

$$\begin{aligned} e^{\tau A} \cdot e^{\tau B} \cdot e^{\tau C}\boldsymbol{v}(t) = (I &+ \tau(A + B + C) \\ &+ \frac{\tau^2}{2}(A^2 + B^2 + C^2 + 2(AC + BC + AB)))\boldsymbol{v}(t) + O(\tau^3), \end{aligned} \tag{3.6}$$

for all $t \in \mathcal{I}$. Let $\boldsymbol{v} : \mathcal{I} \to \mathbb{R}^n$ be $p + 1$ continuously differentiable function ($\boldsymbol{v} \in C^{p+1}(\mathcal{I})$). Then the Taylor expansion of the function $\boldsymbol{v}$ can be defined as:

$$\boldsymbol{v}(t+\tau) = \sum_{j=0}^{p} \frac{\tau^j}{j!}\boldsymbol{v}^{(j)}(t) + \frac{\tau^{p+1}}{(p+1)!}\boldsymbol{v}^{(p+1)}(t+\theta\tau), \qquad \forall \tau > 0\ (t+\tau \in \mathcal{I}), \tag{3.7}$$

where

$$\begin{aligned} \boldsymbol{v}^{(j)}(t) &= [v_i^{(j)}]_{i=1}^n \in \mathbb{R}^n, \qquad j = 1, \ldots, p, \\ \boldsymbol{v}^{(p+1)}(t + \theta\tau) &\equiv [v_i^{(p+1)}(t + \theta_i\tau)]_{i=1}^n \in \mathbb{R}^n, \qquad \theta_i \in (0, 1), \quad i = 1, \ldots, n. \end{aligned}$$

Using the introduced notation of $O(\tau^p)$ (cf. (3.1)), we can rewrite Taylor series (3.7) as

$$\boldsymbol{v}(t + \tau) = \sum_{j=0}^{p} \frac{\tau^j}{j!}\boldsymbol{v}^{(j)}(t) + O(\tau^{p+1}). \tag{3.8}$$

Let $\boldsymbol{f} : [0, T] \to \mathbb{R}^n$ be a given vector function and $A \in \mathbb{R}^{n\times n}$. The solution of the initial value problem

$$\begin{cases} \boldsymbol{w}'(t) = A\boldsymbol{w}(t) + \boldsymbol{f}(t), & t \in [0, T], \\ \boldsymbol{w}(0) \text{ is given}, \end{cases} \tag{3.9}$$

reads

$$\boldsymbol{w}_{\mathsf{exact}}(t) = e^{tA}\boldsymbol{w}(0) + \int_0^t e^{(t-s)A}\boldsymbol{f}(s)ds, \qquad t \in [0, T]. \tag{3.10}$$

3.2 Splitting of the ODE system

Spatial discretization methods described in the previous section yield ODE system (3.9) which we split into the following two ODE systems:

$$\boldsymbol{w}_1' = A_1\boldsymbol{w}_1 + \boldsymbol{f}_1, \qquad \boldsymbol{w}_2' = A_2\boldsymbol{w}_2 + \boldsymbol{f}_2, \qquad \text{with} \quad A_1 + A_2 = A, \quad \boldsymbol{f}_1 + \boldsymbol{f}_2 = \boldsymbol{f}. \tag{3.11}$$

3.3 Strang-Marchuk splitting

Consider the Strang-Marchuk splitting scheme [27,35] where, at every time step, a step for subproblem 1 with a step size $\tau/2$ is followed by a step τ for subproblem 2 and, again, by a step $\tau/2$ for subproblem 1. Assuming that time integration at every split step is done exactly, we can write the solution of this splitting scheme after one time step as

$$\boldsymbol{w}_{\mathsf{strang}}(\tau) = e^{\frac{\tau}{2}A_1}\left[e^{\tau A_2}\boldsymbol{w}_1(\tau/2) + \int_0^\tau e^{(\tau-s)A_2}\boldsymbol{f}_2(s)ds\right] + \int_{\tau/2}^\tau e^{(\tau-s)A_1}\boldsymbol{f}_1(s)ds, \tag{3.12}$$

where $\boldsymbol{w}_1(\tau/2)$ is the solution of the first substep for subproblem 1:

$$\boldsymbol{w}_1(\tau/2) = e^{\frac{\tau}{2}A_1}\boldsymbol{w}_1(0) + \int_0^{\tau/2} e^{(\tau/2-s)A_1}\boldsymbol{f}_1(s)ds,$$

with $\boldsymbol{w}_1(0) \equiv \boldsymbol{w}(0)$ being the initial data of the original problem (3.9). Substituting the last expression for $\boldsymbol{w}_1(\tau/2)$ into (3.12), we obtain:

$$\begin{aligned}\boldsymbol{w}_{\mathsf{strang}}(\tau) &= e^{\frac{\tau}{2}A_1}\left[e^{\tau A_2}\left(e^{\frac{\tau}{2}A_1}\boldsymbol{w}(0) + \int_0^{\tau/2} e^{(\tau/2-s)A_1}\boldsymbol{f}_1(s)ds\right) + \int_0^{\tau} e^{(\tau-s)A_2}\boldsymbol{f}_2(s)ds\right] \\ &\quad + \int_{\tau/2}^{\tau} e^{(\tau-s)A_1}\boldsymbol{f}_1(s)ds \\ &= e^{\frac{\tau}{2}A_1}e^{\tau A_2}e^{\frac{\tau}{2}A_1}\boldsymbol{w}(0) + e^{\frac{\tau}{2}A_1}e^{\tau A_2}\int_0^{\tau/2} e^{(\tau/2-s)A_1}\boldsymbol{f}_1(s)ds \\ &\quad + e^{\frac{\tau}{2}A_1}\int_0^{\tau} e^{(\tau-s)A_2}\boldsymbol{f}_2(s)ds + \int_{\tau/2}^{\tau} e^{(\tau-s)A_1}\boldsymbol{f}_1(s)ds.\end{aligned} \tag{3.13}$$

Theorem 3.3.1 *Assume that the functions $\boldsymbol{f}_1$, $\boldsymbol{f}_2$ are three times continuously differentiable vector functions: $\boldsymbol{f}_i : [0,T] \to \mathbb{R}^n$, $\boldsymbol{f}_i \in C^3([0,T])$, $i = 1, 2$. Then the Strang-Marchuk splitting scheme* (3.13) *applied to the inhomogeneous ODE system* (3.9) *with splitting* (3.11) *has third order local error, i.e. the scheme has second order accuracy:*

$$\begin{aligned}\boldsymbol{w}_{\mathsf{strang}}(\tau) - \boldsymbol{w}_{\mathsf{exact}}(\tau) = -\frac{\tau^3}{12}\Bigg(&\left[\frac{1}{2}A_1 + A_2, [A_1, A_2]\right]\boldsymbol{w}(0) \\ &+ \left(\frac{1}{2}A_2A_1 - A_1A_2 - A_2^2\right)\boldsymbol{f}_1\left(\frac{\tau}{2}\right) \\ &+ \left(2A_2A_1 - A_1A_2 + \frac{1}{2}A_1^2\right)\boldsymbol{f}_2\left(\frac{\tau}{2}\right) \\ &- A_1\boldsymbol{f}_2'\left(\frac{\tau}{2}\right) + \frac{1}{2}A_2\boldsymbol{f}_1'\left(\frac{\tau}{2}\right)\Bigg) + O(\tau^4),\end{aligned} \tag{3.14}$$

where $\boldsymbol{w}_{\mathsf{exact}}$ is the exact solution of (3.9) *defined by* (3.10) *and $[A_1, A_2]$ is the commutator of A_1 and A_2 (cf.* (3.3)*).*

Proof Comparing (3.13) and (3.10), we first note that [9]

$$(e^{\frac{\tau}{2}A_1}e^{\tau A_2}e^{\frac{\tau}{2}A_1} - e^{\tau A})\boldsymbol{w}(0) = -\frac{\tau^3}{12}\left(\left[\frac{1}{2}A_1 + A_2, [A_1, A_2]\right]\right)\boldsymbol{w}(0) + O(\tau^4). \tag{3.15}$$

The rest of the proof consists of estimating the differences in the terms containing $\boldsymbol{f}_1$ and $\boldsymbol{f}_2$ in (3.13) and (3.10). We first rewrite the terms of (3.13) containing $\boldsymbol{f}_1$ as

$$\begin{aligned}&e^{\frac{\tau}{2}A_1}e^{\tau A_2}\int_0^{\tau/2} e^{(\tau/2-s)A_1}\boldsymbol{f}_1(s)ds + \int_{\tau/2}^{\tau} e^{(\tau-s)A_1}\boldsymbol{f}_1(s)ds \\ &= \int_0^{\tau/2} e^{\frac{\tau}{2}A_1}e^{\tau A_2}e^{(\tau/2-s)A_1}\boldsymbol{f}_1(s)ds + \int_{\tau/2}^{\tau} e^{(\tau-s)A_1}\boldsymbol{f}_1(s)ds\end{aligned}$$

and, using (3.2) and (3.4), we arrive at

$$= \int_0^\tau \boldsymbol{f}_1(s)ds + \int_0^\tau (\tau - s)A_1\boldsymbol{f}_1(s)ds + \int_0^\tau \frac{(\tau-s)^2}{2}A_1^2\boldsymbol{f}_1(s)ds \qquad (3.16)$$

$$+ \int_0^{\tau/2} \left(\tau A_2 + \frac{\tau^2}{2}\left(A_2^2 + A_1A_2 + A_2A_1\right) - \tau s A_2A_1\right)\boldsymbol{f}_1(s)ds + O(\tau^4). \qquad (3.17)$$

We now introduce the notations

$$\boldsymbol{f}_{i,0} = \boldsymbol{f}_i(\tau/2) \in \mathbb{R}^n, \quad \boldsymbol{f}_{i,1} = \boldsymbol{f}_i'(\tau/2) \in \mathbb{R}^n, \quad \boldsymbol{f}_{i,2} = \boldsymbol{f}_i''(\tau/2) \in \mathbb{R}^n \qquad i = 1, 2,$$

and define the Taylor expansions of $\boldsymbol{f}_1$ and $\boldsymbol{f}_2$:

$$\boldsymbol{f}_i(s) = \boldsymbol{f}_{i,0} + (s-\tau/2)\boldsymbol{f}_{i,1} + \frac{(s-\tau/2)^2}{2}\boldsymbol{f}_{i,2} + O(s-\tau/2)^3, \qquad i = 1, 2. \quad (3.18)$$

Replacing $\boldsymbol{f}_1$ in (3.17) by its Taylor expansion (3.18) and taking into account (3.2), we obtain

$$\int_0^\tau \boldsymbol{f}_1(s)ds = \int_0^\tau \left[\boldsymbol{f}_{1,0} + (s-\tau/2)\boldsymbol{f}_{1,1} + \frac{(s-\tau/2)^2}{2}\boldsymbol{f}_{1,2}\right]ds + O(\tau^4)$$

$$= \int_0^\tau ds \cdot \boldsymbol{f}_{1,0} + \underbrace{\int_0^\tau (s-\tau/2)ds}_{=0} \cdot \boldsymbol{f}_{1,1} + \int_0^\tau \frac{(s-\tau/2)^2}{2}ds\boldsymbol{f}_{1,2} + O(\tau^4) =$$

$$= \tau\boldsymbol{f}_{1,0} + \frac{\tau^3}{24}\boldsymbol{f}_{1,2} + O(\tau^4).$$

Similarly, we have

$$\int_0^\tau (\tau - s)A_1\boldsymbol{f}_1(s)ds = \frac{\tau^2}{2}A_1\boldsymbol{f}_{1,0} - \frac{\tau^3}{12}A_1\boldsymbol{f}_{1,1} + O(\tau^4),$$

$$\int_0^\tau \frac{(\tau-s)^2}{2}A_1^2\boldsymbol{f}_1(s)ds = \frac{\tau^3}{6}A_1^2\boldsymbol{f}_{1,0} + O(\tau^4),$$

$$\int_0^{\tau/2} \tau A_2\boldsymbol{f}_1(s)ds = \frac{\tau^2}{2}A_2\boldsymbol{f}_{1,0} - \frac{\tau^3}{8}A_2\boldsymbol{f}_{1,1} + O(\tau^4),$$

$$\int_0^{\tau/2} \frac{\tau^2}{2}(A_2^2 + A_1A_2 + A_2A_1)\boldsymbol{f}_1(s)ds = \frac{\tau^3}{4}(A_2^2 + A_1A_2 + A_2A_1)\boldsymbol{f}_{1,0},$$

and $$\int_0^{\tau/2} \tau s A_2A_1\boldsymbol{f}_1(s)ds = \frac{\tau^3}{6}A_2A_1\boldsymbol{f}_{1,0}.$$

Hence, we get

$$e^{\frac{\tau}{2}A_1} \cdot e^{\tau A_2}\int_0^{\tau/2} e^{(\tau/2-s)A_1}\boldsymbol{f}_1(s)ds + \int_{\tau/2}^\tau e^{(\tau-s)A_1}\boldsymbol{f}_1(s)ds$$

$$= \tau \boldsymbol{f}_{1,0} + \frac{\tau^2}{2}(A_1 + A_2)\boldsymbol{f}_{1,0} \tag{3.19}$$

$$+\frac{\tau^3}{12}\left(\frac{1}{2}\boldsymbol{f}_{1,2} - A_1\boldsymbol{f}_{1,1} + 2A_1^2\boldsymbol{f}_{1,0} + 3(A_2^2 + A_1A_2 + A_2A_1)\boldsymbol{f}_{1,0} - \frac{3}{2}A_2\boldsymbol{f}_{1,1} - \frac{3}{2}A_2A_1\boldsymbol{f}_{1,0}\right).$$

Next, we estimate the term with $\boldsymbol{f}_2$ in (3.13):

$$e^{\frac{\tau}{2}A_1}\int_0^\tau e^{(\tau-s)A_2}\boldsymbol{f}_2(s)ds =^{(3.5)} \int_0^\tau \boldsymbol{f}_2(s)ds + \int_0^\tau \left(\frac{\tau}{2}A_1 + (\tau-s)A_2\right)\boldsymbol{f}_2(s)ds$$
$$+ \int_0^\tau \left(\frac{\tau^2}{8}A_1^2 + \frac{(\tau-s)^2}{2}A_2^2 + \frac{\tau(\tau-s)}{2}A_1A_2\right)\boldsymbol{f}_2(s)ds + O(\tau^4).$$

Replacing here $\boldsymbol{f}_2(s)$ by its Taylor expansion (3.18), we have

$$\int_0^\tau \boldsymbol{f}_2(s)ds =^{(3.19)} \tau\boldsymbol{f}_{2,0} + \frac{\tau^3}{24}\boldsymbol{f}_{2,2} + O(\tau^4),$$

$$\int_0^\tau \left(\frac{\tau}{2}A_1 + (\tau-s)A_2\right)\boldsymbol{f}_2(s)ds =^{(3.2)} \frac{\tau^2}{2}(A_1+A_2)\boldsymbol{f}_{2,0} - \frac{\tau^3}{12}A_2\boldsymbol{f}_{2,1} + O(\tau^4),$$

$$\int_0^\tau \left(\frac{\tau^2}{8}A_1^2 + \frac{(\tau-s)^2}{2}A_2^2 + \frac{\tau(\tau-s)}{2}A_1A_2\right)\boldsymbol{f}_2(s)ds$$
$$=^{(3.2)} \frac{\tau^3}{8}\left(A_1^2\boldsymbol{f}_{2,0} + \frac{3}{4}A_2^2\boldsymbol{f}_{2,0} + 2A_1A_2\boldsymbol{f}_{2,0}\right) + O(\tau^4).$$

Thus, the $\boldsymbol{f}_2$-term in (3.13) can be estimated as

$$e^{\frac{\tau}{2}A_1}\int_0^\tau e^{(\tau-s)A_2}\boldsymbol{f}_2(s)ds = \tau\boldsymbol{f}_{2,0} + \frac{\tau^2}{2}(A_1+A_2)\boldsymbol{f}_{2,0} \tag{3.20}$$

$$\frac{\tau^3}{12}\left(\frac{1}{2}\boldsymbol{f}_{2,2} - A_2\boldsymbol{f}_{2,1} + \frac{3}{2}A_1^2\boldsymbol{f}_{2,0} + 2A_2^2\boldsymbol{f}_{2,0} + 3A_1A_2\boldsymbol{f}_{2,0}\right) + O(\tau^4).$$

This, together with (3.19), yields

$$\boldsymbol{w}_{\mathsf{strang}}(\tau) = e^{\frac{\tau}{2}A_1}e^{\tau A_2}e^{\frac{\tau}{2}A_1}\boldsymbol{w}(0) + \tau(\boldsymbol{f}_{1,0}+\boldsymbol{f}_{2,0}) + \frac{\tau^2}{2}(A_1+A_2)(\boldsymbol{f}_{1,0}+\boldsymbol{f}_{2,0})$$
$$+\tau^3\left(\frac{1}{24}\boldsymbol{f}_{1,2} - \left(\frac{1}{12}A_1 + \frac{1}{8}A_2\right)\boldsymbol{f}_{1,1} + \frac{1}{24}(4A_1^2 + 6A_2^2 + 6A_1A_2 + 3A_2A_1)\boldsymbol{f}_{1,0}\right.$$
$$\left.+\frac{1}{24}\boldsymbol{f}_{2,2} - \frac{1}{12}A_2\boldsymbol{f}_{2,1} + \frac{1}{24}(3A_1^2 + 4A_2^2 + 6A_1A_2)\boldsymbol{f}_{2,0}\right) + O(\tau^4). \tag{3.21}$$

Consider now the exact solution $\boldsymbol{w}_{\mathsf{exact}}(\tau)$ given by (3.10). Using again the Taylor series of $\boldsymbol{f}(s)$, we can rewrite the integral term in (3.10) as

$$\int_0^\tau e^{(\tau-s)A}\boldsymbol{f}(s)ds =^{(3.4),(3.2)} \int_0^\tau \left[I + (\tau-s)A + \frac{(\tau-s)^2}{2}A^2\right]\boldsymbol{f}(s)ds + O(\tau^4)$$
$$= \tau(\boldsymbol{f}_{1,0}+\boldsymbol{f}_{2,0}) + \frac{\tau^2}{2}(A_1+A_2)(\boldsymbol{f}_{1,0}+\boldsymbol{f}_{2,0})$$
$$+\tau^3\left(\frac{1}{6}A^2(\boldsymbol{f}_{1,0}+\boldsymbol{f}_{2,0}) - \frac{1}{12}A(\boldsymbol{f}_{1,1}+\boldsymbol{f}_{2,1}) + \frac{1}{24}(\boldsymbol{f}_{1,2}+\boldsymbol{f}_{2,2})\right) + O(\tau^4),$$

so that

$$\boldsymbol{w}_{\mathsf{exact}}(\tau) = e^{\tau A}\boldsymbol{w}(0) + \tau(\boldsymbol{f}_{1,0} + \boldsymbol{f}_{2,0}) + \frac{\tau^2}{2}(A_1 + A_2)(\boldsymbol{f}_{1,0} + \boldsymbol{f}_{2,0}) + \tau^3\left(\frac{1}{6}A^2(\boldsymbol{f}_{1,0} + \boldsymbol{f}_{2,0}) - \frac{1}{12}A(\boldsymbol{f}_{1,1} + \boldsymbol{f}_{2,1}) + \frac{1}{24}(\boldsymbol{f}_{1,2} + \boldsymbol{f}_{2,2})\right) + O(\tau^4). \tag{3.22}$$

Subtracting the last expression from (3.21) and taking into account (3.15), we arrive at the required statement given by (3.14). □

3.4 Symmetrically weighted sequential (SWS) splitting

We consider now the symmetrically weighted sequential (SWS) splitting [34]. In this splitting scheme, solution after one time step is defined as

$$\boldsymbol{w}_{\mathsf{sws}}(\tau) = \frac{1}{2}(\boldsymbol{w}_{\mathsf{seq12}}(\tau) + \boldsymbol{w}_{\mathsf{seq21}}(\tau)), \tag{3.23}$$

where $\boldsymbol{w}_{\mathsf{seq12}}$ is solution of the sequential splitting method, i.e. it is obtained by performing a step τ for subproblem 1 and then a step τ for subproblem 2 (for $\boldsymbol{w}_{\mathsf{seq21}}$, the order of the substeps is the opposite):

$$\boldsymbol{w}_{\mathsf{seq12}}(\tau) = e^{\tau A_2}\left[e^{\tau A_1}\boldsymbol{w}(0) + \int_0^\tau e^{(\tau-s)A_1}\boldsymbol{f}_1(s)ds\right] + \int_0^\tau e^{(\tau-s)A_2}\boldsymbol{f}_2(s)ds. \tag{3.24}$$

The following result holds:

Theorem 3.4.1 *Assume that the functions $\boldsymbol{f}_1$, $\boldsymbol{f}_2$ are three times continuously differentiable vector functions: $\boldsymbol{f}_i : [0,T] \to \mathbb{R}^n$, $\boldsymbol{f}_i \in C^3([0,T])$, $i = 1, 2$. Then the symmetrically weighted sequential (SWS) splitting scheme* (3.23) *applied to the inhomogeneous ODE system* (3.9) *with splitting* (3.11) *has third order local error, i.e. the scheme has second order accuracy:*

$$\begin{aligned}\boldsymbol{w}_{\mathsf{sws}}(\tau) - \boldsymbol{w}_{\mathsf{exact}}(\tau) = \tau^3\,[A_1 - A_2, [A_1, A_2]]\,\boldsymbol{w}(0) \\ + \frac{\tau^3}{12}\Big((A_2A_1 - 2A_1A_2 + A_2^2)\boldsymbol{f}_1(\tau/2) \\ + (A_1A_2 - 2A_2A_1 + A_1^2)\boldsymbol{f}_2(\tau/2) \\ + A_2\boldsymbol{f}_1'(\tau/2) + A_1\boldsymbol{f}_2'(\tau/2)\Big) + O(\tau^4),\end{aligned} \tag{3.25}$$

where $\boldsymbol{w}_{\mathsf{exact}}$ is the exact solution of (3.9) *defined by* (3.10) *and $[A_1, A_2]$ is the commutator of A_1 and A_2 (cf.* (3.3)*).*

Proof The first term in (3.24) containing the integral can be rewritten as

$$
\begin{aligned}
e^{\tau A_2}\int_0^\tau e^{(\tau-s)A_1}\boldsymbol{f}_1(s)ds &= \int_0^\tau e^{\tau A_2}e^{(\tau-s)A_1}\boldsymbol{f}_1(s)ds \\
&=^{(3.5),(3.18)} \int_0^\tau \Big[I+\tau A_2+(\tau-s)A_1+\frac{\tau^2}{2}A_2^2+\frac{(\tau-s)^2}{2}A_1^2+\tau(\tau-s)A_2A_1 \\
&\quad +O(\tau^3)+O(\tau-s)^3\Big]\left(\boldsymbol{f}_{1,0}+(s-\frac{\tau}{2})\boldsymbol{f}_{1,1}+\frac{1}{2}(s-\frac{\tau}{2})^2 f_{1,2}+O(s-\frac{\tau}{2})^3\right)ds \\
&=^{(3.2)} \int_0^\tau \left[I+\tau A_2+(\tau-s)A_1+\frac{\tau^2}{2}A_2^2+\frac{(\tau-s)^2}{2}A_1^2+\tau(\tau-s)A_2A_1\right]\boldsymbol{f}_{1,0}ds \\
&\quad +\int_0^\tau (s-\frac{\tau}{2})(I+\tau A_2+(\tau-s)A_1)\boldsymbol{f}_{1,1}ds+\int_0^\tau \frac{1}{2}(s-\frac{\tau}{2})^2\boldsymbol{f}_{1,2}ds+O(\tau^4) \\
&= \tau\boldsymbol{f}_{1,0}+\tau^2A_2\boldsymbol{f}_{1,0}+\frac{\tau^2}{2}A_1\boldsymbol{f}_{1,0}+(\frac{\tau^3}{2}A_2^2+\frac{\tau^3}{6}A_1^2)\boldsymbol{f}_{1,0}+\frac{\tau^3}{2}A_2A_1\boldsymbol{f}_{1,0} \\
&\quad -\frac{\tau^3}{12}A_1\boldsymbol{f}_{1,1}+\frac{\tau^3}{24}\boldsymbol{f}_{1,2}+O(\tau^4).
\end{aligned}
\tag{3.26}
$$

Next, we evaluate the second integral term in (3.24) as

$$
\begin{aligned}
\int_0^\tau e^{(\tau-s)A_2}\boldsymbol{f}_2(s)ds &=^{(3.4),(3.18)} \int_0^\tau \left[\left(I+(\tau-s)A_2+\frac{(\tau-s)^2}{2}A_2^2\right)\boldsymbol{f}_2(s)+O(\tau-s)^3\right]ds \\
&=^{(3.2),(3.18)} \int_0^\tau \left(I+(\tau-s)A_2+\frac{(\tau-s)^2}{2}A_2^2\right) \\
&\qquad \times\left(\boldsymbol{f}_{2,0}+(s-\frac{\tau}{2})\boldsymbol{f}_{2,1}+\frac{1}{2}(s-\frac{\tau}{2})^2\boldsymbol{f}_{2,2}\right)ds+O(\tau^4), \\
&= \int_0^\tau \left[I+(\tau-s)A_2+\frac{(\tau-s)^2}{2}A_2^2\right]\boldsymbol{f}_{2,0}ds \\
&\quad +\int_0^\tau (s-\frac{\tau}{2})(I+(\tau-s)A_2)\boldsymbol{f}_{2,1}ds+\frac{1}{2}\int_0^\tau (s-\frac{\tau}{2})^2\boldsymbol{f}_{2,2}ds \\
&= \tau\boldsymbol{f}_{2,0}+\frac{\tau^2}{2}A_2\boldsymbol{f}_{2,0}+\frac{\tau^3}{6}A_2^2\boldsymbol{f}_{2,0}+\underbrace{\int_0^\tau (s-\frac{\tau}{2})ds}_{=0}\boldsymbol{f}_{2,1} \\
&\quad -\frac{\tau^3}{12}A_2\boldsymbol{f}_{2,1}+\frac{\tau^3}{24}\boldsymbol{f}_{2,2}+O(\tau^4).
\end{aligned}
\tag{3.27}
$$

Substitution of (3.26),(3.27) into (3.24) leads to

$$
\begin{aligned}
\boldsymbol{w}_{\mathsf{seq12}}(\tau) &= e^{\tau A_2}e^{\tau A_1}\boldsymbol{w}(0)+\tau\boldsymbol{f}(\tau/2)+\frac{\tau^2}{2}\left[A_1\boldsymbol{f}_{1,0}+A_2\boldsymbol{f}_{2,0}\right]+\tau^2A_2\boldsymbol{f}_{1,0} \\
&\quad +\frac{\tau^3}{2}(A_2^2+\frac{1}{3}A_1^2+A_2A_1)\boldsymbol{f}_{1,0}+\frac{\tau^3}{6}A_2^2\boldsymbol{f}_{2,0} \\
&\quad -\frac{\tau^3}{12}(A_1\boldsymbol{f}_{1,1}+A_2\boldsymbol{f}_{2,1})+\frac{\tau^3}{24}\boldsymbol{f}''(\tau/2)+O(\tau^4),
\end{aligned}
\tag{3.28}
$$

where we have used the fact that $\boldsymbol{f}_{1,0}+\boldsymbol{f}_{2,0}=\boldsymbol{f}(\tau/2)$ and $\boldsymbol{f}_{1,2}+\boldsymbol{f}_{2,2}=\boldsymbol{f}''(\tau/2)$ (see (3.18)). By swapping 1 and 2 in the formula above, a similar expression

for $\boldsymbol{w}_{\mathsf{seq21}}(\tau)$ can be obtained:

$$\begin{aligned}\boldsymbol{w}_{\mathsf{seq21}}(\tau) = e^{\tau A_1}e^{\tau A_2}\boldsymbol{w}(0) + \tau\boldsymbol{f}(\tau/2) + \frac{\tau^2}{2}\left[A_2\boldsymbol{f}_{2,0} + A_1\boldsymbol{f}_{1,0}\right] + \tau^2 A_1\boldsymbol{f}_{2,0} \\ + \frac{\tau^3}{2}(A_1^2 + \frac{1}{3}A_2^2 + A_1A_2)\boldsymbol{f}_{2,0} + \frac{\tau^3}{6}A_1^2\boldsymbol{f}_{1,0} \\ - \frac{\tau^3}{12}(A_2\boldsymbol{f}_{2,1} + A_1\boldsymbol{f}_{1,1}) + \frac{\tau^3}{24}\boldsymbol{f}''(\tau/2) + O(\tau^4).\end{aligned} \tag{3.29}$$

With (3.28),(3.29), expression (3.23) can be rewritten as

$$\begin{aligned}\boldsymbol{w}_{\mathsf{sws}}(\tau) = \frac{1}{2}\left[e^{\tau A_1}e^{\tau A_2} + e^{\tau A_2}e^{\tau A_1}\right]\boldsymbol{w}(0) + \tau\boldsymbol{f}(\tau/2) + \frac{\tau^2}{2}A\boldsymbol{f}(\tau/2) \\ + \tau^3\left(\frac{1}{12}(2A_1^2 + 3A_2A_1 + 3A_2^2)\boldsymbol{f}_{1,0} + \frac{1}{12}(2A_2^2 + 3A_1A_2 + 3A_1^2)\boldsymbol{f}_{2,0}\right. \\ \left. -\frac{1}{12}(A_1\boldsymbol{f}_{1,1} + A_2\boldsymbol{f}_{2,1}) + \frac{1}{24}(\boldsymbol{f}_{1,2} + \boldsymbol{f}_{2,2})\right) + O(\tau^4)\end{aligned} \tag{3.30}$$

Subtracting (3.22) from the last expression, we obtain

$$\begin{aligned}\boldsymbol{w}_{\mathsf{sws}}(\tau) - \boldsymbol{w}_{\mathsf{exact}}(\tau) = \left(\frac{1}{2}(e^{\tau A_1}e^{\tau A_2} + e^{\tau A_2}e^{\tau A_1}) - e^{\tau A}\right)\boldsymbol{w}(0) \\ + \frac{\tau^3}{12}\left((A_2A_1 - 2A_1A_2 + A_2^2)\boldsymbol{f}_{1,0}\right. \\ \left. + (A_1A_2 - 2A_2A_1 + A_1^2)\boldsymbol{f}_{2,0} + A_2\boldsymbol{f}_{1,1} + A_1\boldsymbol{f}_{2,1}\right) + O(\tau^4).\end{aligned}$$

It is shown in [4] that

$$\left(\frac{1}{2}(e^{\tau A_1}e^{\tau A_2} + e^{\tau A_2}e^{\tau A_1}) - e^{\tau A}\right)\boldsymbol{w}(0) = \tau^3\left[A_1 - A_2, [A_1, A_2]\right]\boldsymbol{w}(0) + O(\tau^4),$$

and this finishes the proof. □

4 Numerical experiments

In this section we present numerical experiments with the splitting methods discussed in Section 3. In the experiments, both the finite difference and the finite element space discretizations described in Section 2 have been used. We split space-discretized problem (3.9) by taking in (3.11)

$$\text{splitting f-A-f:} \quad A_1 = 0, \quad \boldsymbol{f}_1 = \boldsymbol{f}, \quad A_2 = A, \quad \boldsymbol{f}_2 = 0, \tag{4.1}$$

or

$$\text{splitting A-f-A:} \quad A_1 = A, \quad \boldsymbol{f}_1 = 0, \quad A_2 = 0, \quad \boldsymbol{f}_2 = \boldsymbol{f}. \tag{4.2}$$

Due to the symmetry of the SWS splitting with respect to the order of the split subproblems (see (3.23)), the choice between (4.1) and (4.2) does not matter for the SWS splitting. For the Strang-Marchuk splitting, (4.1) means that each time step consists of a half time step advance for the first problem $\boldsymbol{w}_1' = \boldsymbol{f}$, a whole time step advance for the second problem $\boldsymbol{w}_2' = A\boldsymbol{w}_2$ and, again, a half time advance for the first problem—we refer to this splitting as f-A-f. Similarly, the A-f-A splitting is given by (4.2).

4.1 Experiments with the finite difference space discretization

In order to justify the theoretical results obtained in the previous section, we investigate the time integration of the semi-discretized two-dimensional system

$$\begin{aligned} \frac{\partial E_z}{\partial t} &= \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - E_z + \exp(-t^2), \\ \frac{\partial H_x}{\partial t} &= -\frac{\partial E_z}{\partial y}, \\ \frac{\partial H_y}{\partial t} &= \frac{\partial E_z}{\partial x}, \end{aligned} \tag{4.3}$$

where, for the sake of simplicity, the material parameters ε_r, μ_r and σ_r are chosen to be one. We solve the problem on the unit square. On the domain boundary the component E_z is supposed to be zero (perfect conductor boundary), and the initial condition is given in the form

$$\begin{aligned} E_z(x, y, 0) &= 0, \\ H_x(x, y, 0) &= -\sin(\pi x)\cos(\pi y)/\sqrt{2}, \\ H_y(x, y, 0) &= \cos(\pi x)\sin(\pi y)/\sqrt{2}. \end{aligned}$$

The semi-discrete system, which has the form (2.10), is obtained with the partition of the edges of the unit square into eight equidistant intervals, that is the mesh sizes are chosen as $\Delta x = \Delta y = 1/8$. As discussed in Section 2.3, the matrix A can be written as the sum of a skew-symmetric matrix S and a diagonal matrix D. The matrix S can be written as $S = S_1 + S_2$, where S_1 and S_2 are obtained by zeroing the rows of S that belong to the magnetic and the electric field components, respectively. A similar splitting, $D = D_1 + D_2$ holds for the matrix D. In view of (4.3), the matrix D_2 is zero and all nonzero entries of D_1 are equal to -1.

We investigate the splitting when the matrix A and the source term $\boldsymbol{f}$ in (3.11) are split with the choice given by (4.2). Thus we have the subproblems

$$\boldsymbol{w}_1' = A\boldsymbol{w}_1, \qquad \boldsymbol{w}_2' = \boldsymbol{f}. \tag{4.4}$$

Like in real applications, we do not solve these subproblems exactly. The

second problem is solved with the trapezoidal rule and the first one with the Strang-Marchuk splitting. More specifically, using the relation $A = S_1 + S_2 + D_1$, we split the system $\boldsymbol{w}_1' = A\boldsymbol{w}_1$ as

$$\boldsymbol{w}_{11}' = S_1\boldsymbol{w}_{11}, \qquad \boldsymbol{w}_{12}' = S_2\boldsymbol{w}_{12}, \qquad \boldsymbol{w}_{13}' = D_1\boldsymbol{w}_{13} \tag{4.5}$$

and solve it in the order 11-12-13-12-11. It can be easily seen that $S_i^2 = 0$, $i = 1, 2$, which implies that $\exp(S_i) = I + S_i$, $i = 1, 2$, with I being the identity matrix. Moreover, the matrix $\exp(D_1)$ is a diagonal matrix that has the exponentials of the diagonal entries of D_1 on its diagonal. From these facts it follows that the three systems in (4.5) can be solved exactly, thus the time integration error in the solution of $\boldsymbol{w}_1' = A\boldsymbol{w}_1$ is caused only by splitting. Let us notice that, in cases when the components of $\boldsymbol{f}$ have primitive functions in a closed form, the system $\boldsymbol{w}_2' = \boldsymbol{f}$ can be also solved exactly. However, this is not the case for the source function $\exp(-t^2)$ in (4.3), this is why we integrate the system with the trapezoidal rule.

Because we do not solve the subproblems exactly, the theoretical results of the previous section cannot be applied directly. However, the combination of the second order numerical methods with the second order splitting will result in a second order global accuracy. Indeed, both the exact solution $\boldsymbol{w}_{\mathsf{exact}}$ of (2.10) and the split numerical solution $\boldsymbol{w}_{\mathsf{numerical}}$ given in the previous paragraph can be written at the first time step as

$$\boldsymbol{w}_{\mathsf{numerical,exact}}(\tau) = \left(I + \tau A + \frac{\tau^2}{2}A^2\right)\boldsymbol{w}(0) + \tau\boldsymbol{f}\left(\frac{\tau}{2}\right) + \frac{\tau^2}{2}A\boldsymbol{f}\left(\frac{\tau}{2}\right) + O(\tau^3).$$

To prove this, the same technique can be employed that was used in Section 3. Thus $\boldsymbol{w}_{\mathsf{numerical}} - \boldsymbol{w}_{\mathsf{exact}} = O(\tau^3)$, which shows the second order accuracy of the method.

In our numerical tests the error of the H_x field is measured in the maximum norm at the time level $t = 1/2$. We compare the numerical solution obtained by the use of splittings described in the previous section with a variable step-size Runge-Kutta method solution of the semi-discretized problem. The last one is accepted as the exact reference solution of the semi-discrete system.

First, we apply the Strang-Marchuk-splitting in two different orders (4.1),(4.2). The error versus time-step plot is shown in Figure 2. The results clearly demonstrate the second order accuracy of the method. We can also see that for this test case the setting f-A-f produces about four times greater error than the setting A-f-A.

Next, we present the results obtained with the SWS splitting in Figure 3. They confirm the second order accuracy of the method.

Finally, we compare the Strang-Marchuk and SWS splittings with the classical

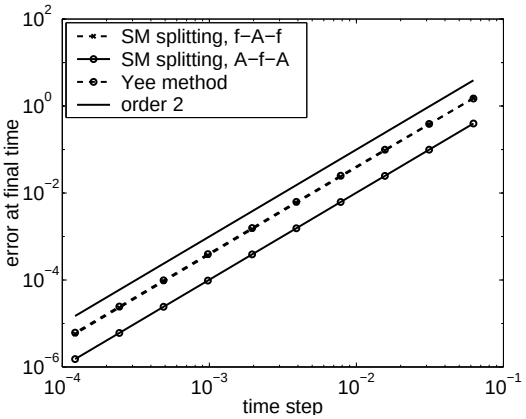

Fig. 2. Errors of the Strang-Marchuk f-A-f and A-f-A splittings (4.1),(4.2) and the Yee method (4.6). The errors of the f-A-f splitting and the Yee method can hardly be distinguished from each other.

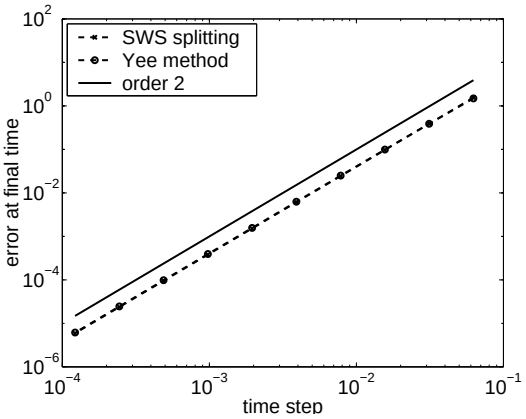

Fig. 3. Errors of the SWS splitting and the Yee method (4.6). The errors of the two schemes can hardly be distinguished from each other.

Yee method:

$$\begin{aligned}(1+\tau/2)\mathcal{E}^{n+1/2} &= (1-\tau/2)\mathcal{E}^{n-1/2} + \tau\nabla\times\mathcal{H}^{n} - \tau\mathcal{J}^{n+1/2},\\ \mathcal{H}^{n} &= \mathcal{H}^{n-1} - \tau\nabla\times\mathcal{E}^{n-1/2}, \quad n=1,2,\ldots,\end{aligned} \tag{4.6}$$

where the material parameters are taken, as in problem (4.3), to be one, the superscripts indicate the time levels at which the fields are approximated and the symbols $\nabla\times$ denote the finite difference approximations of the curl operator. As we can see in Figure 2, the Strang-Marchuk splitting f-A-f behaves very similarly to the Yee method. The A-f-A splitting gives a smaller error. Figure 3 shows that the SWS splitting yields nearly the same error as the Yee method. Comparing the CPU times of the schemes used in the test, we find that

$$t_{\mathsf{A-f-A}} \approx t_{\mathsf{f-A-f}} \approx \frac{3}{4}t_{\mathsf{Yee}}, \quad t_{\mathsf{SWS}} \approx \frac{5}{4}t_{\mathsf{Yee}},$$

where $t_{\mathsf{A-f-A}}$ and $t_{\mathsf{f-A-f}}$ are the CPU times of the A-f-A and f-A-f Strang-Marchuk splittings, respectively, t_{Yee} is the CPU time of the Yee method and

t_{SWS} the CPU time of the SWS splitting. Note that the SWS splitting is ideally parallelizable for two processors. For this parallel implementation of the SWS splitting, we would have $t_{\mathsf{SWS,par}} \approx (5/8)t_{\mathsf{Yee}}$. These relations of the CPU times, together with the error measurements of the schemes, show that the proposed splitting methods outperform the classical Yee method.

4.2 Experiments with the finite element space discretization

In this section, results of numerical experiments with initial-value problem (3.9),(2.17) are presented.

Description of the test problem

This test problem is taken from [1]: the domain $\Omega = [0,1]^3 \subset \mathbb{R}^3$ (where $\varepsilon_r = \mu_r = 1$) is partitioned into a non-structured tetrahedral mesh with $N_{\mathsf{edge}} = 2627$ internal edges. The electric current function $\boldsymbol{J}$ (cf. (2.11)), which determines the source term $\boldsymbol{f}(t)$, is chosen such that the analytical solution of (2.11) is given by

$$\boldsymbol{E}_{\mathsf{an}}(x,y,z,t) = \left(\sum_{i=0}^{100} \cos(\omega_i t)\right) \cdot \begin{bmatrix} \sin \pi y \sin \pi z \\ \sin \pi x \sin \pi z \\ \sin \pi x \sin \pi y \end{bmatrix}, \qquad \omega_i = 1{+}0.1i, \quad i = 0, \ldots, 100.$$

The initial conditions are taken in correspondence with the chosen analytical solution. The problem is solved on the time interval $t \in [0,T]$, $T = 50$.

Gautschi-Krylov time integration scheme

One time integration scheme for solving (3.9),(2.17) is the Gautschi scheme [11,17,16,13]:

$$\begin{cases} \dfrac{\boldsymbol{y}^{n+1/2} - \boldsymbol{y}^n}{\tau/2} = \boldsymbol{v}^n, \\ \dfrac{\boldsymbol{v}^{n+1} - \boldsymbol{v}^n}{\tau} = \psi(\tau^2 \tilde{A}_{\varepsilon,\mu})(-\tilde{A}_{\varepsilon,\mu}\boldsymbol{y}^{n+1/2} + \tilde{\boldsymbol{j}}^{n+1/2}), \\ \dfrac{\boldsymbol{y}^{n+1} - \boldsymbol{y}^{n+1/2}}{\tau/2} = \boldsymbol{v}^{n+1}, \end{cases} \qquad (4.7)$$

$$\psi(x^2) = 2\frac{1-\cos x}{x^2},$$

where τ is the time step size, the superindex n indicates the time level $t_n = n\tau$. The Gautschi scheme with no splitting is a second-order accurate unconditionally stable symplectic time integrator which is able to accurately resolve a wave behavior of the solution even if the time step size exceeds the shortest wave length [17,16,13]. We evaluate the matrix function ψ with the help of the Krylov subspace techniques (see [37,6,22,32,7,15,8,17] and Chapter 11 in book [38]). This results in the Gautschi-Krylov scheme which was shown to be promising for solving finite element space discretized Maxwell equations [1]. Krylov matrix function evaluations can be done efficiently in such a way that the following attractive properties of the Gautschi scheme are preserved in the Gautschi-Krylov scheme [1]: unconditional stability, good accuracy (small dispersion error) and exactness for the case $\boldsymbol{f} = \text{const}(t)$. Numerical experiments presented in [1] demonstrate efficiency of the scheme as compared to the popular Newmark β-scheme. For implementation details of the Gautschi-Krylov scheme, we refer to [1].

Gautschi-Krylov scheme with the source term $\boldsymbol{f}$ split off

The property of being exact for the stationary source term makes the Gautschi-Krylov scheme an ideal candidate for use within splitting methods. In particular, taking the Strang-Marchuk or SWS splitting with (4.1) or (4.2) in combination with the Gautschi-Krylov scheme applied to the subproblem with $\boldsymbol{f}_i = 0$, we obtain splitting schemes where the split substeps are done exactly. Indeed, the subproblem with $A_i = 0$, $\boldsymbol{f}_i = \boldsymbol{f}$ can be solved as accurate as needed by using a higher order quadrature rule. The question then arises whether such splitting schemes will perform better (in terms of achieved accuracy and required computational work) than the Gautschi-Krylov scheme applied to the unsplit problem (3.9),(2.17).

The local time integration error of the Gautschi-Krylov scheme with the f-A-f and A-f-A splittings (which consists only of the splitting error) is given by Theorem 3.3.1. Indeed, substituting the values of A_i and $\boldsymbol{f}_i$ given by (4.1),(4.2) into (3.14), we obtain

$$\text{splitting f-A-f:} \quad \boldsymbol{w}_{\mathsf{strang}}(\tau) - \boldsymbol{w}_{\mathsf{exact}}(\tau) = -\frac{\tau^3}{12}\left(-A^2\boldsymbol{f}\left(\frac{\tau}{2}\right) + \frac{1}{2}A\boldsymbol{f}'\left(\frac{\tau}{2}\right)\right) + O(\tau^4),$$

$$\text{splitting A-f-A:} \quad \boldsymbol{w}_{\mathsf{strang}}(\tau) - \boldsymbol{w}_{\mathsf{exact}}(\tau) = -\frac{\tau^3}{12}\left(\frac{1}{2}A^2\boldsymbol{f}\left(\frac{\tau}{2}\right) - A\boldsymbol{f}'\left(\frac{\tau}{2}\right)\right) + O(\tau^4).$$

Taking into account that (cf. (2.17))

$$A\boldsymbol{f}' = \begin{bmatrix} 0 \\ \tilde{\boldsymbol{j}}' \end{bmatrix}, \qquad A^2\boldsymbol{f} = \begin{bmatrix} -\tilde{A}_{\varepsilon,\mu}\tilde{\boldsymbol{j}} \\ 0 \end{bmatrix},$$

the expressions for the local errors can be further simplified as

$$\begin{aligned} &\text{splitting f-A-f:} \quad \boldsymbol{w}_{\mathsf{strang}}(\tau) - \boldsymbol{w}_{\mathsf{exact}}(\tau) = -\frac{\tau^3}{24} \begin{bmatrix} 2\tilde{A}_{\varepsilon,\mu}\tilde{\boldsymbol{j}} \\ \tilde{\boldsymbol{j}}' \end{bmatrix} + O(\tau^4), \\ &\text{splitting A-f-A:} \quad \boldsymbol{w}_{\mathsf{strang}}(\tau) - \boldsymbol{w}_{\mathsf{exact}}(\tau) = \frac{\tau^3}{24} \begin{bmatrix} \tilde{A}_{\varepsilon,\mu}\tilde{\boldsymbol{j}} \\ 2\tilde{\boldsymbol{j}}' \end{bmatrix} + O(\tau^4). \end{aligned} \tag{4.8}$$

Thus, choices (4.1) and (4.2) yield comparable local errors. For this test problem, the choice f-A-f turns out to be slightly more accurate (see Table 1) and we use this f-A-f order henceforth. The errors reported in the Table and throughout this subsection are measured as

$$\frac{\|\boldsymbol{y}(T) - \boldsymbol{y}_{\mathsf{ref}}(T)\|_2}{\|\boldsymbol{y}_{\mathsf{ref}}(T)\|_2}, \tag{4.9}$$

where $\boldsymbol{y}(T)$ is the numerical solution and $\boldsymbol{y}_{\mathsf{ref}}(T)$ is the reference solution obtained by time integration of the problem with a tiny time step size.

Table 1
Errors of the Gautschi-Krylov scheme with the Strang-Marchuk splitting for different orders of the operators (cf. (4.1) and (4.2)). The errors are measured as shown in (4.9).

step size τ	0.1	0.05	0.025	0.0125	0.00625
Gautschi/Strang, splitting f-A-f	3.93e-01	6.09e-02	1.48e-02	3.73e-03	1.06e-03
Gautschi/Strang, splitting A-f-A	3.53e-01	8.78e-02	2.19e-02	5.51e-03	1.46e-03

Gautschi-Krylov scheme with and without splitting

The answer to the question whether the Gautschi-Krylov scheme with the split off source term is more efficient than without splitting is given in Figure 4. There, the following three schemes are compared for solution of (3.9),(2.17):
(i) Gautschi-Krylov scheme applied to the unsplit problem,
(ii) Gautschi-Krylov scheme with splitting (4.1) in the Strang-Marchuk way (see Section 3.3),
(iii) Gautschi-Krylov scheme with splitting (4.1) in the SWS way (see Section 3.4).
All the three schemes are implemented in such a way that computational costs per time step are nearly the same (except for the SWS splitting where the costs are twice as large). In the experiments, we perform the substeps for subproblem 1 (with $\boldsymbol{f}_1 = \boldsymbol{f}$ and $A_1 = 0$) exactly, by integrating the given source function $\boldsymbol{f}$ analytically. Of course, we could also have used a (higher-order) quadrature rule instead (see Table 2 and discussion below). As one can

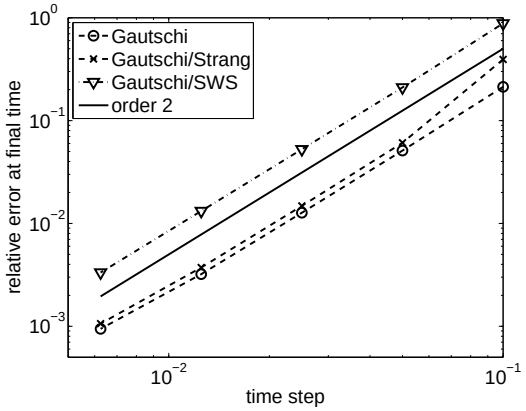

Fig. 4. Errors of Gautschi-Krylov scheme applied without splitting and with the Strang-Marchuk and SWS splittings. The errors are measured as shown in (4.9).

see from Figure 4, the splitting schemes perform a bit worse than the unsplit Gautschi-Krylov scheme. The SWS splitting is twice as expensive per time step as the other two schemes and less accurate for the same step size.

We do not have a thorough explanation for this slightly disappointing performance of the Gautschi-Krylov scheme with splittings. However, the following argumentation can certainly be given. As pointed out above, the Gautschi-Krylov scheme is able to accurately handle time scales shorter than the time step size used. In this test problem, the characteristic time scale of the source function $\boldsymbol{f}$ is approximately $2\pi/(\max_i \omega_i) \approx 0.6$ which is rather small compared to the time step sizes used. Splitting the source term off, we make the task of the Gautschi-Krylov scheme easier, the scheme is then exact per split step. The error is, however, now transferred to the splitting level, whereas the ability of the scheme to accurately treat the fast time scales in the source term is not exploited anymore. On the other hand, we can expect that the splitting error is significant (cf. (4.8)), also because the time step size is taken large with respect to the characteristic time scale of the source term.

This argumentation is confirmed by the experiments with the leap-frog scheme where the time step size is restricted due to the CFL condition (see subsection on the leap frog scheme below and Figure 5). Note that the time step used here exceeds the maximal time step allowable by the CFL condition up to a factor of six.

Integrating the split off source term approximately

Results presented in Figure 4 are obtained with exact analytical integration of the source term $\boldsymbol{f}$. This would not be possible if the time dependence of $\boldsymbol{f}$ was not known explicitly. In that case a quadrature rule could be used. To see the effect of the approximate solution of the source subproblem on the attained

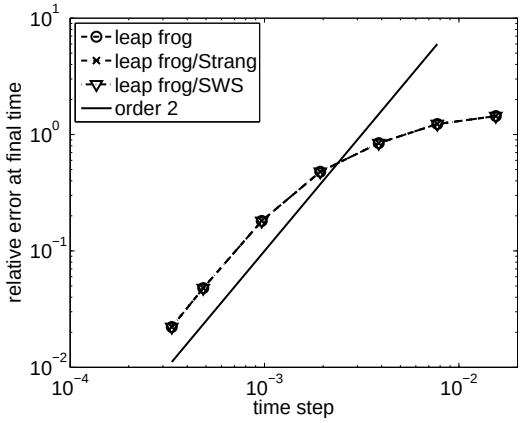

Fig. 5. Errors of the leap frog scheme applied without splitting and with the Strang–Marchuk and SWS splittings. The errors are measured as shown in (4.9).

accuracy, we run the Gautschi-Krylov scheme with the split off source term handled by the midpoint quadrature rule. Surprisingly, this leads to a higher accuracy (see Table 2). We do not have any explanation for this phenomenon.

Table 2
Errors of the Gautschi-Krylov scheme with the Strang-Marchuk splitting (4.1) for the exactly integrated source term and source term integrated with the midpoint quadrature rule. The errors are measured as shown in (4.9).

step size τ	0.1	0.05	0.025	0.0125	0.00625
Gautschi/Strang, exact source	3.93e-01	6.09e-02	1.48e-02	3.73e-03	1.06e-03
Gautschi/Strang, midpoint rule	3.66e-01	4.89e-02	1.16e-02	2.95e-03	8.89e-04

Leap frog scheme with and without splitting

Another time integration scheme that is used for time integration of the Maxwell equation is the leap frog scheme. For this model problem (cf. (3.9), (2.17)), the scheme is given by (4.7) with the matrix function ψ replaced by the identity matrix. The leap frog scheme is second order accurate but, unlike the Gautschi scheme, is not exact for the case $\boldsymbol{f} = \text{const}(t)$ and conditionally stable [1]. We apply the leap-frog scheme in combination with splitting (4.1) in both the Strang-Marchuk and SWS ways (see Sections 3.3 and 3.4). We compare these two splitting schemes with the unsplit leap frog scheme. In this implementation, the computational costs of the leap frog and leap frog/Strang schemes per time step are nearly identical, and the costs of the leap frog/SWS are twice as large. The results of the comparisons are presented in Figure 5: the error plots of the three schemes hardly differ from each other.

5 Conclusions: to split or not split

We have analyzed the splitting error of the Strang-Marchuk and SWS splitting schemes for numerical solution of linear inhomogeneous systems of differential equations (3.9) with operator splitting (3.11). Expressions for the leading term of the local error are derived which show the second order global accuracy of the splitting schemes.

Several relevant numerical tests have been done with the time-dependent Maxwell equations discretized in space by either finite differences or finite elements. An interesting case is when the source term $\boldsymbol{f}(t)$ is split off. For the Maxwell equations discretized in space with staggered central finite differences, the Strang-Marchuk splitting has been shown to be equally or more efficient (in terms of accuracy and computational times) than the classical Yee method. The SWS splitting, ideally suited for parallel implementation on two processors, outperforms the Yee method when implemented in parallel.

For the Maxwell equations discretized in space with edge vector finite elements (cf. (2.17)), we have tested the Gautschi-Krylov scheme applied without splitting and with both the Strang-Marchuk and SWS splitting where the inhomogeneous source term $\boldsymbol{f}(t)$ is split. The time integration error of these two splitting schemes consists solely of the splitting error. The comparisons show that the Gautschi-Krylov scheme with splitting is slightly less accurate than with no splitting. This can be explained by the fact that splitting off the source term, though making the scheme exact per split step, moves the error to the splitting level. This error can be significant since the time step size in the experiments is chosen large with respect to the characteristic time scale of the source term and the CFL restriction. In addition, if the source term is split off, no advantage is taken of the ability of the scheme to accurately handle fast time scales [16,13]. The loss in accuracy due to splitting is, however, marginal. The computational costs of the unsplit Gautschi-Krylov scheme and Gautschi-Krylov scheme with the Strang-Marchuk splitting are nearly the same, the costs of Gautschi-Krylov scheme with the SWS splitting are twice as large. (Note, again, that the parallel SWS splitting has the same costs as the other schemes.) For the leap frog scheme, no difference in performance is observed when the scheme is applied without and with both the Strang-Marchuk and SWS splitting.

Thus, for considered test problems, the splitting methods do not lead to a deterioration in accuracy or performance and in some cases perform better. As such, they can be recommended for use in appropriate cases (e.g., when convenient for programming purposes or when coupling different physical processes into one model).

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