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Department of Mathematics and Computing Science

RANA 02-15
May 2002

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Reports on Applied and Numerical Analysis
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P.O. Box 513
5600 MB Eindhoven, The Netherlands
ISSN: 0926-4507

Investigation of Numerical Time-Integrations of the Maxwell Equations Using the Staggered Grid Spatial Discretization

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Abstract

The YEE-method is a simple and elegant way of solving the time dependent MAXWELL equations. On the other hand this method has some inherent drawbacks too. The main one is that its stability requires a very strict upper bound for the possible time-steps. This is why, during the last decade, the main goal was to construct such methods that are unconditionally stable. This means that the time-step can be chosen based only on accuracy instead of stability considerations. In this paper we give a *uniform treatment* of methods that use the same spatial staggered grid approximation as the classical YEE-method. Three other numerical methods are discussed: the NAMIKI-ZHENG-CHEN-ZHANG (NZCZ) ADI method, the KOLE-FIGGE-DERAEDT-method (KFR) and a KRYLOV-space method. All methods are discussed with non-homogeneous material parameters. We show how the existing finite difference numerical methods are *based on the approximation of a matrix exponential.* With this formulation we prove the unconditional stability of the NZCZ-method without any computer algebraic tool. Moreover, we accelerate the KRYLOV-space method in the approximation of the matrix exponential with a skew-symmetric formulation of the semi-discretized equations. Our main goal is to compare the methods from the point of view of the computational speed. This question is investigated in 1D numerical tests.

1 Introduction

The 3D MAXWELL equations, which describe the behavior of time dependent electromagnetic fields, in the absence of free charges and currents, can be written in the form

$$-\nabla \times \mathbf{H} + \varepsilon \partial_t \mathbf{E} = \mathbf{0}, \tag{1.1}$$

$$\nabla \times \mathbf{E} + \mu \partial_t \mathbf{H} = \mathbf{0}, \tag{1.2}$$

$$\nabla(\varepsilon \mathbf{E}) = 0, \tag{1.3}$$

$$\nabla(\mu \mathbf{H}) = 0, \tag{1.4}$$

where

$$\mathbf{E} = (E_x(t,x,y,z), E_y(t,x,y,z), E_z(t,x,y,z)) \tag{1.5}$$

is the electric field strength,

$$\mathbf{H} = (H_x(t,x,y,z), H_y(t,x,y,z), H_z(t,x,y,z)) \tag{1.6}$$

is the magnetic field strength, ε is the electric permittivity and μ is the magnetic permeability. It is well-known that the divergence equations (1.3) and (1.4) follow from the curl equations if we suppose that the fields in question were divergence-free at the initial point of time. This means that we must solve only the curl equations applying divergence-free initial conditions for $\mathbf{E}$ and $\mathbf{H}$.

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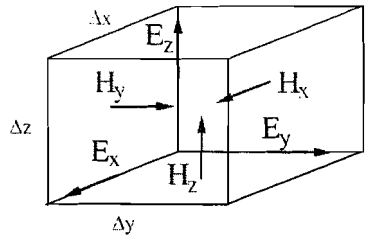

Figure 1.1: *Standard* YEE *cell.*

The first and still extensively applied method to solve the equations (1.1), (1.2) numerically was constructed by YEE in 1966 ([12]). This method starts with the definition of a generally rectangular mesh (with the choice of the step-sizes $\Delta x, \Delta y$ and Δz) for the electric field and another staggered (by $\Delta x/2, \Delta y/2$ and $\Delta z/2$) grid for the magnetic field in the computational domain. The building blocks of this mesh are the so-called YEE-cells (see Figure 1.1). Defining the approximations of the field strengths at the points shown in Figure 1.1, we calculate the first spatial derivatives in the curl operator using central differences. These approximations of the spatial derivatives produce second order accuracy, this is why this discretization is so common. The methods investigated in this paper all use this type of approximation. The only difference between the methods will be only in the time discretization. In the following we formulate the semi-discretized system.

Let us suppose that the computational space has been divided into N YEE-cells and let us introduce the notation

$$\mathcal{I} = \{(i/2, j/2, k/2) \mid i, j, k \in \mathbb{Z}, \text{ not all odd and not all even,} \tag{1.7}$$

$$(i\Delta x/2, j\Delta y/2, k\Delta z/2)^\top \text{ is in the computational domain}\}.$$

We define the functions $\Psi_{i/2,j/2,k/2} : \mathbb{R} \to \mathbb{R}$ $((i/2, j/2, k/2) \in \mathcal{I})$ as

$$\Psi_{i/2,j/2,k/2}(t) = \begin{cases} \sqrt{\varepsilon_{i/2,j/2,k/2}} E_x(t, i\Delta x/2, j\Delta y/2, k\Delta z/2), & \text{if } i \text{ is odd and } j,k \text{ are even,} \\ \sqrt{\varepsilon_{i/2,j/2,k/2}} E_y(t, i\Delta x/2, j\Delta y/2, k\Delta z/2), & \text{if } j \text{ is odd and } i,k \text{ are even,} \\ \sqrt{\varepsilon_{i/2,j/2,k/2}} E_z(t, i\Delta x/2, j\Delta y/2, k\Delta z/2), & \text{if } k \text{ is odd and } i,j \text{ are even,} \\ \sqrt{\mu_{i/2,j/2,k/2}} H_x(t, i\Delta x/2, j\Delta y/2, k\Delta z/2), & \text{if } j,k \text{ are odd and } i \text{ is even,} \\ \sqrt{\mu_{i/2,j/2,k/2}} H_y(t, i\Delta x/2, j\Delta y/2, k\Delta z/2), & \text{if } i,k \text{ are odd and } j \text{ is even,} \\ \sqrt{\mu_{i/2,j/2,k/2}} H_z(t, i\Delta x/2, j\Delta y/2, k\Delta z/2), & \text{if } i,j \text{ are odd and } k \text{ is even,} \end{cases} \tag{1.8}$$

where $\varepsilon_{i/2,j/2,k/2}$ and $\mu_{i/2,j/2,k/2}$ denote the electric permittivity and magnetic permeability at the points $(i\Delta x/2, j\Delta y/2, k\Delta z/2)^\top$, respectively. This setting corresponds to the staggered grid spatial discretization. Starting from the rearranged form of the MAXWELL equations

$$\partial_t(\sqrt{\varepsilon}\mathbf{E}) = \frac{1}{\sqrt{\varepsilon}} \nabla \times \frac{(\sqrt{\mu}\mathbf{H})}{\sqrt{\mu}}, \tag{1.9}$$

$$\partial_t(\sqrt{\mu}\mathbf{H}) = -\frac{1}{\sqrt{\mu}} \nabla \times \frac{(\sqrt{\varepsilon}\mathbf{E})}{\sqrt{\varepsilon}}, \tag{1.10}$$

we can obtain the semi-discretized system

$$\begin{aligned} \frac{\mathrm{d}\Psi_{i/2,j/2,k/2}(t)}{\mathrm{d}t} = \frac{1}{\varepsilon_{i/2,j/2,k/2}} \Bigg[& \frac{\Psi_{i/2,(j+1)/2,k/2}(t)}{\Delta y \sqrt{\mu_{i/2,(j+1)/2,k/2}}} - \frac{\Psi_{i/2,(j-1)/2,k/2}(t)}{\Delta y \sqrt{\mu_{i/2,(j-1)/2,k/2}}} - \\ & \frac{\Psi_{i/2,j/2,(k+1)/2}(t)}{\Delta z \sqrt{\mu_{i/2,j/2,(k+1)/2}}} + \frac{\Psi_{i/2,j/2,(k-1)/2}(t)}{\Delta z \sqrt{\mu_{i/2,j/2,(k-1)/2}}} \Bigg], \text{ if } i \text{ is odd and } j,k \text{ are even,} \end{aligned} \tag{1.11}$$

$$\frac{\mathrm{d}\Psi_{i/2,j/2,k/2}(t)}{\mathrm{d}t} = \frac{1}{\varepsilon_{i/2,j/2,k/2}}\left[\frac{\Psi_{i/2,j/2,(k+1)/2}(t)}{\Delta z\sqrt{\mu_{i/2,j/2,(k+1)/2}}} - \frac{\Psi_{i/2,j/2,(k-1)/2}(t)}{\Delta z\sqrt{\mu_{i/2,j/2,(k-1)/2}}} - \right. \tag{1.12}$$
$$\left.\frac{\Psi_{(i+1)/2,j/2,k/2}(t)}{\Delta x\sqrt{\mu_{(i+1)/2,j/2,k/2}}} + \frac{\Psi_{(i-1)/2,j/2,k/2}(t)}{\Delta x\sqrt{\mu_{(i-1)/2,j/2,k/2}}}\right], \text{ if } j \text{ is odd and } i,k \text{ are even,}$$

$$\frac{\mathrm{d}\Psi_{i/2,j/2,k/2}(t)}{\mathrm{d}t} = \frac{1}{\varepsilon_{i/2,j/2,k/2}}\left[\frac{\Psi_{(i+1)/2,j/2,k/2}(t)}{\Delta x\sqrt{\mu_{(i+1)/2,j/2,k/2}}} - \frac{\Psi_{(i-1)/2,j/2,k/2}(t)}{\Delta x\sqrt{\mu_{(i-1)/2,j/2,k/2}}} - \right. \tag{1.13}$$
$$\left.\frac{\Psi_{i/2,(j+1)/2,k/2}(t)}{\Delta y\sqrt{\mu_{i/2,(j+1)/2,k/2}}} + \frac{\Psi_{i/2,(j-1)/2,k/2}(t)}{\Delta y\sqrt{\mu_{i/2,(j-1)/2,k/2}}}\right], \text{ if } k \text{ is odd and } i,j \text{ are even,}$$

$$\frac{\mathrm{d}\Psi_{i/2,j/2,k/2}(t)}{\mathrm{d}t} = \frac{1}{\mu_{i/2,j/2,k/2}}\left[\frac{\Psi_{i/2,j/2,(k+1)/2}(t)}{\Delta z\sqrt{\varepsilon_{i/2,j/2,(k+1)/2}}} - \frac{\Psi_{i/2,j/2,(k-1)/2}(t)}{\Delta z\sqrt{\varepsilon_{i/2,j/2,(k-1)/2}}} - \right. \tag{1.14}$$
$$\left.\frac{\Psi_{i/2,(j+1)/2,k/2}(t)}{\Delta y\sqrt{\varepsilon_{i/2,(j+1)/2,k/2}}} + \frac{\Psi_{i/2,(j-1)/2,k/2}(t)}{\Delta y\sqrt{\mu_{i/2,(j-1)/2,k/2}}}\right], \text{ if } j,k \text{ are odd and } i \text{ is even,}$$

$$\frac{\mathrm{d}\Psi_{i/2,j/2,k/2}(t)}{\mathrm{d}t} = \frac{1}{\mu_{i/2,j/2,k/2}}\left[\frac{\Psi_{(i+1)/2,j/2,k/2}(t)}{\Delta x\sqrt{\varepsilon_{(i+1)/2,j/2,k/2}}} - \frac{\Psi_{(i-1)/2,j/2,k/2}(t)}{\Delta x\sqrt{\varepsilon_{(i-1)/2,j/2,k/2}}} - \right. \tag{1.15}$$
$$\left.\frac{\Psi_{i/2,j/2,(k+1)/2}(t)}{\Delta z\sqrt{\varepsilon_{i/2,j/2,(k+1)/2}}} + \frac{\Psi_{i/2,j/2,(k-1)/2}(t)}{\Delta z\sqrt{\mu_{i/2,j/2,(k-1)/2}}}\right], \text{ if } i,k \text{ are odd and } j \text{ is even,}$$

$$\frac{\mathrm{d}\Psi_{i/2,j/2,k/2}(t)}{\mathrm{d}t} = \frac{1}{\mu_{i/2,j/2,k/2}}\left[\frac{\Psi_{i/2,(j+1)/2,k/2}(t)}{\Delta y\sqrt{\varepsilon_{i/2,(j+1)/2,k/2}}} - \frac{\Psi_{i/2,(j-1)/2,k/2}(t)}{\Delta y\sqrt{\varepsilon_{i/2,(j-1)/2,k/2}}} - \right. \tag{1.16}$$
$$\left.\frac{\Psi_{(i+1)/2,j/2,k/2}(t)}{\Delta x\sqrt{\varepsilon_{(i+1)/2,j/2,k/2}}} + \frac{\Psi_{(i-1)/2,j/2,k/2}(t)}{\Delta x\sqrt{\mu_{(i-1)/2,j/2,k/2}}}\right], \text{ if } i,j \text{ are odd and } k \text{ is even,}$$

which can be written in a shorter form as

$$\frac{\mathrm{d}\Psi(t)}{\mathrm{d}t} = \mathbf{A}\Psi(t),\ t > 0. \tag{1.17}$$

The vector-scalar function $\Psi : \mathbb{R} \to \mathbb{R}^{6N}$, $\Psi(t) = (\ldots, \Psi_{i/2,j/2,k/2}(t), \ldots)^\top$ can be obtained from an arbitrary ordering of the functions $\Psi_{i/2,j/2,k/2}$ into a vector and $\mathbf{A} \in \mathbb{R}^{6N\times 6N}$. From equations (1.11)-(1.16) follow some important properties of $\mathbf{A}$ directly.

Lemma 1.1 *Every row of* $\mathbf{A}$ *consists at most four nonzero elements in the forms* $1/(\sqrt{\varepsilon_{\cdot,\cdot,\cdot}\mu_{\cdot,\cdot,\cdot}}\Delta_\cdot)$, *that is* $\mathbf{A}$ *is a sparse matrix.* $\mathbf{A}$ *is a skew-symmetric matrix* ($\mathbf{A}^\top = -\mathbf{A}$).

The system (1.17) must be solved applying a divergence-free initial condition for $\Psi(0)$. The solution can be written in the form

$$\Psi(t) = \exp(t\mathbf{A})\Psi(0), \tag{1.18}$$

where $\exp(t\mathbf{A})$ denotes the exponential matrix and it is well-defined with the TAYLOR-series of the exponential function. This matrix exponential cannot be computed directly because $\mathbf{A}$ is a very large matrix. According to this representation, usually, the numerical methods for the MAXWELL equations are based on some approximation of the matrix exponential $\exp(t\mathbf{A})$. With the choice of a time-step $\Delta t > 0$

$$\Psi(t + \Delta t) = \exp(\Delta t\mathbf{A})\Psi(t) \tag{1.19}$$

follows from (1.18). Using this equality the one-step iteration

$$\Psi^{n+1} = U_n(\Delta t\mathbf{A})\Psi^n,\ \Psi^0 \text{ is given} \tag{1.20}$$

can be defined, where $U_n(\Delta t\mathbf{A})$ is the approximation of the exponential $\exp(\Delta t\mathbf{A})$ (this approximation may depend on n) and Ψ^n is the approximation of the function Ψ at time-level $n\Delta t$.

In the next section we give the $U_n(\Delta t\mathbf{A})$ approximations of the matrix exponential $\exp(\Delta t\mathbf{A})$ for the classical YEE-method, for the NAMIKI-ZHENG-CHEN-ZHANG-method (NZCZ, [6, 15]) and for the KOLE-FIGGE-DE RAEDT-method (KFR, [5]), which show that the existing methods are based on the approximation of the matrix exponential $\exp(\Delta t\mathbf{A})$ (for these methods $U_n(\Delta t\mathbf{A})$ is independent of n). Moreover, we describe a method that does not compute the approximation of the matrix exponential itself, but the approximation of the product of the matrix exponential and the iteration vector (that is here $U_n(\Delta t\mathbf{A})$ depends on n). This KRYLOV-space approximation has very nice properties because of the skew-symmetricity of the matrix $\mathbf{A}$. The stability of the NZCZ-method was proven with the help of significant use of computer algebra, namely, MAPLE V was applied in showing that the magnitudes of the eigenvalues of the iteration matrix are equal unity. Using our formulation this proof can be done on pure mathematical basis. Furthermore, our proof does not suppose that the material parameters (ε, μ) are constants (compare with [15]). Our main goal is to compare the methods from the point of view of the numerical computational time. This will be investigated in the last section in 1D numerical tests.

2 Uniform treatment of methods using the Yee space discretization

As we wrote in the previous section the time integration of the MAXWELL equations, using a staggered grid spatial approximation, means the approximation of the matrix exponential $\exp(\Delta t\mathbf{A})$. The better is this approximation the better is the numerical scheme. The matrix $\mathbf{A}$ is very large (usualy $6N \geq 10^6$) and although it is sparse the matrix $\exp(\Delta t\mathbf{A})$ is a full matrix, which is due its definition. These facts necessitate the approximation of the matrix exponential. These approximations are given for the classical YEE-method, for the NZCZ-method and for the KFR-method in this section. The approximations are based on some splitting of the matrix $\mathbf{A}$ in the form $\mathbf{A} = \mathbf{A}_1 + \mathbf{A}_2$. Then the exponential $\exp(\mathbf{A})$ can be approximated by the exponentials $\exp(\mathbf{A}_1)$ and $\exp(\mathbf{A}_2)$. Naturally, if $\mathbf{A}_1$ and A_2 commute, then the relation $\exp(\mathbf{A}) = \exp(\mathbf{A}_1)\exp(\mathbf{A}_2)$ is true, but in our settings this is not the case.

2.1 Classical Yee-method

The classical YEE-method uses a so-called leap-frog time integration scheme, for which the electric field at $t = 0$ and the magnetic field at $t = \Delta t/2$ must be given. This is why this method starts with the computation (from the initial data) of the approximation of the magnetic field at time level $\Delta t/2$ using some numerical method in the form $\hat{\Psi}^0 = \mathbf{B}\Psi^0$, where the matrix $\mathbf{B} \in \mathbb{R}^{6N\times 6N}$ corresponds to some appropriate one-step numerical scheme. Then we update the values of the electric field at $t = \Delta t$ from the electric field given at time level $t = 0$ and the magnetic field at $t = \Delta t/2$ approximating the time derivatives by forward differences. In the next step we update the magnetic field at time level $t = 3\Delta t/2$ similar manner.

This method can be written in matrix iteration form. To do this, we define two matrices, $\mathbf{A}_{1Y}$ and $\mathbf{A}_{2Y}$, as follows. The matrix $\mathbf{A}_{1Y}$ is composed from the matrix $\mathbf{A}$ changing the rows belonging to the electric field variables (indexed by $(i/2, j/2, k/2) \in \mathcal{I}$, two of i, j and k are even, one is odd) to zero rows. $\mathbf{A}_{2Y}$ can be derived, in similar manner, zeroing the rows belonging to the magnetic field variables (indexed by $(i/2, j/2, k/2) \in \mathcal{I}$, two of i, j and k are odd, one is even). From equations (1.11)-(1.16) follow some important properties of the matrices $\mathbf{A}_{1Y}$ and $\mathbf{A}_{2Y}$.

Lemma 2.1 *Matrices $\mathbf{A}_{1Y}$ and $\mathbf{A}_{2Y}$ do not commute and the equality $\mathbf{A} = \mathbf{A}_{1Y} + \mathbf{A}_{2Y}$ is fulfilled. Moreover, the relation $\mathbf{A}_{1Y}^\top = -\mathbf{A}_{2Y}$ is valid.*

REMARK 2.2. According to the lemma above, $\mathbf{A} = \mathbf{A}_{1Y} + \mathbf{A}_{2Y}$ is a splitting of $\mathbf{A}$. Furthermore, the splitting is based on the physical background, namely, according to the electric and magnetic components.

Using the matrices $\mathbf{A}_{1Y}, \mathbf{A}_{2Y}$ the YEE-method has the form

$$\Psi^n = [(\mathbf{I} + \Delta t \mathbf{A}_{1Y})(\mathbf{I} + \Delta t \mathbf{A}_{2Y})]^n \mathbf{B}\Psi^0 = [(\mathbf{I} + \Delta t \mathbf{A}_{1Y})(\mathbf{I} + \Delta t \mathbf{A}_{2Y})]^n \hat{\Psi}^0, \quad n = 1, 2, \ldots. \tag{2.21}$$

(as a simple example the matrix $\mathbf{B}$ can be chosen in the form $\mathbf{B} = \mathbf{I} + (\Delta t/2)\mathbf{A}_{1Y}$) and in this manner it applies the explicit exponential approximation

$$\exp(\Delta t \mathbf{A}) = \exp(\Delta t(\mathbf{A}_{1Y} + \mathbf{A}_{2Y})) \approx \exp(\Delta t \mathbf{A}_{1Y}) \exp(\Delta t \mathbf{A}_{2Y}) \approx (\mathbf{I} + \Delta t \mathbf{A}_{1Y})(\mathbf{I} + \Delta t \mathbf{A}_{2Y}). \tag{2.22}$$

This approximation of the exponential is identical with the TAYLOR-series of $\exp(\Delta t \mathbf{A})$ up to the first order term, which can be seen from the form $\mathbf{I} + \Delta t \mathbf{A} - \Delta t^2 \mathbf{A}_{1Y} \mathbf{A}_{1Y}^{\top}$ of the iteration matrix. It can be proven applying VON NEUMANN analysis, that the YEE-method can be kept to be stable choosing the time-step sufficiently small.

Theorem 2.3 *(e.g. [11]) The numerical solution of the* MAXWELL *equations using staggered spatial discretization and leap-frog time integration (*YEE*-method) is stable if and only if the condition*

$$\Delta t < \frac{1}{c\sqrt{(1/\Delta x)^2 + (1/\Delta y)^2 + (1/\Delta z)^2}} \tag{2.23}$$

is fulfilled, where c is the maximal speed of light in the computational domain.

This means that if we solve a problem with 10^6 cells, where $\Delta x = \Delta y = \Delta z = 10^{-6}(m)$ with the YEE-algorithm (9 operations are needed to update each variable) the upper bound for the time-step would be $\Delta t = 2 \times 10^{-15}(s)$. This means that we have to execute 2.7×10^{19} operations to evaluate the field quantities after 1 microsecond. Using a fast computer with 10^{12} operations per second this procedure would take 6×10^7 seconds, that is 7.44 hours. This huge computational time is unacceptable in real-life problems.

2.2 Namiki-Zheng-Chen-Zhang-method

A lot of effort has been invested during the last decade to bridge the stability problem of the YEE-method. The main goal was to construct methods, where Δt can be chosen based on accuracy considerations instead of stability reason. The first paper which showed an unconditionally stable method, with a detailed proof of the stability, was appeared in 2000 and was written by the authors ZHENG, CHEN and ZHANG (see paper [15]). This method is also mentioned by NAMIKI for more general problems in paper [6], but the stability was showed only on test-problems. This is why we call this method NAMIKI-ZHENG-CHEN-ZHANG-method (NZCZ) in this paper. We divide the time-steps into two equal parts. In the first half time-step we handle the first terms of the curl operator approximation implicitly (applying the implicit Euler method), the second ones explicitly (applying the explicit Euler method), in the next half time-step this is done in reverse order. Applying this method suitably we must solve two systems of linear equations with symmetric tridiagonal matrices in one iteration step. Now we show that the NZCZ-method can be also derived from the approximation of the matrix exponential $\exp(\Delta t \mathbf{A})$. Let us define the matrices $\mathbf{A}_{1N}, \mathbf{A}_{2N}$ such a way that $\mathbf{A}_{1N}$ comes from the discretization of the first items in the curl operator, and $\mathbf{A}_{2N}$ comes from the second ones.

Lemma 2.4 *The matrices $\mathbf{A}_{1N}$ and $\mathbf{A}_{2N}$ are skew-symmetric and do not commute, moreover, $\mathbf{A} = \mathbf{A}_{1N} + \mathbf{A}_{2N}$.*

With the matrices $\mathbf{A}_{1N}$, $\mathbf{A}_{2N}$ we can define an exponential approximation as follows

$$\exp(\Delta t \mathbf{A}) = \exp(\Delta t(\mathbf{A}_{1N} + \mathbf{A}_{2N})) \approx \tag{2.24}$$

$$\approx \exp((\Delta t/2)\mathbf{A}_{2N}) \cdot \exp((\Delta t/2)\mathbf{A}_{1N}) \cdot \exp((\Delta t/2)\mathbf{A}_{1N}) \cdot \exp((\Delta t/2)\mathbf{A}_{2N}) = \tag{2.25}$$

$$= (\exp(-(\Delta t/2)\mathbf{A}_{2N}))^{-1} \cdot \exp((\Delta t/2)\mathbf{A}_{1N}) \cdot (\exp(-(\Delta t/2)\mathbf{A}_{1N}))^{-1} \cdot \exp((\Delta t/2)\mathbf{A}_{2N}) \approx \tag{2.26}$$

$$\approx (\mathbf{I} - (\Delta t/2)\mathbf{A}_{2N})^{-1} \cdot (\mathbf{I} + (\Delta t/2)\mathbf{A}_{1N}) \cdot (\mathbf{I} - (\Delta t/2)\mathbf{A}_{1N})^{-1} \cdot (\mathbf{I} + (\Delta t/2)\mathbf{A}_{2N}). \quad (2.27)$$

At the first approximation we used the fact that the TAYLOR-series of $\exp(\Delta t(\mathbf{A}_{1N} + \mathbf{A}_{2N}))$ and $\exp((\Delta t/2)\mathbf{A}_{2N}) \cdot \exp((\Delta t/2)\mathbf{A}_{1N}) \cdot \exp((\Delta t/2)\mathbf{A}_{1N}) \cdot \exp((\Delta t/2)\mathbf{A}_{2N})$ are identical up to the term with Δt^2. At the second approximation the first two terms were used from the TAYLOR-series of the exponential function. Thus we can define the one-step iteration

$$\Psi^{n+1} = (\mathbf{I} - (\Delta t/2)\mathbf{A}_{2N})^{-1} \cdot (\mathbf{I} + (\Delta t/2)\mathbf{A}_{1N}) \cdot (\mathbf{I} - (\Delta t/2)\mathbf{A}_{1N})^{-1} \cdot (\mathbf{I} + (\Delta t/2)\mathbf{A}_{2N})\Psi^n, \quad (2.28)$$

(Ψ^0 is given) which can also be obtained from the usual form of the NZCZ-method

$$\frac{\Psi^{n+1/2} - \Psi^n}{\Delta t/2} = \mathbf{A}_{1N}\Psi^{n+1/2} + \mathbf{A}_{2N}\Psi^n, \quad (2.29)$$

$$\frac{\Psi^{n+1} - \Psi^{n+1/2}}{\Delta t/2} = \mathbf{A}_{1N}\Psi^{n+1/2} + \mathbf{A}_{2N}\Psi^{n+1}. \quad (2.30)$$

REMARK 2.5. The above system shows that the NZCZ-method is similar to the Alternating Direction Implicit (ADI) methods (see [3] and [4]), but here the alteration is applied in the two terms of the curl operator.

In the eighties, when ADI methods were constructed for the MAXWELL equations, a lot of effort has been devoted to the verification of their stability. This effort remained without results. As we have mentioned earlier, the first unconditionally stable method was constructed in 2000 and the stability was proven by computer algebraic tools. Employing the iteration form (2.28) we are able to give the pure mathematical proof of the stability of the NZCZ-method (with non-homogeneous material parameters). The next lemma will play a key-role in the sequel.

Lemma 2.6 *Assume that* $\mathbf{C}$ *is a skew-symmetric real matrix and* s *is an arbitrary real number. Then*

$$\| (I + s\mathbf{C}) \cdot (I - s\mathbf{C})^{-1} \|_2 = 1. \quad (2.31)$$

Proof. Introducing the notation $\mathbf{D} := (I + s\mathbf{C}) \cdot (I - s\mathbf{C})^{-1}$ we have

$$\mathbf{D}^{-1} = (I - s\mathbf{C}) \cdot (I + s\mathbf{C})^{-1} = (I + s\mathbf{C}^{\mathsf{T}}) \cdot (I - s\mathbf{C}^{\mathsf{T}})^{-1} =$$

$$= (I + s\mathbf{C})^{\mathsf{T}} \cdot (I - s\mathbf{C})^{-\mathsf{T}} = \mathbf{D}^{\mathsf{T}}. \quad (2.32)$$

Hence $\mathbf{D}$ is orthogonal and consequently, $\| \mathbf{D} \|_2 = 1$. ■

Theorem 2.7 *Let* $h = \min\{\Delta x, \Delta y, \Delta z\}$ *and let* $q = c\Delta t/h$ *be an arbitrary fixed number. The numerical solution of the* MAXWELL *equations is unconditionally stable in 2-norm using staggered spatial discretization and using the* NAMIKI-ZHENG-CHEN-ZHANG *time integration method.*

Proof. The unconditional stability means that for all step-sizes satisfying the condition $q = c\Delta t/h$ the relation

$$\| \Psi^n \|_2 \leq K \| \Psi^0 \|_2 \quad (2.33)$$

is true for all $n \in \mathbb{N}$ with a constant K independent on n. From (2.28) follows the relation

$$\| \Psi^n \|_2^2 = \quad (2.34)$$

$$= \| [(\mathbf{I} - (\Delta t/2)\mathbf{A}_{2N})^{-1} \cdot (\mathbf{I} + (\Delta t/2)\mathbf{A}_{1N}) \cdot (\mathbf{I} - (\Delta t/2)\mathbf{A}_{1N})^{-1} \cdot (\mathbf{I} + (\Delta t/2)\mathbf{A}_{2N}))]^n \Psi^0 \|_2^2 \leq$$

$$\leq \| (\mathbf{I} - (\Delta t/2)\mathbf{A}_{2N})^{-1} \|_2^2 \cdot \| (\mathbf{I} + (\Delta t/2)\mathbf{A}_{2N})) \|_2^2 \cdot \| \Psi^0 \|_2^2 .$$

Here we employed Lemma 2.4 and Lemma 2.6 for the matrices $\mathbf{A}_{1N}$ and $\mathbf{A}_{2N}$. Moreover, because of the skew-symmetry of $\mathbf{A}_{2N}$, its eigenvalues can be written in the form $\pm \mathrm{i}\lambda_k$ ($k = 1, \ldots, 3N$, $\lambda_k \geq 0$, $\mathrm{i} = \sqrt{-1}$). Applying this we have the estimations

$$\| (\mathbf{I} - (\Delta t/2)\mathbf{A}_{2N})^{-1} \|_2^2 = \varrho((\mathbf{I} + (\Delta t/2)\mathbf{A}_{2N})^{-1}(\mathbf{I} - (\Delta t/2)\mathbf{A}_{2N})^{-1}) =$$

$$= \varrho((\mathbf{I} - (\Delta t/2)^2\mathbf{A}_{2N}^2)^{-1}) = \frac{1}{\min_k\{|1 - (\Delta t/2)^2(\pm \mathrm{i}\lambda_k)^2|\}} = \frac{1}{1 + (\Delta t/2)^2\lambda_{min}^2} \leq 1, \tag{2.35}$$

$$\| \mathbf{I} + (\Delta t/2)\mathbf{A}_{2N} \|_2^2 = \varrho((\mathbf{I} - (\Delta t/2)\mathbf{A}_{2N})(\mathbf{I} + (\Delta t/2)\mathbf{A}_{2N})) =$$

$$= \varrho(\mathbf{I} - (\Delta t/2)^2\mathbf{A}_{2N}^2) = 1 + (\Delta t/2)^2\lambda_{max}^2 \leq 1 + \left(\frac{c\Delta t}{h}\right)^2 = 1 + q^2. \tag{2.36}$$

In the previous expressions $\varrho(.)$ denotes the spectral radius, $\lambda_{max} = \max\{\lambda_1, \ldots, \lambda_{3N}\}$ and $\lambda_{min} = \min\{\lambda_1, \ldots, \lambda_{3N}\}$. Furthermore, the GERSCHGOREN-theorem and the form $1/(\sqrt{\varepsilon_{...}\mu_{...}}\Delta.)$ of the elements of $\mathbf{A}_{2N}$ are applied to get an upper bound for λ_{max}. In the long run we get that $\| \Psi^n \|_2^2 \leq (1 + q^2) \| \Psi^0 \|_2^2$, that is the choice $K = \sqrt{1 + q^2}$ is satisfactory. ■

REMARK 2.8. We remark that the constant q must be chosen according to the inequality $q < 1/\sqrt{3}$ (here $h = \Delta x = \Delta y = \Delta z$) in 3D problems in the case of the classical YEE-method to guarantee the stability of the method. According to the previous theorem in the NZCZ-method the parameter q can be set arbitrarily, which shows the unconditional stability of the method.

REMARK 2.9. We also remark that in 1D problems the splitting $\mathbf{A} = \mathbf{A} + \mathbf{0}$ can be applied. That is $\mathbf{A}_{1N} = \mathbf{A}$ and $\mathbf{A}_{2N} = \mathbf{0}$. This means that $U_n(\Delta t\mathbf{A}) = (\mathbf{I} + (\Delta t/2)\mathbf{A})(\mathbf{I} - (\Delta t/2)\mathbf{A})^{-1}$, and because of Lemma 2.6 $\| U_n(\Delta t\mathbf{A}) \|_2 = 1$. In the general 3D case we have $\| U_n(\Delta t\mathbf{A}) \|_2 \neq 1$.

2.3 Kole-Figge-de Raedt-method

According to the previous two subsections we can generalize the time integration methods as follows. In order to compute the matrix exponential $\exp(\Delta t\mathbf{A})$ efficiently we split the matrix $\mathbf{A}$ into the from $\mathbf{A} = \mathbf{A}_1 + \ldots + \mathbf{A}_p$ ($p \in \mathbb{N}$), where the matrices $\mathbf{A}_1, \ldots, \mathbf{A}_p$ are skew-symmetric matrices. Then we write the matrix exponential $\exp(\Delta t\mathbf{A})$ as a product of matrices in the form $\exp(\xi_{i_l}\Delta t\mathbf{A}_i)$, where ξ_{i_l} is some suitable chosen real constant, $i \in \{1, \ldots, p\}$. If the matrices $\mathbf{A}_1, \ldots, \mathbf{A}_p$ do not commute then this product is only an approximation of the original exponential. Then we usually approximate the matrices $\exp(\xi_{i_l}\Delta t\mathbf{A}_i)$ again (e.g. by their truncated TAYLOR-series).

The third method investigated in this paper was firstly described by KOLE, FIGGE and DE RAEDT (KFR-method, [5]). In this work special splittings are found such a way that the exponentials $\exp(\xi_{i_l}\Delta t\mathbf{A}_i)$ could be computed exactly using the fact

$$\exp\left(\begin{bmatrix} 0 & \alpha \\ -\alpha & 0 \end{bmatrix}\right) = \begin{bmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{bmatrix}, \tag{2.37}$$

where α is an arbitrary constant. We demonstrate this method on a simple example. Let us consider the skew-symmetric, block-diagonal matrix

$$\mathbf{K} = \begin{bmatrix} 0 & q & 0 & 0 & 0 & 0 & 0 \\ -q & 0 & q & 0 & 0 & 0 & 0 \\ 0 & -q & 0 & q & 0 & 0 & 0 \\ 0 & 0 & -q & 0 & q & 0 & 0 \\ 0 & 0 & 0 & -q & 0 & q & 0 \\ 0 & 0 & 0 & 0 & -q & 0 & q \\ 0 & 0 & 0 & 0 & 0 & -q & 0 \end{bmatrix}, \tag{2.38}$$

which can appear in the numerical solution of the 1D MAXWELL equations ($q \in \mathbb{R}$). With the splitting of this matrix in the form

$$\mathbf{K} = \mathbf{K}_1 + \mathbf{K}_2 = \begin{bmatrix} 0 & q & 0 & 0 & 0 & 0 & 0 \\ -q & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & q & 0 & 0 & 0 \\ 0 & 0 & -q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & q & 0 \\ 0 & 0 & 0 & 0 & -q & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q & 0 & 0 & 0 & 0 \\ 0 & -q & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & q & 0 & 0 \\ 0 & 0 & 0 & -q & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & q \\ 0 & 0 & 0 & 0 & 0 & -q & 0 \end{bmatrix} \tag{2.39}$$

the exponential $\exp(\mathbf{K})$ can be approximated by means of (2.37) as follows

$$\exp(\mathbf{K}) = \exp(\mathbf{K}_1 + \mathbf{K}_2) \approx \exp(\mathbf{K}_1) \cdot \exp(\mathbf{K}_2) =$$

$$= \begin{bmatrix} cq & sq & 0 & 0 & 0 & 0 & 0 \\ -sq & cq & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & cq & sq & 0 & 0 & 0 \\ 0 & 0 & -sq & cq & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & cq & sq & 0 \\ 0 & 0 & 0 & 0 & -sq & cq & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & cq & sq & 0 & 0 & 0 & 0 \\ 0 & -sq & cq & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & cq & sq & 0 & 0 \\ 0 & 0 & 0 & -sq & cq & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & cq & sq \\ 0 & 0 & 0 & 0 & 0 & -sq & cq \end{bmatrix}, \tag{2.40}$$

where sq and cq denote $\cos(q)$ and $\sin(q)$, respectively. Because $\mathbf{K}_1$ and $\mathbf{K}_2$ are block-diagonal matrices, the product of them can be written using the products of their blocks.

Since matrices $\mathbf{A}_1, \ldots, \mathbf{A}_p$ are skew-symmetrical and only the products of the exponents of these matrices are used in the approximation, the iteration matrix will be orthogonal. That is its 2-norm is exactly one. Thus this method is also unconditionally stable.

Theorem 2.10 *The numerical solution of the* MAXWELL *equations using staggered spatial discretization and using products of exactly calculated matrix exponentials of skew-symmetric matrices in the time integration (*KOLE, FIGGE, DE RAEDT*-method) is unconditionally stable.*

2.4 Application of the Krylov-space method using a modified Arnoldi orthogonalisation method

In the previous methods we approximated the matrix exponential $\exp(\Delta t\mathbf{A})$ and used this approximation to generate a matrix iteration. Changing the philosophy of the matrix exponential approximation we can proceed as follows. We do not approximate the matrix exponential itself but the product of the matrix exponential with the previous state vector. The building blocks of this method are not new (see for example [2, 7, 9, 10, 14]), but the way is new as we combine the numerical solution of the MAXWELL-equations and the KRYLOV-space methods for skew-symmetric matrices to achieve a sufficiently accurate and stable numerical method.

If the initial vector Ψ^0 and a natural number m are given, then we can construct the Krylov-subspace as follows

$$\mathcal{K}(\Delta t\mathbf{A}, \Psi^0, m) = \text{span}\{\Psi^0, \Delta t\mathbf{A}\Psi^0, \ldots, (\Delta t\mathbf{A})^{m-1}\Psi^0\}. \tag{2.41}$$

(span{} denotes the set of all possible linear combinations of the vectors.) We are going to choose the best approximation to $\exp(\Delta t\mathbf{A})\Psi^0$ from this subspace. To do this, first we construct an orthonormal basis $\mathbf{v}_1, \mathbf{v}_2, \ldots$ for the space $\mathcal{K}(\Delta t\mathbf{A}, \Psi^0, m)$ with the well-known ARNOLDI-algorithm 1 (naturally we can leave the constant Δt).

According to the results of the algorithm we can introduce the notations $\mathbf{V}_m = [\mathbf{v}_1, \ldots, \mathbf{v}_m]$, $\mathbf{V}_{m+1} = [\mathbf{v}_1, \ldots, \mathbf{v}_m, \mathbf{v}_{m+1}]$, $\tilde{\mathbf{T}}_m \in \mathbb{R}^{(m+1)\times m}$ is an upper HESSENBERG matrix with the elements

Algorithm 1 ARNOLDI-algorithm

$\beta := \| \mathbf{v} \|_2$
$\mathbf{v}_1 := \Psi^0/\beta$
for j:=1:m **do**
  $\mathbf{p} := \mathbf{A}\mathbf{v}_j$
  for i:=1:j **do**
    $t_{ij} := \mathbf{v}_i^\top \mathbf{p}$
    $\mathbf{p} := \mathbf{p} - t_{ij}\mathbf{v}_i$
  end for
  $t_{j+1,j} := \| \mathbf{p} \|_2$
  $\mathbf{v}_{j+1} := \mathbf{p}/t_{j+1,j}$
end for

t_{ij}, $\mathbf{T}_m = \tilde{\mathbf{T}}(1:m, 1:m) \in \mathbb{R}^{m\times m}$ is also an upper HESSENBERG matrix, and let $\mathbf{e}_j$ be the jth unit vector. Then the relations

$$\mathbf{V}_m^\top \mathbf{V}_m = \mathbf{I}, \ (\mathbf{v}_1, \ldots, \mathbf{v}_m \text{ is an orthonormal basis}) \tag{2.42}$$

$$\mathbf{A}\mathbf{V}_m = \mathbf{V}_{m+1}\tilde{\mathbf{T}}_m = \mathbf{V}_m\mathbf{T}_m + t_{m+1,m}\mathbf{v}_{m+1}\mathbf{e}_m^\top, \tag{2.43}$$

$$\mathbf{V}_m^\top \mathbf{A}\mathbf{V}_m = \mathbf{T}_m \tag{2.44}$$

are satisfied ([1]). We remark that in case of $t_{j+1,j} = 0$ $(j \leq m)$ we terminate the algorithm. Then the subspace $\mathcal{K}(\Delta t\mathbf{A}, \Psi^0, m)$ is invariant regarding the multiplication with $\mathbf{A}$. This means that the matrix exponential can be computed exactly. We suppose for a while that this is not the case. Later we will investigate the modifications arisen by the termination. From the equality (2.44), applying the skew-symmetricity of $\mathbf{A}$ we have

$$\mathbf{T}_m^\top = (\mathbf{V}_m^\top \mathbf{A}\mathbf{V}_m)^\top = \mathbf{V}_m^\top \mathbf{A}^\top \mathbf{V}_m = -\mathbf{T}_m, \tag{2.45}$$

which means that $\mathbf{T}_m$ is a skew-symmetric matrix. Combining this fact with the HESSENBERG structure of $\mathbf{A}$ we obtain, that $\mathbf{T}_m$ is a skew-symmetric tridiagonal matrix with zeros in the main-diagonal. Based on our observation, the ARNOLDI-iteration can be simplified leaving out the inner loop.

Algorithm 2 ARNOLDI-algorithm for skew-symmetric matrices

$\beta_1 := 0, \mathbf{v}_0 = \mathbf{0}, \mathbf{v}_1 = \Psi^0/\| \Psi^0 \|_2$
for j:=1:m **do**
  $\mathbf{p} := \mathbf{A}\mathbf{v}_j + \beta_j\mathbf{v}_{j-1}$
  $\beta_{j+1} := \| \mathbf{p} \|_2$
  $\mathbf{v}_{j+1} := \mathbf{p}/\beta_{j+1}$
end for

In the algorithm the notation $\beta_j = t_{j,j-1}$ $(j = 2, \ldots, m+1)$ is used. This algorithm is much faster than the original ARNOLDI-algorithm. We have to execute only one matrix-vector multiplication (with a sparse matrix, at most four nonzero elements per row) and one vector-vector addition in every step.

After the construction of the basis of the KRYLOV-space $\mathcal{K}(\Delta t\mathbf{A}, \Psi^0, m)$ the best approximation (Ψ^1) to $\exp(\Delta t\mathbf{A})\Psi^0$ can be obtained by the formula

$$\Psi^1 = \beta\mathbf{V}_m \exp(\Delta t\mathbf{T}_m)\mathbf{e}_1 = \mathbf{V}_m \exp(\Delta t\mathbf{T}_m)\mathbf{V}_m^\top \Psi^0. \tag{2.46}$$

Here the notation $\beta = \| \Psi^0 \|_2$ and the fact $\beta\mathbf{V}_m\mathbf{e}_1 = \Psi^0$ have been employed. The main advantage of this method is that we need to compute the matrix exponential only for the small matrix $\Delta t\mathbf{T}_m$

($m << 6N$) and we get the next approximation as a linear combination of the m columns of $\mathbf{V}_m$. This method is encapsulated in the first expression in (2.46), while the second expression writes the method in a vector iteration form. Let us introduce the notation $\mathbf{Q}_0 = \mathbf{V}_m \exp(\Delta t \mathbf{T}_m)\mathbf{V}_m^\top$. Then we have the first step as $\Psi^1 = \mathbf{Q}_0 \Psi^0$. After this we construct the space $\mathcal{K}(\Delta t\mathbf{A}, \Psi^1, m)$ getting a new iteration matrix $\mathbf{Q}_1$. That is $\Psi^2 = \mathbf{Q}_1 \Psi^1$, and so on $\Psi^{n+1} = \mathbf{Q}_n \Psi^n$ $(n = 0, 1, \ldots)$.

Theorem 2.11 *The numerical solution of the* MAXWELL *equations using staggered spatial discretization and using the* KRYLOV*-method with a modified* ARNOLDI *orthogonalization in the time integration is unconditionally stable.*

Proof. The matrices $\mathbf{Q}_i$ $(i = 0, 1, \ldots)$ have the property $\| \mathbf{Q}_i \|_2 = 1$. We show this fact for $\mathbf{Q}_0$. We have

$$\| \mathbf{Q}_0 \|_2^2 = \varrho(\mathbf{Q}_0^\top \mathbf{Q}_0) = \varrho(\mathbf{V}_m \exp(-\Delta t \mathbf{T}_m)\mathbf{V}_m^\top \mathbf{V}_m \exp(\Delta t \mathbf{T}_m)\mathbf{V}_m^\top) = \varrho(\mathbf{V}_m \mathbf{V}_m^\top). \tag{2.47}$$

We see that $\mathbf{V}_m \mathbf{V}_m^\top \mathbf{V}_m = \mathbf{V}_m$, which shows that the spectral radius of $\mathbf{V}_m \mathbf{V}_m^\top$ is one. In the long run we obtain that $\| \Psi^n \|_2 = \| \Psi^0 \|_2$ for all $n = 1, 2, \ldots$. ■

REMARK 2.12. Let us denote the smallest integer m for which $\mathbf{A}^m \Psi^0 \in \mathcal{K}(\Delta t\mathbf{A}, \Psi^0, m)$ is fulfilled by m_0. This number exists because the set of integer numbers for which the above statement is valid is not empty ($m = 6N$ is its element). In this case Ψ^1 gives the exact value of $\exp(\Delta t\mathbf{A})\Psi^0$, which means that $\exp(\Delta t\mathbf{A})$ can be computed exactly with the formula $\exp(\Delta t\mathbf{A}) = \mathbf{V}_{m_0} \exp(\Delta t \mathbf{T}_{m_0})\mathbf{V}_{m_0}^\top$. Moreover, $\mathbf{Q}_0 = \mathbf{Q}_1 = \ldots = \exp(\Delta t\mathbf{A})$ and we have $\exp(n\Delta t\mathbf{A})\Psi^0 = \Psi^n = \mathbf{V}_{m_0} \exp(n\Delta t \mathbf{T}_{m_0})\mathbf{V}_{m_0}^\top \Psi^0$. The exact solution of (1.17) can be obtained at arbitrary time-level $n\Delta t$. This shows that the KRYLOV-space method in special cases ($m_0 << 6N$) can be a very efficient one.

REMARK 2.13. Considering Theorem 4 in [2] we can give an estimation for the error of this method in the form

$$\| \exp(\Delta t\mathbf{A})\Psi^0 - \beta \mathbf{V}_m \exp(\Delta t \mathbf{T}_m)\mathbf{e}_1 \|_2 \leq 12 e^{-(2q)^2/m} \left(\frac{2eq}{m}\right)^m, \quad m \geq 4q \ (q = c\Delta t/h). \tag{2.48}$$

With this relation we are able to choose m or Δt to guarantee a certain accuracy level of the computations. For 1D cases we have the error estimation

$$\| \exp(\Delta t\mathbf{A})\Psi^0 - \beta \mathbf{V}_m \exp(\Delta t \mathbf{T}_m)\mathbf{e}_1 \|_2 \leq 12 e^{-q^2/m} \left(\frac{eq}{m}\right)^m, \quad m \geq 2q \ (q = c\Delta t/h). \tag{2.49}$$

Finally, we summarize the basic properties of the discussed methods in Table 2.1.

3 Comparison of the methods

In the previous section we listed four time-integration methods for the MAXWELL equations. We showed that these methods all based on the approximation of a matrix exponential and we discussed their stability properties. Naturally the NZCZ-, KFR- and KRYLOV-methods need more computational time to advance the values with one time-step than in the YEE-method. At the same time in these methods arbitrarily large Δt can be chosen, so in the long run these methods compute the approximation at a certain time level faster than the YEE-method. Naturally, because of the larger Δt these methods can be less accurate comparing with the YEE-method. In this section we investigate the methods from the point of view of the accuracy and the speed of the numerical algorithms.

YEE	
$U_n(\Delta t\mathbf{A})$	$(\mathbf{I}+\Delta t\mathbf{A}_{1Y})(\mathbf{I}+\Delta t\mathbf{A}_{2Y})$
Stability	$\Delta t < 1/(c\sqrt{(1/\Delta x)^2+(1/\Delta y)^2+(1/\Delta z)^2})$, $\parallel U(\Delta t\mathbf{A}) \parallel_2 \neq 1$
Remark	The splitting $\mathbf{A}=\mathbf{A}_{1Y}+\mathbf{A}_{2Y}$ is done according to the rows belonging to electric and magnetic fields, respectively.
NZCZ	
$U_n(\Delta t\mathbf{A})$	$(\mathbf{I}-(\Delta t/2)\mathbf{A}_{2N})^{-1}\cdot(\mathbf{I}+(\Delta t/2)\mathbf{A}_{1N})\cdot(\mathbf{I}-(\Delta t/2)\mathbf{A}_{1N})^{-1}\cdot(\mathbf{I}+(\Delta t/2)\mathbf{A}_{2N}))$
Stability	unconditionally stable, $\parallel U(\Delta t\mathbf{A}) \parallel_2 \neq 1$ (in 1D $\parallel U(\Delta t\mathbf{A}) \parallel_2 = 1$)
Remark	The splitting $\mathbf{A}=\mathbf{A}_{1N}+\mathbf{A}_{2N}$ is done according to the two space derivative terms of the curl operator, respectively.
KFdR	
$U_n(\Delta t\mathbf{A})$	product of exactly computed matrix exponentials $\exp(\xi\Delta t\mathbf{A}_i)$, $i\in\{1,\ldots,p\}$
Stability	unconditionally stable, $\parallel U(\Delta t\mathbf{A}) \parallel_2 = 1$
Remark	In the splitting $\mathbf{A}=\mathbf{A}_1+\ldots+\mathbf{A}_p$ the matrices are skew-symmetric, for which the matrix exponential can be computed easily.
Krylov	
$U_n(\Delta t\mathbf{A})$	$\mathbf{V}_m\exp(\Delta t\mathbf{T}_m)\mathbf{V}_m^{\dagger}$, this can be different in all iteration steps
Stability	unconditionally stable, $\parallel U(\Delta t\mathbf{A}) \parallel_2 = 1$
Remark	The matrices $\mathbf{V}_m$ and $\mathbf{T}_m$ come from the construction of an orthonormal basis of the KRYLOV-space generated by the modified ARNOLDI-method.

Table 2.1: *Overview of the discussed methods.*

We consider a model example to demonstrate and investigate the properties of the methods. Although, we study only 1D problems, our considerations regarding the benefits and drawbacks of the methods can be extended directly for higher dimensional problems, too. Another goal is to investigate the properties of the matrix exponential approximations.

Let us consider the 1D Maxwell equations

$$\frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial x} \tag{3.50}$$

$$\frac{\partial E_z}{\partial t} = \frac{\partial H_y}{\partial x}, \tag{3.51}$$

on the interval $[0,1]$. In the sequel, we suppose that this interval is bounded by perfect conductor materials (this yields the boundary condition $E_z=0$ at $x=0$ and $x=1$), moreover let $\varepsilon=\mu=1$. In this case $c=1$. Using the staggered grid technique we discretize the equations on the grid depicted in Figure 3.2. The semidiscretized system has the form

$$\frac{\mathrm{d}\Psi}{\mathrm{d}t} = \frac{1}{\Delta x}\mathrm{tridiag}\,[-1,0,1]\Psi, \tag{3.52}$$

where $1/\Delta x = N \in \mathbb{N}$ is the number of the YEE-cells, tridiag $[-1,0,1] \in \mathbb{R}^{(2N-1)\times(2N-1)}$, tridiag $[-1,0,1]$ is a short notation for tridiagonal matrices and $\Psi(t)$ is the approximation of the vector

$$= (H_y(t,\Delta x/2), E_z(t,\Delta x),\ldots,E_z(t,1-\Delta x),H_y(t,1-\Delta x/2))^{\mathsf{T}}. \tag{3.53}$$

In the first example let the initial function for the electric field be

$$E_z(0,x) = -2|x-1/2|+1, \quad x\in[0,1], \tag{3.54}$$

which is not differentiable at $x=1/2$. (The graph of the function is depicted in Figure 3.3.) The initial function for the magnetic field is the constant zero function. We determine the numerical

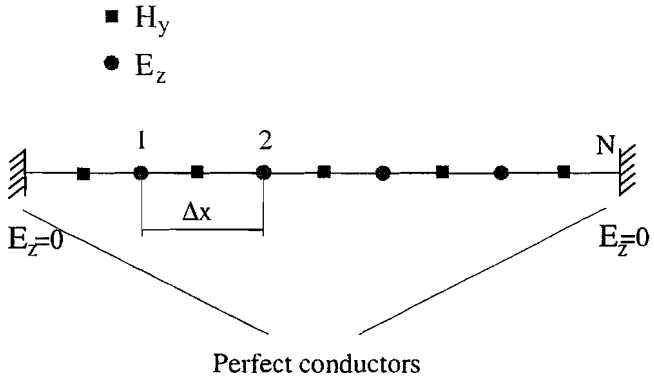

Figure 3.2: *The grid-points in the 1D example.*

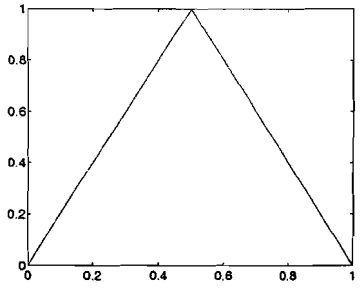

Figure 3.3: *The initial function for E_z.*

solution at time-level $t = 0.8$ using the step-size $\Delta x = 1/500$. The errors of the electric field are measured with the maximum norm ($\|\cdot\|_\infty$) and with the l_2 norm ($\|\cdot\|_{l_2}$). The exact solution can be written in the form of FOURIER-series as follows

$$E_z(t,x) = \frac{8}{\pi^2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{(2k-1)^2}\sin((2k-1)\pi x)\cos((2k-1)\pi t), \tag{3.55}$$

$$H_y(t,x) = \frac{8}{\pi^2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{(2k-1)^2}\cos((2k-1)\pi x)\sin((2k-1)\pi t). \tag{3.56}$$

First we apply the classical YEE-method. The numerical results are listed in Table 3.2. Theorem 2.3 gives the maximal time-step $\Delta t_{max} = 0.002$. Although, Theorem 2.3 ensures the stability only for step-sizes $\Delta t < \Delta t_{max}$ we also applied the value $\Delta t = \Delta t_{max}$. With these time-step (which is called magic step-size, [11]) we have got very accurate numerical solution. The accuracy decreases dramatically decreasing the time-step. In spite of this, we have to be very careful, because the methods with the magic step-size are not stable. (See Section 10.2 in book [8].) According to Table 3.2 we cannot solve our original problem with the YEE-method faster than 0.36 seconds, even if we are not interested in very accurate numerical solution. Moreover, let us observe that the decreasing time-step does not decrease the error, but increases the solution time. This is why the time-steps are suggested to be chosen close to the stability bound both from the accuracy and from the solution speed point of view.

Now we solve the problem with the NZCZ method. As we know from the previous section this method is unconditionally stable, specially, in 1D case the 2-norm of the iteration matrix is one

Δt	Nr. of time-steps	error $\| \cdot \|_{l_2}$	error $\| \cdot \|_\infty$	CPU time (sec.)
0.002005	399	1.7273×10^{8}	3.9252×10^{8}	0.35
0.002051	390	8.1889×10^{59}	2.3142×10^{60}	0.35
0.002	400	5.5153×10^{-15}	1.1435×10^{-14}	0.36
0.001995	401	1.0649×10^{-5}	7.6057×10^{-5}	0.36
0.00199	402	2.1136×10^{-5}	1.5416×10^{-4}	0.36
0.001985	403	3.1337×10^{-5}	2.3357×10^{-4}	0.36
0.00198	404	4.1534×10^{-5}	3.1354×10^{-4}	0.36
0.001333	600	4.3790×10^{-4}	2.9581×10^{-3}	0.54
0.001	800	5.1596×10^{-4}	3.0257×10^{-3}	0.70
0.0005	1600	5.7134×10^{-4}	3.3323×10^{-3}	1.42
0.00005	16000	5.8973×10^{-4}	3.4268×10^{-3}	13.96
0.000005	160000	5.8991×10^{-4}	3.4276×10^{-3}	140.13

Table 3.2: *Computational results with the* YEE*-method.*

Δt	Nr. of time-steps	error $\| \cdot \|_{l_2}$	error $\| \cdot \|_\infty$	CPU time (sec.)
0.08	10	2.9216×10^{-2}	5.7967×10^{-2}	0.04
0.016	50	6.6669×10^{-2}	1.7493×10^{-2}	0.21
0.008	100	3.3758×10^{-3}	1.1446×10^{-2}	0.43
0.004	200	1.7722×10^{-3}	6.9855×10^{-3}	0.88
0.002	400	1.0242×10^{-3}	4.8251×10^{-3}	1.83
0.001	800	7.2343×10^{-4}	3.7563×10^{-3}	3.67
0.0005	1600	6.2641×10^{-4}	3.5141×10^{-3}	7.34

Table 3.3: *Computational results with the NZCZ-method.*

Δt	Nr. of time-steps	error $\|\|\ .\ \|\|_{l_2}$	error $\|\|\ .\ \|\|_{\infty}$	CPU time (sec.)
0.0005	1600	3.0649×10^{-2}	5.7587×10^{-2}	0.72
0.00005	16000	1.9252×10^{-3}	5.0141×10^{-3}	7.14
0.00001	80000	6.9278×10^{-4}	3.4210×10^{-3}	36.12

Table 3.4: *Computational results with the KFR-method applying sequential splitting.*

Δt	Nr. of time-steps	error $\|\|\ .\ \|\|_{l_2}$	error $\|\|\ .\ \|\|_{\infty}$	CPU time (sec.)
0.001	800	4.2613×10^{-2}	6.5893×10^{-2}	0.54
0.0005	1600	1.0583×10^{-2}	1.7226×10^{-2}	1.07
0.00005	16000	6.0946×10^{-4}	3.4252×10^{-3}	10.96
0.00001	80000	5.9035×10^{-4}	3.4275×10^{-3}	54.29

Table 3.5: *Computational results with the KFR-method applying* STRANG*-splitting.*

(see Remark 2.9). This means that the time-step can be chosen arbitrarily. The results are in Table 3.3. We see that the NZCZ method is slower with a factor about five than the YEE-method. Moreover, the accuracy of the method is a little bit poorer. Because this method is implicit we have to invert a tridiagonal matrix in every time-step (the so-called THOMAS-algorithm has been used, a special GAUSS elimination method). However, the YEE-method breaks down after $\Delta t = 0.002$, while the NZCZ method behaves adequately after this bound too. We can choose even $\Delta t = 0.08 = 40\Delta t_{max}$ solving the problem almost nine times faster than with the YEE-method. The decrease of the computational time is at the expense of the accuracy.

In the third place we investigate the KFR-method. Let us introduce the notation

$$\mathbf{K} = \Delta t/\Delta x \cdot \text{tridiag}\,[-1, 0, 1]. \tag{3.57}$$

This matrix has the same structure like in (2.38) and we use the same procedure as in (2.39) to split this matrix into the form $\mathbf{K} = \mathbf{K}_1 + \mathbf{K}_2$. For the matrices $\mathbf{K}_1$ and $\mathbf{K}_2$ the matrix exponential can be computed exactly. How could we get an adequate approximation for $\exp(\mathbf{K})$ using the matrices $\exp(\mathbf{K}_1)$ and $\exp(\mathbf{K}_2)$? From the comparison of the TAYLOR-series of these exponentials we get the accuracy of approximations as follows. The approximation

$$\exp(\mathbf{K}) \approx \exp(\mathbf{K}_1)\exp(\mathbf{K}_2) \tag{3.58}$$

(so-called sequential splitting) has first,

$$\exp(\mathbf{K}) \approx \exp(\mathbf{K}_1/2)\exp(\mathbf{K}_2)\exp(\mathbf{K}_1/2) \tag{3.59}$$

(so-called STRANG-splitting) has second and

$$\exp(\mathbf{K}) \approx \exp(\alpha_1\mathbf{K}_1)\exp(\beta_1\mathbf{K}_2)\exp(\alpha_2\mathbf{K}_1)\exp(\beta_2\mathbf{K}_2)\exp(\alpha_2\mathbf{K}_1)\exp(\beta_1\mathbf{K}_2)\exp(\alpha_1\mathbf{K}_1), \tag{3.60}$$

$$\alpha_1 = \frac{1}{2(2-2^{1/3})},\ \alpha_2 = (1-2^{1/3})\alpha_1,\ \beta_1 = 2\alpha_1,\ \beta_2 = -2^{4/3}\alpha_1$$

has fourth order accuracy (see [13]). The computational results are listed in Tables 3.4, 3.5 and 3.6. In the tables we do not show the time-steps that produce larger error than 0.1 in maximum norm. For example, in the case of the first order method, we could not choose the time-step 0.001 and of course any larger time-step either.

We can notice that in spite of the exact computation of the matrix exponentials with matrices $\mathbf{K}_1$ and $\mathbf{K}_2$ this method behaves relatively poorer than the YEE- or NZCZ-methods from the point of view of the accuracy. Moreover, increasing the accuracy of the method the computational costs

Δt	Nr. of time-steps	error $\|\,.\,\|_{l_2}$	error $\|\,.\,\|_\infty$	CPU time (sec.)
0.002	400	4.0329×10^{-2}	6.2563×10^{-2}	0.62
0.001	800	2.7462×10^{-3}	5.8719×10^{-3}	1.22
0.0005	1600	6.2340×10^{-4}	3.3982×10^{-3}	2.49
0.00005	16000	5.8991×10^{-4}	3.4276×10^{-3}	25.31
0.00001	80000	5.8991×10^{-4}	3.4276×10^{-3}	126.96

Table 3.6: *Computational results with the KFR-method applying fourth order splitting.*

m	error $\|\,.\,\|_{l_2}$	error $\|\,.\,\|_\infty$	CPU time (sec.)
30	5.2785×10^{-1}	1.8928×10^{0}	0.41
60	4.3976×10^{-1}	9.6640×10^{-1}	1.19
70	2.0309×10^{-1}	4.4442×10^{-1}	1.56
80	3.8035×10^{-3}	1.7060×10^{-2}	2.00
90	5.8973×10^{-4}	3.4262×10^{-3}	2.60
120	5.8991×10^{-4}	3.4276×10^{-3}	4.78
150	5.8991×10^{-4}	3.4276×10^{-3}	8.27

Table 3.7: *Computational results with different m values for the* KRYLOV*-method with $\Delta t = 0.08$.*

also increased. This yields that we cannot solve the problem faster than 0.54 seconds (to keep the accuracy acceptable), which makes this method not too efficient (compare with the 0.36 seconds in the case of the YEE-method).

We explain this phenomenon as follows. Let us consider the YEE-scheme and the first order KFR-scheme. In both cases we apply matrix splitting for the matrix $\mathbf{K}$. In the first case we approximate the matrix exponentials by the first two terms of the series of the exponential function (see (2.22)), while in the second one we calculate the matrix exponential exactly with sinus and cosine functions (see (3.58)). As it can be seen from the computational results, the exact calculation of the exponentials does not mean directly that the KFR-method is generally more accurate. The accuracy is determined by the splitting of the matrix $\mathbf{K}$ and the initial vector of the iteration, too. The splitting in the YEE-method is more natural (corresponds to the electric and magnetic fields) than in the KFR-method (where a tricky splitting is used to compute the exponentials exactly). Let us see an example taking the matrix $\mathbf{K} = \text{tridiag}\,[-1, 0, 1] \in \mathbb{R}^{99\times 99}$ and the vector

$$\mathbf{v} = [\cos(\pi/100), 0, \cos(3\pi/100), 0, \cos(5\pi/100), 0, \cos(7\pi/100), \ldots, 0, \cos(99\pi/100)]^\top. \qquad (3.61)$$

Then with the YEE-method splitting approximates $\exp(K)\mathbf{v}$ with the 2-norm error 9.8718×10^{-3}. The KFR-method does the same with the error 7.0501×10^{-1}, which is 71 times greater than in the YEE-method. For the second order KFR- method we have the error 1.2773×10^{-1}, while for the fourth order one 6.3142×10^{-2}.

Finally, we apply the KRYLOV-method. We expect this method to be more accurate than the previous methods, because new iteration matrix is calculated in every time-step. Moreover, we can notice that the speed of the method depends strongly on the number m, because the KRYLOV-basis with m elements must be generated also in every time-step. First we choose the time-step $\Delta t = 0.08$ and compute the error of the method depending on m. The results are in Table 3.7.

We can observe that the error of the method is acceptable if m is about 80 or greater. Generally, we can apply Remark 2.13 to estimate m to get a sufficiently accurate solution. In this way we obtain the (naturally) greater $m \approx 110$ ($q = 40$) value. Moreover, as we can see, the computational time does not depend linearly on the value of m. The reason is that the number of operations in one time-step has the form $d_1 m^2 + d_2 N m$, where the first term comes from the computation of the exponential of matrix $\mathbf{T}_m$ and the second one comes from other computations ($d_1, d_2 \in \mathbb{R}$).

Δt	Nr. of time-steps	m computed	error $\|\cdot\|_{l_2}$	error $\|\cdot\|_\infty$	CPU time (sec.)
0.08	10	110	5.8991×10^{-4}	3.4276×10^{-3}	4.05
0.008	100	20	5.8991×10^{-4}	3.4276×10^{-3}	2.43
0.0008	1000	7	5.8991×10^{-4}	3.4276×10^{-3}	9.85
0.00008	10000	5	5.8991×10^{-4}	3.4276×10^{-3}	77.19

Table 3.8: *Computational results with the* KRYLOV*-method.*

For relatively large values of m the first term is comparable with the second one. We compute the errors for several time-steps (see Table 3.8). The values m come from the expressions in Remark 2.13.

For the time-step $\Delta t = 0.8$ we would have $m = 960$. In this case the relation $m << 2N-1 = 999$ (where $2N-1$ means the number of unknowns) does not yield, and the KRYLOV-method is very expensive. The fastest method in the table is the method with $\Delta t = 0.008$. This method has the same computational speed as the NZCZ-method with $\Delta t = 0.002$ or the fourth order KFR-method with $\Delta t = 0.0005$, but the method is more accurate.

REMARK 3.1. The errors in Table 3.8 are the same for every time-step. This is why for the given m values we get a very accurate approximation for the vector

$$\exp((0.8/500)\text{tridiag}\,[-1,0,1])\Psi^0, \tag{3.62}$$

but we compare this vector with the exact solution of the MAXWELL equations. That is the errors in the table come from the spatial discretization and not from the time one. The error could be decreased by increasing the number of the grid points. (See the last two rows in Table 3.6.)

We consider another exact solution of the 1D MAXWELL equations in the form

$$E_z(t,x) = \sin(\pi x)\sin(\pi t), \tag{3.63}$$
$$H_y(t,x) = -\cos(\pi x)\cos(\pi t). \tag{3.64}$$

The numerical results are in Table 3.9. We denoted the fourth order KFR-method by KFR4 and the sign $-$ means that the error of the method is very large (≥ 0.1). In the heads the error in l_2-norm, in maximum norm and the CPU-time is listed, respectively. As in the previous example, when the YEE-method is stable then it is more accurate comparing with the other methods. Furthermore, this method is also the fastest one, because this is a cheap explicit method. In the case of the KFR4-method the time-step cannot increased above the maximal time-step of the YEE-method ($\Delta t = 0.002$) because the accuracy of it is unacceptably small. We have experienced that the choice $m = 8$ is suitable in the KRYLOV-method. This method solves the equations in a quickest way, namely 0.01 seconds is enough. This shows that the KRYLOV-method in special cases can be very efficient.

4 Conclusions

We described and investigated three methods, the NZCZ, KFR and Krylov-method. The methods passes the nice properties of the YEE-method: easy understandability, solution of a wide frequency range with one simulation (time domain methods), animation displays, specification of the material properties at all points within the computational domain and the computation of the electric and magnetic fields directly. The most important reason why these methods have been constructed is to speed up the numerical computations. Naturally, the increase in the time-step necessitates decrease in the accuracy, that is we have to find the balance between the accuracy and the computational speed.

Δt	YEE	NZCZ	KFR4	KRYLOV, $m = 8$
0.8	-	-	-	2.3650×10^{-6} 3.3446×10^{-6} 0.01
0.08	-	7.4635×10^{-3} 1.0555×10^{-2} 0.04	-	2.3751×10^{-6} 3.3446×10^{-6} 0.11
0.008	-	7.8034×10^{-5} 1.1036×10^{-4} 0.43	-	2.3702×10^{-6} 3.6623×10^{-6} 1.14
0.004	-	2.1285×10^{-5} 3.0100×10^{-5} 0.88	-	2.3650×10^{-6} 3.3446×10^{-6} 2.27
0.002	2.0510×10^{-15} 2.9006×10^{-15} 0.36	7.0949×10^{-6} 1.0034×10^{-5} 1.33	5.4022×10^{-2} 7.6333×10^{-2} 0.62	2.3650×10^{-6} 3.3446×10^{-6} 4.53
0.001	2.2865×10^{-6} 3.2336×10^{-6} 0.70	3.5475×10^{-6} 5.0169×10^{-6} 3.67	3.7922×10^{-3} 5.3431×10^{-3} 1.22	2.3650×10^{-6} 3.3446×10^{-6} 9.01
0.0005	2.3454×10^{-6} 3.3169×10^{-6} 1.42	2.6606×10^{-6} 3.7627×10^{-6} 7.34	2.4440×10^{-4} 3.4578×10^{-4} 2.49	2.3650×10^{-6} 3.3446×10^{-6} 18.30
0.00005	2.3648×10^{-6} 3.3443×10^{-6} 14.14	2.3680×10^{-6} 3.3488×10^{-6} 72.15	2.3893×10^{-6} 3.3788×10^{-6} 25.31	2.3650×10^{-6} 3.3446×10^{-6} 181.12
0.000005	2.3648×10^{-6} 3.3446×10^{-6} 148.48	2.3652×10^{-6} 3.3450×10^{-6} 735.51	2.3415×10^{-6} 3.3111×10^{-6} 247.87	2.3650×10^{-6} 3.3446×10^{-6} 1794.86

Table 3.9: *Computational results with the exact solutions in (3.64).*

We observed that the NZCZ-method is slower with a factor about five than the YEE-method, but the method is unconditionally stable and in the long run it computes the solution faster. The accuracy of the method is acceptable. In the KFR-method we experienced that the method is relatively inaccurate, and to make it much more accurate costs a lot computational time. The KRYLOV-space method is generally slow, but in special cases behaves much better than the NZCZ-method, and the accuracy of the method is considerable.

We see that the behavior of the methods are determined by the properties of the matrix splitting. The investigation of other matrix splitting methods could show the way to a more efficient MAXWELL-solver.

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