ENERGY EVOLUTION OF MULTI-SYMPLECTIC METHODS FOR MAXWELL EQUATIONS WITH PERFECTLY MATCHED LAYER BOUNDARY

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In this paper, we consider the energy evolution of multi-symplectic methods for three-dimensional (3D) Maxwell equations with perfectly matched layer boundary, and present the energy evolution laws of Maxwell equations under the discretization of multi-symplectic Yee method and general multi-symplectic Runge-Kutta methods.

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I. INTRODUCTION

Maxwell equations are the most foundational equations in electromagnetism and are widely applied to many application fields, such as aeronautics, electronics, and biology, etc. They are mathematical expressions of the natural laws correlating fields, such as Ampère’s law and Faraday’s law. On the other hand, in lossless medium, the electromagnetic energy of the wave is constant at different times. As we all know, to preserve the energy is greatly important in constructing numerical schemes for different physical problems. However, numerical methods, with some boundary conditions, can not preserve the energy exactly in general cases. Therefore, it is important and necessary to investigate the energy evolution of Maxwell equations under numerical discretization with some boundary conditions. The purpose of this paper is to study the energy evolution of multi-symplectic methods for 3D Maxwell’s equations with perfectly matched layer (PML) boundary.

It has been recognized that symplectic structure-preserving numerical methods have significant superiority than non-symplectic methods in numerical solving Hamiltonian ordinary differential equations (ODEs) and Hamiltonian partial differential equations (PDEs). At the end of last century, symplectic integrators have been generalized to multi-symplectic one. And multi-symplectic integrators have been applied to Maxwell equations. For example, discussed the self-adjointness of the Maxwell equations with variable coefficients and , and showed that the equations have the multi-symplectic structure. firstly proposed an unconditionally stable, energy-conserved, and computational efficient scheme for two-dimensional (2D) Maxwell equations with an isotropic and lossless medium. The further analysis in the case of 3D was studied in. Meanwhile, proposed a kind of splitting multi-symplectic integrators method for Maxwell equations in three dimensions, which was proved to be unconditionally stable, non-dissipative, and of first order accuracy in time and second order accuracy in space.

It is well known that the PML boundary conditions are widely applied to the numerical simulation Maxwell equations. In 1993, Berenger firstly proposed the PML technique, which is based on modifying the PDEs away from all physical boundaries such that absorbing outgoing waves from the computation domain. It is a simple and straightforward technique, easily implemented for both two and three space dimensions using either cartesian or cylindrical coordinates. However, to the best of our knowledge, the investigation of multi-symplectic methods for Maxwell equations with PML boundary does not exist. In this paper, inspired by this problem, we investigate the energy evolution of general multi-symplectic methods for Maxwell equations with Berenger’s PML boundary.

The rest of this paper is organized as follows. In Section 2, we begin with some preliminary results about 3D Maxwell equations and Berenger’s PML systems. An equivalent formulation to Berenger’s PML systems is introduced in Section 3. In Section 4, we present the energy evolution laws of multi-symplectic Yee method and general multi-symplectic Runge-Kutta methods for 3D Maxwell equations with PML boundary.

II. PRELIMINARY RESULTS

Notations. We denote by the $L^2$ scalar product, the norm in $H^s$.

A. 3D Maxwell equations

For a linear homogeneous medium within linear isotropic material with the permittivity and the permeability , the
scattering of electromagnetic waves without the charges or the currents can be described by the 3D Maxwell equations in curl formulation

\[
\frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \mathbf{H},
\]

(1)

\[
\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \mathbf{E},
\]

(2)

where \( \mathbf{E} = (E_x, E_y, E_z)^T \) and \( \mathbf{H} = (H_x, H_y, H_z)^T \) represent the electric field and the magnetic field, respectively. The domain \( \Omega \times [0,T] = [0,a] \times [0,b] \times [0,c] \times [0,T] \) under consideration is occupied by this medium and surrounded by perfect conductors.

The curl equations (1) and (2) can be written as the componentwise formula

\[
\frac{\partial}{\partial t} \begin{bmatrix}
E_x \\
E_y \\
E_z \\
H_x \\
H_y \\
H_z
\end{bmatrix} =
\begin{bmatrix}
\frac{1}{\varepsilon} \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \\
\frac{1}{\varepsilon} \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \\
\frac{1}{\varepsilon} \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \\
\frac{1}{\mu} \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \\
\frac{1}{\mu} \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \\
\frac{1}{\mu} \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}
\end{bmatrix}.
\]

(3)

When the medium is lossless, then by Green’s formula it gets the following invariants:

**Energy I**: \( \int_{\Omega} \left( \varepsilon |\mathbf{E}(\mathbf{x}, t)|^2 + \mu |\mathbf{H}(\mathbf{x}, t)|^2 \right) \, d\Omega = \text{Constant} \),

**Energy II**: \( \int_{\Omega} \left( \frac{1}{\varepsilon} |\nabla \times \mathbf{E}(\mathbf{x}, t)|^2 + \frac{1}{\mu} |\nabla \times \mathbf{H}(\mathbf{x}, t)|^2 \right) \, d\Omega = \text{Constant} \).

The first invariant is called Poynting theorem in electromagnetism and it can be easily verified, and the second is a little more complex. For more details, see [2].

In the 2D transverse electric (TE) polarization case, the electric and magnetic field read \( \mathbf{E} = (E_x, E_y, 0)^T \), \( \mathbf{H} = (0, 0, H_z)^T \). Therefore, the Maxwell equations (1) and (2) become

\[
\begin{align*}
\frac{\partial E_x}{\partial t} &= \frac{1}{\varepsilon} \frac{\partial H_z}{\partial y}, \\
\frac{\partial E_y}{\partial t} &= \frac{1}{\varepsilon} \frac{\partial H_x}{\partial z}, \\
\frac{\partial H_z}{\partial t} &= \frac{1}{\mu} \frac{\partial E_y}{\partial x},
\end{align*}
\]

(4)

Let \( \mathbf{Z} = (H_x, H_y, H_z, E_x, E_y, E_z)^T \). Then the componentwise formula (3) is multi-symplectic, i.e.,

\[
\mathbf{M} \mathbf{Z}_t + \mathbf{K}_1 \mathbf{Z}_x + \mathbf{K}_2 \mathbf{Z}_y + \mathbf{K}_3 \mathbf{Z}_z = 0,
\]

(5)

where

\[
\mathbf{M} = \begin{pmatrix}
0 & -I_{3 \times 3} \\
I_{3 \times 3} & 0
\end{pmatrix}, \quad \mathbf{K}_p = \begin{pmatrix}
\varepsilon^{-1} R_p & 0 \\
0 & \mu^{-1} R_p
\end{pmatrix}, \quad \forall p = 1, 2, 3.
\]

The sub-matrix \( I_{3 \times 3} \) is a \( 3 \times 3 \) identity matrix and

\[
\begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & -1 \\
0 & 1 & 0
\end{bmatrix}, \quad \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
-1 & 0 & 0
\end{bmatrix}, \quad \begin{bmatrix}
0 & -1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}.
\]

The multi-symplectic formulation in (5) preserves the following multi-symplectic structure

\[
\frac{\partial}{\partial t} \mathbf{dZ} \wedge \mathbf{M} \mathbf{dZ} + \sum_{p=1}^3 \frac{\partial}{\partial \mathbf{x}_p} \mathbf{dZ} \wedge K_p \mathbf{dZ} = 0,
\]

(6)

where \( \mathbf{dZ} \) is the solution of the variational equation associated with (5).

Let \( \partial \] \( \int_{\Omega} \) \( \mathbf{E}(\mathbf{x}, t) \) \( \frac{\partial}{\partial t} \) \( \mathbf{H}(\mathbf{x}, t) \) \( \frac{\partial}{\partial t} \) \( \mathbf{dZ} \wedge \mathbf{M} \mathbf{dZ} + \sum_{p=1}^3 \frac{\partial}{\partial \mathbf{x}_p} \mathbf{dZ} \wedge K_p \mathbf{dZ} = 0,
\]

(7)

**Definition 1** The numerical method (7) is multi-symplectic if it preserves the discrete version of the multi-symplectic structure in (5). That is,

\[
\partial_n^{l_{i,j,k}} \left( \mathbf{dZ}_{i,j,k}^n \wedge \mathbf{M} \mathbf{dZ}_{i,j,k}^n \right) + \sum_{p=1}^3 \partial_n^{l_{i,j,k}} \left( \mathbf{dZ}_{i,j,k}^n \wedge K_p \mathbf{dZ}_{i,j,k}^n \right) = 0.
\]

(8)

From the multi-symplectic Hamiltonian formulation given by (5), of which its solution preserves the multi-symplectic structure (6). Now, we list several multi-symplectic numerical schemes applied to Maxwell equations given in this section.

- **Yee method**
  This method is the basis of the highly popular numerical methods known as the FDTD methods [2]. Yee method is constructed by central difference in both space and time based on a half-step staggered grid. It is a second-order method and is conditionally stable. Recently [10] showed that Yee method is multi-symplectic by the discrete variational principle, so we call it the multi-symplectic Yee method.

- **Multi-symplectic Runge-Kutta methods**
  Applying the symplectic Runge-Kutta methods in both time and space to Maxwell equations (5) leads to the multi-symplectic Runge-Kutta methods. [2] presented the sufficient conditions of multi-symplecticity Runge-Kutta methods for Hamiltonian PDEs.

B. Berenger’s PML system for 3D Maxwell equations

In the PML medium, each component of electromagnetic field is split into two parts. In cartesian coordinates, the six components yield 12 subcomponents denoted by \( E_{xy}, E_{xz}, E_{yz}, \)
where the parameters \((\sigma_x, \sigma_y, \sigma_z, \sigma^*_x, \sigma^*_y, \sigma^*_z)\) are homogeneous to electric and magnetic conductivities.

If \(\sigma_x = \sigma_y = \sigma_z \neq \sigma^*_x = \sigma^*_y = \sigma^*_z \neq 0\), then \((9)-(20)\) yield the classical Maxwell equations \((1)-(2)\). Thus, the absorbing medium defined by \((9)-(20)\) holds as particular cases of all usual media (vacuum, conductive media).

The 3D PML technique is a straightforward generalization of the 2D case. The Maxwell equations are solved by the FDTD method within a computational domain surrounded by an absorbing layer which is an aggregate of PML media.

### III. ONE FORMULATION EQUIVALENT TO BERENGER’S FORMULATION

Berenger’s formulation involves a splitting of the unknown electromagnetic fields. The idea of this is to restore the usual operator by introducing a new variable.

Let us consider the Berenger’s PML parrel \(xoy\)-plane, i.e., \(\sigma_x = \sigma^*_x = 0\) and \(\sigma_y = \sigma^*_y = 0\). For simplicity, we assume that \(\varepsilon = \mu = 1\) and \(\sigma_z = \sigma^*_z \equiv \sigma\), where \(\sigma\) is a constant that does not depend on \(x, y, z, t\). Then Berenger’s systems \((9)-(20)\) of the 3D Maxwell equations can be rewritten as

\[
\begin{align*}
\frac{\partial E_{xy}}{\partial t} &= \frac{\partial (H_{x} + H_{z})}{\partial y}, \\
\frac{\partial E_{xz}}{\partial t} &= \frac{\partial (H_{x} + H_{y})}{\partial z}, \\
\frac{\partial E_{yz}}{\partial t} &= -\frac{\partial (H_{y} + H_{x})}{\partial z}, \\
\frac{\partial E_{yx}}{\partial t} &= -\frac{\partial (H_{y} + H_{z})}{\partial y}, \\
\frac{\partial E_{zx}}{\partial t} &= -\frac{\partial (H_{z} + H_{x})}{\partial y}, \\
\frac{\partial E_{zy}}{\partial t} &= -\frac{\partial (H_{z} + H_{y})}{\partial y}.
\end{align*}
\]

Let \(E_{xy}, E_{xz}, E_{yz}, E_{yx}, E_{zx}, E_{zy}, H_{x}, H_{y}, H_{z}, H_{x}, H_{y}, H_{z}\) be a solution of Berenger’s system \((21)-(32)\) with initial conditions \(E^0, H^0\). Adding \((25)\) and \((26), (31)\) and \((32)\), respectively, we can obtain that

\[
\begin{align*}
\frac{\partial E_{xy}}{\partial t} &= \frac{\partial H_{x}}{\partial y} - \frac{\partial H_{z}}{\partial y}, \\
\frac{\partial E_{xz}}{\partial t} &= \frac{\partial H_{x}}{\partial z} - \frac{\partial H_{y}}{\partial z}, \\
\frac{\partial E_{yz}}{\partial t} &= \frac{\partial H_{y}}{\partial z} - \frac{\partial H_{x}}{\partial z}, \\
\frac{\partial E_{yx}}{\partial t} &= \frac{\partial H_{y}}{\partial y} - \frac{\partial H_{z}}{\partial y}, \\
\frac{\partial E_{zx}}{\partial t} &= \frac{\partial H_{z}}{\partial y} - \frac{\partial H_{x}}{\partial y}, \\
\frac{\partial E_{zy}}{\partial t} &= \frac{\partial H_{x}}{\partial y} - \frac{\partial H_{z}}{\partial y}.
\end{align*}
\]

Applying \(\partial_t + \sigma\) to \((21), \partial_{yx}\) to \((22)\), and adding the two terms give

\[
\partial_t [(\partial_t + \sigma) E_{xy} + \partial_y (\partial_t + \sigma) E_{xz}] + \partial_t H_{x} - (\partial_t + \sigma) H_{z} = 0.
\]

Since \(\sigma\) does not depend on \(y\), the operators \(\partial_t + \sigma\) and \(\partial_y\) commute, we get by setting \(E_{xy} = E_{xy} + E_{xz}\)

\[
\partial_t [(\partial_t + \sigma) E_{xy} + \partial_y H_{y}] - \partial_y [(\partial_t + \sigma) H_{z}] = 0.
\]

In order to transform the last term into a time derivative, we introduce a new variable \(\tilde{H}_{z}\) satisfying

\[
(\partial_t + \sigma) H_{z} = \tilde{H}_{z},
\]

then

\[
\partial_t [(\partial_t + \sigma) E_{xy} + \tilde{H}_{x} - \partial_y \tilde{H}_{z}] = 0.
\]

If we make the assumption that at \(t = 0\),

\[
(\partial_t E_{x} + \sigma E_{x}^0 + \partial_y H_{y}^0 - \partial_y \tilde{H}_{z}^0 = 0.
\]
it follows
\[(\partial_t + \sigma)E_x + \partial_x H_y - \partial_y H_z = 0.\] (37)

Note that (35) can not completely determine \(\tilde{H}_z\). We have to prescribe an initial value of \(\tilde{H}_z\), say
\[\tilde{H}_z^0 = H_z^0,\] (38)

which in particular implies that \(\tilde{H}_z \equiv H_z\) if \(\sigma = 0\).

A similar process, it implies
\[(\partial_t + \sigma)E_y + \partial_y H_x - \partial_x H_y = 0.\] (39)

Similarly, it follows from introducing a new variable \(\tilde{E}_z\) satisfying
\[(\partial_t + \sigma)\tilde{E}_z = \partial_t \tilde{E}_z,\] (40)

that
\[(\partial_t + \sigma)H_x - \partial_x E_z + \partial_z \tilde{E}_z = 0,\] (41)
\[(\partial_t + \sigma)H_y + \partial_y E_z - \partial_y \tilde{E}_z = 0.\] (42)

In order to make the calculations of the next sections more readable, it is useful to adopt new notations for \(E_z\) and \(\tilde{E}_z\), \(H_z\) and \(\tilde{H}_z\).

- \(E_z\) is denoted by \(E_z^x\), \(\tilde{E}_z\) is denoted by \(E_z^y\);
- \(H_z\) is denoted by \(H_z^x\), \(\tilde{H}_z\) is denoted by \(H_z^y\).

Then the un-splitting formulation (21)-(32) can be rewritten as
\[
\begin{align*}
(\partial_t + \sigma)E_z^x + \partial_x H_y - \partial_y H_z &= 0, \quad (a) \\
(\partial_t + \sigma)E_z^y + \partial_y H_x - \partial_x H_z &= 0, \quad (b) \\
\partial_t E_z^x + \partial_x H_y - \partial_y H_z &= 0, \quad (c) \\
(\partial_t + \sigma)E_z^y &= \partial_t E_z^y, \quad (d) \\
(\partial_t + \sigma)H_z^x + \partial_x E_z^y - \partial_y E_z^y &= 0, \quad (e) \\
(\partial_t + \sigma)H_z^y + \partial_y E_z^x - \partial_x E_z^x &= 0, \quad (f) \\
\partial_t H_z^x + \partial_x E_z^y - \partial_y E_z^y &= 0, \quad (g) \\
(\partial_t + \sigma)H_z^y &= \partial_t H_z^y. \quad (h)
\end{align*}
\]

\[\text{We introduce the difference operators \((k = n, or k = n + \frac{1}{2})\)}
\[
\begin{align*}
(D_{\Delta t} U)^k &= \frac{U_{k+\frac{1}{2}} - U_k - \frac{1}{2}}{\Delta t}, \quad (D_{\Delta t} U)_k &= \frac{U_{k+\frac{1}{2}} - U_k - \frac{1}{2}}{\Delta t}, \\
(D_{\Delta t} U)_{\alpha,\beta,\gamma} &= \frac{U^{\alpha+\frac{1}{2}} - U^{\alpha-\frac{1}{2}} - \sigma U^{\alpha+\frac{1}{2}} + \sigma U^{\alpha-\frac{1}{2}}}{\Delta t} \\
&= (D_{\Delta t} U)_{\alpha,\beta,\gamma}^+ + \sigma U^{\alpha,\beta,\gamma}. \quad (44)
\end{align*}
\]

With these notations, multi-symplectic Yee method for (43) is
\[
\begin{align*}
(D_{\Delta t} E_x^x)_{i+1/2,j,k} + (D_{\Delta t} H_x^x)_{i+1/2,j,k} &= (D_{\Delta t} E_x^x)_{i+1/2,j,k} + (D_{\Delta t} H_x^x)_{i+1/2,j,k}, \quad (45) \\
(D_{\Delta t} E_y^y)_{i,j+1/2,k} + (D_{\Delta t} H_y^y)_{i,j+1/2,k} &= (D_{\Delta t} E_y^y)_{i,j+1/2,k} + (D_{\Delta t} H_y^y)_{i,j+1/2,k}, \quad (46) \\
(D_{\Delta t} E_z^x)_{i,j+1/2,k+1/2} + (D_{\Delta t} H_z^x)_{i,j+1/2,k+1/2} &= (D_{\Delta t} E_z^x)_{i,j+1/2,k+1/2} + (D_{\Delta t} H_z^x)_{i,j+1/2,k+1/2}, \quad (47) \\
(D_{\Delta t} E_z^y)_{i,j+1/2,k+1/2} + (D_{\Delta t} H_z^y)_{i,j+1/2,k+1/2} &= (D_{\Delta t} E_z^y)_{i,j+1/2,k+1/2} + (D_{\Delta t} H_z^y)_{i,j+1/2,k+1/2}, \quad (48) \\
(D_{\Delta t} H_z^x)_{i,j+1/2,k+1/2} + (D_{\Delta t} E_z^x)_{i,j+1/2,k+1/2} &= (D_{\Delta t} H_z^x)_{i,j+1/2,k+1/2} + (D_{\Delta t} E_z^x)_{i,j+1/2,k+1/2}, \quad (49) \\
(D_{\Delta t} H_z^y)_{i,j+1/2,k+1/2} + (D_{\Delta t} E_z^y)_{i,j+1/2,k+1/2} &= (D_{\Delta t} H_z^y)_{i,j+1/2,k+1/2} + (D_{\Delta t} E_z^y)_{i,j+1/2,k+1/2}, \quad (50) \\
(D_{\Delta t} H_z^y)_{i,j+1/2,k+1/2} + (D_{\Delta t} E_z^x)_{i,j+1/2,k+1/2} &= (D_{\Delta t} H_z^y)_{i,j+1/2,k+1/2} + (D_{\Delta t} E_z^x)_{i,j+1/2,k+1/2}. \quad (51)
\end{align*}
\]

We define the one-dimensional (1D) discrete scalar product
\[
(U, V)_h = \sum_{\alpha} U_{\alpha} V_{\alpha}, \quad \forall (U, V) \in (l^2(\alpha))^2,
\]
where \(\alpha\) is either an integer or a half-integer. The 3D discrete scalar product will be denoted \(((U, V))_h\) (or when needed with an index \(l^2(\alpha) \times l^2(\beta) \times l^2(\gamma)\)).

Discrete integrations by parts yields
\[
\begin{align*}
(D_{\Delta t} U)_{\alpha} &= -(U, D_{\Delta t} V)_{\alpha} = -(U_{\alpha+1/2}, V), \quad \forall U \in l^2(\alpha), \quad (52) \\
(D_{\Delta t} U)_{\beta} &= -(U, D_{\Delta t} V)_{\beta} = -(U_{\beta+1/2}, V), \quad \forall U \in l^2(\beta), \quad (53) \\
(D_{\Delta t} U)_{\gamma} &= -(U, D_{\Delta t} V)_{\gamma} = -(U_{\gamma+1/2}, V), \quad \forall U \in l^2(\gamma), \quad (54)
\end{align*}
\]

Since \(\sigma\) is constant,
\[
\begin{align*}
D_{\Delta t}^2 D_{\Delta t} &= D_{\Delta t} D_{\Delta t}^2, \\
D_{\Delta t}^2 D_{\Delta x} &= D_{\Delta x} D_{\Delta t}^2, \\
D_{\Delta t} D_{\Delta y} &= D_{\Delta y} D_{\Delta t}, \\
D_{\Delta t} D_{\Delta z} &= D_{\Delta z} D_{\Delta t}. \quad (55)
\end{align*}
\]

**Theorem 1** For any integer \(n \geq 0\), let \(E_{\alpha,\beta,\gamma}^x = (E_{\alpha,\beta,\gamma}^x)^n\) and \(H_{\alpha,\beta,\gamma}^x = (H_{\alpha,\beta,\gamma}^x)^n\).
the solution of (53)-(54), then the discrete version of the energy evolution law is,
\[
e_{1+1/2}^n - e_{1-1/2}^n + 2\sigma ||D_{\Delta t}E_{\Delta t}^n||^2 + 2\sigma ||D_{\Delta t}E_{\Delta t}^{n+1/2}||^2 + \sigma (||D_{\Delta t}E_{\Delta t}^{n+1/2} - D_{\Delta t}E_{\Delta t}^{n+1/2}||^2_h)
\]
where
\[
e_{1+1/2}^n = \frac{1}{2\Delta t} \left( ||D_{\Delta t}E_{\Delta t}^{n+1/2}||^2_h + ||D_{\Delta t}E_{\Delta t}^{n+1/2} - D_{\Delta t}E_{\Delta t}^{n+1/2}||^2_h + ||\sigma E_{\Delta t}^{n+1/2} + \sigma E_{\Delta t}^{n+1/2}||^2_h \right) + \sigma (||D_{\Delta t}E_{\Delta t}^{n+1/2} - D_{\Delta t}E_{\Delta t}^{n+1/2}||^2_h)
\]

Proof 1 We divide it into seven parts

(i) By applying \(D_{\Delta t}^2\) to (43), we get
\[
(D_{\Delta t}^2 E_{\Delta t}^n) + (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) - (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) = 0.
\]
We multiply (60) with \((D_{\Delta t} E_{\Delta t}^n)\) to get
\[
((D_{\Delta t}^2 E_{\Delta t}^n) + (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) - (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n))_h = 0.
\]

(ii) By applying \(D_{\Delta t}^2\) to (46). Since \(\sigma\) is constant, we get
\[
(D_{\Delta t}^2 E_{\Delta t}^n) + (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) - (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) = 0.
\]
Multiplying (62) with \((D_{\Delta t} E_{\Delta t}^n)\) yields
\[
(((D_{\Delta t}^2 E_{\Delta t}^n) + (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) - (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n))_h = 0.
\]

(iii) After applying \(D_{\Delta t}^2\) to (47), then the equation (47) be shift to time \(n\)
\[
(D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) + (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) - (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) = 0.
\]
Using (57), (55) and (48), this is equivalent to
\[
((D_{\Delta t}^2 E_{\Delta t}^n) + (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) - (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n))_h = 0.
\]
We multiply (64) with \((D_{\Delta t} E_{\Delta t}^n)\) to get
\[
(((D_{\Delta t}^2 E_{\Delta t}^n) + (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n) - (D_{\Delta t} D_{\Delta t}^2 H_{\Delta t}^n))_h = 0.
\]

(iv) Equation (49) is written as (43), (46) and (47) not at time \(n + 1/2\) but at time \(n\). It is thus necessary to consider the mean-value of (49) at \(n\) and \(n + 1\):}
\[
(D_{\Delta t}^2 H_{\Delta t}^n + 1/2) + (D_{\Delta t}^2 E_{\Delta t}^n) + 1/2 - (D_{\Delta t}^2 E_{\Delta t}^n + 1/2) = 0.
\]
We apply \(D_{\Delta t}\) to this equation and multiply it by \((D_{\Delta t}^2 H_{\Delta t}^n)\) to get
\[
(((D_{\Delta t}^2 H_{\Delta t}^n) + 1/2 + (D_{\Delta t} D_{\Delta t}^2 E_{\Delta t}^n + 1/2) - (D_{\Delta t} D_{\Delta t}^2 E_{\Delta t}^n + 1/2), (D_{\Delta t}^2 H_{\Delta t}^n))_h = 0.
\]
Concerning the second term, we first develop
\[
((D_M^2)^2 E_x)^n = (D_M^2(D_M E_x))^n + \sigma(D_M^2 E_x) \\
= (D_M^2 E_x)^n + 2\sigma(D_M E_x)^n + \sigma^2 \frac{E_x^{n+1/2} + E_x^{n-1/2}}{2}.
\]
We multiply this expression by \((D_M E_x)^n\), and rearrange the last term
\[
\sigma^2 \left( \frac{E_x^{n+1/2} + E_x^{n-1/2}}{2} (D_M E_x)^n \right) = \frac{\sigma^2}{2\Delta} \left( \frac{E_x^{n+1/2}}{2} - \frac{E_x^{n-1/2}}{2} \right)^2.
\]
and get
\[
S^2 = \frac{1}{2\Delta} \left( \frac{E_x^{n+1/2}}{2} - \frac{E_x^{n-1/2}}{2} \right)^2 - \sigma^2 \left( \frac{E_x^{n+1/2}}{2} - \frac{E_x^{n-1/2}}{2} \right)^2 + 2\sigma \left( \frac{E_x^{n+1/2}}{2} - \frac{E_x^{n-1/2}}{2} \right)^2.
\]
The same as \(S^3\), we can get
\[
S^3 = \frac{1}{2\Delta} \left( \frac{E_x^{n+1/2}}{2} - \frac{E_x^{n-1/2}}{2} \right)^2 - \sigma^2 \left( \frac{E_x^{n+1/2}}{2} - \frac{E_x^{n-1/2}}{2} \right)^2 + 2\sigma \left( \frac{E_x^{n+1/2}}{2} - \frac{E_x^{n-1/2}}{2} \right)^2.
\]
Due to \(S^1 + S^2 + S^3 + S^4 + S^5 + S^6 = 0\), then we can obtain the energy evolution law \((59)\). The proof is finished.

2) General multi-symplectic Runge-Kutta methods.

The Runge-Kutta methods for Maxwell equations \((5)\) are
\[
Z_{i,j,k,n} = \hat{Z}_{i,j,k} + \Delta \sum_{s=1}^{r} \partial_n \partial Z_{i,j,k,s},
\]
\[
\hat{Z}_{i,j,k} = \hat{Z}_{i,j,k} + \Delta \sum_{s=1}^{r} \partial_t \partial Z_{i,j,k,s},
\]
\[
Z_{i,j,k,n} = \hat{Z}_{i,j,k} + \Delta \sum_{s=1}^{r} \partial_n \partial Z_{i,j,k,n},
\]
\[
\hat{Z}_{i,j,k} = \hat{Z}_{i,j,k} + \Delta \sum_{s=1}^{r} \partial_t \partial Z_{i,j,k,n},
\]
\[
Z_{i,j,k,n} = \hat{Z}_{i,j,k} + \Delta \sum_{s=1}^{r} \partial_n \partial Z_{i,j,k,n},
\]
\[
\hat{Z}_{i,j,k} = \hat{Z}_{i,j,k} + \Delta \sum_{s=1}^{r} \partial_t \partial Z_{i,j,k,n},
\]
\[
Z_{i,j,k,n} = \hat{Z}_{i,j,k} + \Delta z \sum_{s=1}^{r} \partial_n \partial Z_{i,j,k,n},
\]
\[
\hat{Z}_{i,j,k} = \hat{Z}_{i,j,k} + \Delta z \sum_{s=1}^{r} \partial_t \partial Z_{i,j,k,n},
\]
\[
Z_{i,j,k,n} = \hat{Z}_{i,j,k} + \Delta z \sum_{s=1}^{r} \partial_n \partial Z_{i,j,k,n},
\]
\[
\hat{Z}_{i,j,k} = \hat{Z}_{i,j,k} + \Delta z \sum_{s=1}^{r} \partial_t \partial Z_{i,j,k,n},
\]

Theorem 2 (Hong et al. 2005) If in the methods \((73)-(82)\)
\[
b_j b_n - b_j a_n - b_n a_j = 0,
\]
\[
\hat{b}_j b_n - \hat{b}_n a_j - \hat{b}_n a_j = 0,
\]
\[
\tilde{b}_j b_n - \tilde{b}_n a_j - \tilde{b}_n a_j = 0.
\]

and
\[
\hat{b}_n \hat{b}_n - \hat{b}_n \tilde{a}_w - \hat{b}_w \tilde{a}_w = 0, \quad (86)
\]
hold for \(s, n = 1, 2, ..., r, u, i = 1, 2, ..., r_1, v, j = 1, 2, ..., r_2\)
and \(w, k = 1, 2, ..., r_3\), then the method \((73)-(82)\) is multi-symplectic.

Let \(U = (E_x, E_y, E_z, E_{xy}, E_{xz}, E_{yx}, H_x, H_y, H_z, H_{xy}, H_{xz}, H_{yx}, H_{xz})^T\),
then the 3D Maxwell equations with PML \((21)-(32)\) can be rewritten as
\[
\partial_t U + \Sigma U = P(\nabla)U, \quad (87)
\]
with
\[
\Sigma = \begin{pmatrix} A_{6 \times 6} & 0 \\ 0 & A_{6 \times 6} \end{pmatrix}, \quad P(\nabla) = \begin{pmatrix} 0 & B_{6 \times 6} \\ -B_{6 \times 6} & 0 \end{pmatrix},
\]
where
\[
B_{6 \times 6} = \begin{pmatrix} \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} \end{pmatrix}.
\]

Based on theorem \((2)\), we apply an \(s\)-stage symplectic Runge-Kutta method to the \(t\)-direction, of form \((87)\), to obtain the following scheme,
\[
U^n = u^0 + \Delta \sum_{m=1}^{s} a_{nm} (\Sigma U^n + P(\nabla)U^n), \quad (88)
\]
\[
u^1 = u^0 + \Delta \sum_{m=1}^{s} b_{m} (\Sigma U^n + P(\nabla)U^n), \quad (89)
\]
where the coefficients of the equations \((88)-(89)\) satisfy the following symplectic condition:
\[
b_m a_{nm} + b_n a_{nm} = b_m b_n, \quad m, n = 1, 2, ..., s. \quad (90)
\]

Now, we introduce the following difference operators and apply Yee method to the \(x\)-direction, \(y\)-direction and \(z\)-direction respectively, of form \((88)-(89)\),
\[
\delta_x V_{i,j,k}^n = \frac{V_{i-1/2,j,k}^n - V_{i+1/2,j,k}^n}{\Delta z},
\]
\[
\delta_y V_{i,j,k}^n = \frac{V_{i,j+1/2,k}^n - V_{i,j-1/2,k}^n}{\Delta y},
\]
\[
\delta_z V_{i,j,k}^n = \frac{V_{i,j,k+1/2}^n - V_{i,j,k-1/2}^n}{\Delta z}.
\]
Then, we obtain that,

\[ U_{i,j,k}^n = u_{i,j,k}^0 + \Delta t \sum_{m=1}^{s} a_{nm} \left( - \Sigma U_{i,j,k}^m + \hat{P}(\nabla) \nabla U_{i,j,k}^m \right), \]  

(91)

\[ u_{i,j,k}^0 = u_{i,j,k}^0 + \Delta t \sum_{m=1}^{s} b_{mn} \left( - \Sigma U_{i,j,k}^m + \hat{P}(\nabla) U_{i,j,k}^m \right), \]  

(92)

with

\[
\hat{P}(\nabla) = \begin{pmatrix}
\delta z & -\delta z & \delta y & \delta y \\
\delta z & -\delta z & -\delta x & -\delta x \\
\delta y & -\delta y & \delta x & \delta x \\
\end{pmatrix}.
\]

**Theorem 3** For and integer \( n \geq 0 \), set \( E_{i,j,k}^n = (E_{i,j,k}^n, E_{j,i,k}^n, E_{k,i,j}^n) \) and \( H_{i,j,k}^n = (H_{i,j,k}^n, H_{j,i,k}^n, H_{k,i,j}^n) \) be the solution of the discrete scheme (91)–(92), then the discrete version of the energy law is,

\[
\|E_{i,j,k}^{n+1}\|^2_h + \|H_{i,j,k}^{n+1}\|^2_h = \|E_{i,j,k}^n\|^2_h + \|H_{i,j,k}^n\|^2_h - 2\Delta t \sum_{m=1}^{s} b_{mn} \left( E_{i,j,k}^m \right)^2 + \left( H_{i,j,k}^m \right)^2,
\]

(93)

where

\[
\|E_{i,j,k}^n\|^2_h = h_i h_j h_k \sum_{l=1}^{s} \sum_{r=0}^{s} \left( (E_{i,j,k}^n)^2 + (E_{j,i,k}^n)^2 + (E_{k,i,j}^n)^2 \right),
\]

\[
\|H_{i,j,k}^n\|^2_h = h_i h_j h_k \sum_{l=1}^{s} \sum_{r=0}^{s} \left( H_{i,j,k}^n \right)^2 + \left( H_{j,i,k}^n \right)^2 + \left( H_{k,i,j}^n \right)^2.
\]

**Proof 2** For simplicity, we introduce the following notation

\[ f_{i,j,k}^m = -\Sigma U_{i,j,k}^m + \hat{P}(\nabla) U_{i,j,k}^m. \]

(94)

From the discrete scheme (92), we can get the following relation between \( u_{i,j,k}^1 \) and \( u_{i,j,k}^0 \):

\[
(u_{i,j,k}^1)^T u_{i,j,k}^1 = (u_{i,j,k}^0)^T u_{i,j,k}^0 + \Delta t \sum_{m=1}^{s} b_{mn} f_{i,j,k}^m (u_{i,j,k}^0)^T U_{i,j,k}^m + \Delta t \sum_{m=1}^{s} b_{mn} f_{i,j,k}^m (u_{i,j,k}^1)^T U_{i,j,k}^m
\]

\[
= ((u_{i,j,k}^0)^T U_{i,j,k}^0 + \Delta t \sum_{m=1}^{s} b_{mn} f_{i,j,k}^m (u_{i,j,k}^0)^T U_{i,j,k}^m + \Delta t \sum_{m=1}^{s} b_{mn} f_{i,j,k}^m (u_{i,j,k}^1)^T U_{i,j,k}^m)
\]

Note that the discrete scheme (91) and the notation (94), it can be rewritten as

\[ u_{i,j,k}^0 = U_{i,j,k}^n - \Delta t \sum_{m=1}^{s} a_{nm} f_{i,j,k}^m. \]

(95)

Then, we insert the relation between \( u_{i,j,k}^1 \) and \( u_{i,j,k}^0 \) into (95), we obtain that

\[
(u_{i,j,k}^1)^T u_{i,j,k}^1 = (u_{i,j,k}^0)^T U_{i,j,k}^n + \Delta t \sum_{m=1}^{s} b_{mn} ((U_{i,j,k}^n)^T f_{i,j,k}^m + (f_{i,j,k}^m)^T U_{i,j,k}^n) + (\Delta t)^2 \sum_{m,n=1}^{s} b_{mn} b_{mn} a_{nm} - b_{mn} a_{nm}) (f_{i,j,k}^m)^T f_{i,j,k}^m.
\]

(96)

Due to the symplectic condition (90), we have

\[
(u_{i,j,k}^1)^T u_{i,j,k}^1 = (u_{i,j,k}^0)^T U_{i,j,k}^n + \Delta t \sum_{m=1}^{s} b_{mn} ((U_{i,j,k}^n)^T f_{i,j,k}^m + (f_{i,j,k}^m)^T U_{i,j,k}^n)
\]

(97)

Since the Maxwell equations energy conserving law in lossless medium, we obtain

\[
(U_{i,j,k}^n)^T (\hat{P}(\nabla) U_{i,j,k}^n) = 0.
\]

Therefore, (92) becomes the following form

\[
(u_{i,j,k}^1)^T u_{i,j,k}^1 = (u_{i,j,k}^0)^T U_{i,j,k}^n - 2\Delta t \sum_{m=1}^{s} b_{mn} ((U_{i,j,k}^n)^2 + (H_{i,j,k}^n)^2).
\]

(98)

From the presentation of \( \Sigma \) and \( U \), we have

\[
(u_{i,j,k}^1)^T u_{i,j,k}^1 = (u_{i,j,k}^0)^T U_{i,j,k}^n - 2\Delta t \sum_{m=1}^{s} b_{mn} ((E_{i,j,k}^n)^2 + (H_{i,j,k}^n)^2).
\]

(99)

Summing all terms in the above equation (99) over all spatial indices \( i, j, k \), then we can get the energy evolution law (93). The proof is finished.
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