Numerical dispersion analysis of a multi-symplectic scheme for the three dimensional Maxwell’s equations

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ABSTRACT

In this paper, we study a multi-symplectic scheme for three dimensional Maxwell’s equations in a simple medium. This is a system of PDEs with multi-symplectic structures. We prove that this multi-symplectic scheme preserves the discrete version of local and global energy conservation law and the discrete divergence. Furthermore, we extend the discussion to several dispersion properties of the multi-symplectic scheme including the numerical dispersion relation, the numerical group velocity, the effect of large time steps and the CFL condition.

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1. Introduction

Maxwell’s equations are very important in the electromagnetic world and are widely applied to many application fields. They are mathematical expressions of the natural laws correlative fields, such as Ampère’s law and Faraday’s law, etc. Recently, it is of special importance to develop efficient numerical methods for effective and accurately simulating Maxwell’s equations in large scale and long time computations. The famous time-domain technique in computational electromagnetic (CEM) was developed by Yee [1]. The method, generally referred as the finite-difference time-domain method (FDTD), is based on the staggered central difference in space and staggered leapfrog integration in time for Cartesian coordinates. Yee’s method is an explicit second-order method. It is considered that the CFL condition reveals the stability of numerical methods, and to reach a precise solution is guaranteed by a numerical method with high accuracy. In most cases, Yee’s scheme gives a very accurate numerical solutions though it is restricted by the CFL condition.

Symplectic integrators, which preserve the symplectic property of the original differential equations, have received much attention over the last two decades [2–4]. The source-less Maxwell’s equations with constant scalar parameters have the symplectic property [5]. Thus, based on the method of line for Hamiltonian partial differential equations (PDEs) [6], they can be integrated by the symplectic algorithms. As is expected, the symplectic algorithms for the Maxwell’s equations are much superior to standard methods in the performance of numerical stability and long-time computing [7,8]. The concept of multi-symplectic schemes for multi-symplectic PDEs, which can be viewed as the extension of symplectic schemes for Hamiltonian ODEs to Hamiltonian PDEs, was proposed by Bridges and Reich [9] and Marsden et al. [10] respectively. Now, the multi-symplectic schemes have been applied to lots of important equations such as nonlinear wave equation, the nonlinear Schrödinger equation, the Korteweg-de Vries equation, the Zakharov-Kuznetsov equation, etc. (Please see the review paper [11,12] and references therein.) The Maxwell’s equations also have the multi-symplectic structure [13–15] and two multi-symplectic schemes for two-dimensional Maxwell’s equations were proposed and experimented
respectively in Refs. [14,15]. The corresponding theoretical analysis of the two above schemes, as well as some comparative schemes are carried in Refs. [16,17], where we can see some impressive merits of the multi-symplectic schemes for the two dimensional Maxwell’s equations. Another positive news for the multi-symplectic schemes is that the famous Yee’s scheme for the Maxwell’s equations is multi-symplectic [18] which gives a new explanation for many of its previously observed notable numerical qualities. However, there is no numerical experiments reported of the multi-symplectic schemes for the three dimensional Maxwell’s equations due to the limitation of memory and the performance of CPU, because it is required to solve at least one $10^6$ scale algebraic equations at every time step provided that the considered spatial domain is divided into $100 \times 100 \times 100$ cells. To save the computing memory, Kong [19] developed the splitting technology, which can use the multi-symplectic schemes for one dimensional equations to simulate three dimensional Maxwell’s equations. Such technology has also been applied to the nonlinear Schrödinger equation [20].

In this paper, we study a multi-symplectic scheme for the three dimensional Maxwell’s equations. From the aspect of the numerical dispersion, we show that the multi-symplectic scheme has some nice properties. The outline of this paper is organized as follows. In Section 2, the multi-symplectic formulation of Maxwell’s equations is introduced and a multi-symplectic scheme as well as its discrete multi-symplectic conservation law are proposed in Section 3. In Section 4, the discrete version of energy conservation law and the discrete property of divergence-free are proved. In Section 5, the dispersion relation of the scheme and some comparisons with Yee’s method are given. Non-dissipation property of the multi-symplectic scheme is proved. In Section 6, some analyses based on the dispersion relation are presented. Finally, we draw some conclusions in Section 7.

2. Multi-symplectic formulation for Maxwell’s equations

The Maxwell’s equations in an isotropic, homogeneous, non-dispersive medium are

\[
\begin{align*}
\frac{\partial \mathbf{E}}{\partial t} + \nabla \times \mathbf{H} &= 0 \quad \text{(Faraday's Law),} \\
\frac{\partial \mathbf{B}}{\partial t} - \nabla \times \mathbf{E} &= 0 \quad \text{(Ampere's Law),} \\
\mathbf{B} &= \mu \mathbf{H}, \\
\mathbf{D} &= \varepsilon \mathbf{E}.
\end{align*}
\tag{2.1}
\]

In the absence of impressed electric charge, the magnetic induction and electric displacement fields satisfy the constraints (Gauss’s Law)

\[
\begin{align*}
\nabla \cdot \mathbf{B} &= 0, \\
\nabla \cdot \mathbf{D} &= 0.
\end{align*}
\tag{2.2}
\]

Scattering obstacles will be modeled by a spatial variation of $\varepsilon$ and $\mu$. In free space, $\varepsilon$ and $\mu$ are two constants, $\varepsilon_0, \mu_0$. The speed of light in free space is $c = 1/\sqrt{\varepsilon_0 \mu_0}$.

Introduce two vector functions $\mathbf{U}$ and $\mathbf{V}$ satisfying $\mathbf{U}_t = \mathbf{E}$ and $\mathbf{V}_t = \mathbf{H}$, respectively, then the Lagrangian density for Eq. (2.1) can be written as

\[
\mathcal{L} = \frac{1}{2} \mu \langle \mathbf{V}_t, \mathbf{V}_t \rangle + \frac{1}{2} \langle \nabla \times \mathbf{V}, \nabla \times \mathbf{U} \rangle + \frac{1}{2} \varepsilon \langle \mathbf{U}_t, \mathbf{U}_t \rangle - \frac{1}{2} \langle \mathbf{U}_t, \nabla \times \mathbf{V} \rangle,
\tag{2.3}
\]

where $\langle \cdot, \cdot \rangle$ represents the standard inner production of vector space. The generalized conjugate momenta can be derived by covariant Legendre transform correspondingly,

\[
\begin{align*}
P &= \frac{\partial \mathcal{L}}{\partial \mathbf{V}_t} = \mu \mathbf{V}_t + \frac{1}{2} \nabla \times \mathbf{U}, \\
Q &= \frac{\partial \mathcal{L}}{\partial \mathbf{U}_t} = \varepsilon \mathbf{U}_t - \frac{1}{2} \nabla \times \mathbf{V},
\end{align*}
\tag{2.4}
\]

further the covariant Hamiltonian by

\[
\mathcal{S} = \langle P, V_t \rangle + \langle Q, U_t \rangle + \langle \frac{\partial \mathcal{L}}{\partial \nabla \times \mathbf{V}}, \nabla \times \mathbf{V} \rangle + \langle \frac{\partial \mathcal{L}}{\partial \nabla \times \mathbf{U}}, \nabla \times \mathbf{U} \rangle - \mathcal{L} = \langle P, H \rangle + \langle Q, E \rangle - \frac{1}{2} \mu \langle H, H \rangle - \frac{1}{2} \varepsilon \langle E, E \rangle.
\tag{2.5}
\]

Set $Z = [\mathbf{H}, \mathbf{E}, \mathbf{V}, \mathbf{U}, \mathbf{P}, \mathbf{Q}]^T$, then Eq. (2.1) is transformed into the following form:

\[
\begin{align*}
-\frac{1}{2} \nabla \times \mathbf{E} &= \mathbf{P} - \mu \mathbf{H}, \\
-\frac{1}{2} \nabla \times \mathbf{H} &= \mathbf{Q} - \varepsilon \mathbf{E}, \\
\mathbf{P}_t - \frac{1}{2} \nabla \times \mathbf{E} &= 0, \\
\mathbf{Q}_t + \frac{1}{2} \nabla \times \mathbf{H} &= 0, \\
\mathbf{V}_t &= \mathbf{H}, \\
\mathbf{U}_t &= \mathbf{E}.
\end{align*}
\]
The above equations can be organized into Bridges’ multi-symplectic form as

\[ MZ_t + N\nabla \times Z = \nabla_2 S(Z), \]  

(2.6)

where

\[
M = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 1/2 R_1 & 0 & 0 \\
0 & 0 & 0 & -1/2 R_1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1/2 R_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
\]

where

\[
F = \begin{pmatrix}
0 & 0 & 0 & 1/2 R_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1/2 R_2 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1/2 R_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
\]

and

\[
L = \begin{pmatrix}
0 & 0 & 0 & 0 & 1/2 R_3 & 0 & 0 & 0 \\
0 & 0 & 0 & -1/2 R_3 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1/2 R_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
\]

\[
W = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

Thus, we easily find that matrices \( M, F, L, \) and \( W \) (\( \in \mathbb{R}^{18 \times 18} \)) are skew symmetric. Additionally, the rotation operator may be simplified as \( \nabla \times = R_1 \frac{\partial}{\partial x} + R_2 \frac{\partial}{\partial y} + R_3 \frac{\partial}{\partial z} \).

The representation Eq. (2.6) is a simplified expression in vector form. In three dimensions, Eq. (2.6) can be written as follows:

\[ MZ_t + NZ_x + LZ_y + WZ_z = \nabla_2 S(Z). \]  

(2.9)

Since matrices \( M, F, L, \) and \( W \) are skew symmetric and \( S : \mathbb{R}^n \rightarrow \mathbb{R} \) is a smooth function of the state variable \( Z(x, y, t) \), it can be shown that the multi-symplectic PDEs (2.9) satisfy the following multi-symplectic conservation law according to Bridges’ theory:

\[
\frac{\partial \omega}{\partial t} + \frac{\partial \phi}{\partial x} + \frac{\partial \psi}{\partial y} + \frac{\partial \phi}{\partial z} = 0,
\]  

(2.10)

where
We can not explain theoretically the benefit of the multi-symplectic formulation (2.6). But we can show the benefit from the numerical experiments. Applying the multi-symplectic Preissmann scheme to the multi-symplectic formulation (2.9) leads to multi-symplectic integrators which have good numerical behavior for 1 + 1 dimensional problem [13] and 2 + 1 dimensional problem [15]. Applying the multi-symplectic Euler-box scheme to (2.9) leads to a multi-symplectic integrator which also gives very accurate numerical solutions for 2 + 1 dimensional problem [14]. So we believe that the multi-symplectic formulation (2.9) indeed gives us much benefit. In the following discussion, we will apply the multi-symplectic Euler-box scheme to the multi-symplectic formulation (2.9) for the three dimensional problem and investigate whether the corresponding scheme still has some nice properties.

3. Multi-symplectic Euler-box scheme for the three dimensional Maxwell’s equations

Since Eq. (2.9) preserves the multi-symplectic conservation law, naturally, when discretizing Hamiltonian PDEs (2.9) by a numerical scheme, we also expect that the multi-symplectic conservation law (2.10) should be preserved. Bridges and Reich defined a numerical scheme as a multi-symplectic scheme if the scheme preserved a discrete multi-symplectic conservation law.

In the conventional schemes, the Preissmann scheme [9] and the Euler-box scheme [21] for the PDEs (2.9) are shown to be multi-symplectic. The multi-symplectic Preissmann scheme has been applied to many classical equations in the last few years [22–28], and the multi-symplectic Euler-box scheme for two dimensional Maxwell’s equations was investigated in Ref. [14] and Ref. [17]. Here we investigate the multi-symplectic Euler-box scheme for the three dimensional Maxwell’s equations.

Set $t_n, n = 1, 2, \ldots, i = 1, 2, \ldots, M, j = 1, 2, \ldots, N, k = 1, 2, \ldots, L$ be the regular grids of the integral domain, $Z_{ijk}$ is an approximation to $Z(x_i, y_j, z_k, t_n)$, $\Delta t = t_{n+1} - t_n$ is the time step, $\Delta x = x_{i+1} - x_i$ is the $x$-direction step, $\Delta y = y_{j+1} - y_j$ is the $y$-direction step and $\Delta z = z_{k+1} - z_k$ is the $z$-direction step.

We take the following splitting for the matrix $M, F, L$ and $W$ in the multi-symplectic PDEs (2.9):

$$M = M_+ + M_-, \quad F = F_+ + F_-, \quad L = L_+ + L_-, \quad W = W_+ + W_-,$$

where $M_+ = M_-, F_+ = -F_-, L_+ = -L_-$ and $W_+ = -W_-$, then rewrite the PDEs as

$$M_+ Z_1 + M_ Z_1 + F_+ Z_x + F_ Z_x + L_+ Z_y + L_ Z_y + W_+ Z_z + W_ Z_z = \nabla S(Z).$$

Consider the following so-called Euler box scheme for the above PDEs (2.9):

$$M_+ \delta_x^1 Z_{1ijk} + M_- \delta_x Z_{1ijk} + F_+ \delta_x^1 Z_{1ijk} + F_- \delta_x Z_{1ijk} + L_+ \delta_y^1 Z_{1ijk} + L_- \delta_y Z_{1ijk} + W_+ \delta_z^1 Z_{1ijk} + W_- \delta_z Z_{1ijk} = \nabla S(Z_{1ijk}),$$

where

$$\delta_x^1 Z_{1ijk} = \pm \frac{Z_{1ijk+1} - Z_{1ijk}}{\Delta t}, \quad \delta_x Z_{1ijk} = \pm \frac{Z_{1ijk} - Z_{1ijk-1}}{\Delta x},$$

$$\delta_y^1 Z_{1ijk} = \pm \frac{Z_{1ijk+1} - Z_{1ijk}}{\Delta t}, \quad \delta_y Z_{1ijk} = \pm \frac{Z_{1ijk} - Z_{1ijk-1}}{\Delta x},$$

with the special matrices splitting as

$$M_+ = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -I & 0 & 0 \\ 0 & 0 & 0 & 0 & -I & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad F_+ = \begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} R_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} R_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$L_+ = \begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} R_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad W_+ = \begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} R_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$
Theorem 3.1. The Euler box scheme (3.1) is multi-symplectic with the following discrete multi-symplectic conservation law:

$$\delta_t \omega^m_{ij,k} + \delta_x \psi^m_{ij,k} + \delta_y \phi^m_{ij,k} + \delta_z \phi^m_{ij,k} = 0,$$

(3.2)

where

$$\omega^m_{ij,k} = dZ_{ij,k}^{n+1} \wedge M, \quad \omega^m_{ij,k} = dZ_{ij,k}^{n+1} \wedge F, \quad \phi^m_{ij,k} = dZ_{ij,k}^{n+1} \wedge W.$$ 

The proof is similar to that of Theorem 3.1 in [14], where the discrete multi-symplectic conservation law in the two-dimensional form can be easily extended to the three-dimensional form.

We can eliminate the auxiliary variables $V, U, P$ and $Q$, the procedure is trivial but rather tedious, so we omit it here and give the final multi-symplectic scheme directly as follows:

$$
\begin{align*}
2\mu \delta_t H^m_{x_{ij,k}} &= \delta_x^2 E^m_{y_{ij,k}} + \delta_y^2 E^m_{z_{ij,k}} - \delta_z^2 E^m_{x_{ij,k}}, \\
2\mu \delta_t H^m_{y_{ij,k}} &= \delta_y^2 E^m_{x_{ij,k}} + \delta_x^2 E^m_{z_{ij,k}} - \delta_z^2 E^m_{y_{ij,k}}, \\
2\mu \delta_t H^m_{z_{ij,k}} &= \delta_z^2 E^m_{x_{ij,k}} + \delta_x^2 E^m_{y_{ij,k}} - \delta_y^2 E^m_{z_{ij,k}}, \\
-2\mu \delta_t E^m_{x_{ij,k}} &= \delta_x H^m_{y_{ij,k}} + \delta_y H^m_{z_{ij,k}} - \delta_z H^m_{x_{ij,k}}, \\
-2\mu \delta_t E^m_{y_{ij,k}} &= \delta_y H^m_{x_{ij,k}} + \delta_x H^m_{z_{ij,k}} - \delta_z H^m_{y_{ij,k}}, \\
-2\mu \delta_t E^m_{z_{ij,k}} &= \delta_z H^m_{x_{ij,k}} + \delta_x H^m_{y_{ij,k}} - \delta_y H^m_{z_{ij,k}},
\end{align*}

(3.3)

This is an implicit scheme that involves solving a linear system of $H^m_{x_{ij,k}}, H^m_{y_{ij,k}}, H^m_{z_{ij,k}}, E^m_{x_{ij,k}}, E^m_{y_{ij,k}}, E^m_{z_{ij,k}}$ at each time step. Suppose the computational space domain is $[0, T_x] \times [0, T_y] \times [0, T_z]$, $T_x$ is period of $x$ direction, $T_y$ is period of $y$ direction and $T_z$ is period of $z$ direction. $[0, T_x]$ is averagely divided by $M$, $[0, T_y]$ is averagely divided by $N$ and $[0, T_z]$ is averagely divided by $L$. We take numerical periodic boundary conditions as

$$
\begin{align*}
H_{m_{ij,0}} &= H_{m_{ij,k}}, \\
H_{y_{ij,0}} &= H_{y_{ij,k}}, \\
H_{z_{ij,0}} &= H_{z_{ij,k}},
\end{align*}

(3.4)

and same periodic boundary conditions are taken for $E^m_{x_{ij,k}}, E^m_{y_{ij,k}}, E^m_{z_{ij,k}}$.

We arrange variables in the order of equations in scheme (3.3).

$$x^n = [x^n_1, x^n_2, x^n_3, x^n_4, x^n_5, x^n_6]^T,$$

$$x^n_1 = [H^n_{x_{1,1}}, H^n_{x_{1,2}}, \ldots, H^n_{x_{1,M}}, H^n_{x_{2,1}}, H^n_{x_{2,2}}, \ldots, H^n_{x_{2,M}}, H^n_{x_{3,1}}, H^n_{x_{3,2}}, \ldots, H^n_{x_{3,M}}, H^n_{x_{4,1}}, H^n_{x_{4,2}}, \ldots, H^n_{x_{4,M}}, H^n_{x_{5,1}}, H^n_{x_{5,2}}, \ldots, H^n_{x_{5,M}}]^T,$$

and $x^n_2, x^n_3, x^n_4, x^n_5, x^n_6$ are vectors of $H^n_{y}, H^n_{z}, E^n_{x}, E^n_{y}, E^n_{z}$ respectively which are defined similarly to $x^n_1$. Then the resulting linear system for (3.3) is

$$M_1(\Delta t, \Delta x, \Delta y, \Delta z)x^{n+1} = M_2(\Delta t, \Delta x, \Delta y, \Delta z)x^n,$$

(3.5)

where

$$M_1(\Delta t, \Delta x, \Delta y, \Delta z) = \begin{pmatrix}
E & 0 & 0 & 0 & -C & B \\
0 & E & 0 & C & 0 & -A \\
0 & 0 & E & -B & A & 0 \\
0 & C^T & -B^T & F & 0 & 0 \\
-C^T & 0 & A^T & 0 & F & 0 \\
B^T & -A^T & 0 & 0 & 0 & F
\end{pmatrix}.$$
Obviously $M_1(\Delta t, \Delta x, \Delta y, \Delta z)$ is symmetric. Moreover the coefficient matrix $M_1(\Delta t, \Delta x, \Delta y, \Delta z)$ is a strictly diagonally dominant matrix, if $\Delta t$, $\Delta x$, $\Delta y$ and $\Delta z$ satisfy the following conditions:

\[
\begin{align*}
\frac{\Delta t}{\Delta x} + \frac{\Delta t}{\Delta y} &< \mu, \quad \frac{\Delta t}{\Delta x} + \frac{\Delta t}{\Delta z} < \mu, \quad \frac{\Delta t}{\Delta y} + \frac{\Delta t}{\Delta z} < \mu, \\
\frac{\Delta t}{\Delta y} + \frac{\Delta t}{\Delta z} &< \epsilon, \quad \frac{\Delta t}{\Delta x} + \frac{\Delta t}{\Delta z} < \epsilon, \quad \frac{\Delta t}{\Delta y} + \frac{\Delta t}{\Delta z} < \epsilon,
\end{align*}
\]

which lead to

\[
\Delta t < \min \left\{ \frac{1}{2} \mu \min(\Delta x, \Delta y, \Delta z), \frac{1}{2} \epsilon \min(\Delta x, \Delta y, \Delta z) \right\}.
\]
Thus, we can use various efficient iterative methods such as Jacobi method, Gauss–Seidel method and GMRES method to solve the system (3.5) which will be discussed in our future work.

**Remark 3.1.** Maxwell’s equations in (2.1) have another natural multi-symplectic formulation [16,19] which require no extra variables,

\[
MZ_t + K_1 Z_x + K_2 Z_y + K_3 Z_z = \nabla S(Z),
\]

where \( Z = (H_x, H_y, H_z, E_x, E_y, E_z)^T \) and \( M, K_1, K_2, K_3 \) are skew-symmetric matrices given by

\[
M = \begin{pmatrix}
0 & -I_{3 \times 3} & 0 \\
I_{3 \times 3} & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad K_i = \begin{pmatrix}
\varepsilon^{-1} R_i & 0 \\
0 & \mu^{-1} R_i
\end{pmatrix}, \quad \forall i = 1, 2, 3.
\]

The sub-matrix \( I_{3 \times 3} \) is a \( 3 \times 3 \) identity matrix and \( R_1, R_2, R_3 \) are the same as (2.8).

We can also consider the multi-symplectic Euler-box scheme for this multi-symplectic formulation (3.8)

\[
M, Z_t + M, Z_x + K_1, Z_x + K_2, Z_y + K_3, Z_z = \nabla S(Z),
\]

with the matrices splitting as

\[
M_+ = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0
\end{pmatrix}, \quad K_{1+} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
\]

\[
K_{2+} = \begin{pmatrix}
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \quad K_{3+} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
\]

and \( M_-, K_{1-}, K_{2-}, K_{3-} \) are defined similarly as above. Substituting the matrices into (3.9), we get another multi-symplectic Euler-box scheme for the three dimensional Maxwell’s equations,

\[
\begin{align*}
\mu \partial_t H^n_{ij,k} &= \partial_x E^n_{y_{ij,k}} - \partial_y E^n_{z_{ij,k}}, \\
\mu \partial_t^2 H^n_{y_{ij,k}} &= \partial_y E^n_{ij,k} - \partial_z E^n_{z_{ij,k}}, \\
\mu \partial_t^2 H^n_{z_{ij,k}} &= \partial_y E^n_{ij,k} - \partial_z E^n_{ij,k}, \\
-\varepsilon \partial_t^2 E^n_{ij,k} &= \partial_x H^n_{y_{ij,k}} - \partial_y H^n_{z_{ij,k}}, \\
-\varepsilon \partial_t^2 E^n_{y_{ij,k}} &= \partial_x H^n_{ij,k} - \partial_j H^n_{z_{ij,k}}, \\
-\varepsilon \partial_t^2 E^n_{z_{ij,k}} &= \partial_y H^n_{ij,k} - \partial_z H^n_{y_{ij,k}}.
\end{align*}
\]

Note that the multi-symplectic scheme (3.10) is different from (3.3), i.e., applying the multi-symplectic Euler-box scheme to two different multi-symplectic formulations for the Maxwell’s equations results in two different multi-symplectic schemes. It is obvious that formulation (3.8) is more natural and the resulting discretization (3.10) based on (3.8) is more simple than (3.3). But the numerical experiences show that the discretizations according to the formulation (2.6) perform very well for the two dimensional problem [14,15,17]. Thus we believe that the multi-symplectic discretization (3.3) can also simulate the three dimensional problem well. That is why we focus on the scheme (3.3) in this paper. Further comparing the two multi-symplectic formulations for the three dimensional Maxwell’s equations is worthy to be investigated.

4. **Discrete energy conservation law and divergence preservation**

4.1. **Discrete energy conservation law**

In this section, we consider the property of energy conservation of the scheme (3.3). For grid functions defined on the uniform grids: \( U := \{U_{ijk}\} \), the discrete energy norm is defined as
The following theorem proves that the multi-symplectic scheme (3.3) preserves the discrete energy conservation law.

**Theorem 4.1.** (Discrete local energy conservation law). For the integers \( n \geq 0 \), let \( E^n := (E^n_{x_{i,j,k}}, E^n_{y_{i,j,k}}, E^n_{z_{i,j,k}}) \) and \( H^n := (H^n_{x_{i,j,k}}, H^n_{y_{i,j,k}}, H^n_{z_{i,j,k}}) \) be the solutions of the scheme (3.3), there exist the discrete local energy conservation properties

\[
2\delta_t \left( (E^n_{x_{i,j,k}})^2 + (E^n_{y_{i,j,k}})^2 + (E^n_{z_{i,j,k}})^2 \right) + 2\mu \delta_t \left( (H^n_{x_{i,j,k}})^2 + (H^n_{y_{i,j,k}})^2 \right)
\]

The above equations yields

\[
\delta_t U^n_{i,j,k} = \frac{U^n_{i,j,k} - U^n_{i,j,k-1}}{\Delta t}, \quad \delta_t U^n_{i,j,k} = \frac{U^n_{i,j,k} - U^n_{i,j,k-1}}{\Delta t}
\]

The following theorem proves that the multi-symplectic scheme (3.3) preserves the discrete energy conservation law.

**Proof.** The scheme (3.3) is equivalent to the following equations

\[
2\delta_t \left( (E^n_{x_{i,j,k}})^2 + (E^n_{y_{i,j,k}})^2 + (E^n_{z_{i,j,k}})^2 \right) + 2\mu \delta_t \left( (H^n_{x_{i,j,k}})^2 + (H^n_{y_{i,j,k}})^2 \right)
\]

Multiplying by \( (H^n_{x_{i,j,k}} + H^n_{y_{i,j,k}}), (H^n_{x_{i,j,k}} + H^n_{y_{i,j,k}}), (E^n_{x_{i,j,k}} + E^n_{y_{i,j,k}}), (E^n_{x_{i,j,k}} + E^n_{y_{i,j,k}}), (E^n_{x_{i,j,k}} + E^n_{y_{i,j,k}}) \) respectively to both sides of the above equations yields

\[
2\delta_t \left( (E^n_{x_{i,j,k}})^2 + (E^n_{y_{i,j,k}})^2 + (E^n_{z_{i,j,k}})^2 \right) + 2\mu \delta_t \left( (H^n_{x_{i,j,k}})^2 + (H^n_{y_{i,j,k}})^2 \right)
\]

Summing the above Eqs. (4.2), we can get the discrete local energy conservation law (4.1).

**Remark 4.1**

Summing over all terms with respect to \( i, j, k \) in the local discrete energy conservation law (4.1) and according to the periodic boundary conditions (3.4), the summation of right terms of the above equations vanishes, thus we get the discrete global energy conservation law

\[
\|\delta_t E^{n+1}\|^2 + \|\delta_t H^{n+1}\|^2 = \|\delta_t E^n\|^2 + \|\delta_t H^n\|^2.
\]

From the scheme (3.3), \( \delta_t E \) and \( \delta_t H \) satisfy the equations

\[
2\mu(\delta_t H_{x_{i,j,k}} - \delta_t E_{y_{i,j,k}}) = -\frac{\Delta t}{\Delta y} \left( (\delta_t E_{x_{i,j,k}} + \delta_t E_{y_{i,j,k}}) - (\delta_t E_{x_{i,j,k}} + \delta_t E_{y_{i,j,k}}) \right) + \frac{\Delta t}{\Delta z} \left( (\delta_t E_{x_{i,j,k}} + \delta_t E_{y_{i,j,k}}) - (\delta_t E_{x_{i,j,k}} + \delta_t E_{y_{i,j,k}}) \right)
\]

\[
2\mu(\delta_t H_{y_{i,j,k}} - \delta_t E_{x_{i,j,k}}) = -\frac{\Delta t}{\Delta y} \left( (\delta_t E_{x_{i,j,k}} + \delta_t E_{y_{i,j,k}}) - (\delta_t E_{x_{i,j,k}} + \delta_t E_{y_{i,j,k}}) \right) + \frac{\Delta t}{\Delta z} \left( (\delta_t E_{x_{i,j,k}} + \delta_t E_{y_{i,j,k}}) - (\delta_t E_{x_{i,j,k}} + \delta_t E_{y_{i,j,k}}) \right)
\]
The multi-symplectic scheme (3.3) for the three dimensional Maxwell’s equations with periodic boundary conditions is unconditionally stable.

**Remark 4.2.** The multi-symplectic Preissmann scheme for the 2 + 1 dimensional Maxwell’s equations is proved to be unconditionally stable [15]. Following the similar procedures to the proof in [15], we can derive that the multi-symplectic Preissmann scheme for the three dimensional Maxwell’s equations is also unconditionally stable. But from the expression of the Preissmann scheme in [15], we can find it is already very complicated for the 2 + 1 dimensional problem. When applying the Preissmann scheme to the three dimensional problem, we believe the corresponding scheme is more complicated than the multi-symplectic scheme (3.3) for calculation.

### 4.2. Divergence preservation

For Maxwell’s Eq. (2.1), the magnetic field and electronic field are divergence-free if the media is lossless.

\[
\text{div}(\mu H) = 0, \quad \text{div}(\varepsilon E) = 0. \tag{4.5}
\]

In Ref. [29], Chen et al. discussed electronic field divergence-free of the numerical algorithms for two dimensional Maxwell’s equations, and showed that the discrete divergence of an energy-conserved splitting FDTD methods was a first order approximation to the exact divergence-free condition. They extended the discussion to three dimensional Maxwell’s equations in their later work [30]. Two schemes named EC-S-FDTD-I, EC-S-FDTDII-1 were introduced and proved that the EC-S-FDTD-I scheme had one order approximation to the divergence-free fields, while the EC-S-FDTDII-1 scheme had two order approximations. In this subsection, we show that the divergence-free condition (4.5) holds exactly if the multi-symplectic scheme (3.3) is used.

**Theorem 4.2.** For the scheme (3.3), the following identity holds

\[
\mu (\delta_x H^n_{z,jk} + \delta_y H^n_{y,jk} + \delta_z H^n_{x,jk}) = \mu (\delta_x H^0_{z,jk} + \delta_y H^0_{y,jk} + \delta_z H^0_{x,jk}),
\]

\[
\varepsilon (\delta_x E^n_{z,jk} + \delta_y E^n_{y,jk} + \delta_z E^n_{x,jk}) = \varepsilon (\delta_x E^0_{z,jk} + \delta_y E^0_{y,jk} + \delta_z E^0_{x,jk}).
\]

**Proof.** The equivalent scheme (3.3) is

\[
\delta_x H^n_{z,jk} = \frac{1}{2\mu} \delta_x (E^n_{y,jk} + E^{n-1}_{y,jk}) - \frac{1}{2\mu} \delta_y (E^n_{z,jk} + E^{n-1}_{z,jk}),
\]

\[
\delta_y H^n_{y,jk} = \frac{1}{2\mu} \delta_y (E^n_{x,jk} + E^{n-1}_{x,jk}) - \frac{1}{2\mu} \delta_z (E^n_{y,jk} + E^{n-1}_{y,jk}),
\]

\[
\delta_z H^n_{x,jk} = \frac{1}{2\mu} \delta_z (E^n_{y,jk} + E^{n-1}_{y,jk}) - \frac{1}{2\mu} \delta_y (E^n_{x,jk} + E^{n-1}_{x,jk}).
\]
\[-\delta_t E^n_{x_{ijk}} = \frac{1}{2\mu} \delta_y (H^n_{x_{ijk}} + H^{n-1}_{x_{ijk}}) - \frac{1}{2\mu} \delta_z (H^n_{x_{ijk}} + H^{n-1}_{y_{ijk}}),\]

\[-\delta_t E^n_{y_{ijk}} = \frac{1}{2\mu} \delta_z (H^n_{y_{ijk}} + H^{n-1}_{z_{ijk}}) - \frac{1}{2\mu} \delta_x (H^n_{y_{ijk}} + H^{n-1}_{x_{ijk}}),\]

\[-\delta_t E^n_{z_{ijk}} = \frac{1}{2\mu} \delta_x (H^n_{z_{ijk}} + H^{n-1}_{y_{ijk}}) - \frac{1}{2\mu} \delta_y (H^n_{z_{ijk}} + H^{n-1}_{x_{ijk}}).\]

Note that \(\delta_x^t, \delta_y^t, \delta_z^t\) are interchangeable, from the above equations, we get

\[\delta_t \left( \delta_x H^n_{x_{ijk}} + \delta_y H^n_{y_{ijk}} + \delta_z H^n_{z_{ijk}} \right) = \delta_x^t \delta_x H^n_{x_{ijk}} + \delta_y^t \delta_y H^n_{y_{ijk}} + \delta_z^t \delta_z H^n_{z_{ijk}}\]

\[= \delta_x^t \left[ \frac{1}{2\mu} \delta_y (E^n_{x_{ijk}} + E^{n-1}_{x_{ijk}}) - \frac{1}{2\mu} \delta_z (E^n_{y_{ijk}} + E^{n-1}_{y_{ijk}}) \right]\]

\[+ \delta_y^t \frac{1}{2\mu} \delta_z (E^n_{y_{ijk}} + E^{n-1}_{y_{ijk}}) - \frac{1}{2\mu} \delta_x (E^n_{z_{ijk}} + E^{n-1}_{z_{ijk}})\]

\[+ \delta_z^t \frac{1}{2\mu} \delta_x (E^n_{z_{ijk}} + E^{n-1}_{z_{ijk}}) - \frac{1}{2\mu} \delta_y (E^n_{x_{ijk}} + E^{n-1}_{x_{ijk}}) = 0.\]

Similarly

\[-\delta_t \left( \delta_x E^n_{x_{ijk}} + \delta_y E^n_{y_{ijk}} + \delta_z E^n_{z_{ijk}} \right) = -\delta_x^t \delta_x E^n_{x_{ijk}} - \delta_y^t \delta_y E^n_{y_{ijk}} - \delta_z^t \delta_z E^n_{z_{ijk}}\]

\[= -\delta_x^t \frac{1}{2\mu} \delta_y (H^n_{x_{ijk}} + H^{n-1}_{x_{ijk}}) - \frac{1}{2\mu} \delta_z (H^n_{y_{ijk}} + H^{n-1}_{y_{ijk}})\]

\[-\delta_y^t \frac{1}{2\mu} \delta_z (H^n_{y_{ijk}} + H^{n-1}_{y_{ijk}}) - \frac{1}{2\mu} \delta_x (H^n_{z_{ijk}} + H^{n-1}_{z_{ijk}})\]

\[-\delta_z^t \frac{1}{2\mu} \delta_x (H^n_{z_{ijk}} + H^{n-1}_{z_{ijk}}) - \frac{1}{2\mu} \delta_y (H^n_{x_{ijk}} + H^{n-1}_{x_{ijk}}) = 0.\]

By summing over \(n\), we have

\[\mu(\delta_x^t H^n_{x_{ijk}} + \delta_y^t H^n_{y_{ijk}} + \delta_z^t H^n_{z_{ijk}}) = \mu(\delta_x^t H^0_{x_{ijk}} + \delta_y^t H^0_{y_{ijk}} + \delta_z^t H^0_{z_{ijk}}),\]

\[\varepsilon(\delta_x^t E^n_{x_{ijk}} + \delta_y^t E^n_{y_{ijk}} + \delta_z^t E^n_{z_{ijk}}) = \varepsilon(\delta_x^t E^0_{x_{ijk}} + \delta_y^t E^0_{y_{ijk}} + \delta_z^t E^0_{z_{ijk}}).\]

This completes the proof. \(\square\)

Thus, if the numerical initial value is divergence-free, so is the numerical solution of the multi-symplectic scheme (3.3) at any time level.

5. Dispersion and non-dissipation property

5.1. Dispersion relation of the multi-symplectic scheme

In this section, we follow the dispersion analysis for the two dimensional Maxwell’s equations in [16]. There is a large amount of literature on the dispersion analysis of numerical methods for Maxwell’s equations (for example, see [31,32] for the dispersion analysis of FDTD methods and ADI methods). In the multi-symplectic literature, dispersion analysis has been applied to scalar PDEs such as the KdV equation in [33,34] and the Sine–Gordon equation in [35]. In this section, we will investigate the dispersion relation of the multi-symplectic scheme (3.3) and the non-dissipation property.

Suppose a linear PDE has a solution of the form

\[u(x, t) = \exp \left( \sum_{j=1}^{3} k\kappa_j + i\omega t \right) U_0,\]  

where \(U_0\) denotes an arbitrary constant vector, \(\omega\) is frequency and \(\kappa_j\) the vector wave number. Substituting (5.1) into Maxwell’s Eq. (2.9) yields,

\[\left( i\omega M + i\sum_{j=1}^{3} k\kappa_j \right) U_0 = 0,\]

where \(K_1 = F, K_2 = L, K_3 = W.\) Since this equality holds for nonzero \(U_0,\) this implies that a relation must exist between \(\omega\) and \(\kappa_i.\) This relation is called the exact dispersion relation, given by
In order to derive the numerical dispersion relation, we take the numerical solutions of (2.9) to be
\[ u^j_{n-1} = \exp \left( i \sum p k_p \Delta x_p + i \omega l \Delta t \right), \]
where \( \Delta y \approx j_p \Delta x_p, \ t \approx l \Delta t. \)

Associated with the dispersion relations are two important quantities: phase velocity \( v_p \) and group velocity \( v_g \)
\[ v_p = \left. \frac{\partial \omega}{\partial k} \right|_{k = 0}, \quad v_g = \nabla_{k} \omega(\mathbf{k}), \]
where \( \mathbf{k} = k/|k| \) is the unit vector. The phase velocity \( v_p \) describes the speed at which the phase of a wave propagates and the direction of the normal vector to the propagating wavefront. The group velocity \( v_g \) describes the speed at which the envelope of a wave packet propagates and gives the direction of the normal vector to the constant \( \omega \)-surface of the dispersion relation. In particular, a PDE is said to be dispersive if the magnitude of \( v_g \) depends on the vector wave number \( k \). That is, a wave-packet of this PDE with different \( k \) will spread out.

Similarly, a numerical dispersion relation \( \omega(\mathbf{k}, \Delta x, \Delta t) \) from a numerical integrator can be derived by substituting a solution of the form
\[ u^j_{n-1} = \exp \left( i \sum p k_p \Delta x_p + i \omega l \Delta t \right), \]
into a linear PDE. Regardless of whether the PDE is dispersive or not, any numerical finite difference discretizations introduce numerical dispersion [36].

In the following, we discuss the three dimensional problem in \((x,y,z)\). The exact group velocity \( v_g \) and the vector wave number \( k \) are expressed in spherical coordinates,
\[ v_g = |v_g| \left( \sin \alpha \cos \beta, \sin \alpha \sin \beta, \cos \alpha \right), \]
\[ k = (k_x, k_y, k_z) = |k| \left( \sin \phi \cos \theta, \sin \phi \sin \theta, \cos \phi \right), \]
where \( |v_g| \) and \( \alpha, \beta \) are the magnitude and angles of \( v_g \), \( |k| \) and \( \phi, \theta \) are the magnitude and angles of \( k \).

For the Maxwell’s Eqs. (2.9), the exact dispersion relation (5.2) between \( \omega \) and \( k \) with \( \mu = \varepsilon = 1 \) is
\[ \omega^2 = k_x^2 + k_y^2 + k_z^2. \]

In order to derive the numerical dispersion relation, we take the numerical solutions of (2.9) to be
\[ E^n_{ijk} = E_0 e^{i(k_x \xi_i + k_y \eta_j + k_z \zeta_k + \omega t)}, \quad H^n_{ijk} = H_0 e^{i(k_x \xi_i + k_y \eta_j + k_z \zeta_k + \omega t)} \]
where
\[ -\pi \leq \Delta x k_x \leq \pi, \ -\pi \leq \Delta y k_y \leq \pi, \ -\pi \leq \Delta z k_z \leq \pi, \ -\pi \leq \Delta t \omega \leq \pi \]
\[ \xi_i = i \Delta x, \ \eta_j = j \Delta y, \ \zeta_k = k \Delta z, \ t_n = n \Delta t. \]

Inserting the definition (5.6) into the scheme (3.3), we can obtain
\[ \tan^2 \frac{\omega l \Delta t}{2} = \frac{\Delta t^2}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} + \frac{\Delta t^2}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2} + \frac{\Delta t^2}{\Delta z^2} \sin^2 \frac{k_z \Delta z}{2}. \]

This is the numerical dispersion relation of the scheme (3.3) with \( \mu = \varepsilon = 1 \). In the limit when \( \Delta t, \Delta x, \Delta y, \Delta z \to 0 \), the numerical dispersion relation (5.7) converges to the exact dispersion relation (5.5).

In the following discussion, uniform cells are considered \((\Delta x = \Delta y = \Delta z = \Delta)\). For fixed stepsizes \( \Delta t = 0.01, \Delta = 0.1 \), we first plot the dispersion relation for the frequency \( \omega \) as a function of the vector wave number \((k_x, k_y, k_z)\) in Fig. 1. Since \( \omega \) is a three variables function of \( k_x, k_y, k_z \), we use the function “slice” to plot the dispersion relation and the slice planes are \( k_x = 5, 15, 25; \ k_y = 5, 15, 25; \ k_z = 5, 15, 25 \), respectively.

In order to see the relation clearly, we plot the contours of constant \( \omega \) values of the dispersion relation projecting on the \((k_x, k_y)\)-plane in Fig. 2. We omit the contour figures projecting on the \((k_x, k_z)\)-plane and \((k_y, k_z)\)-plane, because they are identical to that of \((k_x, k_y)\)-plane due to the symmetric property of the numerical dispersion relation. Fig. 2(b) shows that the numerical contours are almost circle for small values of \( k \). For large \( k \) however, the distances can vary. Since a faster wavefront will have closer contour lines in the dispersion figure, here we can infer that the numerical propagation speed \( |v_g| \) is direction-dependent.

5.2 Comparing with Yee’s method

Yee’s method [1] is constructed by central difference in both space and time based on a half-step staggered grid and is a second-order method. The numerical dispersion relation for Yee’s method is
\[
\sin^2 \frac{\omega \Delta t}{2} = \frac{\Delta t^2}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} + \frac{\Delta t^2}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2} + \frac{\Delta t^2}{\Delta z^2} \sin^2 \frac{k_z \Delta z}{2}.
\]

The difference of dispersion relations between the multi-symplectic scheme (3.3) and Yee’s method appears only in the \(t\) direction. Here we take the two dimensional problem to describe it. In the two dimensional problem, the dispersion relations for the two schemes are

\begin{align*}
\text{Euler – boxscheme:} & \quad \tan^2 \frac{\omega \Delta t}{2} = \frac{\Delta t^2}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} + \frac{\Delta t^2}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2}, \\
\text{Yee’s method:} & \quad \sin^2 \frac{\omega \Delta t}{2} = \frac{\Delta t^2}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} + \frac{\Delta t^2}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2}.
\end{align*}

\textbf{Fig. 3} shows the dispersion relations for the multi-symplectic scheme (3.3) and Yee’s method. When the CFL condition \(\gamma = \Delta t/\Delta\) is small, the dispersion relation figures for the two method are nearly the same. So the numerical behavior of the two schemes should be close when \(\gamma\) is small. But when \(\gamma\) is greater than \(\sqrt{2}/2\), the frequency \(\omega\) for Yee’s method is a imaginary number which is coincide with that Yee’s method is conditionally stable with \(\gamma = \sqrt{2}/2\). This conclusion can
be extended directly to the three dimensional problem. From this, we can infer that the numerical behavior of the multi-
symplectic scheme (3.3) is as good as Yee’s method when $c$ is less than $\sqrt{2}/2$. Moreover, it is also suitable for the case when $c > \sqrt{2}/2$ due to the unconditional stability which Yee’s method can not handle with.

### 5.3. Non-dissipation property

Taking the stability factor $\xi = e^{i\omega T}$ and defining $a_x$, $b_y$ and $c_z$ respectively by

$$a_x = \frac{1}{\Delta x} \sin \left( \frac{1}{2} k_x \Delta x \right), \quad b_y = \frac{1}{\Delta y} \sin \left( \frac{1}{2} k_y \Delta y \right), \quad c_z = \frac{1}{\Delta z} \sin \left( \frac{1}{2} k_z \Delta z \right).$$

similar procedures to that of the numerical dispersion relation, we can obtain the equation of the stability factor $\xi$ for the multi-symplectic scheme,

$$(\xi - 1)^2 + \frac{(\Delta T)^2}{\mu e} (a_x^2 + b_y^2 + c_z^2)(\xi + 1)^2 = 0,$$

or

$$d_0 \xi^2 + 2d_1 \xi + d_0 = 0,$$

where $d_0$ and $d_1$ are defined as

$$d_0 = 1 + \frac{(\Delta T)^2}{\mu e} (a_x^2 + b_y^2 + c_z^2), \quad d_1 = -1 + \frac{(\Delta T)^2}{\mu e} (a_x^2 + b_y^2 + c_z^2).$$

The roots of (5.10) are

$$\xi_1 = -\frac{d_1}{d_0} + i \frac{\sqrt{d_0^2 - d_1^2}}{d_0}, \quad \xi_2 = -\frac{d_1}{d_0} - i \frac{\sqrt{d_0^2 - d_1^2}}{d_0}.$$  

Clearly, the modulus of the two roots are both equal to one, which means that the scheme is non-dissipative, and it is consistent with the energy conservation property discussed in the above section.

### 6. Some analyses on the numerical dispersion relation

To verify the above inference, we calculate the magnitude $|v_g|$ of the group velocity by

$$|v_g| = \sqrt{(v_{g,x})^2 + (v_{g,y})^2 + (v_{g,z})^2},$$

where

$$(v_{g,x}) = \frac{\partial \omega}{\partial k_x}, \quad (v_{g,y}) = \frac{\partial \omega}{\partial k_y}, \quad (v_{g,z}) = \frac{\partial \omega}{\partial k_z}. $$

---

**Fig. 3.** The dispersion relation figures with stepsizes $\Delta t = 0.01, \Delta = 0.1$ for Maxwell’s Eqs. (2.9) from (a) scheme (3.3); (b) Yee’s method.
The exact group velocity of Maxwell’s Eqs. (2.9) is $|v_g| = 1$ and for the multi-symplectic scheme (3.3), substituting into (6.1) the vectors $\kappa$ in spherical coordinates (5.4), and let $a = |\kappa|/\Delta t$, this yields the propagation speed $|v_g|$ in terms of $a$ and $\phi, \theta$.

Define $\Psi_x = \frac{1}{2} a \sin \phi \cos \theta, \Psi_y = \frac{1}{2} a \sin \phi \sin \theta, \Psi_z = \frac{1}{2} a \cos \phi$, then the numerical group velocity can be written as follows:

$$|v_g| = \frac{1}{1 + \frac{a^2}{\Delta t^2} (\sin^2 \Psi_x + \sin^2 \Psi_y + \sin^2 \Psi_z)} \sqrt{\frac{\sin^2 2\Psi_x + \sin^2 2\Psi_y + \sin^2 2\Psi_z}{4(\sin^2 \Psi_x + \sin^2 \Psi_y + \sin^2 \Psi_z)}}$$ (6.3)

In the following discussion, several aspects of the numerical dispersion relation will be studied based on the group velocity (6.3).

(1) **Effect of the Frequency on the Group Velocity:** We plot the numerical dispersion at different wave number $|\kappa| = 2.5\pi, 5\pi, 7.5\pi$ with $\phi \in [0, \pi], \theta \in [0, 2\pi]$ in Fig. 4. The numerical group velocity in all $|\kappa|$ experiences a lag behind the exact group velocity. The lag increases as $|\kappa|$ increases. In other words, for a given grid spacing, the error $(1 - |v_g|)$ for the high frequency modes is greater than that for the low frequency modes.

These properties can be verified again by the spherical figures of $|v_g|$ as Fig. 5 shows which is made by transforming spherical coordinates into Cartesian coordinates. The group velocity is represented by the radius of the ball. The hollowed ball is a unit ball which represents the exact group velocity while the inner ball represents the numerical group velocity.

(2) **Effect of the Wave Number Angles $\phi, \theta$ on the Group Velocity:** Fig. 6 shows the relation between the numerical group velocity and wave number angle $\theta$ at different $a$ and $\phi$. We make three observations from the figures:

1. By dividing the domain of $\theta$ into four equal parts $[0, \frac{\pi}{2}], [\frac{\pi}{2}, \pi], [\pi, \frac{3\pi}{2}], [\frac{3\pi}{2}, 2\pi]$, we can find that whatever $a$ and $\phi$ choose, $|v_g|$ is symmetric with respect to $\theta = \frac{\pi}{2}, \frac{3\pi}{2}$ in each part of the domain.

2. Furthermore, transforming the spherical coordinates into the Cartesian coordinates, $|v_g|$ is symmetric with respect to $(x, z)$-plane, $(y, z)$-plane and the diagonal planes $x = \pm y$ which can be see clearly from Fig. 5(c).

---

![Fig. 4. Numerical group velocity at different $|\kappa|$ with $\Delta t = 0.01, \Delta = 0.1$. (a) $|\kappa| = 2.5\pi$; (b) $|\kappa| = 5\pi$; (c) $|\kappa| = 7.5\pi$.](image-url)
3. For fixed $v_g$ reaches the maximum and equal value when $h = \frac{p}{4}, \frac{3p}{4}, \frac{5p}{4}$ while the minimum and equal value when $h = 0, \frac{p}{2}, \frac{3p}{2}$.

Next we investigate the relation between the numerical group velocity and wave number angle $\alpha$ at different $\alpha$ and $h$ in Fig. 7. Here we only choose such $h$ belong to $\left[0, \frac{p}{2}\right]$ due to the symmetry plotted in Fig. 6. We can also make some observations as follows:

1. Whatever $\alpha$ chooses, $|v_g|$ is symmetric with respect to $\phi = \frac{p}{2}$ which means the $(x,y)$-plane.
2. According to the result in the second observation above, the largest $|v_g|$ turns up at $\theta = \frac{p}{4}$ which is corresponding to the top lines in each of Fig. 7. By calculation, we find the maximum point appears at $\phi = \frac{3p}{10}, \theta = \frac{3p}{10}$ which means the fastest propagating direction of the numerical group velocity in the first quadrant is $\theta = \frac{3p}{10}$.
3. Similarly, we can draw the conclusion from the bottom lines in Fig. 7 that $|v_g|$ reaches minimum when $\phi = 0, \frac{p}{2}, \pi$ and $\theta = 0$. Due to the symmetry of $|v_g|$, we can see further that the lowest propagating directions are the axes and the velocities along such directions are the same.
4. When $\theta$ varies from $0$ to $\frac{p}{4}$, the fastest traveling direction of $|v_g|$ varies from $\phi = \frac{p}{4} \rightarrow \frac{3p}{10}$ which can be seen from the left parts of Fig. 7, and the right parts is an opposite procedure due to the symmetry about $\phi = \frac{p}{2}$.

(3) Effect of the Large Time Step on the Group Velocity: Since the time step in the unconditionally stable scheme (3.3) is no longer restricted by the CFL condition, it is important and meaningful to see how a large time step impacts on numerical dispersion. Fig. 8 illustrates the group velocities with different time steps. It is obvious that the error $(1 - |v_g|)$ increases when the time step increases. It is conformed again by the spherical figures, Fig. 9. This is an indication that the time step can not be made too large.

(4) Propagation Angles of the Group Velocity: The propagation angles of the group velocity are $\alpha$ and $\beta$ in the definition of (5.3), and we can rewrite them as a function of $\alpha$, $\phi$, and $\theta$. For the exact dispersion relation (5.5),
then we can obtain $\alpha = \phi$ and $\beta = \theta$. Similarly, we can also derive the functions for the numerical dispersion relation:

$$
\alpha = \arctan \left( \sqrt{\frac{\sin^2 2\Psi_x + \sin^2 2\Psi_y}{\sin^2 2\Psi_z}} \right),
$$

$$
\beta = \arctan \left( \frac{\sin 2\Psi_y}{\sin 2\Psi_x} \right),
$$

where $\Psi_x, \Psi_y, \Psi_z$ are defined as above.

The relation between propagation angle $\alpha$ and wave number angles $\phi, \theta$ is plotted in Fig. 10 with $\theta \in [0, 2\pi]$ and $\phi \in [0, \pi/2]$ due to the fact that the range value of the function arctan is $[-\pi/2, \pi/2]$.

In order to see the relations more clearly, we give the contour plot in Fig. 11 which shows the relation between $\alpha$ and $\theta$ with $a = \pi/2$ at different $\phi$. We can find the similar results about symmetry with respect to $\theta$. With these results, we just need to discuss the relation between $\alpha$ and $\phi$ in the domain $[0, \pi/2]$ of $\theta$ which is represented by the contour plot Fig. 12.

The black lines in Fig. 12 is the exact angle relation between $\alpha$ and $\phi$, which is $\alpha = \phi$. We can see that for small $a$, $\alpha$ is lag behind $\phi$, as $a$ increases, the left curves are upward bending while the right curves are downward bending. When $a$ is large enough, for example, $a = 3\pi/4$, $\alpha$ is greater than $\phi$ for small $\phi$. Moreover, the lower degree of upward bending, the greater
Fig. 7. Numerical group velocity versus wave number angles $\phi$ at different $\theta$ (labeled) with $\Delta t = 0.01, \Delta = 0.1$ for (a) $a = \pi/4$; (b) $a = \pi/2$; (c) $a = 3\pi/4$.

Fig. 8. Numerical group velocity for $a = \pi/4, \Delta = 0.1$ with (a) $\Delta t = 0.02$; (b) $\Delta t = 0.08$. 
Fig. 9. Numerical group velocity for $a = \pi/4, \Delta = 0.1$ with (a) $\Delta t = 0.02$, (b) $\Delta t = 0.08$.

Fig. 10. Wave propagation angle $\alpha$ versus wave number angle $\phi$ and $\theta$ for (a) $a = \pi/4$, (b) $a = \pi/2$, (c) $a = 3\pi/4$. 

Fig. 11. Wave propagation angle $\alpha$ versus wave number angle $\theta$ with $\alpha = \frac{\pi}{4}$ at different $\phi$ (labeled).

Fig. 12. Wave propagation angle $\alpha$ versus wave number angle $\phi$ at different $\theta$ (labeled) for (a) $\alpha = \frac{\pi}{4}$; (b) $\alpha = \frac{\pi}{2}$; (c) $\alpha = \frac{3\pi}{4}$.
Fig. 13. Wave propagation angle $\beta$ versus wave number angle $\phi$ and $\theta$ for (a) $a = \frac{\pi}{4}$; (b) $a = \frac{\pi}{2}$; (c) $a = \frac{3\pi}{4}$.

Fig. 14. Wave propagation angle $\beta$ versus wave number angle $\phi$ with $a = \frac{3\pi}{4}$ at different $\theta$ (labeled).
degree of downward bending. From Fig. 12(c), it is obvious that the lowest degree of upward bending as well as the greatest degree of downward bending occurs at $\theta = \frac{\pi}{2}$.

Similarly, in Fig. 13, we present the relation between propagation angle $\beta$ and wave number angle $\theta$ with $\phi \in [0, \pi], \theta \in [0, \frac{\pi}{2}]$. We also plot the contour lines at different $\theta$ in Fig. 14 which shows that whatever $\theta$ chooses, $\beta$ is symmetric with respect to $\phi = \frac{\pi}{2}$. So we only need to discuss the relation between $\beta$ and $\theta$ in the domain $[0, \frac{\pi}{2}]$ of $\phi$ which is represented by the contour plot Fig. 15. It is seen that as $\alpha$ increases, $\beta$ is upward bending when $\theta < \frac{\pi}{4}$ and downward bending when $\theta \geq \frac{\pi}{4}$. Moreover, the degree of upward and downward bending are the same, and the largest bending degree occurs at $\phi = \frac{\pi}{2}$.

Although we do not give the fully analysis of $\alpha$ and $\beta$, i.e., only the domain $[0, \frac{\pi}{2}]$ is discussed for both $\alpha$ and $\beta$, we can infer the properties of the rest parts due to the symmetry of the period trigonometric function, the definition of $\alpha$, $\beta$ (6.5), (6.6) and the spherical plot Fig. 5.

(5) **Effect on the CFL Condition**: In order to view dispersion characteristics more closely and precisely, the dispersion relation is shown on the cut of the $(\kappa_x, \kappa_y)$-plane ($\phi = \pi/2, \kappa_z = |\kappa| \cos \phi = 0$). Now we investigate what happens to the numerical contours as we increase the ratio $\gamma$ towards 1. Fig. 16 displays sections of dispersion contours at $\omega = 6$. In this figure, three different mesh sizes are considered: $\Delta = 0.1, 0.05, 0.01$ which means $\gamma = 0.1, 0.2, 1$ respectively. We can see from the magnified part of the figure that as $\gamma \rightarrow 1$, the contours tend towards the exact dispersion contour which is also conformed the unconditional stability of the multi-symplectic scheme (3.3).
7. Conclusion

In this paper, based on the Euler-box scheme, we investigate a multi-symplectic scheme for the three dimensional Maxwell’s equations. For calculation, we present a linear system for the scheme whose coefficient matrix is a symmetric and strictly diagonally dominant matrix under some conditions. Thus we can use various efficient iterative methods to solve it. We derive the discrete multi-symplectic conservation law and the discrete local and global energy conservation law which represents the unconditional stability of the scheme. We also prove that the discrete divergence is preserved exactly by the scheme. Furthermore, we present the numerical dispersion relation and some analyses on it. The dispersion relation for the multi-symplectic Euler-box scheme applied to the three dimensional Maxwell’s equations is a direct extension of the 2 + 1 dimensional problem which has studied in Ref. [17] and we give some new results for the three dimensional problem as follows.

We find that the dispersion relation of the scheme is close to that of Yee’s scheme with small CFL number. Although our multi-symplectic scheme need to use iterative methods to solve a linear system while Yee’s scheme is more efficient since it is an explicit scheme, our multi-symplectic scheme is unconditional stable and we can use larger time step than that of Yee’s scheme which is restricted by the CFL condition. But for the concrete numerical efficiency comparing with the classical Yee’s scheme, we still need to do widely numerical experiments which will be investigated in our future work.

The error between the numerical group velocity and the exact one grows as the increment of the magnitude of the wave number κ. Moreover, we give the symmetric property of the numerical group velocity which have several symmetric planes in the Cartesian coordinates. We also investigate the relation between the propagating angles and the wave number angles which gives further understanding of the numerical group velocity. Finally, we analyze the effect of the large time step and CFL condition which can instruct the choice of spatial and time steps.

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