Symplectic Discretization for Spectral Element Solution of Maxwell's Equations

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Abstract

Based on the GLL-spectral element discretization of time-dependent Maxwell's equations introduced recently, we obtain a Poisson system or a Poisson system with a little oscillation. We prove that any symplectic partitioned Runge-Kutta method preserves the Poisson structure and the implied symplectic structure. Numerical examples show the efficiency of the symplectic spectral-element method.

Keywords: *Maxwell's Equations; Spectral Element Method; Poisson System; Symplectic Partitioned Runge-Kutta Method*

1. Introduction

Maxwell's equations are very important and the fundamental laws governing electromagnetic fields. With the increasing concern of electromagnetic fields, especially in time-domain simulations for wide-band applications, more and more research on numerical solutions of time-domain Maxwell's equations is produced. Recently, Liu et. al. adopted the spectral element time-domain method based on Gauss-Lobatto-Legendre (GLL) polynomials for the spatial discretization and Runge-Kutta method for the temporal discretization to solve Maxwell's equations. The GLL-spectral element time-domain

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method has high accuracy and geometric flexibility, and due to the orthogonality of the basis functions, we can obtain a diagonal or block diagonal mass matrix by using of the GLL quadrature with little cost. Here we utilize the GLL-spectral element time-domain method to discretize Maxwell's equations first to obtain a system of ODEs, which is a Poisson system to be solved by symplectic methods on temporal direction in this paper.
Maxwell's equations can be written as a infinite dimensional Hamiltonian system. So, its solution is a Hamiltonian flow in functional space which preserves the symplectic structure in the time direction. Recently, some scholars propose the symplectic method (see[10-13]) on temporal discretization of time-domain Maxwell's equations.
Symplectic methods preserve exactly the inherent canonical property of the continuous Hamiltonian flow. Extensive numerical tests have indicated that the symplectic integrators are superior to the non-symplectic ones, especially for longtime simulations and conservations of invariants. Obviously, these features of symplectic methods are very important during the design of numerical methods for time-domain Maxwell's equations. For an infinite dimensional Hamiltonian system, the most popular approach to construct the symplectic methods is dimension reduction, in order to receive a finite dimensional Hamiltonian system. However, it is difficult to achieve the aim because of the nonconsistency between the numbers of edges and faces obtained via discretizing electric and magnetic fields respectively. Actually, the obtained ODEs is a general Poisson system or a Poisson system with an oscillation rather than a Hamiltonian system. Fortunately, it can be proved that any symplectic partitioned Runge-Kutta (PRK) method preserves the Poisson structure and the implied symplectic structure of the Poisson system. Finally we present some numerical examples to test the high efficiency of the symplectic spectral element method.

2. Maxwell's Equations and Spatial Discretization

Assuming the medium is isotropic and linear, we can write Maxwell's equations as follows:

$$\begin{cases} \epsilon \dfrac{\partial \mathbf{E}}{\partial t} & = & \nabla \times \mathbf{H} - \mathbf{J} \\ \mu \dfrac{\partial \mathbf{H}}{\partial t} & = & -\nabla \times \mathbf{E}, \end{cases} \tag{1}$$

where ϵ and μ are the permittivity and permeability of the medium, respectively. The coefficients ϵ and μ are bounded $L^\infty(\Omega)$ functions and physically there exist constants $\epsilon_0, \epsilon_1, \mu_0, \mu_1$ in Ω, such that

$$\begin{cases} 0 < \epsilon_0 \leq \epsilon \leq \epsilon_1 < \infty \\ 0 < \mu_0 \leq \mu \leq \mu_1 < \infty. \end{cases}$$

For simplicity, let ϵ, μ be constant. If there are finite types of medium in Ω, the above Maxwell's equations can be written as Hamiltonian system

$$\begin{cases} \frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\epsilon}\nabla \times \mathbf{H} - \frac{1}{\epsilon}\mathbf{J} = \frac{\delta \mathbb{H}}{\delta \mathbf{H}} \\ \frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu}\nabla \times \mathbf{E} = -\frac{\delta \mathbb{H}}{\delta \mathbf{E}} \end{cases} \tag{2}$$

where $\mathbb{H}[\mathbf{E}, \mathbf{H}] = \int_\Omega \frac{1}{2\mu}\mathbf{E} \cdot \nabla \times \mathbf{E} + \frac{1}{2\epsilon}\mathbf{H} \cdot \nabla \times \mathbf{H} - \frac{1}{\epsilon}\mathbf{H} \cdot \mathbf{J} d\mathbf{V}.$

In spatial direction, the weak form of (1): find $\mathbf{E}, \mathbf{H}$ in relevant finite element space U_h, V_h, such that

$$\begin{cases} \frac{\partial}{\partial t}\langle \epsilon \mathbf{E}, \mathbf{E}^* \rangle = \langle \nabla \times \mathbf{H} - \mathbf{J}, \mathbf{E}^* \rangle \\ \frac{\partial}{\partial t}\langle \mu \mathbf{H}, \mathbf{H}^* \rangle = -\langle \nabla \times \mathbf{E}, \mathbf{H}^* \rangle \end{cases} \tag{3}$$

where $\langle \mathbf{U}, \mathbf{W} \rangle = \int_\Omega \mathbf{U} \cdot \mathbf{W} d\mathbf{V}$.

Let U_h= span $\{\mathbf{\Phi}_1, \cdots, \mathbf{\Phi}_{N_e}\}$, V_h= span $\{\mathbf{\Psi}_1, \cdots, \mathbf{\Psi}_{N_h}\}$, where N_e, N_h are the numbers of unknowns for the electric and magnetic fields, respectively. Then, we can gain that

$$\mathbf{E}(\mathbf{X}, t) = \sum_{i=1}^{N_e} e_i(t)\mathbf{\Phi}_i(\mathbf{X}), \qquad \mathbf{H}(\mathbf{X}, t) = \sum_{j=1}^{N_h} h_j(t)\mathbf{\Psi}_j(\mathbf{X}).$$

Assuming $\{\Gamma_1, \cdots, \Gamma_k\}$ is a regular subdivision on Ω, we will focus our discussion on any one of the subdivisional elements denoted by Ω_k.

The matrix form of (3) is:

$$\begin{cases} A\frac{de(t)}{dt} = Kh(t) - f(t) \\ B\frac{dh(t)}{dt} = Ge(t) \end{cases} \tag{4}$$

where $e(t) = (e_1(t), \cdots, e_{N_e}(t))^T, \qquad h(t) = (h_1(t), \cdots, h_{N_h}(t))^T$;

$$f_i(t) = (\langle \mathbf{J}, \mathbf{\Phi}_1 \rangle, \cdots, \langle \mathbf{J}, \mathbf{\Phi}_{N_e} \rangle);\; A_{ij} = \langle \epsilon \mathbf{\Phi}_i, \mathbf{\Phi}_j \rangle;$$

$$B_{ij} = \langle \mu \mathbf{\Psi}_i, \mathbf{\Psi}_j \rangle;\; K_{ij} = \langle \nabla \times \mathbf{\Psi}_j, \mathbf{\Phi}_i \rangle;\; G_{ij} = -\langle \nabla \times \mathbf{\Phi}_j, \mathbf{\Psi}_i \rangle.$$

If $\int_{\partial \Omega_k} (\mathbf{\Psi}_i \times \mathbf{\Phi}_j) \cdot \vec{\mathbf{n}} dS = 0$, $\vec{\mathbf{n}}$ is unit outward normal vector of the boundary of Ω_k, then $G = -K^T$.

With $\mathbf{J} = 0$, (4) yields a Poisson system

$$\begin{cases} A\dfrac{de(t)}{dt} = Kh(t) = K\nabla_h \hat{H}(e,h) \\ B\dfrac{dh(t)}{dt} = - K^T e(t) = - K^T \nabla_e \hat{H}(e,h) \end{cases} \tag{5}$$

where $\hat{H}(e,h) = \dfrac{1}{2}(e^2 + h^2)$. If $\mathbf{J} \neq 0$, (5) is a Poisson system with a oscillation.

3. Symplectic Structure of Poisson System

Equations (5) is a particular case of the following equations

$$\begin{cases} \dfrac{dq}{dt} = M\nabla_p H(q,p) \\ \dfrac{dp}{dt} = -M^T \nabla_q H(q,p) \end{cases} \tag{6}$$

where $q \in \mathbb{R}^{m_1 \times 1}, p \in \mathbb{R}^{m_2 \times 1}, M \in \mathbb{R}^{m_1 \times m_2}, rank(M) = r$.
Let $m = m_1 + m_2$, (6) can be written as a form of Poisson system

$$\frac{dz}{dt} = B(z)\nabla H(z)$$

where $z = (q^T, p^T) \in \mathbb{R}^m, B(z) = \begin{bmatrix} 0_{m_1} & M \\ -M^T & 0_{m_2} \end{bmatrix}$, 0_{m_i} denotes m_i order zero matrix.
Now, we analysis the symplectic structure of the semi-discrete equation (5). As we known, a differential scheme is a normal symplectic scheme or method if the corresponding step-transition operator is a normal symplectic transformation for Hamiltonian system. Although the definition of symplectic system depends on Hamiltonian system, the system itself can be used in different equations. No more than the corresponding step-transition operator is not symplectic transformation for a non-Hamiltonian system. In this section we prove that the Poisson system (6) embodies symplectic structure implicitly. Whereas the symplectic method will be chosen to solve (6), and the numerical solutions will preserve its symplectic structure.
For depiction easily, we set

$$M = \begin{bmatrix} K \\ CK \end{bmatrix} = \begin{bmatrix} \hat{K} & \hat{K}\hat{C} \\ C\hat{K} & C\hat{K}\hat{C} \end{bmatrix}, \tag{7}$$

where $K \in \mathbb{R}^{r \times m_2}$, $C \in \mathbb{R}^{(m_1 - r) \times r}$, $\hat{K} \in \mathbb{R}^{r \times r}$, $\hat{C} \in \mathbb{R}^{r \times (m_2 - r)}$. $\hat{K}$ is a non degenerate matrix. For M, we assume that the $r \times r$ order sub-matrix on the top left corner is a non degenerate matrix. Or else, it can be adjusted to a non degenerate one by some techniques.

View $q_0 = q(t_0)$, $p_0 = p(t_0)$ as the initial values of (6), let $q = [\hat{q}^T, \hat{\hat{q}}^T]^T$, $p = [\hat{p}^T, \hat{\hat{p}}^T]^T$, $\hat{H}(\hat{q}, \hat{p}) = H(q, p)$, $\hat{\hat{q}} = C\hat{q} + (\hat{\hat{q}}_0 - C\hat{q}_0)$, $\hat{\hat{p}} = \hat{C}^T\hat{p} + (\hat{\hat{p}}_0 - \hat{C}^T\hat{p}_0)$.

Theorem 1. Equations (6) is equal to the following equations

$$\begin{cases} \dot{\hat{q}} &= \hat{K}\nabla_{\hat{p}}\hat{H}(\hat{q}, \hat{p}) \\ \dot{\hat{p}} &= -\hat{K}^T\nabla_{\hat{q}}\hat{H}(\hat{q}, \hat{p}) \\ \hat{\hat{q}} &= C\hat{q} + (\hat{\hat{q}}_0 - C\hat{q}_0) \\ \hat{\hat{p}} &= \hat{C}^T\hat{p} + (\hat{\hat{p}}_0 - \hat{C}^T\hat{p}_0) \end{cases} \tag{8}$$

Proof: According to the first equation of (6)

$$\dot{q} = M\nabla_p H(q, p),$$

we get

$$\begin{cases} \dot{\hat{q}} &= K\nabla_p H(q, p) \\ \dot{\hat{\hat{q}}} &= CK\nabla_p H(q, p) \end{cases}$$

So $\dot{\hat{\hat{q}}} = C\dot{\hat{q}}$, $\hat{\hat{q}}(t) = C\hat{q}(t) + (\hat{\hat{q}}_0 - C\hat{q}_0)$. Similarly, $\dot{p} = -K^T(\nabla_{\hat{q}}H(q, p) + C^T\nabla_{\hat{\hat{q}}}H(q, p))$. Let $\bar{H}(\hat{q}, p) = H(q, p)|_{\hat{\hat{q}} = C\hat{q} + (\hat{\hat{q}}_0 - C\hat{q}_0)}$, then

$$\begin{cases} \nabla_{\hat{q}}\bar{H}(\hat{q}, p) &= (\nabla_{\hat{q}}H(q, p) + C^T\nabla_{\hat{\hat{q}}}H(q, p))|_{\hat{\hat{q}} = C\hat{q} + (\hat{\hat{q}}_0 - C\hat{q}_0)}, \\ \nabla_p\bar{H}(q, p) &= \nabla_p H(q, p)|_{\hat{\hat{q}} = C\hat{q} + (\hat{\hat{q}}_0 - C\hat{q}_0)}, \end{cases}$$

We gain that

$$\begin{cases} \dot{\hat{q}} &= K\nabla_p\bar{H}(\hat{q}, p) \\ \dot{p} &= -K^T\nabla_{\hat{q}}\bar{H}(\hat{q}, p) \end{cases}$$

(6) is equal to

$$\begin{cases} \dot{\hat{q}} &= K\nabla_p\bar{H}(q, p) \\ \dot{p} &= -K^T\nabla_{\hat{q}}\bar{H}(q, p) \\ \hat{\hat{q}}(t) &= C\hat{q}(t) + (\hat{\hat{q}}_0 - C\hat{q}_0) \end{cases} \tag{9}$$

According to the first and second equation of (9), we respectively have $\dot{\hat{q}} = \hat{K}(\nabla_{\hat{p}}\bar{H}(\hat{q}, p) + \hat{C}\nabla_{\hat{\hat{p}}}\bar{H}(\hat{q}, p))$, and

$$\begin{cases} \dot{\hat{p}} &= -\hat{K}^T\nabla_{\hat{q}}H(\hat{q}, p) \\ \dot{\hat{\hat{p}}} &= -\hat{C}^T\hat{K}^T\nabla_{\hat{q}}H(\hat{q}, p) \end{cases}$$

Thereby $\dot{\hat{\hat{p}}} = \hat{C}^T\dot{\hat{p}}$, $\hat{\hat{p}}(t) = \hat{C}^T\hat{p}(t) + (\hat{\hat{p}}_0 - \hat{C}^T\hat{p}_0)$.

Let $\hat{p}(t)$, $\hat{\hat{p}}_0$, $\hat{p}_0$ substitute $\hat{\hat{p}}$, then (9) can be simply written as differential equations only on $\hat{q}(t)$ and $\hat{p}(t)$. Considering the above proof, we know that

$$\begin{cases} \dot{\hat{q}} &= \hat{K}(\nabla_{\hat{p}}\bar{H}(\hat{q}, p) + \hat{C}\nabla_{\hat{\hat{p}}}\bar{H}(\hat{q}, p))|_{\hat{\hat{p}} = \hat{C}^T\hat{p} + (\hat{\hat{p}}_0 - \hat{C}^T\hat{p}_0)} \\ \dot{\hat{p}} &= -\hat{K}^T\nabla_{\hat{q}}\bar{H}(\hat{q}, p)|_{\hat{\hat{p}} = \hat{C}^T\hat{p} + (\hat{\hat{p}}_0 - \hat{C}^T\hat{p}_0)} \end{cases}$$

From the definition of $\hat{H}$, we can obtain $\hat{H}(\hat{q},\hat{p}) = \bar{H}(\hat{q},p)|_{\hat{\hat{p}}=\hat{C}^T\hat{p}+(\hat{\hat{p}}_0-\hat{C}^T\hat{p}_0)}$, then
$\nabla_{\hat{q}}\hat{H}(\hat{q},\hat{p}) = \nabla_{\hat{q}}\bar{H}(\hat{q},p)|_{\hat{\hat{p}}=\hat{C}^T\hat{p}+(\hat{\hat{p}}_0-\hat{C}^T\hat{p}_0)}$,
$\nabla_{\hat{p}}\hat{H}(\hat{q},\hat{p}) = (\nabla_{\hat{p}}\bar{H}(\hat{q},p) + \hat{C}\nabla_{\hat{\hat{p}}}\bar{H}(\hat{q},p)|_{\hat{\hat{p}}=\hat{C}^T\hat{p}+(\hat{\hat{p}}_0-\hat{C}^T\hat{p}_0)}$, so,

$$\left\{\begin{array}{lll} \dot{\hat{q}} & = & \hat{K}\nabla_{\hat{p}}\hat{H}(\hat{q},\hat{p}) \\ \dot{\hat{p}} & = & -\hat{K}^T\nabla_{\hat{q}}\hat{H}(\hat{q},\hat{p}). \end{array}\right. \tag{10}$$

Sequentially, equations (9) is equal to (8), then (6) is equal to (8). ■

Based on the theorem, we know that the Poisson system can be divided into two parts: one is the Hamiltonian system (10) with symplectic structure $d\hat{p} \dot{\wedge} \hat{K}^{-1}d\hat{q}$, the other is a simple algebraic system

$$\left\{\begin{array}{lll} \hat{\hat{q}} & = & C\hat{q} + (\hat{\hat{q}}_0 - C\hat{q}_0) \\ \hat{\hat{p}} & = & \hat{C}^T\hat{p} + (\hat{\hat{p}}_0 - \hat{C}^T\hat{p}_0). \end{array}\right. \tag{11}$$

Hence symplectic algorithms stand in the breach among various numerical methods for Maxwell's equations. Generally, the phase flow of Poisson itself is Poisson mapping, therefore its structure-preserving algorithms should be Poisson integrator. For a linear system, i.e., $B(z)$ is a constant matrix, Zhu and Qin [15] have shown that any symplectic implicit diagonal Runge-Kutta method is a Poisson scheme. Actually in this case, all of the symplectic Runge-Kutta method are Poisson integrators. Here the Poisson system (6) is a linear and separable system.

4. Symplectic PRK Methods and Poisson Schemes

In this section, we apply the symplectic PRK method to equation (6) and present some important conclusions which provide dependence in theory for application of symplectic algorithms to Maxwell's equations. The coefficients of s-order PRK methods are given out as follows

Table 1: Table of Butcher for PRK method

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \qquad \begin{array}{c|ccc} \bar{c}_1 & \bar{a}_{11} & \cdots & \bar{a}_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ \bar{c}_s & \bar{a}_{s1} & \cdots & \bar{a}_{ss} \\ \hline & \bar{b}_1 & \cdots & \bar{b}_s \end{array}$$

Usually, it is used for the following ordinary differential equations

$$\left\{\begin{array}{l} \dfrac{dq}{dt} = f(q,p) \\ \dfrac{dp}{dt} = g(q,p) \end{array}\right. \tag{12}$$

i.e. q, p the two sets variable of equations (12) will be expressed by using the R-K methods of the left and right table in table 1, respectively. The result is

$$\begin{cases} Q_i &= q_0 + h\sum_{j=0}^{s} a_{ij} f(Q_j, P_j) \\ P_i &= p_0 + h\sum_{j=0}^{s} \bar{a}_{ij} g(Q_j, P_j) \\ q_1 &= q_0 + h\sum_{j=0}^{s} b_j f(Q_j, P_j) \\ p_1 &= p_0 + h\sum_{j=0}^{s} \bar{b}_j g(Q_j, P_j) \end{cases}$$

The symplectic conditions of PRK method [16] are

$$\begin{cases} b_i\bar{a}_{ij} + \bar{b}_j a_{ji} - b_i\bar{b}_j &= 0 \\ b_i &= \bar{b}_i \end{cases} \tag{13}$$

If (12) is a separable system, the symplectic conditions of PRK method will be only the first formula of (13).

Next we introduce a definition and some theorems to analyze the numerical solutions of (6).

Definition 1. The variables $\hat{q}$ and $\hat{p}$ in Hamiltonian equations (10) are called the symplectic components of q and p, respectively; the other part variables $\hat{\hat{q}}$ and $\hat{\hat{p}}$ are called their non-symplectic components.

Theorem 2. Let u denote the numerical solution of PRK method for (6), then the symplectic components of u are numerical solutions of PRK method for (10) and the non-symplectic components of u are numerical solutions of the PRK method for (11).

Proof : The numerical solution of s order PRK method according to table 1 for (6) is $(q_0, p_0), (q_1, p_1), \cdots, (q_N, p_N)$. The details of the computation is

$$\begin{cases} Q_i^n &= q_n + h\sum_{j=1}^{s} a_{ij} M\nabla_p H(Q_j^n, P_j^n) \\ P_i^n &= p_n - h\sum_{j=1}^{s} \bar{a}_{ij} M^T\nabla_q H(Q_j^n, P_j^n) \\ q_{n+1} &= q_n + h\sum_{j=1}^{s} b_j M\nabla_p H(Q_j^n, P_j^n) \\ p_{n+1} &= p_n - h\sum_{j=1}^{s} \bar{b}_j M^T\nabla_q H(Q_j^n, P_j^n) \end{cases}, \quad \begin{array}{l} i = 1, 2, \cdots, s. \\ n = 0, 1, \cdots, N-1. \end{array} \tag{14}$$

Considering $M = \begin{bmatrix} K \\ CK \end{bmatrix}$, for $n = 0, 1, \cdots, N-1$, from $q_{n+1} = q_n + h\sum_{j=1}^{s} b_j M\nabla_p H(Q_j^n, P_j^n)$, we get $\hat{\hat{q}}_{n+1} - \hat{\hat{q}}_n = C(\hat{q}_{n+1} - \hat{q}_n)$ then

$$\hat{\hat{q}}_{n+1} = C\hat{q}_{n+1} + (\hat{\hat{q}}_n - C\hat{q}_n) \tag{15}$$

Furthermore, we recursively have

$$\hat{\hat{q}}_n = C\hat{q}_n + (\hat{\hat{q}}_0 - C\hat{q}_0), \qquad n = 1, 2, \cdots, N. \tag{16}$$

For $i = 1, 2, \cdots, s; \quad n = 0, 1, \cdots, N-1$, from

$$Q_i^n = q_n + h\sum_{j=1}^{s} a_{ij} M \nabla_p H(Q_j^n, P_j^n)$$

we get

$$\hat{\hat{Q}}_i^n - \hat{\hat{q}}_n = C(\hat{Q}_i^n - \hat{q}_n). \tag{17}$$

Based on (16), we have

$$\hat{\hat{Q}}_i^n = C\hat{Q}_i^n + (\hat{\hat{q}}_0 - C\hat{q}_0). \tag{18}$$

By using (18) and the definition of $\bar{H}(\hat{q}, p)$, we know that $\bar{H}(\hat{Q}_j^n, P_j^n) = H(Q_j^n, P_j^n)|_{\hat{\hat{Q}}_j^n = C\hat{Q}_j^n + (\hat{\hat{q}}_0 - C\hat{q}_0)}$, and

$$\begin{aligned}
K^T\nabla_{\hat{q}}\bar{H}(\hat{Q}_j^n, P_j^n) &= K^T(\nabla_{\hat{q}}H(Q_j^n, P_j^n) + C^T\nabla_{\hat{\hat{q}}}H(Q_j^n, P_j^n))|_{\hat{\hat{Q}}_j^n = C\hat{Q}_j^n + (\hat{\hat{q}}_0 - C\hat{q}_0)} \\
&= M^T\nabla_q H(Q_j^n, P_j^n)|_{\hat{\hat{Q}}_j^n = C\hat{Q}_j^n + (\hat{\hat{q}}_0 - C\hat{q}_0)}, \\
\nabla_p\bar{H}(\hat{Q}_j^n, P_j^n) &= \nabla_q H(Q_j^n, P_j^n)|_{\hat{\hat{Q}}_j^n = C\hat{Q}_j^n + (\hat{\hat{q}}_0 - C\hat{q}_0)}.
\end{aligned}$$

Combining (14), we drive the following schemes

$$\left\{\begin{aligned}
\hat{Q}_i^n &= \hat{q}_n + h\sum_{j=1}^{s} a_{ij} K\nabla_p\bar{H}(\hat{Q}_j^n, P_j^n) \\
P_i^n &= p_n - h\sum_{j=1}^{s} \bar{a}_{ij} K^T\nabla_{\hat{q}}\bar{H}(\hat{Q}_j^n, P_j^n) \\
\hat{q}_{n+1} &= \hat{q}_n + h\sum_{j=1}^{s} b_j K\nabla_p\bar{H}(\hat{Q}_j^n, P_j^n) \\
p_{n+1} &= p_n - h\sum_{j=1}^{s} \bar{b}_j K^T\nabla_{\hat{q}}\bar{H}(\hat{Q}_j^n, P_j^n) \\
\hat{\hat{q}}_{n+1} &= C\hat{q}_{n+1} + (\hat{\hat{q}}_n - \hat{q}_n)
\end{aligned}\right. \tag{19}$$

Similarly, according to (19), we drive the following schemes

$$\left\{\begin{array}{lcl} \hat{Q}_i^n & = & \hat{q}_n + h\sum_{j=1}^{s} a_{ij}\hat{K}\nabla_{\hat{p}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{P}_i^n & = & \hat{p}_n - h\sum_{j=1}^{s} \bar{a}_{ij}\hat{K}^T\nabla_{\hat{q}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{q}_{n+1} & = & \hat{q}_n + h\sum_{j=1}^{s} b_j\hat{K}\nabla_{\hat{p}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{p}_{n+1} & = & \hat{p}_n - h\sum_{j=1}^{s} \bar{b}_j\hat{K}^T\nabla_{\hat{q}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{\hat{q}}_{n+1} & = & C\hat{q}_{n+1} + (\hat{\hat{q}}_0 - C\hat{q}_0) \\ \hat{\hat{p}}_{n+1} & = & \hat{C}^T\hat{p}_{n+1} + (\hat{\hat{p}}_0 - \hat{C}^T\hat{p}_0) \end{array}\right. \tag{20}$$

(23) can be divided into two parts, one is PRK discretization of (10), the other is

$$\left\{\begin{array}{lcl} \hat{\hat{q}}_n & = & C\hat{q}_n + (\hat{\hat{q}}_0 - C\hat{q}_0) \\ \hat{\hat{p}}_n & = & \hat{C}^T\hat{p}_n + (\hat{\hat{p}}_0 - \hat{C}^T\hat{p}_0) \end{array}\right. \tag{21}$$

Obviously, (21) is the discretize form of (11). ■

Let $L = \begin{bmatrix} 0 & \hat{K} \\ -\hat{K}^T & 0 \end{bmatrix}^{-1}$, since the accuracy flow of (10) is $L-$symplectic transform, we have the following theorem:

Theorem 3. The step-transition operator of symplectic PRK method for (10) is $L-$symplectic transform.

Proof: Let $\hat{z} = [\hat{q}^T, \hat{p}^T]^T$, (10) is equal to

$$\frac{d\hat{z}}{dt} = L^{-1}\nabla_{\hat{z}}\hat{H}(\hat{z}). \tag{22}$$

Let $D = \begin{bmatrix} \hat{K}^{-1} & 0 \\ 0 & I_r \end{bmatrix}$; $w = [u^T, v^T]^T = \phi(\hat{z}) = C\hat{z}$ $S(w) = \hat{H} \circ \phi^{-1}(w)$ i.e. $\hat{H}(\hat{z}) = S \circ \phi(\hat{z})$, then

$$\hat{H}(\hat{q}, \hat{p}) = S(\hat{K}^{-1}\hat{q}, \hat{p}) \tag{23}$$

and

$$\nabla_{\hat{z}}\hat{H}(\hat{z}) = \nabla_{\hat{z}}(S \circ \phi)(\hat{z}) = \left[\frac{\partial\phi(\hat{z})}{\partial\hat{z}}\right]^T \nabla_w S(w)|_{w=\phi(\hat{z})} = D^T\nabla_w S(w)|_{w=C\hat{z}},$$

that is

$$\left\{\begin{array}{lcl} \nabla_{\hat{q}}\hat{H}(\hat{q}, \hat{p}) & = & \hat{K}^{-T}\nabla_u S(\hat{K}^{-1}\hat{q}, \hat{p}) \\ \nabla_{\hat{p}}\hat{H}(\hat{q}, \hat{p}) & = & \nabla_v S(\hat{K}^{-1}\hat{q}, \hat{p}) \end{array}\right. \tag{24}$$

Then, for $w = D\hat{z}$ we have

$$\frac{dw}{dt} = \frac{\partial w}{\partial \hat{z}} \frac{d\hat{z}}{dt} = DL^{-1}\nabla_{\hat{z}}\hat{H}(\hat{z}) = DL^{-1}D^T\nabla_w S(w),$$

and

$$DL^{-1}D^T = \begin{bmatrix} 0 & I_r \\ -I_r & 0 \end{bmatrix}.$$

For $J = \begin{bmatrix} 0 & I_r \\ -I_r & 0 \end{bmatrix}$, we get $\frac{dw}{dt} = J^{-1}\nabla_w(-S)(w)$, namely

$$\begin{cases} \frac{du}{dt} &= \nabla_v S(u, v) \\ \frac{dv}{dt} &= -\nabla_u S(u, v) \end{cases} \tag{25}$$

By using PRK method satisfied (13) to solve (10), we get

$$\begin{cases} \hat{Q}_i^n &= \hat{q}_n + h\sum_{j=1}^{s} a_{ij}\hat{K}\nabla_{\hat{p}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{P}_i^n &= \hat{p}_n - h\sum_{j=1}^{s} \bar{a}_{ij}\hat{K}^T\nabla_{\hat{q}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{q}_{n+1} &= \hat{q}_n + h\sum_{j=1}^{s} b_j\hat{K}\nabla_{\hat{p}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{p}_{n+1} &= \hat{p}_n - h\sum_{j=1}^{s} \bar{b}_j\hat{K}^T\nabla_{\hat{q}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) \end{cases}$$

From (24) we know that

$$\begin{cases} \nabla_{\hat{q}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) &= \hat{K}^{-T}\nabla_u S(\hat{K}^{-1}\hat{Q}_j^n, \hat{P}_j^n) \\ \nabla_{\hat{p}}\hat{H}(\hat{Q}_j^n, \hat{P}_j^n) &= \nabla_v S(\hat{K}^{-1}\hat{Q}_j^n, \hat{P}_j^n) \end{cases}$$

So, we get

$$\begin{cases} \hat{K}^{-1}\hat{Q}_i^n &= \hat{K}^{-1}\hat{q}_n + h\sum_{j=1}^{s} a_{ij}\nabla_v S(\hat{K}^{-1}\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{P}_i^n &= \hat{p}_n - h\sum_{j=1}^{s} \bar{a}_{ij}\nabla_u S(\hat{K}^{-1}\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{K}^{-1}\hat{q}_{n+1} &= \hat{K}^{-1}\hat{q}_n + h\sum_{j=1}^{s} b_j\nabla_v S(\hat{K}^{-1}\hat{Q}_j^n, \hat{P}_j^n) \\ \hat{p}_{n+1} &= \hat{p}_n - h\sum_{j=1}^{s} \bar{b}_j\nabla_u S(\hat{K}^{-1}\hat{Q}_j^n, \hat{P}_j^n) \end{cases}$$

Let $U_i^n,\ V_i^n$ replace $\hat{K}^{-1}\hat{Q}_i^n,\ \hat{K}^{-1}\hat{Q}_i^n\hat{P}_i^n$ respectively, we have

$$\left\{\begin{array}{rcl} U_i^n &=& \hat{K}^{-1}\hat{q}_n + h\sum_{j=1}^{s} a_{ij}\nabla_v S(U_j^n, V_j^n) \\ V_i^n &=& \hat{p}_n - h\sum_{j=1}^{s} \bar{a}_{ij}\nabla_u S(U_j^n, V_j^n) \\ \hat{K}^{-1}\hat{q}_{n+1} &=& \hat{K}^{-1}\hat{q}_n + h\sum_{j=1}^{s} b_j\nabla_v S(U_j^n, V_j^n) \\ \hat{p}_{n+1} &=& \hat{p}_n - h\sum_{j=1}^{s} \bar{b}_j\nabla_u S(U_j^n, V_j^n) \end{array}\right. \tag{26}$$

From (29), we know that $(\hat{K}^{-1}\hat{q}_n, \hat{p}_n)$ is the numerical solution of the same symplectic PRK method for (25) with initial value $(\hat{K}^{-1}\hat{q}_0, \hat{p}_0)$. Since (25) is normal Hamiltonian system, the step-transition operator of symplectic PRK method for (25) is symplectic transform, i.e. the transform $(\hat{K}^{-1}\hat{q}_n, \hat{p}_n) \mapsto (\hat{K}^{-1}\hat{q}_{n+1}, \hat{p}_{n+1})$ is normal symplectic transform, then

$$\left[\frac{\partial(\hat{K}^{-1}\hat{q}_{n+1}, \hat{p}_{n+1})}{\partial(\hat{K}^{-1}\hat{q}_n, \hat{p}_n)}\right]^T J \left[\frac{\partial(\hat{K}^{-1}\hat{q}_{n+1}, \hat{p}_{n+1})}{\partial(\hat{K}^{-1}\hat{q}_n, \hat{p}_n)}\right] = J. \tag{27}$$

Moreover

$$\begin{aligned} \frac{\partial(\hat{K}^{-1}\hat{q}_{n+1}, \hat{p}_{n+1})}{\partial(\hat{K}^{-1}\hat{q}_n, \hat{p}_n)} &= \left[\frac{\partial(\hat{K}^{-1}\hat{q}_{n+1}, \hat{p}_{n+1})}{\partial(\hat{q}_{n+1}, \hat{p}_{n+1})}\right]\left[\frac{\partial(\hat{q}_{n+1}, \hat{p}_{n+1})}{\partial(\hat{q}_n, \hat{p}_n)}\right]\left[\frac{\partial(\hat{q}_n, \hat{p}_n)}{\partial(\hat{K}^{-1}\hat{q}_n, \hat{p}_n)}\right] \\ &= \begin{bmatrix} \hat{K}^{-1} & 0 \\ 0 & I_r \end{bmatrix}\left[\frac{\partial(\hat{q}_{n+1}, \hat{p}_{n+1})}{\partial(\hat{q}_n, \hat{p}_n)}\right]\begin{bmatrix} \hat{K} & 0 \\ 0 & I_r \end{bmatrix}, \end{aligned} \tag{28}$$

Combining (27) and (28), we have

$$\left[\frac{\partial(\hat{q}_{n+1}, \hat{p}_{n+1})}{\partial(\hat{q}_n, \hat{p}_n)}\right]^T L \left[\frac{\partial(\hat{q}_{n+1}, \hat{p}_{n+1})}{\partial(\hat{q}_n, \hat{p}_n)}\right] = L. \tag{29}$$

That is the transform: $(\hat{q}_n, \hat{p}_n) \mapsto (\hat{q}_{n+1}, \hat{p}_{n+1})$ is $L-$symplectic transform. ■

From *theorem* 2. and *theorem* 3. we see that when the symplectic PRK method is applied to Poisson system (6), the corresponding numerical mapping of (10) is an $L-$ symplectic mapping. In fact, the symplectic scheme is Poisson integrator of the Poisson system (6). The following theorem proves it.

Theorem 4. The corresponding step-transition is Poisson mapping of symplectic PRK method for Poisson system (6).

Proof: The only work we need to do is the proof of the transform $(q_0, p_0) \mapsto (q_1, p_1)$ is Poisson mapping, that is

$$\left[\frac{\partial(q_1, p_1)}{\partial(q_0, p_0)}\right]\begin{bmatrix} 0_{m\times m} & M \\ -M^T & 0_{m\times m} \end{bmatrix}\left[\frac{\partial(q_1, p_1)}{\partial(q_0, p_0)}\right]^T = \begin{bmatrix} 0_{m\times m} & M \\ -M^T & 0_{m\times m} \end{bmatrix}. \tag{30}$$

The Jacobi matrix is $\dfrac{\partial(q_1,p_1)}{\partial(q_0,p_0)} = \dfrac{\partial(\hat{q}_1,\hat{\hat{q}}_1,\hat{q}_1,\hat{\hat{q}}_1)}{\partial(\hat{q}_0,\hat{\hat{q}}_0,\hat{q}_0,\hat{\hat{q}}_0)}$.

From (20), we can know that $\hat{q}_1,\ \hat{p}_1$ are independent of $\hat{\hat{q}}_0,\ \hat{\hat{p}}_0,\ \hat{\hat{q}}_1,\ \hat{\hat{p}}_0,\ \hat{\hat{p}}_1,\ \hat{\hat{q}}_0$. Therefore, the correlative partial derivatives are all zeroes. Let $\hat{q}_0,\ \hat{p}_1$ replace $\hat{q}_1,\ \hat{p}_1$ in (21), then

$$\frac{\partial(q_1,p_1)}{\partial(q_0,p_0)} = \begin{bmatrix} \dfrac{\partial\hat{q}_1}{\partial\hat{q}_0} & 0_{r\times(m_1-r)} & \dfrac{\partial\hat{q}_1}{\partial\hat{p}_0} & 0_{r\times(m_2-r)} \\ C(\dfrac{\partial\hat{q}_1}{\partial\hat{q}_0}-I_r) & I_{m_1-r} & C\dfrac{\partial\hat{q}_1}{\partial\hat{p}_0} & 0_{(m_1-r)\times(m_2-r)} \\ \dfrac{\partial\hat{p}_1}{\partial\hat{q}_0} & 0_{r\times(m_1-r)} & \dfrac{\partial\hat{p}_1}{\partial\hat{p}_0} & 0_{r\times(m_2-r)} \\ \hat{C}^T\dfrac{\partial\hat{p}_1}{\partial\hat{q}_0} & 0_{(m_2-r)\times(m_2-r)} & \hat{C}^T(\dfrac{\partial\hat{p}_1}{\partial\hat{p}_0}-I_r) & I_{m_2-r} \end{bmatrix},$$

thus

$$\begin{aligned} &\frac{\partial(q_1,p_1)}{\partial(q_0,p_0)}\begin{bmatrix} 0_{m\times m} & M \\ -M^T & 0_{m\times m}\end{bmatrix}\left[\frac{\partial(q_1,p_1)}{\partial(q_0,p_0)}\right]^T \\ =& \begin{bmatrix} \Lambda_1 & \Lambda_1 C^T & \Lambda_3 & \Lambda_3\hat{C} \\ C\Lambda_1 & C\Lambda_1 C^T & C\Lambda_3 & C\Lambda_3\hat{C} \\ -{\Lambda_3}^T & -{\Lambda_3}^T C^T & \Lambda_2 & \Lambda_2\hat{C} \\ -\hat{C}^T{\Lambda_3}^T & -\hat{C}^T{\Lambda_3}^T C^T & \hat{C}^T\Lambda_2 & \hat{C}^T\Lambda_2\hat{C}\end{bmatrix}, \end{aligned} \tag{31}$$

where

$$\begin{aligned} \Lambda_1 =& -\frac{\partial\hat{q}_1}{\partial\hat{p}_0}\hat{K}^T\left[\frac{\partial\hat{q}_1}{\partial\hat{q}_0}\right]^T + \frac{\partial\hat{q}_1}{\partial\hat{q}_0}\hat{K}\left[\frac{\partial\hat{q}_1}{\partial\hat{p}_0}\right]^T; \\ \Lambda_2 =& -\frac{\partial\hat{p}_1}{\partial\hat{p}_0}\hat{K}^T\left[\frac{\partial\hat{p}_1}{\partial\hat{q}_0}\right]^T + \frac{\partial\hat{p}_1}{\partial\hat{q}_0}\hat{K}\left[\frac{\partial\hat{p}_1}{\partial\hat{p}_0}\right]^T; \\ \Lambda_3 =& -\frac{\partial\hat{p}_1}{\partial\hat{p}_0}\hat{K}^T\left[\frac{\partial\hat{q}_1}{\partial\hat{q}_0}\right]^T + \frac{\partial\hat{p}_1}{\partial\hat{q}_0}\hat{K}\left[\frac{\partial\hat{q}_1}{\partial\hat{p}_0}\right]^T. \end{aligned}$$

For L is non degenerate, from (32) we get $\left[\dfrac{\partial(\hat{q}_1,\hat{p}_1)}{\partial(\hat{q}_0,\hat{p}_0)}\right]L^{-1}\left[\dfrac{\partial(\hat{q}_1,\hat{p}_1)}{\partial(\hat{q}_0,\hat{p}_0)}\right]^T = L^{-1}$, i.e.

$$\left[\frac{\partial(\hat{q}_1,\hat{p}_1)}{\partial(\hat{q}_0,\hat{p}_0)}\right]\begin{bmatrix} 0 & \hat{K} \\ -\hat{K}^T & 0\end{bmatrix}\left[\frac{\partial(\hat{q}_1,\hat{p}_1)}{\partial(\hat{q}_0,\hat{p}_0)}\right]^T = \begin{bmatrix} 0 & \hat{K} \\ -\hat{K}^T & 0\end{bmatrix}.$$

Outspread the above formula, we have

$$\begin{aligned} \Lambda_1 =& \ 0_{r\times r} \\ \Lambda_2 =& \ 0_{r\times r} \\ \Lambda_3 =& \ \hat{K}. \end{aligned}$$

Put them into (31), we get (30). ■

5. Numerical Results and Conclusions

The symplectic partitioned Runge-Kutta (PRK) method is a Poisson scheme. In this section, we want to put it into solving equation (5). In (5), we choose the spectral element space based on Gauss-Lobatto-Legendre polynomials as the finite element space. First, we introduce the 1-D case: N-th order Legendre polynomial is

$$L_N(\xi) = \frac{1}{2^N N!}\frac{d^N}{d\xi^N}(\xi^2-1)^N,$$

GLL points $\{\xi_j, \quad j=0,1,\cdots,N\}$ are the zero points of $(1-\xi^2)L'_N(\xi)$.
On reference element $[-1,1]$, N-th order GLL basic functions are

$$\phi_j(\xi) = -\frac{1}{N(N+1)L_N(\xi_j)}\,\frac{(1-\xi^2)L'_N(\xi)}{\xi-\xi_j}, \quad j=0,1,\cdots,N. \tag{32}$$

such that $\phi_j(\xi_k)=\delta_{jk}, \qquad \forall\ j,k=0,\cdots,N.$
For polynomial $P(x)$ whose order is not more than $2N-1$, we have
$\int_{-1}^{1} P(\xi)d\xi = \sum_{k=0}^{N}\omega_k P(\xi_k)$, where the weight is $\omega_k = \frac{2}{N(N+1)[L_N(\xi_k)]^2}$.
$\forall f(\xi)\in[-1,1]$, f is a smooth function, its interpolation formula can be written as

$$f(\xi) = \sum_{j=0}^{N}\phi_j(\xi)f(\xi_j) + \mathcal{O}(\Delta\xi^{N+1}).$$

As for 3-D case, on reference element $[-1,1]\times[-1,1]\times[-1,1]$, we can choose $\Psi_i = \Phi_r(\xi)\Phi_s(\eta)\Phi_t(\zeta), \quad i=0,\cdots,N$, where $N=(N_\xi+1)(N_\eta+1)(N_\zeta+1), \quad N_\xi,\ N_\eta,\ N_\zeta$ are the number of GLL points in $\xi,\ \eta,\ \zeta$ directions, respectively.
Make the best use of properties of the basic functions for spectral element and some techniques [9] , we can arrive at a diagonal mass matrix. Accordingly, we can achieve high order accuracy in spatial discretization and the cost of computation is not increased. For simplicity, in this paper, we discuss the problem only for the 1-D case. Take a plane wave equation for example:

$$\begin{cases} \dfrac{\partial\varepsilon}{\partial t} &= & -c_0\dfrac{\partial\mathcal{H}}{\partial x} \\ \dfrac{\partial\mathcal{H}}{\partial t} &= & -c_0\dfrac{\partial\varepsilon}{\partial x} \end{cases} \tag{33}$$

where c_0 is the speed of light in vacuum.
Because we use the GLL spectral element to discretize equation in space, it yields a separable system. Then in temporal discretization, we can choose 4th-order explicit symplectic PRK method to deal with the resulting PDE. Its Butcher table is Table 2. We present several numerical examples to show superiority of the PRK method. Combined with the

Table 2: Table of Butcher for 4th-order symplectic PRK method

$$\begin{array}{c|cccc} \frac{\gamma_1}{2} & \frac{\gamma_1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & \frac{\gamma_1}{2} & \frac{\gamma_1+\gamma_2}{2} & 0 & 0 \\ \frac{3\gamma_1+2\gamma_2}{2} & \frac{\gamma_1}{2} & \frac{\gamma_1+\gamma_2}{2} & \frac{\gamma_1+\gamma_2}{2} & 0 \\ 1 & \frac{\gamma_1}{2} & \frac{\gamma_1}{2} & \frac{\gamma_1+\gamma_2}{2} & \frac{\gamma_1}{2} \\ \hline & \frac{\gamma_1}{2} & \frac{\gamma_1}{2} & \frac{\gamma_1}{2} & \frac{\gamma_1}{2} \end{array} \qquad \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \gamma_1 & \gamma_1 & 0 & 0 & 0 \\ \gamma_1+\gamma_2 & \gamma_1 & \gamma_2 & 0 & 0 \\ 1 & \gamma_1 & \gamma_2 & \gamma_1 & 0 \\ \hline & \gamma_1 & \gamma_2 & \gamma_1 & 0 \end{array}$$

spectral element method, we can gain more accurate numerical solutions but the computational cost dose not increase. And we compare it with a 4th-order non-symplectic RK method [9], its non-dissipative property is more and more obvious with the time increasing.

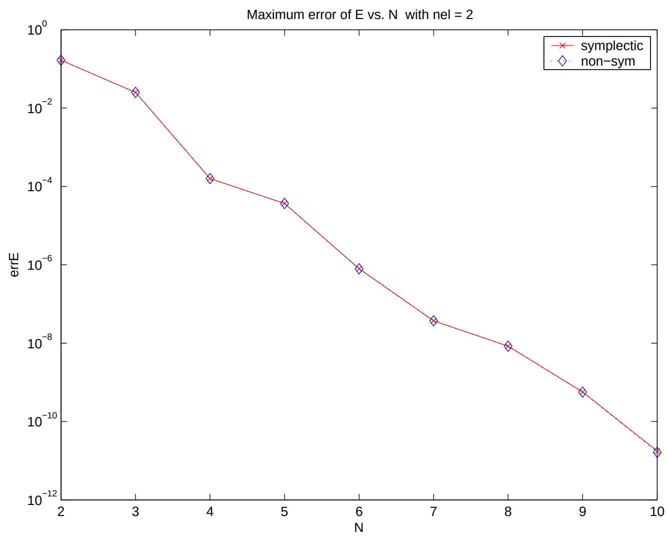

Fig. 1. Errors of Electric Field at $2.125T$(prt=1/64)

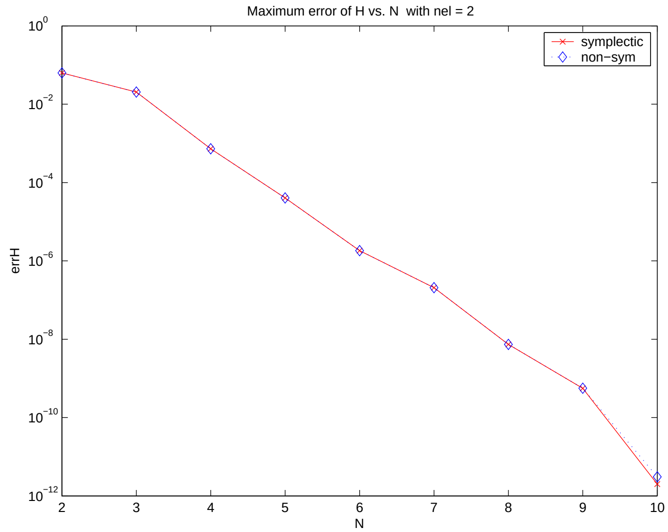

Fig. 2. Errors of Magnetic Field at $2.125T$(prt=1/64)

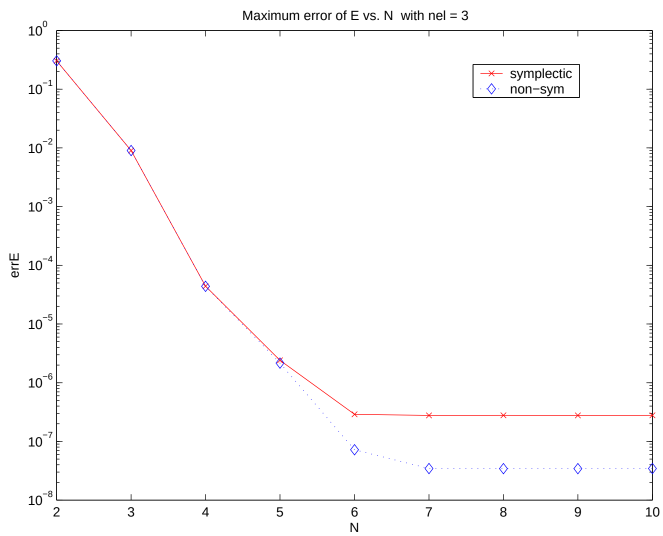

Fig. 3. Errors of Electric Field at $102.125T$(prt=1/8)

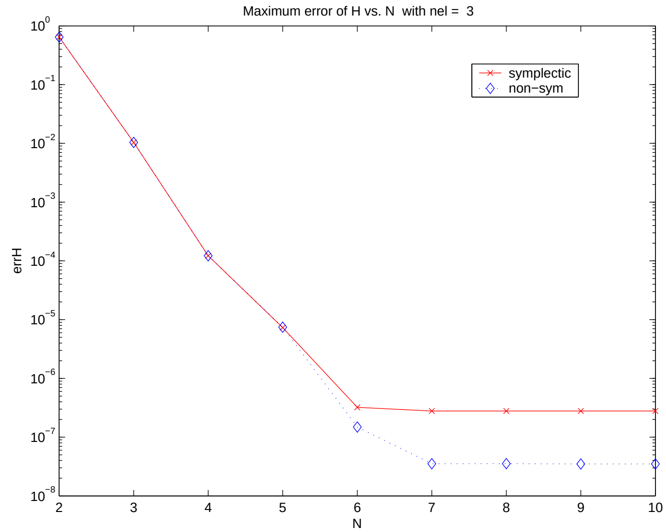

Fig. 4. Errors of Magnetic Field at $102.125T$(prt=1/8)

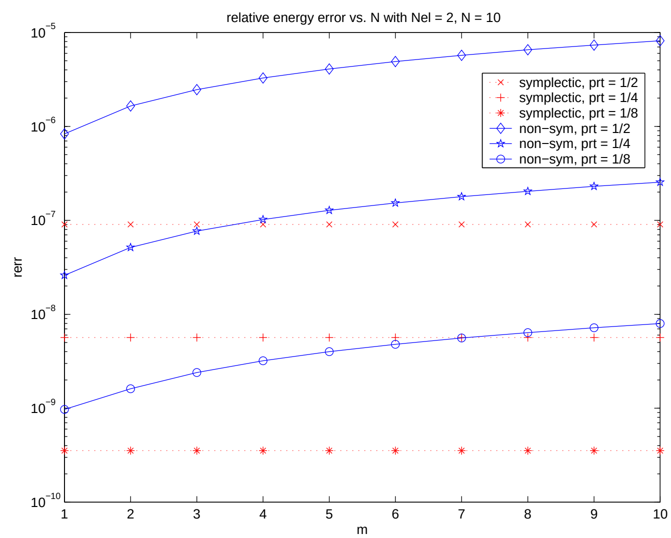

Fig. 5. Comparison of The Errors of Relative Energy between Symplectic and Non-Symplectic Method

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