Compatible Subdomain Level Isotropic/Anisotropic Discontinuous Galerkin Time Domain (DGTD) Method for Multiscale Simulation

by

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Dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the Department of Electrical and Computer Engineering in the Graduate School of Duke University

2015
Abstract

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Abstract

Domain decomposition method provides a solution for the very large electromagnetic system which are impossible for single domain methods. Discontinuous Galerkin (DG) method can be viewed as an extreme version of the domain decomposition, i.e., each element is regarded as one subdomain. The whole system is solved element by element, thus the inversion of the large global system matrix is no longer necessary, and much larger system can be solved with the DG method compared to the continuous Galerkin (CG) method.

In this work, the DG method is implemented on a subdomain level, that is, each subdomain contains multiple elements. The numerical flux only applies on the interfaces between adjacent subdomains. The subdomain level DG method divides the original large global system into a few smaller ones, which are easier to solve, and it also provides the possibility of parallelization. Compared to the conventional element level DG method, the subdomain level DG has the advantage of less total DoFs and flexibility in interface choice. In addition, the implicit time stepping is relatively much easier for the subdomain level DG, and the total CPU time can be much less for the electrically small or multiscale problems.

The hybrid of elements are employed to reduce the total DoF of the system. Low-order tetrahedrons are used to catch the geometry fine parts and high-order hexahedrons are used to discretize the homogeneous and/or geometry coarse parts. In addition, the non-conformal mesh not only allow different kinds of elements but
also sharp change of the element size, therefore the DoF can be further decreased.

The DGTD method in this research is based on the **EB** scheme to replace the previous **EH** scheme. Different from the requirement of mixed order basis functions for the field variables \( E \) and \( H \) in the **EH** scheme, the **EB** scheme can suppress the spurious modes with same order of basis functions for \( E \) and \( B \). One order lower in the basis functions in \( B \) brings great benefits because the DoFs can be significantly reduced, especially for the tetrahedrons parts.

With the basis functions for both \( E \) and \( B \), the **EB** scheme upwind flux and **EB** scheme Maxwellian PML, the eigen-analysis and numerical results shows the effectiveness of the proposed DGTD method, and multiscale problems are solved efficiently combined with the implicit-explicit hybrid time stepping scheme and multiple kinds of elements.

The **EB** scheme DGTD method is further developed to allow arbitrary anisotropic media via new anisotropic **EB** scheme upwind flux and anisotropic **EB** scheme Maxwellian PML. The anisotropic M-PML is long time stable and absorb the outgoing wave effectively. A new TF/SF boundary condition is brought forward to simulate the half space case. The negative refraction in \( \text{YVO}_4 \) bicrystal is simulated with the anisotropic DGTD and half space TF/SF condition for the first time with numerical methods.
To my beloved parents ...
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# List of Abbreviations and Symbols

## Abbreviations

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<tr>
<td>CFL</td>
<td>Courant-Friedrichs-Levy condition.</td>
</tr>
<tr>
<td>CG</td>
<td>continuous Galerkin.</td>
</tr>
<tr>
<td>CN</td>
<td>Crank-Nicolson method.</td>
</tr>
<tr>
<td>DDM</td>
<td>domain decomposition method.</td>
</tr>
<tr>
<td>DG</td>
<td>discontinuous Galerkin.</td>
</tr>
<tr>
<td>DGTD</td>
<td>discontinuous Galerkin time domain.</td>
</tr>
<tr>
<td>DoF</td>
<td>degree of freedom.</td>
</tr>
<tr>
<td>ExRK</td>
<td>explicit Runge-Kutta.</td>
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<tr>
<td>FDTD</td>
<td>finite-difference time-domain.</td>
</tr>
<tr>
<td>FEM</td>
<td>finite element method.</td>
</tr>
<tr>
<td>FETD</td>
<td>finite-element time-domain.</td>
</tr>
<tr>
<td>FVTD</td>
<td>finite-volume time-domain.</td>
</tr>
<tr>
<td>GLL</td>
<td>Gauss-Lobatto-Legendre polynomial.</td>
</tr>
<tr>
<td>GS</td>
<td>Gauss-Seidel iteration.</td>
</tr>
<tr>
<td>Im-ExRK</td>
<td>implicit / explicit Runge-Kutta method.</td>
</tr>
<tr>
<td>LT/QN</td>
<td>linear tangential / quadratic normal basis functions.</td>
</tr>
<tr>
<td>MoM</td>
<td>method of moments.</td>
</tr>
<tr>
<td>ODE</td>
<td>ordinary differential equations.</td>
</tr>
<tr>
<td>PDE</td>
<td>partial differential equations.</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
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<tr>
<td>---------</td>
<td>--------------------------------------------------</td>
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<tr>
<td>PEC</td>
<td>perfect electric conductor.</td>
</tr>
<tr>
<td>PMC</td>
<td>perfect magnetic conductor.</td>
</tr>
<tr>
<td>PML</td>
<td>perfectly matched layer.</td>
</tr>
<tr>
<td>PSTD</td>
<td>pseudospectral time-domain method.</td>
</tr>
<tr>
<td>SETD</td>
<td>spectral-element time-domain method.</td>
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I thank my parents for their endless love in me. They live in frugality and use their limited income to foster me for more than twenty years. Finally, I thank my wife, Dr. He Zhu, for her love, support, sacrifice and the kind and gentle disposition.
Even the frequency domain solver in electromagnetic wave modeling has gain much development in recent years (Chew et al., 2002; Song et al., 1997; Peng et al., 2013; Li and Jin, 2007; Peng et al., 2011), the requirements of a fast and reliable time domain solver has never been less. The advantages of time domain methods are mainly threefold. First, it can obtain the broad-band response just in one shot. Second, the time domain method can handle the non-linear process, including the EM-IC hybrid problem. In addition, the time domain solvers can simulate the transient problems which are difficult for the frequency domain solvers. These properties guarantee the time domain methods are irreplaceable in AD/DA hybrid IC design and chip packaging, EMC research, signal integrity analysis and etc.

The multiscale problems are on the frontier of both of the academic research and engineering. The coarse objects (or the homogeneous background media) can be very large compared to the wavelength, while the fine structures can be very small in size. The ratio of size between the whole computing region and the finest geometry structures may be thousands, or even larger. The property results in incremental complexity of the problem which can not be solved by traditional numerical methods
in computational electromagnetics. Therefore, an EM forward solver, which can handle the multi-scale problems in time domain both efficiently and accurately, is of great importance. It is also the main aim of this research. In addition, this research is further extended to deal with anisotropic media, in which the permittivity, permeability, electrical and magnetic conductivities can be arbitrary positive definite tensors.

To attain the goals stated above, an appropriate choice of numerical methods is crucial. A popular time domain method to solve first order Maxwell’s equations is Finite Difference Time Domain (FDTD) method brought forward by Yee (Yee et al., 1966) originally. The FDTD method is relatively easy to implement, robust and computationally cheap per cubic wavelength. Therefore, it is widely used in almost all the partial differential equations (PDEs) based problems (Taflove and Brodwin, 1975; Taflove, 1980; Holland, 1977; Mur, 1981; Maloney et al., 1990; Zheng et al., 2000). However, FDTD has the intrinsic weakness in mesh flexibility, which has a relative larger geometric error, especially for the curved or tilted structures. In addition, it can only preserve second order accuracy, which will bring significant numerical dispersion for electrically large problems. In addition, constrained by the CFL condition, the multi-scale problems usually have a very small time step interval, which will lead to an unacceptable CPU time sometimes.

Another time domain technique to solve Maxwell’s equations is the Finite Volume Time Domain (FVTD) method, which was first applied to computational fluid dynamics, and later adapted in the electromagnetic analysis (Shankar et al., 1990; Madsen and Ziolkowski, 1990; Holland et al., 1991; Madsen, 1995; Baumann et al., 2004, 2005; Fumeaux et al., 2004). Rather than pointwise approximations on a grid, finite volume scheme approximates the average integral value on a reference volume. It can use the unstructured mesh which can also enjoy the modeling flexibility. The field in each volume is linked with the adjacent volumes via the fluxes. The FVTD
method is free of grid dispersion, however, it is numerically dissipative which is not suitable for simulating the wave traveling in a long distance due to the attenuation.

The Finite Element Method (FEM) (Jin, 2007; Demkowicz and Vardapetyan, 1998) has been paid more attention in recent years. Compared to Finite Different (FD) methods, it has mesh flexibility with unstructured elements, thus can treat complex structures with good geometry approximation, this is the most attractive point of FEM. In addition, unlike methods based on Integral Equations (IEs), it allow arbitrary background media, therefore, it has a larger scope of applications; one general code is enough to solve the metal scattering objects, homogeneous and inhomogeneous scattering objects. Finite Element Time Domain (FETD) method can be regarded as a time domain version of FEM, which inherits the advantages from both finite element scheme and time domain methods. According to the governing equations, FETD can be divided into two class. One is to solve the second order curl-curl wave equations (Jiao et al., 2003; Lee et al., 1997; Gedney and Navsariwala, 1995) and the other is to deal with the first order Maxwell’s equations. The former class can use the conclusions and imitate the research methods from the well-developed frequency domain FEM. However, it is relatively difficult to add the Perfectly Matched Layer (PML). In this research, we concentrate on the later class, in which PML is easier to implement.

In the FETD method, mixed vector basis functions are employed to guarantee the continuity conditions be satisfied on the interfaces of adjacent elements. The well-studied and widely used scheme in FETD is based on the variables $\mathbf{E}$ and $\mathbf{H}$ (EH scheme), that is, the electric and magnetic field intensities. However, EH scheme has the problem of spurious modes which refer to the non-physical frequency components (Chen and Liu, 2009; Chen et al., 2010; Peterson et al., 1998; Jiang et al., 1996). The origins of these spurious solutions have been studied in (Bermúdez and Pedreira, 1992; Ikeuchi et al., 1981; Winkler and Brian Davies, 1984; Rahman and
Davies, 1984; Monk, 2003; Tonti, 2003). These non-physical solutions appear when
same order of basis functions for $E$ and $H$ are used, for example, $E1H1$ (first order
basis functions for both $E$ and $H$) (Cohen et al., 2007; Winkler and Brian Davies,
1984). To suppress the spurious modes, different order interpolation polynomials
should be employed, for example, $E1H2$ (first order basis functions for $E$ and second
order basis functions for $H$) (Chen and Liu, 2009; Chen et al., 2010, 2011). Com-
pared to $E1H1$, $E1H2$ has the same error convergence rate but more unknowns,
thus the computation load will increase dramatically. One promising way to solve
this problem is to use the variables $E$ and $B$ ($EB$ scheme) instead of $E$ and $H$. $EB$
scheme is supposed to be capable of suppressing spurious modes with same order
basis functions, thus the total unknowns can be reduced (Ren et al., 2013). This is
one key point of this research.

For the 3D multiscale problems, the number of unknowns can be very large,
usually at the level of million or even larger. Thus it is difficult or impossible to
solve the whole problem just in one domain because the system matrix is too large
to be inverted either explicitly or implicitly. Therefore, a new paradigm, domain
decomposition method (DDM), has been recently investigated for electromagnetic
problems (Cangellaris and Wu, 2005; Chen et al., 2010; Peng and Lee, 2010; Wang
et al., 2012; Xue and Jin, 2014). This computational strategy is to break a large
difficult problem into a few smaller ones which are easier to solve. One of the widely
used scheme for domain decomposition is discontinous Galerkin method, which is a
non-overlapping domain decomposition method.

The main objective of this research is to develop a new scheme discontinuous
Galerkin time domain (DGTD) method, that is, $EB$ scheme DGTD method, which
allows different kinds of elements according to the characteristic of the geometry
structures. It should be applied to solve the multiscale problems and other problems
with large number of unknowns. In addition, this DGTD method should be extended
to anisotropic media. The detailed specific aims are as follows:

- **Derive and implement new basis functions of the variable B for different kinds of elements:** When the Maxwell’s equations are solved with DGTD methods, we can use either EH scheme or EB scheme. In EH scheme, curl-conforming vector basis functions are used to discretize both E and H fields, they are from the first family of the Nédélec elements, i.e., the edge elements. However, in the EB scheme, besides the curl-conforming basis functions used for E, div-conforming vector basis functions are used to discretize B, they are from the second family of Nédélec elements, i.e., the face elements (Nédélec, 1986, 1980). The basis functions of the B field should be derived and implemented for tetrahedron, hexahedron and prism elements.

- **Extend the single domain EB scheme Galerkin method to multi-domain DGTD method:** The single domain EB scheme Galerkin method should be extended to the multi-domain situation. The EB scheme domain decomposition should not only allow same kind of elements for different sub-domains, but also different types of elements to maximize the efficiency. That is, the DGTD method can be not only tetrahedron-tetrahedron, hexahedron-hexahedron, prism-prism but also tetrahedron-hexahedron, tetrahedron-prism, hexahedron-prism and any other combination of these elements. The numerical flux, that is, Riemann Solver or central flux, should be modified to be compatible with the divergence-conforming basis functions. In addition, the splitting of the shared interface should be generalized, not related to the element type.

- **Derive and Implement Perfectly Matched Layer (PML) in EB scheme:** An effective and efficient EB scheme time domain Perfectly Matched Layer (PML) should be developed for the open boundary condition. It should use the high order basis functions to use as few as unknowns to maximize the
efficiency. In addition, the late time stability is required for the EB scheme PML. And the computational load for the updating the extra equations in the PML region should be light. The PML should be in a Maxwellian form to be compatible for the DGTD method, as split-form is not easy to implement is the Galerkin scheme based method.

- **Derive and Implement EB scheme DGTD for arbitrary anisotropic medium**: Based on the DGTD method for isotropic media, the anisotropic DGTD method should inherit all the advantages of the isotropic DGTD method, including the EB scheme, the hybrid of element types, the multiple solvers in time integration, the non-conformal mesh. In addition, it should allow permittivity, permeability and electric and magnetic conductivities of full tensors. Thus the anisotropic DGTD method needs a new EB scheme numerical fluxes for anisotropic media. In addition, the anisotropic EB scheme PML should be proposed to simulate the unbounded problems, it should also be Maxwellian, accurate and long time stable.

- **Code Package**: The code should provide a general strategy for the DGTD method, and it should not be sensitive either to the element type or to the time integration scheme. In addition, the main three parts of the code, i.e., preprocessing, spatial discretization and time stepping, should be well-separated, thus it is suitable to be developed simultaneously by different people. The preprocessing part is mainly to obtain the geometry information from the mesh files, generate the edges and faces to denote the basis functions, assign the material information and boundary conditions to these generated edges and faces, and count the DoFs of each subdomain for the field variables \( \mathbf{E} \) and \( \mathbf{B} \). The spatial discretization part assigns the basis functions for each edge and face generated from preprocessing part and assemble the global system matrices.
from the element matrices. The time stepping part takes the assembled system matrices from the spatial discretization part, apply different time integration scheme at a subdomain level including post-processing of the results.
Discontinuous Galerkin Time Domain (DGTD) method involves the studies of finite element method (FEM), spectral element method (SEM), Prism-Spectral element method and discontinuous Galerkin (DG) methods and time integration. These aspects are not isolated, they need to be considered simultaneously to achieve overall good performance of the DGTD method.

2.1 Governing Equations

According to the governing equations to be solved, the discontinuous Galerkin method in computational electromagnetics can be divided into two classes. One is based on the second order wave equation, either on subdomain level (Lou and Jin, 2006b; Tuncer et al., 2014) or element level (Lou and Jin, 2006a), and the other is based on the Maxwell’s equations (Alvarez et al., 2010; Fahs, 2009; Gedney et al., 2008; Li et al., 2015; Tobón et al., 2015; Chen et al., 2011; Ren et al., 2015). The former form has the advantage of symmetric mass matrix and implicit time stepping at same cost of explicit time stepping, however, it needs dual fields to handle the
boundary condition between subdomains, or it is relative complex to construct PML. The latter form is relatively expensive for implicit time stepping, however, it is much easier to approximate the numerical flux between adjacent subdomains and to derive the PML. In this research, the latter form is preferred, and the first order Maxwell’s equations are shown as follows:

\[
\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}_c - \mathbf{J}_i \tag{2.1}
\]

\[
\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} - \mathbf{M}_c - \mathbf{M}_i \tag{2.2}
\]

\[
\nabla \cdot \mathbf{D} = \rho_e \tag{2.3}
\]

\[
\nabla \cdot \mathbf{B} = \rho_m \tag{2.4}
\]

\[
\mathbf{D} = \varepsilon \mathbf{E} \tag{2.5}
\]

\[
\mathbf{B} = \mu \mathbf{H} \tag{2.6}
\]

\[
\mathbf{J}_c = \sigma_e \mathbf{E} \tag{2.7}
\]

\[
\mathbf{M}_c = \sigma_m \mathbf{H} \tag{2.8}
\]

where \( \mathbf{E} \), \( \mathbf{H} \), \( \mathbf{D} \) and \( \mathbf{B} \) are the electric field intensity, magnetic field intensity, the electric flux density and the magnetic flux density, respectively; \( \mathbf{J}_c \) and \( \mathbf{M}_c \) are the electric and magnetic current densities due to conductive properties of the medium; \( \mathbf{J}_i \)
and $\mathbf{M}_i$ are the electric and magnetic current densities due to imposed sources, while $\epsilon, \mu, \sigma_e, \text{ and } \sigma_m$ are the material’s permittivity, permeability, electric conductivity, and magnetic conductivity, respectively. Equations (2.1)-(2.4) are the topological laws and equations (2.5)-(2.8) are the constitutive laws.

2.2 Finite Element Method and Spectral Element Method

The finite element method is one of the most popular numerical tool to approximate the boundary value problems by transforming the partial differential equations to the system of linear algebra equations. The finite element method has been widely used in various disciplines, such as solid and fluid mechanics, thermodynamics, it was introduced to electromagnetics engineering since 1970s. According to the origin definition by Ciarlet (Ciarlet, 1978; Monk, 2003), the finite element can be regarded as a triad $(K, \mathcal{P}, \mathcal{N})$. $K \subset \mathbb{R}^d$ is a bounded closed set with nonempty interior and piecwise smooth boundary. $\mathcal{P}$ is a finite-dimensional space of functions on $K$, while $\mathcal{N} = \{N_1, N_2, \ldots, N_k\}$ is the set of basis functions for $\mathcal{P}$.

Recent research has shown that the finite element should be understood as a sequence of scalar and vector elements satisfying the De Rham diagram, which relates the Hilbert function spaces $H^1$, $\mathbf{H}(\text{curl})$, $\mathbf{H}(\text{div})$, and $L^2$ (Solín et al., 2004; Bossavit, 1998) with differential operators, is as shown below:

\begin{equation}
H^1 \xrightarrow{\nabla} \mathbf{H}(\text{curl}) \xrightarrow{\nabla \times} \mathbf{H}(\text{div}) \xrightarrow{\nabla} L^2
\end{equation}

where

\begin{equation}
H^1(\Omega) = \left\{ u \in L^2(\Omega) ; \frac{\partial u}{\partial x_i} \in L^2(\Omega), 1 \leq i \leq d \right\}
\end{equation}

\begin{equation}
\mathbf{H}(\Omega; \text{curl}) = \left\{ \mathbf{u} \in [L^2(\Omega)]^d ; \nabla \times \mathbf{u} \in [L^2(\Omega)]^d \right\}
\end{equation}
\[
\mathbf{H}(\Omega; \text{div}) = \left\{\mathbf{u} \in [L^2(\Omega)]^d; \nabla \cdot \mathbf{u} \in L^2(\Omega)\right\} \quad (2.12)
\]

\[
L^2(\Omega) = \left\{u : \Omega \rightarrow \mathbb{R} \left| \int_{\Omega} |u|^2 \, dx < \infty \right.\right\} \quad (2.13)
\]

with \(d\) being the dimension of the geometry.

In computational electromagnetics, the space \(\mathbf{H}(\text{curl})\) and \(\mathbf{H}(\text{div})\) forms a mathematical foundation for the analysis of stability and convergence of Maxwell’s equations, and it also provides the guidance of the choice of the vector basis functions for the field variables.

The research of the spaces \(\mathbf{H}(\text{curl})\) and \(\mathbf{H}(\text{div})\) causes a breakthrough of EM simulation in FEM, in which the vector basis functions are introduced (Bossavit and Verite, 1982; Barton and Cendes, 1987; Demkowicz et al., 2000). The field intensities, \(\mathbf{E}\) and \(\mathbf{H}\), should be discretized by the basis functions from space \(\mathbf{H}(\text{curl})\) and flux densities should be discretized by the basis functions from space \(\mathbf{H}(\text{div})\). These basis functions accurately model the nature of the field intensities and flux densities, thus eliminate many problems associated with the previous nodal basis functions. With the development of the vector basis functions, FEM has become a powerful simulations tool for various applications in electromagnetics.

Spectral element method (SEM) shares the mathematical fundamentals with FEM, however, it is a high order method (Komatitsch and Tromp, 2002; Ostachowicz et al., 2011; Liu et al., 2015; Graglia et al., 1997). Unlike FEM, in which 1st or 2nd order basis functions are employed, the shape function of SEM are usually high order Chebyshev, Laguerre or Lobatto polynomials with non-uniform spaced nodes. The zero points of these interpolation polynomials are denser at the ends of the elements, which allows the oscillations to be avoided. The computational error of
SEM, ε, decreases exponentially with the order of the approximation polynomials n, thus guarantees the fast (spectral) convergence to the exact solution. This property of SEM provides higher computational efficiency over FEM when modeling geometry coarse parts, as high order large elements could be used.

### 2.3 Hodge Operator

The De Rham diagram as shown in (2.9) provides the guidance of the choice of basis functions in FEM and SEM for electromagnetics. The basis functions of potentials, field intensity, flux density and charge density are from the function spaces of $H^1$, $H(curl)$, $H(div)$ and $L^2$, respectively.

In differential geometry, we denote $C^p$ as the three dimensional manifold with the differential forms of degree $p$ (p-form) and $d$ as the exterior derivative (Castillo et al., 2004; Arnold et al., 2010; Kotiuga, 1989). Thus the relationship $C^p \xrightarrow{d} C^{p+1}$ holds. The Hodge star operator, $\ast$, yields an isomorphism between $C^p$ and $C^{3-p}$, therefore, the De Rham complex leads to the following Tonti diagram (Tonti, 2001; Ren and Razek, 1996; Remacle et al., 1998):

$$
\begin{array}{ccccccc}
0 & \xleftarrow{d} & C^3 & \xleftarrow{d} & C^2 & \xleftarrow{d} & C^1 & \xleftarrow{d} & C^0 \\
\downarrow{\ast} & & \downarrow{\ast} & & \downarrow{\ast} & & \downarrow{\ast} & \\
C^0 & \xrightarrow{d} & C^1 & \xrightarrow{d} & C^2 & \xrightarrow{d} & C^3 & \xrightarrow{d} & 0 \\
\end{array}
$$

(2.14)

In discrete electromagnetics, the $\nabla$, $\nabla \times$ and $\nabla \cdot$ can be regarded as operator $d$, then the De Rham with Hodge operator are shown below (Llano, 2013):

$$
\begin{array}{ccccccc}
C^0 & \xrightarrow{d} & C^1 & \xrightarrow{d} & C^2 & \xrightarrow{d} & C^3 \\
H^1 & \xrightarrow{\nabla} & \mathbf{H}(curl) & \xrightarrow{\nabla \times} & \mathbf{B} & \xrightarrow{\nabla \cdot} & \rho_m \\
\Phi_E & \xleftarrow{\nabla \cdot} & \mathbf{D} & \xleftarrow{\nabla \times} & \mathbf{H} & \xleftarrow{\nabla} & \Phi_M \\
\rho_e & \xrightarrow{\nabla \cdot} & \mathbf{D} & \xleftarrow{\nabla \times} & \mathbf{H} & \xrightarrow{\nabla} & \Phi_M \\
L^2 & \xrightarrow{\nabla \cdot} & \mathbf{D} & \xleftarrow{\nabla \times} & \mathbf{H} & \xrightarrow{\nabla} & \Phi_M \\
C^3 & \xleftarrow{d} & C^2 & \xleftarrow{d} & C^1 & \xleftarrow{d} & C^0 \\
\end{array}
$$

(2.15)
In finite and spectral element methods, the field is discretized by the basis functions, the corresponding vector unknowns for $\mathbf{E}, \mathbf{B}, \mathbf{H}, \mathbf{D}$ are $\mathbf{e}, \mathbf{b}, \mathbf{h}, \mathbf{d}$, respectively. We can also call these unknown vectors cochains. The constitutive laws of the physical systems, which is described by the Hodge operators in the continuous world, can find their equivalence in the discrete level. Thus, some properties such as permeability, permittivity, and conductivity, which define the relationship between field intensity and flux density, have their counterparts in the numerical method: $\star_\epsilon, \star_{\epsilon^{-1}}, \star_\mu$ and $\star_{\mu^{-1}}$, in the following, we name them discrete counterparts of Hodge operators (discrete Hodge).

$$
\begin{array}{c}
\mathbf{e} \\
\star_\epsilon \downarrow \star_{\epsilon^{-1}}
\end{array} \quad
\begin{array}{c}
\mathbf{b} \\
\star_{\mu^{-1}} \downarrow \star_\mu
\end{array}
$$

These discrete counterparts are related with the mesh, the element shape, the basis functions and also the frequency, they contains the information of dispersion. A core problem of the numerical methods is the construction of the discrete counterparts, which must be a good approximation of the Hodge operators (Tarhasaari et al., 1999). There is not a canonical way to built it, different schemes to build the discrete Hodge lead to different numerical methods. Some popular Hodges includes the Yee (FDTD) Hodge, Galerkin Hodge, Whitney Hodge and etc. The mass matrix from Yee Hodge is diagonal and it is simple to build, but it only applies for the structured mesh. Galerkin Hodge is theoretically simple, the dual complex can be built via the barycenters of the primal complex, in addition, its system matrices are topological and metric-free. However, it is usually difficult to built a Galerkin Hodge in high order element and to handle some boundary conditions. Therefore, the Whitney Hodge, which uses Whitney elements to connect the continuum differential form and its discrete counterpart, is most widely used in finite element and spectral element
methods.

2.4 Subdomain Level Discontinuous Galerkin Method

Two classical methods are often used to solve the boundary value problems, one is the Ritz variation method, and the other is the Galerkin’s method. Ritz method seeks a stationary point of a functional which is a variation of the boundary value problem. The Galerkin method belongs to the family of the residual methods, which seeks a solution \( \tilde{u} = u \) to make the residual \( R = \mathcal{L}\tilde{u} - f \) to be zero. In general, a solution satisfying everywhere with the computational domain can not be achieved. Thus, an average-fashion solution over the subdomains of the computational region is feasible. Theoretically, any testing functions (also named as weighting function or trial functions) may be used even though the performances are different. If the weighting functions are chosen the same as the basis functions used to expand the fields (expansion functions), it is the popular Galerkin method.

A key point of the numerical simulation of a system is the total number of unknowns (degrees of freedom, DoFs). A traditional direct solver requires \( O(N^2) \) operations and storage units for a system from FEM (SEM) with \( N \) unknowns. Multi-frontal method can reach \( O(N^{4/3}) \) storage units and \( O(N^2) \) operations, while a newly proposed HSS multifrontal requires \( O(N\log N) \) storage units and \( O(N^2) \) operations. No optimal solver, which requires \( O(N) \) storage units and \( O(N) \) operations, has been developed yet for a general case. Because the storage and CPU operation increases faster than a linear rate, an effective and also intuitive solution for the large problem is domain decomposition. If a large system is divided into a few smaller ones each subdomain is much easier to solve. Further if the connections between these subdomains can be calculated at little cost, the total computation cost for the system will be much less. The domain decomposition method has been widely applied to spectral methods, finite element methods, boundary element methods and etc.
The common domain decomposition schemes includes Schwartz alternating method, Steklov-Poincare framework, Lagrange multiplier framework (FETI, mortar, non-overlapping Schwartz) and etc (Mathew, 2008).

In computational electromagnetics, different domain decomposition methods have been employed. Deprés introduced non-overlapping Schwartz scheme with Robin transmission condition to the 2D Helmholtz equations (Benamou and Desprès, 1997), and further developed to 3D (Stupfel and Mognot, 2000) and non-conforming mesh in (Arbogast and Yotov, 1997; Achdou et al., 2002). Further, mortar element, “ce-ment” element and FETI methods have been extended to the vector elements for EM simulation (Ben Belgacem et al., 2001; Lee et al., 2005; Vouvakis et al., 2006).

Discontinuous Galerkin (DG) methods are special finite element methods, in which the function space consists of piecewise polynomials. These polynomials are allowed to be completely discontinuous across element interfaces. The DG methods can be regarded as the most extreme case of nonconforming finite element methods, that is, one-element one-domain scheme. DG is first proposed to solve the hyperbolic in neutron transport (Reed and Hill, 1973), and further developed by Cockburn (Cockburn and Shu, 1989; Cockburn et al., 1989). Extensive applications of DG methods have been found in electromagnetics, fluid dynamics, elastic wave modeling and etc. The spirit of the DG method is using the flux to relax the continuity condition between adjacent elements.

In computational electromagnetics, DG method has been widely used in the finite element method. Most of them are in the time domain based on element level (Gedney et al., 2012; Li and Jiang, 2013a,b; Lu et al., 2005; Hu and Wang, 2012). In contrast, a subdomain level DG scheme is also studied (Chen and Liu, 2013, 2009), in which, each subdomain consists of multiple elements, and the numerical flux exists between adjacent subdomains. Inside a subdomain, the adjacent elements share the basis functions on the interface, which is the same as convention finite
element method. The advantage of the subdomain level DG lies in the following aspects: first, the DoF is less, because only the interface DoFs will double, while all the DoFs on each element’s face need to be doubled in element level DG; second, the choice of the interfaces between subdomains are relatively flexible, thus the area of the shared interface can be further reduced; last, and the most important, implicit time stepping is relatively more mature and easier to achieve for subdomain level DG method. This is very important for the multiscale problems and electrically small problems. However, the shortcoming of the subdomain DG method is the much larger system equations than the element level DG method. Thus controlling the total DoF of the system is very important.

2.5 Time Integration

The time domain method solve the Maxwell’s equations in a 4D manner, i.e., three spatial dimension plus the time dimension. The time stepping schemes can be classified as explicit or implicit according to the relationship between the time interval and the threshold of the Courant-Friedrichs-Levy (CFL) condition. Explicit time stepping schemes in DGTD methods include leap-frog (Lou and Jin, 2006a,b; Fahs and Lanteri, 2010; Ren et al., 2013), explicit Runge-Kutta (Gedney et al., 2012; Ren et al., 2015). Implicit time stepping is rarely used in the element level DGTD method, because even for the fine parts, local time stepping strategy combined with explicit time stepping scheme (Lörcher et al., 2008) can provide an efficient way for the element level DGTD methods. The few attempts for implicit time stepping in element level includes (Catella et al., 2010) for Maxwell’s equation and (Wang and Mavriplis, 2007) for Euler equation in unsteady compressible flow both in 2D. However, in the subdomain level DG, implicit time stepping can be used based on the Crank-Nicolson scheme, including direct methods, such as Block-Thomas method, LDU method, and the iterative solvers, Gauss-Siedel and etc (Chen et al., 2011;
Ye and Wang, 2011; Tobón et al., 2015; Tobon et al., 2015). In addition, hybrid implicit-explicit methods has also been proposed (Kanevsky et al., 2007; Chen et al., 2011; Dolean et al., 2010).
In finite element method (spectral element method), the computational region is broken into elements of simple shapes. The widely used are triangles, rectangles, quadrilateral and polygons in 2D and tetrahedrons, prism, pyramids, bricks, hexahedrons in 3D. Inside each elements, the interpolation polynomials (also termed as basis functions or shape functions) are required to approximate the quantity unknowns.

According to the quantities to be presented, the basis functions can be divided into two classes, one is scalar basis functions (nodal basis functions), and the other is vector basis functions (edge or face basis functions). In finite element methods for electromagnetics, the nodal basis functions are first utilized, and still being used in some aspects, such as potential problems. However, the scalar basis functions produce many problems (Bossavit and Verite, 1982; Webb, 1993; Csendes and Silvester, 1970), such as the contamination of the spurious modes in near fields, inconvenience in handling boundary conditions and singularities. The vector basis functions are introduced and extensively employed in computational electromagnetics later. For vector basis functions, the unknowns are associated with the edges (edge-based basis functions) and faces (face-based basis functions), and they can overcome many of the
problems related to the nodal basis functions. The construction of the edge elements on tetrahedrons and bricks can be found in (Nédélec, 1980). The face basis functions are not used as frequently as edge basis functions. In this research, we will use both of the edge and face basis functions to discretize the field quantities.

3.1 Basis Functions for Hexahedron

To solve (2.1) and (2.2), we use curl-conforming vector basis functions, denoted as \( \Phi \), to discretize \( \mathbf{E} \) (or \( \mathbf{H} \)), and divergence-conforming vector basis functions, denoted as \( \Psi \), to discretize \( \mathbf{B} \) (or \( \mathbf{D} \)). They belong to the first and second families of Nédélec elements, i.e., the edge elements and face elements (Nédélec, 1986, 1980), respectively.

\[
\hat{\Phi}_{ijk}^{(\xi,M)} = \hat{\xi}\phi_{i}^{(M-1)}(\xi)\phi_{j}^{(M)}(\eta)\phi_{k}^{(M)}(\zeta), i = 0, \cdots, M - 1; (j, k) = 0, \cdots, M
\]

\[
\hat{\Phi}_{ijk}^{(\eta,M)} = \hat{\eta}\phi_{i}^{(M)}(\xi)\phi_{j}^{(M-1)}(\eta)\phi_{k}^{(M)}(\zeta), j = 0, \cdots, M - 1; (i, k) = 0, \cdots, M
\] (3.1)

\[
\hat{\Phi}_{ijk}^{(\zeta,M)} = \hat{\zeta}\phi_{i}^{(M)}(\xi)\phi_{j}^{(M)}(\eta)\phi_{k}^{(M-1)}(\zeta), k = 0, \cdots, M - 1; (i, j) = 0, \cdots, M
\]

\[
\hat{\Psi}_{ijk}^{(\xi,M)} = \hat{\xi}\phi_{i}^{(M)}(\xi)\phi_{j}^{(M-1)}(\eta)\phi_{k}^{(M-1)}(\zeta), i = 0, \cdots, M; (j, k) = 0, \cdots, M - 1
\]

\[
\hat{\Psi}_{ijk}^{(\eta,M)} = \hat{\eta}\phi_{i}^{(M-1)}(\xi)\phi_{j}^{(M)}(\eta)\phi_{k}^{(M-1)}(\zeta), j = 0, \cdots, M; (i, k) = 0, \cdots, M - 1
\] (3.2)

\[
\hat{\Psi}_{ijk}^{(\zeta,M)} = \hat{\zeta}\phi_{i}^{(M-1)}(\xi)\phi_{j}^{(M-1)}(\eta)\phi_{k}^{(M)}(\zeta), k = 0, \cdots, M; (i, j) = 0, \cdots, M - 1
\]

The expressions of the \( M \)th order curl-conforming basis functions and divergence-conforming basis functions in a reference cubic element with \( (\xi, \eta, \zeta) \in [-1,1] \times [-1,1] \times [-1,1] \) are in (3.1) and (3.2), where \( \phi_{i}^{(M)} \) is defined as:

\[
\phi_{i}^{(M)}(x) = \frac{-(1 - x^{2})L_{N}'(x)}{N(N + 1)L_{N}(x_{m})(x - x_{m})}, m = 0, \cdots, M
\] (3.3)

\( L_{N}(x) \) is the Legendre polynomial of degree \( N \), and \( x_{m} \) are the GLL points.
The number of the curl-conforming basis functions in an $M$th-order reference element is $3 \times M \times (M + 1) \times (M + 1)$, and the number of the divergence-conforming basis functions is $3 \times M \times M \times (M + 1)$. A third-order reference element is shown in Fig. 3.1. Each curl-conforming basis function corresponds to an edge and each divergence-conforming basis function corresponds to a face. For example, on the front surface (as Fig. 3.1 shows), the number of edge basis functions is 24 and the number of face basis functions is 9. An example of the spatial distribution of the two kinds of vector basis functions in the third-order reference element is shown in Fig. 3.2. One of the curl-conforming basis functions in a third-order reference element is shown in Fig. 3.2(a), and its corresponding edge is in Fig. 3.2(b). One of the divergence-conforming basis functions in a third-order reference element is shown in Fig. 3.2(c), and its corresponding face is in Fig. 3.2(d). Obviously, the main contribution of the vector field of a curl-conforming (divergence-conforming) basis function is in the volume near its corresponding edge (face). The direction of the curl-conforming basis function is parallel to the corresponding edge and the tangential component is continuous across the adjacent elements. The direction of the divergence-conforming basis functions is perpendicular to the corresponding face and the normal component is continuous across the adjacent elements.
Covariant and contravariant transformations are needed Peterson et al. (1998) to transform the basis function from the reference cubic element to the physical domain as follows:

\[
\Phi = J_a^{-1} \hat{\Phi} \quad (3.4)
\]

\[
\nabla \times \Phi = \frac{1}{|J_a|} J_a^T \hat{\nabla} \times \hat{\Phi} \quad (3.5)
\]

\[
\Psi = \frac{1}{|J_a|} J_a^T \hat{\Psi} \quad (3.6)
\]
where
\[ \hat{\nabla} = \frac{\partial}{\partial \xi} \hat{\xi} + \frac{\partial}{\partial \eta} \hat{\eta} + \frac{\partial}{\partial \zeta} \hat{\zeta} \] (3.7)

Here \( J_a \) is the Jacobian matrix of the transformation defined as
\[
J_a = \begin{bmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\
\frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta}
\end{bmatrix}
\] (3.8)

\( J_a^T \) and \( J_a^{-1} \) are the transpose and the inversion of the Jacobian matrix, respectively. \( x, y, z \) are the coordinates in the physical domain, and \( \xi, \eta, \zeta \) are the coordinates in the reference domain. This transformation is also required by other types of elements, such as tetrahedrons and prism, etc.

### 3.2 Basis Functions for Tetrahedron

There are two classes of curl conforming basis functions for \( \mathbf{E} \) or \( \mathbf{H} \) in a reference tetrahedron. The first order one is Constant-tangential/Linear-normal (Ct/Ln); the second order one is Linear-tangential/Quadratic-normal (Lt/Qn). In one tetrahedron, there are 6 Constant-tangential/Linear-normal(Ct/Ln) basis functions and 20 Linear-tangential/Quadratic-normal (Lt/Qn) basis functions. The mathematical expressions are (Tobón et al., 2015):

- **Constant-tangential/Linear-normal (E1 and H1),** one basis function per edge (\( \Phi_{CtLn}^{ij} \)).
  \[
  \Phi_{ij}^{CtLn} = s_i \nabla s_j - s_j \nabla s_i
  \] (3.9)

- **Linear-tangential/Quadratic-normal (E2 and H2),** two basis functions per edge (\( \Phi_{ij}^{LtQn} \)) and two per face (\( \Phi_{ijk}^{LtQn} \)).
Figure 3.3: Reference tetrahedron

\[ \Phi_{ij}^{\text{LQn}} = s_i \nabla s_j \]  
\[ \Phi_{ijk}^{\text{LQn}} = s_is_k \nabla s_j - s_js_k \nabla s_i \]  

where \( s_p \) barycentric coordinate of the \( p \)-th vertex.

The reference tetrahedron we use is as illustrated in Fig. 3.3. Examples of the field distribution of \( \text{Ct/Ln} \) and \( \text{Lt/Qn} \) basis functions in reference tetrahedron are shown in Fig. 3.4.

The newly proposed divergence-conforming basis functions for \( \mathbf{B} \) (also can be \( \mathbf{D} \)) can be divided into Constant-normal/Linear-tangential (Cn/Lt), the divergence component of its vector field is a constant at the corresponding face and its tangential component changes linearly at this face, and Linear-normal/Quadratic-tangential (Ln/Qt), the divergence component its vector field changes linearly at the corresponding face and its tangential component changes quadratically at this correspond-
Figure 3.4: Curl-conforming basis functions in the reference tetrahedron. (a) Constant-tangential/Linear-normal (Ct/Ln) basis function according to the bold edge; (b) Linear-tangential/Quadratic-normal (Lt/Qn) basis function according to the bold line.

In one tetrahedron, there are 4 Constant-normal/Linear-tangential (Cn/Lt) and 15 Linear-normal/Quadratic-tangential (Ln/Qt) basis functions. The mathematical expressions are:

- Constant-normal/Linear-tangential (D1 and B1), one basis function per face ($\Psi_{ijk}^{CnLt}$).

$$\Psi_{ijk}^{CnLt} = 2 (s_i \vec{v}_{jk} + s_j \vec{v}_{ki} + s_k \vec{v}_{ij}) \quad (3.12)$$

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• Linear-normal/Quadratic-tangential (D2 and B2), three basis functions per face ($\Psi_{ij}^{LnQt}$) and three in the volume ($\Psi_{ijkl}^{LnQt}$).

$$\Psi_{ij}^{LnQt} = s_i \vec{\nu}_{jk}$$

(3.13)

$$\Psi_{ijkl}^{LnQt} = 2s_l (s_i \vec{\nu}_{jk} + s_j \vec{\nu}_{ki} + s_k \vec{\nu}_{ij})$$

(3.14)

where $\vec{\nu}_{ij} = \nabla s_i \times \nabla s_j$.

Examples of the vector field distribution of Cn/Lt and Ln/Qt basis functions in the reference tetrahedron are shown in Fig. 3.5.

3.3 Basis Functions for Prism Element

The prism element can be understood as a hybrid form of hexahedron and tetrahedron. In the lateral ($xy$) plane, it is discretized with low-order triangles and then the surface mesh sweeps along the $z$ direction to form a prism mesh. The reference prism element is shown in Fig. 3.6.

Note in the lateral plane, the triangular mesh is used to catch the relatively fine structure. With triangles, high order basis functions are not preferred. Usually, only the first and second order vector basis functions are enough. In the $z$ direction, arbitrary order of GLL polynomial can be employed according to the height of this layer.

The curl-conforming basis functions we use in prism can be divided into two classes (Tobón et al., 2014), the low-order one and high-order one. (Note, here the 'low' and 'high' are referred to the order of basis functions used for the triangles in the lateral mesh, not referred to the $z$ direction). For the low-order one, we can divide the basis functions into two sets according to the directions of these vector basis functions. One group of them are parallel to the lateral plane, and the other group
Figure 3.5: Divergence-conforming basis functions in the reference tetrahedron. (a) Constant-normal/Linear-tangential (Cn/Lt) basis function according to shaded face; (b) Linear-normal/Quadratic-tangential (Lt/Qn) basis function according to the shaded face.

are in the $z$ direction. The first set can be described as the product of Constant-tangential/Linear-normal (Ct/Ln) edge basis functions in the lateral triangles, $\Theta^{(1)}$, and a $N$th-order polynomial $\phi^{(N)}$, with $N + 1$ Gauss–Lobatto–Legendre points, i.e., the roots of the derivative of the Gauss–Lobatto–Legendre polynomials (Lee et al., 2006; Lee and Liu, 2007).

$$\hat{\Omega}^{(1,N)}_{1_{ik}} (\xi, \eta, \varsigma) = \Theta^{(1)}_i (\xi, \eta) \phi^{(N)}_k (\varsigma)$$ (3.15)
with \( i = 1, 2, 3; \quad k = 1, 2, \cdots, N + 1 \) and

\[
\Theta_1^{(1)}(\xi, \eta) = (s_{i+1} \nabla s_{i+2} - s_{i+2} \nabla s_{i+1}) \tag{3.16}
\]

where \( s_i \) is the simplex coordinate of the \( i \)th node of the triangle.

The second set of the low-order basis functions, which are in the \( z \) direction, are the product of the first order nodal basis function \( s \) in the lateral triangle and \((N - 1)\)th-order polynomial \( \phi^{(N-1)} \)

\[
\hat{\Omega}_{2ik}^{(1, N)}(\xi, \eta, \zeta) = \zeta s_i(\xi, \eta) \phi_k^{(N-1)}(\zeta) \tag{3.17}
\]

with \( i = 1, 2, 3; \quad k = 1, 2, \cdots, N \).

The high-order class can also be divided into two sets, which are transverse to and parallel to the height (\( z \) direction) of the prism. The first set can be described as the product of Linear-tangential/Quadratic-normal (Lt/Qu) edge basis functions in the lateral triangles, \( \Theta^{(2)} \), and a \( N \)th-order polynomial in the \( z \) direction, with \( N + 1 \) Gauss–Lobatto–Legendre points.

\[
\hat{\Omega}_{1ijk}^{(2, N)}(\xi, \eta, \zeta) = \Theta_j^{(2)}(\xi, \eta) \phi_k^{(N)}(\zeta) \tag{3.18}
\]

with \( i = 1, 2, 3; \quad j = 1, 2, 3; \quad k = 1, 2, \cdots, N + 1 \) and \( \Theta_j^{(2)}(\xi, \eta) \) have eight terms.
in total, six of them are:

\[ \Theta_{ij}^{(2)} (\xi, \eta) = s_i \nabla s_j, \quad i = 1, 2, 3; \quad j = 1, 2, 3; \quad i \neq j \quad (3.19) \]

and the other two are

\[ \Theta_{ij}^{(2)} (\xi, \eta) = (1 - s_i - s_j) s_j \nabla s_i - (1 - s_i - s_j) s_i \nabla s_j, \quad i = 1, 2; \quad j = 1, 2; \quad i \neq j \quad (3.20) \]

The second set of high-order basis functions, which are along the \( z \) direction, are the product of the second order nodal basis function \( L \) in the lateral triangle and \((N - 1)\)th-order polynomial \( \phi^{(N-1)} \).

\[ \hat{\Omega}_{2ijk}^{(2,N)} (\xi, \eta, \varsigma) = \varsigma L_{ij} (\xi, \eta) \phi_k^{(N-1)} (\varsigma) \quad (3.21) \]

with \( i = 1, 2, 3; \quad j = 1, 2, 3; \quad k = 1, 2, \cdots, N \). The six second order nodal basis functions \( L \) are: \( L_{ij} (\xi, \eta) = (2s_i - 1)s_i, \quad i = 1, 2, 3, \quad L_{ij} (\xi, \eta) = s_i s_j, \quad i, j = 1, 2, 3 \quad i \neq j \).

\[ L_{ij} (\xi, \eta) = (2s_i - 1)s_j, \quad i = 1, 2, 3 \quad (3.22) \]

and

\[ L_{ij} (\xi, \eta) = s_i s_j, \quad i, j = 1, 2, 3; \quad i \neq j \quad (3.23) \]

The sketch of the distributions of the low-order and high order curl-conforming basis functions are shown in Figure 3.7. Every arrow on the edge is corresponding to one curl-conforming basis function.

Similar to the curl-conforming basis functions, the divergence-conforming basis functions we use in prism can also be divided into two classes, the low-order one and high-order one.

For the low-order one, we can also divide the basis functions in two sets according to their directions like what is done for the curl-conforming basis functions. The first
Figure 3.7: Sketch of curl-conforming basis functions in spectral prism elements. (a) Ct/Ln in lateral plane and 4th order in height; (b) Lt/Qn in lateral plane and 5th order in height.

set can be described as the product of a constant $C$, for the triangle face, and a $N$th-order polynomial $\phi^{(N)}$ in the height. Different from the situation in curl-conforming basis functions, the first set divergence-conforming basis functions are in the height direction.

$$\hat{\Xi}_{2ik}^{(1,N)}(\xi, \eta, \varsigma) = \hat{\varsigma} C \phi_k^{(N)}(\varsigma)$$

with $k = 1, 2, \cdots, N + 1$.

The second set is the product of Constant-normal/Linear-tangential (Cn/Lt) edge basis functions in the lateral triangles, and a $N - 1$th-order GLL polynomial $\phi^{(N-1)}$ in the $z$ direction. The second set of divergence-conforming basis functions are parallel to the $xy$ plane.

$$\hat{\Xi}_{1k}^{(1,N)}(\xi, \eta, \varsigma) = \Upsilon_i^{(1)}(\xi, \eta) \phi_k^{(N-1)}(\varsigma)$$

where $i = 1, 2, 3; k = 1, 2, \cdots, N$.

$$\Upsilon_i^{(1)}(\xi, \eta) = \hat{\varsigma} \times (s_{i+1} \nabla s_{i+2} - s_{i+2} \nabla s_{i+1})$$

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Figure 3.8: Sketch of low-order divergence-conforming basis functions in spectral prism elements. (a) Cn/Lt in lateral plane and 3rd order GLL in height; (b) constant in lateral plane and 4th order GLL in height.

For the high order one, the first set is the product of $s_i$ and a $N$th-order polynomial $\phi^{(N)}$ in the height.

$$\hat{\Xi}_{2ik}^{(2,N)}(\xi, \eta, \zeta) = \hat{s}_i \phi_k^{(N)}(\zeta)$$ (3.27)

where $i = 1, 2, 3; k = 1, 2, \ldots, N$. Note that the physical meaning of $s_i$ in the above equation is the flux across the triangle face, it is not corresponding to the nodes even it has the same math expression as the simplex coordinates.

The second set is the product of Linear-normal/Quadratic-tangential (Lt/Qn), $\hat{\zeta} \times \Theta_{i}^{(2)}$, and a $N - 1$th-order polynomial $\phi^{(N-1)}$ in the height.

$$\hat{\Xi}_{1ijk}^{(2,N)}(\xi, \eta, \zeta) = \hat{\zeta} \times \Theta_{ij}^{(2)}(\xi, \eta) \phi_k^{(N-1)}(\zeta)$$ (3.28)

The sketch of the distributions of the low-order and high-order divergence-conforming basis functions are shown in Fig. 3.8 and Fig. 3.9, respectively.

In Fig. 3.9(a), eight of the nine vertical faces in each layer are linked with basis functions, this can be also seen in Fig. 3.9(b). In Fig. 3.9(c), the middle one of the four faces in each layer is not related with basis functions.
Figure 3.9: Sketch of high-order divergence-conforming basis functions in spectral prism elements. (a) $\text{Ln}/\text{Qt}$ in the lateral plane and 3rd order GLL in height; (b) top view of Fig. 3.9(a) (c) simplex in the lateral plane and 4th order GLL in height.

Examples of the field distribution of low-order curl-conforming basis functions in a reference prism are shown in Figure 3.10. Examples of the field distribution of high-order curl-conforming basis functions in a reference prism are shown in Figure 3.11.

Examples of the field distributions of high-order divergence-conforming basis

Figure 3.10: Low-order curl-conforming basis functions in a reference prism element. (a) One horizontal low-order curl-conforming basis function corresponding to the bold edge; (b) one vertical low-order curl-conforming basis function corresponding to the bold edge.
functions in a reference prism element are shown in Fig. 3.12. Examples of the field distribution of high-order divergence-conforming basis functions in a reference prism are shown in Fig. 3.13.

The advantage of prism element is obvious, as in the \( xy \) plane, the triangular mesh guarantees the geometry detail information can be caught, and in the \( z \) direction,
Figure 3.13: High-order divergence-conforming basis function in a reference prism elements: (a) horizontal high-order divergence-conforming basis function corresponding to the the shaded face (b) vertical high-order divergence-conforming basis function corresponding to the the shaded face.

High order interpolation polynomials can provide spectral accuracy. Therefore prism element is a good choice for the cases in which the structures in $xy$ plane are fine and layered media or homogeneous media in the $z$ direction.
EB Scheme v.s. EH Scheme

The DGTD methods in electromagnetics can be implemented with the second-order wave equations, with either $\mathbf{E}$ or $\mathbf{H}$ as the unknowns (Tsai et al., 2002; Lee et al., 1997; Jiao et al., 2002, 2003; Wong et al., 1995; Gedney and Navsariwala, 1995; Gan and Jiao, 2007) or with the first-order Maxwell’s equations, with two unknowns, the EB scheme (Koning et al., 2005; Feliziani and Maradei, 1997; He and Teixeira, 2007; Donderici and Teixeira, 2008; Marais and Davidson, 2008; Guillouard et al., 1999; Sekine and Asai, 2011; Ren et al., 2013) or EH scheme (Lee and Liu, 2009; Cangellaris et al., 1987; Huang et al., 2013). When the second approach is used, the field variables $\mathbf{E}$ and $\mathbf{H}$ are expanded in terms of edge basis functions to satisfy tangential continuity across adjacent elements. However, this scheme yields spurious modes when the same order of interpolation polynomials are used for both fields (denoted as $\mathbf{E}_n\mathbf{H}_n$) Jiang et al. (1996); Cohen et al. (2007); Tobón et al. (2011). Therefore, to suppress the spurious modes, either $\mathbf{E}_{n+1}\mathbf{H}_n$ or $\mathbf{E}_n\mathbf{H}_{n+1}$ scheme ($\mathbf{E}$ and $\mathbf{H}$ differ by one order) is required. However, the solution accuracy is mainly determined by the lower order polynomial of the two field variables. Therefore, spurious modes in EH scheme are avoided at the cost of a higher order interpolation. This will add the number of
unknowns significantly in 3D cases, and consequently increase memory overhead and CPU time. However, the $\text{EB}$ scheme is free of spurious modes even with the same order of interpolation polynomials for $E$ and $B$ (Ren et al., 2013; Llano, 2013), and this advantage will alleviate the computation load.

The root reason for the different performances of these schemes are due to the establishment of the discrete Hodge. The Whitney element we used produce a map from the $p$-form cochain to the $p$-form space. If $\text{EB}$ scheme is used, the system matrix will do the rest of the work, from the $p$-form space to the $(p+1)$-form cochain, thus the exterior operator is simulated. If $\text{EH}$ scheme is used, the discrete Hodge should map a $p$ cochain on the primal complex to the $(3p)$ cochain on the dual complex. Therefore, if $E$ is put on the primal complex, $H$ must be on the dual complex, as shown in Fig. 4.1.

![Diagram](image)

**Figure 4.1:** $\text{EB}$ and $\text{EH}$ schemes by Whitney elements.

A summary of the schemes aforementioned can be summarized as below:

Choice One (Compatible): $E$ and $B$ both one the primal complex, use Whitney 1-form for $E$ and Whitney 2-form for $B$ to construct the Whitney Hodge correctly.
Choice Two (Compatible): \( \mathbf{E} \) on the edge of primal complex, \( \mathbf{H} \) on the edge of the dual complex to construct Galerkin Hodge. Galerkin Hodge does not equal to Whitney Hodge in general. However, for the 2-form in 3-D cases, Galerkin Hodge equals to Whitney Hodge. Thus in the 3D DGTD methods, the face basis function for \( \mathbf{B} \) can be regarded as an edge basis function in its dual complex for \( \mathbf{H} \).

Choice Three (Incompatible): \( \mathbf{E} \) and \( \mathbf{H} \) both on the primal complex (\( \mathbf{E}_n \mathbf{H}_n \)), the discrete Hodge is not constructed correctly, thus it will have spurious modes.

Choice Four (Low efficiency): \( \mathbf{E} \) on the edge of the primal complex, \( \mathbf{H} \) on the edge of another primal complex (\( \mathbf{E}_n \mathbf{H}_{n+1}, \mathbf{E}_{n+1} \mathbf{H}_n, \mathbf{E}_{n+2} \mathbf{H}_n \) and etc). In fact, we have arbitrary number of combinations with different orders for \( \mathbf{E} \) and \( \mathbf{H} \). In this way, the discrete Hodge is almost established totally randomly, thus it may be very low efficient, as will shown later in the numerical parts.

4.1 Spurious Modes

Spurious Modes refer to the frequency components those appear after numerical simulations, thus lead to incorrect answer. They are usually from inappropriate presentation of a physical problem. In the DGTD method, we can use two ways to check whether the spurious modes exist. One way is to record the time domain response and compared to a reference results. If the obvious difference is not from insufficient sampling or bugs, it is from spurious modes. The two results can be compared in the frequency domain as well after Fourier transformation. This way need a full simulation of the case. Another way is to check the eigenvalues of the discretized system. Take a resonant cavity as example, each eigenvalue is corresponding to one resonant frequency. Eigenvalues not related to resonant frequencies will result in spurious modes.

In the DGTD method, the system of equations (2.1) and (2.2) can be transformed into frequency domain assuming time harmonic solutions. After this transformation,
we can calculate out the eigenvalues value and eigenvectors of the system, then, the
spurious modes will be found if they exist, because the spurious modes will be in
the form of non-physical resonant frequencies of the system. If the variables \( e \) and \( b \)
are separated into two vectors, (2.1) and (2.2) can be written in the following forms
(the detailed formulations for the matrices \( M_{ee}, M_{hh}, M_{bb}, K_{eh}, K_{he}, K_{eb} \) and \( K_{be} \)
can be found in (Ren et al., 2015) or in the following chapter, here we can just take
them as known matrices here):

\[
j \omega M_{ee} e - K_{eb} b = 0 \quad (4.1)
\]

\[
j \omega M_{bb} b - K_{be} e = 0 \quad (4.2)
\]

Similarly, if we use \( e \) and \( h \) as variables

\[
j \omega M_{ee} e - K_{eh} h = 0 \quad (4.3)
\]

\[
j \omega M_{hh} h - K_{he} e = 0 \quad (4.4)
\]

Therefore, using equations (4.1) and (4.2) or (4.3) and (4.4), the eigenproblem
can be formulated as follow:

\[
Y e = \chi X e \quad (4.5)
\]

where

\[
Y = K^{eb} [M^{bb}]^{-1} K^{be} \quad (4.6)
\]

or

\[
Y = K^{eh} [M^{hh}]^{-1} K^{he} \quad (4.7)
\]

and

\[
X = M^{ee} \quad (4.8)
\]

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where $e$ and $\chi = (c_0 k)^2$ represent eigenvectors and eigenvalues, respectively, which must be associated with electric field patterns and wavenumbers allowed in the physical system. Consequently, eigensolutions without a physical meaning are spurious ones, and must be removed.

4.2 Advantages of EB scheme

It is found that in EH scheme, $E_n H_n$ suffers from spurious modes. To suppress these spurious modes, either $E_{n+1} H_n$ or $E_n H_{n+1}$ scheme is needed at the cost of more unknowns. However, EB scheme is free of spurious modes even with same order of basis functions for $E$ and $B$. Thus the EB scheme can have less DoFs. The advantage of the EB scheme over the EH scheme is analyzed with different kinds of elements via eigenvalue analysis.

The numerical eigenvalues of a PEC cavity is analyzed to confirm the spectral accuracy of the proposed EB scheme SETD method and to show its advantages in accuracy over the EH scheme SETD method. The size of the cavity is $2 \text{ m} \times 1 \text{ m} \times 4 \text{ m}$ and it is discretized by two elements with the size of $2 \text{ m} \times 1 \text{ m} \times 2 \text{ m}$ as shown in Fig. 4.2. The DoFs, whose corresponding edges lie on the PEC face, are set to zeros and deleted from the unknown vector when solving the linear system. The relationship between the analytical frequency $f_a$ and the corresponding analytical eigenvalue $\sigma_a$ is

$$\sigma_a = (2\pi f_a)^2$$  \hspace{1cm} (4.9)

The relative error of the numerical eigenvalue $\sigma_n$ is defined as

$$e = \frac{|\sigma_n - \sigma_a|}{\sigma_a}$$  \hspace{1cm} (4.10)

The relative errors of eigenvalues versus Degrees of Freedom (DoFs) of three selected modes, TE$_{102}$, TE$_{012}$ and TM$_{110}$, are shown in Fig. 4.3 in a semi-log plot. For both
**EH** scheme and **EB** scheme SETD methods, p-refinement (refinement by increase polynomial order $p$) (Tang and Baeder, 1998; Solín et al., 2004) is employed to enhance the accuracy. The orders of basis functions are 1, 3, 5 and 7, respectively. The relation between the relative error and order of the basis functions (and thus the DoFs) is nearly linear in this semi-log plot, indicating that the relative error decreases nearly exponentially with the increment of DoFs for both the **EH** and **EB** schemes. This confirms that the proposed **EB** scheme SETD method can achieve spectral accuracy. For the same number of unknowns, it always has a smaller error. Therefore, the proposed **EB** scheme SETD method is a good option to replace the **EH** scheme SETD method.

**Figure 4.2**: Mesh of the PEC cavity.

A coaxial cavity is tested for the proposed **EB** scheme SETD method with a non-structured hexahedron mesh. The inner and outer radii of the cavity are $a = 2$ mm and $b = 5$ mm, respectively, and the height is $d = 20$ mm. The first eight analytical resonant frequencies are listed in Table 4.1. The mesh of the cavity is shown in Figure 4.4. In this case, high-order elements, which are large in geometric size, are not good choices because they cannot approximate the curve edges well. So we use $E_1H_2$ and $E_2H_3$ for **EH** scheme and $E_2B_2$ for **EB** scheme. Unlike the rectangular cavity, h-refinement (refinement by decreasing the element size $h$) (Tang and Baeder, 1998) is employed here to study the relative error convergence rate versus the number of unknowns. Under h-refinement, the mesh of the coaxial cavity in the horizontal and
height directions becomes denser at the same time. The four different meshes for this cavity are as follows: the number of the elements on the outer circle of the cavity is 8, 10, 12, 14, respectively, and the number of the elements on the height direction is 5, 6, 7, 8, respectively. The relation between the DoFs and the relative errors from these four different meshes are compared for TEM\(_1\) mode and TE\(_{2,1,1}\) mode. The results are shown in Fig. 4.5 and Fig. 4.6. The proposed E2B2 scheme has smaller error than E1H2 and E2H3 schemes under the same number of unknowns.

The two above-mentioned cases show that the EB scheme is more efficient than the EH scheme under both p-refinement and h-refinement. Thus, the EB scheme is a promising substitution for the EH scheme SETD methods for Maxwell’s equations.

Table 4.1: First eight modes and the corresponding resonant frequencies of the air-filled coaxial cavity

<table>
<thead>
<tr>
<th>Mode</th>
<th>Resonant Frequency (GHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TEM(_1)</td>
<td>7.4948110</td>
</tr>
<tr>
<td>TEM(_2)</td>
<td>14.989622</td>
</tr>
<tr>
<td>TE(_{1,1,1})</td>
<td>15.846394</td>
</tr>
<tr>
<td>TE(_{1,1,2})</td>
<td>20.490442</td>
</tr>
<tr>
<td>TEM(_3)</td>
<td>22.500000</td>
</tr>
<tr>
<td>TE(_{1,1,3})</td>
<td>26.478448</td>
</tr>
<tr>
<td>TE(_{2,1,1})</td>
<td>28.160966</td>
</tr>
<tr>
<td>TEM(_4)</td>
<td>29.979246</td>
</tr>
</tbody>
</table>

A three dimensional cavity with dimensions of 10 mm × 7.5 mm × 5 mm is solved (Figure 4.7). Eigensolutions (i.e., frequency domain solutions) are obtained from (4.5), using both schemes: (i) EH system of ordinary differential equations (4.3) and (4.4); and (ii) EB system of equations (4.1) and (4.2).

E2B2 (Lt/Qn for E field and Ln/Qt for B) has the best performance respect to E1H2 and E1B1 as we can see in Figure 4.8. For same error, E1H2 requires 10 times more unknowns than E1B1, and similarly, E1B1 requires 10 times more unknowns than E2B2. For a given number of unknowns, E2B2 formulation is one and two
orders of magnitude more accurate than $E_1B$ and $E_1H$ formulations, respectively.

The $EB$ scheme is also compared to $EH$ scheme for prism element under the same computation expense. The size of the PEC cavity is $2m \times 1m \times 4m$. The xy plane is discretized with triangles, the average size of which is $0.2m$. In the z direction, only one element with high order GLL interpolation is used. For the $EH$ scheme, mixed order basis functions for $E$ and $H$ is necessary to suppress the spurious modes, however, the $EB$ scheme is not restricted to this requirement. In this case, the basis functions we utilize for $EH$ scheme increase from $E_{11}H_{22}$ to $E_{17}H_{28}$. (The first digit is the order of the basis functions for the horizontal face, and the second digit is the order of the PLL interpolation polynomials, for Example, $E_{14}$ means the 4th order in z direction and 1st order in $xy$ plane). For the $EB$ scheme, we can divide the basis functions into two groups by the interpolation order of the horizontal triangles: one is $E_{1n}B_{1n}$, here we use basis functions from $E_{11}B_{11}$ to $E_{18}B_{18}$; the other is $E_{1(n+1)}B_{1(n+1)}$, we use basis functions from $E_{21}B_{21}$ to $E_{27}B_{27}$. The comparison of relative errors of the eigenvalues versus Degree of Freedoms (DoFs) of two selected modes, $TE_{011}$ and $TE_{201}$, are shown in Fig. 4.9. We can see both $E_{1n}B_{1n}$ and $E_{1(n+1)}B_{1(n+1)}$ have better performance in accuracy than $E_{1n}H_{2(n+1)}$ under the same DoF. The convergence rate of the new $EB$ scheme Prism Element Time Domain method is approximately exponential until the triangular mesh error in the XY plane is reached. This error is the limitation of p-refinement in the Z direction. From Fig. 4.9, it is obvious the error limitation of the $EB$ scheme is smaller, that is, higher accuracy can be obtained if DoF is large enough. $E_{1n}B_{1n}$ is more computational economic than $E_{1(n+1)}B_{1(n+1)}$, however, the error limitation of $E_{1(n+1)}B_{1(n+1)}$ is smaller. This can deliver two choices to make a balance between accuracy and resource. When computational resource is limited, $E_{1n}B_{1n}$ can be used. If the accuracy requirement is very strict, $E_{1(n+1)}B_{1(n+1)}$ can be used.
Figure 4.3: Relative error vs. DoFs in a semi-log plot. (a) TE_{102} mode; (b) TE_{012} mode; (c) TM_{110} mode.
Figure 4.4: Mesh of the coaxial cavity.

Figure 4.5: TEM$_1$ mode eigenvalue error vs. DoF in a log-log plot.

Figure 4.6: TE$_{2,1,1}$ mode eigenvalue error vs. DoF in a log-log plot.
**Figure 4.7**: PEC cavity and single tetrahedral mesh ($\Delta = 1$ mm)

**Figure 4.8**: Error in eigenvalues vs. number of unknowns of first mode ($\text{TE}_{110}$).
Figure 4.9: Relative error vs DoF in log-log scale (a) TE$_{011}$ mode; (b) TE$_{210}$ mode.
Isotropic DGTD Method

Assuming the medium is isotropic (permittivity, permeability and conductivity are scalars), the first-order Maxwell’s equations based on the electric field intensity $E$ and magnetic flux density $B$ from the imposed current densities are:

\[ \varepsilon \frac{\partial E}{\partial t} = \nabla \times \mu^{-1} B - \sigma_e E - J_s \]  
\[ \frac{\partial B}{\partial t} = -\nabla \times E - \sigma_m \mu^{-1} B - M_s \]

\[ \nabla \cdot \varepsilon E = \rho_e \]

\[ \nabla \cdot B = \rho_m \]

where $J_s$ and $M_s$ are the imposed electric and magnetic current density sources, respectively; $\varepsilon$, $\mu$, $\sigma_e$, and $\sigma_m$ denote material’s permittivity, permeability, electric conductivity and magnetic conductivity, respectively.
5.1 DG Scheme Maxwell’s Equations

The DG method is applied for domain decomposition in the proposed EB scheme SETD method. Assume that the number of subdomains is \( N \). Denote the \( i \)th subdomain as the local subdomain and \( j \)th as an adjacent one as shown in Fig. ??.

After testing, the weak form of Maxwell’s equations for the local subdomain is:

\[
\begin{align*}
\int_{V} \Phi_{p}^{i} \cdot (\epsilon \frac{\partial E^{i}}{\partial t} + \sigma_{r} E^{i} + J^{i})dV & = \int_{V} \nabla \times \Phi_{p}^{i} \cdot \mu^{-1} B^{i}dV + \int_{S} \Phi_{p}^{i} \cdot (\hat{n}^{i} \times \mu^{-1} B^{i})dS \\
\int_{V} \Psi_{p}^{i} \cdot (\frac{\partial B^{i}}{\partial t} + \sigma_{m} \mu^{-1} B^{i} + M^{i})dV & = -\int_{V} \nabla \times \Psi_{p}^{i} \cdot E^{i}dV - \int_{S} \Psi_{p}^{i} \cdot (\hat{n}^{i} \times E^{i})dS
\end{align*}
\]

where \( \Phi_{p} \) and \( \Psi_{p} \) are the testing functions, \((\cdot)^{i}\) and \((\cdot)^{t}\) are the vectors for the \( i \)th subdomain field and total field, respectively, and \( \hat{n}^{i} \) is the unit outward vector on the boundary. When the integration region is in the volume, we have \((\cdot)^{t} = (\cdot)^{i}\). However, \((\cdot)^{t}\) is from the contribution of both the \( i \)th subdomain and the \( j \)th subdomain when the integration region is on the shared surfaces.
To obtain the values of \( \hat{n}_i \times E^t \) and \( \hat{n}_i \times \mu^{-1} B^t \), Riemann Solver (upwind flux) is employed,

\[
(\hat{n}_i \times E^t) = \frac{\hat{n}_i \times (Y^i E^i + Y^j E^j)}{Y^i + Y^j} - \frac{\hat{n}_i \times \hat{n}_i \times (\mu^i B^i - \mu^j B^j)}{\mu^i \mu^j (Y^i + Y^j)} \tag{5.7}
\]

\[
(\hat{n}_i \times \frac{B^t}{\mu}) = \frac{\hat{n}_i \times (\mu^i Z^i B^i + \mu^j Z^j B^j)}{\mu^i \mu^j (Z^i + Z^j)} - \frac{\hat{n}_i \times \hat{n}_i \times (E^i - E^j)}{Z^i + Z^j} \tag{5.8}
\]

where \( \mu^i \) and \( \epsilon^i \) are relative permeability and permittivity of the \( i \)th subdomain, respectively. \( Z^i = \sqrt{\mu^i / \epsilon^i} \) and \( Y^i = 1 / Z^i \) are the impedance and admittance. Then we have the discretized linear system for the \( i \)th subdomain:

\[
M_{ee}^{ii} \frac{dE^i}{dt} = K_{ee}^{ii} e^i + C_{ee}^{ii} e^i + j^i + \sum_{j=1}^{N} L_{ee}^{ij} e^j + \sum_{j=1}^{N} L_{ee}^{ij} e^j \tag{5.9}
\]

\[
M_{bb}^{ii} \frac{dB^i}{dt} = K_{bb}^{ii} b^i + C_{bb}^{ii} b^i + m^i + \sum_{j=1}^{N} L_{bb}^{ij} b^j + \sum_{j=1}^{N} L_{bb}^{ij} b^j \tag{5.10}
\]

We can define the inner product of two functions as \( \langle f, g \rangle_{V_e} = \int_{V_e} f^T \cdot g dV \), where \( V_e \) is the volume of the element and \( (\cdot)^T \) denotes the transpose of a vector. Then the elemental form of the matrices are:

\[
(M_{ee})_{pq} = \langle \Phi_p, \epsilon \Phi_q \rangle_{V_e} \tag{5.11}
\]

\[
(M_{bb})_{pq} = \langle \Psi_p, \Psi_q \rangle_{V_e} \tag{5.12}
\]

\[
(C_{ee})_{pq} = \langle \Phi_p, \sigma_e \Phi_q \rangle_{V_e} \tag{5.13}
\]

\[
(C_{bb})_{pq} = \langle \Psi_p, \sigma_m \mu^{-1} \Psi_q \rangle_{V_e} \tag{5.14}
\]
\[(K_{eb})_{pq} = \langle \nabla \times \Phi_p, \mu^{-1} \Psi_q \rangle_{V_e} \quad (5.15)\]

\[(K_{be})_{pq} = -\langle \Psi_p, \nabla \times \Phi_q \rangle_{V_e} \quad (5.16)\]

\[(j)_p = -\langle \Phi_p, J \rangle_{V_e} \quad (5.17)\]

\[(m)_p = -\langle \Psi_p, M \rangle_{V_e} \quad (5.18)\]

\[(L^{ij}_{eb})_{pq} = -\frac{Z_2}{Z_{12}} \langle \Phi_p^i, (\hat{n}^i \times \Psi_q^j) \rangle_{S_{ij}} \quad (5.19)\]

\[(L^{ij}_{be})_{pq} = -\frac{Y_2}{Y_{12}} \langle \Psi_p^i, (\hat{n}^i \times \Phi_q^j) \rangle_{S_{ij}} \quad (5.20)\]

\[(L^{ii}_{eb})_{pq} = -\frac{Z_2}{Z_{12}} \sum_{j=1}^{N} \langle \Phi_p^i, (\hat{n}^i \times \Psi_q^j) \rangle_{S_{ij}} \quad (5.21)\]

\[(L^{ii}_{be})_{pq} = \frac{Y_1}{Y_{12}} \sum_{j=1}^{N} \langle \Psi_p^i, (\hat{n}^i \times \Phi_q^j) \rangle_{S_{ij}} \quad (5.22)\]

\[(L^{ij}_{ee})_{pq} = \frac{1}{Z_{12}} \langle (\hat{n}^i \times \Phi_p^i), (\hat{n}^i \times \Phi_q^j) \rangle_{S_{ij}} \quad (i \neq j) \quad (5.23)\]

\[(L^{ij}_{bb})_{pq} = \frac{1}{Y_{12}} \langle \Psi_p^i, (\hat{n}^i \times \Psi_q^j) \rangle_{S_{ij}} \quad (i \neq j) \quad (5.24)\]

\[(L^{ii}_{ee})_{pq} = \sum_{j=1}^{N} \frac{-1}{Z_{12}} \langle (\hat{n}^i \times \Phi_p^i), (\hat{n}^i \times \Phi_q^j) \rangle_{S_{ij}} \quad (5.25)\]
\[ (L_{bb}^{ii})_{pq} = \sum_{j=1}^{N} \frac{-1}{Y_{12}} \mathbb{I}((\hat{n}_i^i \times \Psi^j_p, (\hat{n}_i^i \times \Psi^j_q))_{s_{ij}} \]  

where \( S_{ij} \) is the interface between the \( i \)th and \( j \)th subdomains, subscripts \( p \) and \( q \) are the local indexes of basis functions.

5.1.1 The EB Scheme Well-posed PML in DGTD Method

The EB scheme DGTD method is combined with the strongly well-posed PML given by Fan and Liu (Fan and Liu, 2003), to simulate the unbounded problems. The compact vector form of Maxwell’s equations in the PML region is as follows:

\[ \nabla \times \tilde{E} = -\frac{\partial \tilde{B}}{\partial t} - \Lambda_1 \tilde{B} - \Lambda_2 \tilde{B} \]  

and

\[ \nabla \times \mu^{-1} \tilde{B} = \epsilon \frac{\partial \tilde{E}}{\partial t} + \epsilon \Lambda_1 \tilde{E} + \epsilon \Lambda_2 \tilde{E} \]  

where

\[ \tilde{B} = B + \Lambda_0 \tilde{B} \]  

\[ \tilde{E} = E + \Lambda_0 \tilde{E} \]  

\[ \Lambda_0 = diag\{\omega_x, \omega_y, \omega_z\} \]
\Lambda_1 = \text{diag}\{\omega_y + \omega_z - \omega_x, \omega_z + \omega_x - \omega_y, \omega_x + \omega_y - \omega_z\} \quad (5.34)

\Lambda_2 = \text{diag}\{(\omega_x - \omega_y)(\omega_y - \omega_z), (\omega_y - \omega_x)(\omega_z - \omega_y)\} \quad (5.35)

\omega_\eta is the attenuation coefficient in the direction \eta (\eta = x, y, z). \tilde{\mathbf{B}}, \bar{\mathbf{B}} and \mathbf{B} are expanded with the same divergence-conforming basis functions and \tilde{\mathbf{E}}, \bar{\mathbf{E}} and \mathbf{E} are expanded with the same curl-conforming basis functions, that is, \tilde{\mathbf{B}} = \sum \tilde{b}_i \Psi_i, \bar{\mathbf{B}} = \sum \bar{b}_i \Psi_i, \tilde{\mathbf{E}} = \sum \tilde{e}_i \Phi_i, \bar{\mathbf{E}} = \sum \bar{e}_i \Phi_i and \mathbf{E} = \sum e_i \Phi_i.

The PML formulations above can be expanded to the multidomain scenario, which can be expressed in a discretized system as follows:

\begin{align}
M_{ee}^i \frac{d\tilde{e}_i}{dt} &= K_{eb}^i \tilde{b}_i + R_{ee}^i \tilde{e}_i^i + \sum_{j=1}^{N} L_{ei}^{ij} \tilde{b}_j + \sum_{j=1}^{N} L_{e\tilde{e}}^{ij} \tilde{e}_j^i \quad (5.36) \\
M_{bb}^i \frac{d\tilde{b}_i}{dt} &= K_{be}^i \tilde{e}_i + R_{ee}^i \bar{e}_i^i + \sum_{j=1}^{N} L_{be}^{ij} \tilde{e}_j + \sum_{j=1}^{N} L_{b\tilde{b}}^{ij} \bar{b}_j \quad (5.37) \\
M_{ee}^i \frac{d\bar{e}_i}{dt} &= M_{ee}^i \bar{e}_i^i + T_{ee}^i \tilde{e}_i^i \quad (5.38) \\
M_{bb}^i \frac{d\bar{b}_i}{dt} &= M_{bb}^i \bar{b}_i^i + T_{bb}^i \bar{b}_i^i \quad (5.39)
\end{align}

where

\begin{align}
(R_{ee})_{pq} &= -\langle \Phi_p, \epsilon \Lambda_1 \Phi_q \rangle_{V_e} \quad (5.40) \\
(S_{ee})_{pq} &= -\langle \Phi_p, \epsilon \Lambda_2 \Phi_q \rangle_{V_e} \quad (5.41) \\
(T_{ee})_{pq} &= -\langle \Phi_p, \epsilon \Lambda_0 \Phi_q \rangle_{V_e} \quad (5.42)
\end{align}

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\[(\mathbf{R}_{bb})_{pq} = -\langle \Psi_p, \Lambda_1 \Psi_q \rangle_{V_e} \] (5.43)

\[(\mathbf{S}_{bb})_{pq} = -\langle \Psi_p, \Lambda_2 \Psi_q \rangle_{V_e} \] (5.44)

\[(\mathbf{T}_{bb})_{pq} = -\langle \Psi_p, \Lambda_0 \Psi_q \rangle_{V_e} \] (5.45)

The other elemental matrices are the same as (5.11)- (5.26).

A key feature of the DGTD method is the non-conformal mesh, which not only allows different types of elements, but also allows a sharp change of the element size across the interface as shown in . This is very important for controlling the total DoFs of the system.

\[\text{Figure 5.2: 3D non-conformal mesh. (a) Two adjacent subdomains with different types of elements; (b) Interface treatment of the shared interface.}\]
Figure 5.3: 2D non-conformal mesh. (a) Single domain mesh; (b) Multidomain mesh.

5.2 Time Integration Scheme

5.2.1 Explicit Leap-Frog

Explicit leap-frog method use staggered time for $\mathbf{E}$ and $\mathbf{B}$ similar to the FDTD method. In DGTD method, leap-frog time marching based on the upwind flux is as
below:

\[
\text{for } n = 1 : N_t \\
\quad \text{for } i = 1 : N_d \\
\quad \quad b^{(i)}_{n+\frac{1}{2}} = b^{(i)}_{n-\frac{1}{2}} + \Delta t (M_{bb}^{(i)})^{-1}[K_{be}^{(i)}e_n^{(i)} \\
\quad \quad \quad + C_{bb}^{(i)}b_n^{(i)} + M_n^{(i)} + \sum_{j=1}^{N_d} L_{be}^{(ij)}e_n^{(j)}] \\
\quad \quad \quad + C_{ee}^{(i)}e_n^{(i)} + \Delta t (M_{ee}^{(i)})^{-1}[K_{eb}^{(i)}b_{n+\frac{1}{2}}^{(i)} \\
\quad \quad \quad \quad + \sum_{j=1}^{N_d} L_{eb}^{(ij)}b_n^{(j)}] \\
\quad \text{end} \\
\text{end} \\
\] (5.46)

where \(N_t\) is the number of time steps and \(N_d\) is the number of subdomains.

5.2.2 Explicit 4th order Runge-Kutta Method

The fourth-order explicit Runge-Kutta method can be applied to the DGTD method in both physical and PML regions for time integration. For the \(i\)th subdomain, the linear system can be described as

\[
M^i d\ddot{v}^i dt = L^{ii} \ddot{v}^i + \sum_{j=1,j\neq i}^{N} L^{ij} \dddot{v}^j + S^i \ddot{v}^i \\
(5.47)
\]

\[
M^i d\ddot{v}^i dt = M^i \dddot{v}^i + T^i \dddot{v}^i \\
(5.48)
\]

where

\[
L^{ii} = \begin{bmatrix}
R_{ee}^{ii} + L_{ee}^{ii} & K_{eb}^{ii} + L_{eb}^{ii} \\
K_{be}^{ii} & L_{bb}^{ii}
\end{bmatrix}, \quad L^{ij} = \begin{bmatrix}
L_{ee}^{ij} & L_{eb}^{ij} \\
L_{be}^{ij} & L_{bb}^{ij}
\end{bmatrix}, \quad j \neq i
\] (5.49)

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\[
S^i = \begin{bmatrix}
S_{ee}^i & 0 \\
0 & S_{bb}^i
\end{bmatrix},
T^i = \begin{bmatrix}
T_{ee}^i & 0 \\
0 & T_{bb}^i
\end{bmatrix}
\] (5.50)

\[
\tilde{v}^i = \begin{bmatrix}
\tilde{e}^i \\
\tilde{b}^i
\end{bmatrix},
\bar{v}^i = \begin{bmatrix}
\bar{e}^i \\
\bar{b}^i
\end{bmatrix}
\] (5.51)

Assuming that the solutions of the vector unknowns on the \(n\)th time step have already been obtained, the solutions of the \((n+1)\)th time using the \(s\)th-order Runge-Kutta method is

\[
\tilde{v}_{n+1}^i = \tilde{v}_n^i + \Delta t \sum_{k=1}^{s} b_k \tilde{u}_k^i
\] (5.52)

\[
\bar{v}_{n+1}^i = \bar{v}_n^i + \Delta t \sum_{k=1}^{s} b_k \bar{u}_k^i
\] (5.53)

where

\[
M^i \tilde{u}_k^i = \sum_{j=1}^{N} L^{ij}(\tilde{v}_n^i + \Delta t \sum_{l=1}^{k-1} a_{k,l} \tilde{u}_l^j) + S^i(\tilde{v}_n^i + \Delta t \sum_{l=1}^{k-1} a_{k,l} \tilde{u}_l^i) + \tilde{j}(t_n + c_k \Delta t) \] (5.54)

\[
M^i \bar{u}_k^i = M^i(\bar{v}_n^i + \Delta t \sum_{l=1}^{k-1} a_{k,l} \bar{u}_l^i) + T^i(\bar{v}_n^i + \Delta t \sum_{l=1}^{k-1} a_{k,l} \bar{u}_l^i)
\] (5.55)

and the coefficients \(a_{k,l}, b_k\) and \(c_k\) are from the Butcher tableau (Butcher, 2008). Non-PML regions are just a special case, which only needs (5.52) and (5.54) while setting \(\bar{v}\) and \(\bar{u}\) to be zero.

5.2.3 Implicit-Explicit Runge-Kutta

Hybrid implicit-explicit Runge-Kutta (ImExRK) method can be applied for the cases where the computational region contains both geometry fine and coarse parts. For the physical subdomains, either implicit or explicit Runge-Kutta (RK) method can be used depending on whether the it is subdomain with fine mesh or coarse mesh.
Constrained to the Courant-Friedrich-Levy (CFL) condition, explicit Runge-Kutta (EXRK) time stepping is conditional stable and computationally cheap because the mass matrix is sparse and symmetric. The implicit Runge-Kutta (IMRK) time stepping is unconditionally stable, so the time step can be much larger than the explicit scheme and the total CPU time is much less, but at the cost of more memory consumption. Therefore, especially for multiscale cases, a trade-off between CPU time and memory overhead is necessary for the physical region via choosing either implicit or explicit scheme for each subdomain. For the PML region, we only use EXRK because the high order brick elements already allow a large time step interval.

Assume the numbers of the PML subdomains, explicit and implicit physical subdomains are $N_{pml}$, $N_{ex}$ and $N_{im}$, respectively, and the total number of subdomains is $N = N_{pml} + N_{ex} + N_{im}$. Time stepping scheme for the EB scheme DGTD in the PML and physical subdomains are discussed as below.

**Explicit Runge-Kutta Time Integration for PML subdomains**

The linear system of the $i$th subdomain (in PML region) and the stepping scheme is the same as equations (5.47)-(5.53), except the derivatives, $\tilde{u}_k^i$, as below:

$$M^i \tilde{u}_k^i = S^i (\tilde{v}_n^i + \Delta t \sum_{l=1}^{k-1} a_{k,l}^{ex} \tilde{u}_l^i) + j^i (t_n + c_k \Delta t)$$

$$+ \sum_{j=1}^{N_{im}} L^{ij} (\tilde{v}_n^i + \Delta t \sum_{l=1}^{k} a_{k,l}^{im} \tilde{u}_l^i) + \sum_{j=N_{im}+1}^{N} L^{ij} (\tilde{v}_n^i + \Delta t \sum_{l=1}^{k-1} a_{k,l}^{ex} \tilde{u}_l^i)$$

(5.56)

The coefficients $a_{k,l}^{ex}$ and $a_{k,l}^{im}$ are for explicit and implicit subdomains from Butcher tableau (Butcher, 2008; Kværnø, 2004), respectively, $b_k$ and $c_k$ are shared by both explicit and implicit schemes.
Implicit Runge-Kutta Time Integration for physical subdomains

If an implicit physical subdomain is surrounded all by explicit subdomains, the IMRK time stepping is

\[ \tilde{v}_{i,n+1} = \tilde{v}_{i,n} + \Delta t \sum_{k=1}^{s} b_k \tilde{u}_{k}^i \]  

(5.57)

\[ (M_i - \Delta t a_{k,k}^{im} L_i) \tilde{u}_{k}^i = L_i (\tilde{v}_{i,n} + \Delta t \sum_{l=1}^{k-1} a_{k,l}^{im} \tilde{u}_{l}^i) \]

+ \sum_{j=N_{im}+1}^{N} L_{ij} (\tilde{v}_{j,n} + \Delta t \sum_{l=1}^{k-1} a_{k,l}^{ex} \tilde{u}_{l}^j) + j^i (t_n + c_k \Delta t)  

(5.58)

If \( M \) multiple implicit subdomains in physical region couple together, we need to update them together. The \( M \) system equations are assembled in a large matrix system

\[
\begin{bmatrix}
M^1 & 0 & \ldots & 0 \\
0 & M^2 & \ddots & \vdots \\
\vdots & \ddots & \ddots & 0 \\
0 & \ldots & 0 & M^M
\end{bmatrix}
\begin{bmatrix}
\mathbf{u}_1^1 \\
\mathbf{u}_2^1 \\
\vdots \\
\mathbf{u}_M^1
\end{bmatrix}
= \begin{bmatrix}
\mathbf{q}_1^1 \\
\mathbf{q}_2^1 \\
\vdots \\
\mathbf{q}_M^1
\end{bmatrix}
\]

\[
\Delta t a_{k,k}^{im}
\begin{bmatrix}
L^{1,1} & L^{1,2} & \ldots & L^{1,M} \\
L^{2,1} & L^{2,2} & \ddots & \vdots \\
\vdots & \ddots & \ddots & L^{M-1,M} \\
L^{M,1} & \ldots & L^{M,M-1} & L^{M,M}
\end{bmatrix}
\begin{bmatrix}
\mathbf{u}_1^1 \\
\mathbf{u}_2^1 \\
\vdots \\
\mathbf{u}_M^1
\end{bmatrix}
\]

(5.59)

where

\[ \mathbf{q}_i^1 = \sum_{j=1}^{N} L_{ij}^j \left( \tilde{v}_{j,n} + \Delta t \sum_{l=1}^{k-1} a_{k,l}^{ex} \tilde{u}_{l}^j \right) + j^i (t_n + c_k \Delta t) \]  

(5.60)

This system equation could be solved at a subdomain level using iterative method as stated in (Chen et al., 2011).
Explicit Runge-Kutta Time Integration for physical subdomains

Explicit Runge Kutta time stepping scheme for the physical subdomains can be regarded as a special case of explicit Runge-Kutta scheme for PML subdomains, which only needs (5.56) and (5.52) in this article while setting $\bar{v}$ and $\bar{u}$ to be zero.

5.2.4 Implicit Gauss-Siedel

If the implicit time stepping are required by all the subdomains, Crank-Nicolson scheme (Crank and Nicolson, 1947) can be employed for temporal integration, which is shown as below:

$$
M^i v_{n+1}^i - v_n^i = \frac{1}{\Delta t} \sum_{j=1}^{N} L^{ij} v_{n+1}^j + v_n^j + f^i(t + \frac{1}{2} \Delta t); \quad (5.61)
$$

The update form of $v$ is below:

$$
(M^i - \frac{1}{2} \Delta t)v_{n+1}^i = (M^i + \frac{1}{2} \Delta t)v_n^i + f^i(t + \frac{1}{2} \Delta t) \sum_{j=1}^{N} L^{ij}) \quad (5.62)
$$

To solve (5.62), usually two ways are preferred. One is iterative method, such as Gauss-Siedel. The other class non-iterative methods for the sequentially ordered systems, including the Block-Thomas (Chen et al., 2011), which utilize the block tri-diagonal property of the system matrice and the LDU methods (Tobon et al., 2015; Sun and Liu, 2015), which is an advanced version of Block-Thomas method with surface-volume unknowns split.

5.3 Numerical Cases

5.3.1 Microstrip Line Case

The time-domain behavior of a simplified microstrip line is simulated to further confirm the advantages of the EB scheme DGTD method for a multidomain case.
The structure is shown in Fig. 5.5(a). The lower layer and upper layer are PEC, and the middle layer is dielectric with a relative permittivity of 3.4. The outer part is a PEC cavity filled with air; the lower corner of PEC cavity is at (-4.25, -1, -0.1) mm and the upper corner of PEC cavity is at (4.25, 1, 0.65) mm. The detailed dimensions of this microstrip line model are shown in Fig. 5.5(b) and Fig. 5.5(c). The start and end points of the active and passive lumped ports are located at (-3.55, 0, 0) mm, (-3.55, 0, 0.2) mm, (3.55, 0, 0) mm, and (3.55, 0, 0.2) mm, respectively. The source type is Blackman-Harris Window (BHW) pulse (Liu, 1997) with a characteristic frequency of 12 GHz; therefore, the highest frequency at -40 dB below the peak is about 40 GHz. The implementation of the lumped port is depicted in Fig. 5.4. If the original start point (end point) of a lumped port does not lie on the PEC structure or it is not located on a point of the mesh, the nearest PEC point in the mesh will be chosen as the new start point (end point). A path, which is formed by the edges in the associated elements, links the new start and end points. The lumped port voltage is loaded on one of these edges (the red dashed line in Fig. 5.4), while other edges along this path are set as PEC (the black solid lines in Fig. 5.4).

The whole microstrip line is divided into four subdomains with three interfaces at $x = -3.35$ mm, $x = 0$ mm and $x = 3.35$ mm, respectively. As the two subdomains at the two ends contain lumped ports, a dense mesh with low-order brick elements is used. For the two subdomains in the middle, a coarse mesh with high-order brick elements is a good option as it is more economic in DoFs. The mesh is shown in Fig. 5.6, where the orders of basis functions for the four subdomains are 2, 3, 3 and 2, respectively. Riemann Solver is used to deal with the energy communication between adjacent subdomains. Time integration is done by the Block Thomas method (Chen et al., 2011), which is a fast implicit time stepping scheme for the sequential structures. The time interval is 1 ps and total observation window length is 300 ps. The simulation is also executed by the EH scheme SETD method, and the orders of
basis functions are $E_{2H3}$, $E_{3H4}$, $E_{3H4}$ and $E_{2H3}$, respectively.

Note that all the following comparisons, analysis and the consequent conclusions are obtained from results in DGTD method and commercial software Wavenology (denoted as WCT in Fig. 5.7), which use conventional Finite Difference Time Domain (FDTD) method (Yee’s scheme). The comparisons of the total voltage of port 1, the scattered voltages of ports 1 and 2, and the S parameters are shown in Fig. 5.7. It is obvious that $EB$ scheme DGTD method has better agreement with the reference than the $EH$ scheme DGTD method, especially in the S parameters. The comparison of resource consumption is listed in Table 5.1. With only less than half of the unknowns and less than one-seventh of CPU time of $EH$ scheme, the $EB$ scheme can obtain more accurate results. Therefore, for the multidomain case, the advantages of $EB$ scheme SETD method over $EH$ scheme SETD method are maintained, because the Riemann Solver we used to deal with the numerical flux on the interfaces between adjacent subdomains is effective and does not degrade the accuracy of SETD method.
Figure 5.5: A microstrip line model. (a) Isometric view; (b) YZ cross-section; (c) XZ cross-section.

Table 5.1: Resource Consumption of EB scheme DGTD method and EH scheme DGTD method for 300 time steps

<table>
<thead>
<tr>
<th>Scheme</th>
<th>CPU Time (s)</th>
<th>Number of unknowns</th>
<th>Memory (MB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E2B2 SETD</td>
<td>150.8</td>
<td>62878</td>
<td>760</td>
</tr>
<tr>
<td>E2H3 SETD</td>
<td>1140.2</td>
<td>157508</td>
<td>2103</td>
</tr>
</tbody>
</table>
5.3.2 Wireless Multipath Case

A DGETD case with the well-posed PML is simulated for an indoor wireless communication system in a simplified room model with an unbounded region. This solver can be utilized to study wave propagation and field distribution for the design and optimization of communication systems.

The configuration of the room shown in Fig 5.8 has dimensions $4.6 \times 3.6 \times 2.6$ m, and the lower point is located at (-2.3, -1.8, -1.3) m. It is truncated by PML with a side length of 1.2 m in all directions. The thickness of the concrete wall is 0.2 m, and its relative permittivity is 4. The size of the wooden bed is $2 m \times 0.6 m \times 0.4 m$ with the lower corner at (-1.7, -1.2, -0.7) m. The size of the wooden table is $1 m \times 0.6 m \times 1.2 m$ with the lower corner at (0.7, 0.6, -0.7) m, and its relative permittivity is 2. The two wooden chairs, which are discretized with unstructured hexahedrons as shown in Fig. 5.9, are cylinders with the height of 0.4 m and radius of 0.3 m. The centers are located at (0.5, 0.8, -0.5) m and (0.8, -0.6, -0.5) m, respectively. All the other parts are meshed with bricks.

An electrical dipole source is located at (1.81, 1.33, 0.87) m and the BHW function is used as the excitation time function. The highest frequency is 335.1 MHz. It is distributed to the edge DoFs of the element in which the source is located. The dipole receiver is located at (-1.81, -1.33, 0.87) m. The electric field value is synthesized.
from the edge DoFs of the element in which the receiver is located. It is the inverse process of the source distribution.

The whole case is divided into five regions: PML, concrete wall, room with chairs removed, and two chairs. The orders of the interpolation polynomials for the basis functions are $E_4B_4$, $E_2B_2$, $E_3B_3$, $E_2B_2$, and $E_2B_2$, respectively. Each of the first three regions is divided into four subdomains with the interfaces at $x = 0$ and $y = 0$; therefore, the total number of subdomains is 14.

The results from the $EB$ scheme DGTD method for this model are compared with high-accuracy conventional FDTD. The observation window is 200 ns. From the time-domain results in Fig.5.10(a), it is observed that the wave amplitude is very small after 150 ns; therefore, the proposed $EB$ scheme PML is effective in absorbing the incident wave and the result from $EB$ scheme DGTD method agrees very well with the FDTD result. The spectral magnitudes of the received signals from both methods are shown in Fig.5.10(b), and the agreement for the dominant frequency band (above -40 dB) is good.

The computation resource comparison is listed in Table 5.2. The DGTD method uses high-order basis functions, which only require about 4 points per wavelength (PPW), but FDTD requires at least 10 PPW. In addition, the DGTD method (unstructured mesh) can capture the curved faces with elements of moderate size; however, FDTD (structured mesh) has to be implemented with small Yee’s cells. Therefore, the DGTD method needs much fewer unknowns than FDTD. The memory usage of the $EB$ scheme DGTD method is about 90 percents of that from FDTD. FDTD is a matrix-free method, in which only unknowns are stored in the memory. The DGTD method stores not only the unknowns, but also the stiffness matrices, the lower and upper matrices (from the LU decomposition of the mass matrices). Thus the memory performance of the two methods for this case is similar although the DoF of the DGTD method is much smaller. As the DGTD method solves a linear
matrix system, it needs more CPU time than FDTD in one single step; however, the DGTD method allows a larger time step interval than FDTD (62.5 ps vs. 5 ps), and consequently fewer time steps. Therefore, for a fixed observation window, the DGTD method uses only less than half of the total CPU time of FDTD.

Table 5.2: Resource Consumption of the \textbf{EB} scheme DGTD method and FDTD for the unbounded room.

<table>
<thead>
<tr>
<th></th>
<th>\textbf{EB} scheme DGTD</th>
<th>FDTD</th>
<th>Gain</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of unknowns</td>
<td>694712</td>
<td>10167768</td>
<td>14.6</td>
</tr>
<tr>
<td>Memory (MB)</td>
<td>1122</td>
<td>1263</td>
<td>1.126</td>
</tr>
<tr>
<td>$\Delta t$ (ps)</td>
<td>62.5</td>
<td>5</td>
<td>12.5</td>
</tr>
<tr>
<td>CPU Time (s)</td>
<td>6557</td>
<td>16751</td>
<td>2.555</td>
</tr>
</tbody>
</table>

5.3.3 \textit{Dielectric Ring in a Resonant PEC Cavity}

The case of a dielectric ring in a resonant PEC cavity (Gedney and Roden, 2000) is studied to demonstrate the effectiveness and advantage of the proposed \textbf{EB} scheme DGTD method compared to the \textbf{EH} scheme DGTD method. The locations of the six boundaries are [-162 mm, 162 mm, -60.5 mm, 60.5 mm, -21.5 mm, 21.5 mm]. The resonant ring is teflon with a relative permittivity of 2.06. The inner and outer radii of the ring are 16.65 mm and 27.75 mm, respectively, and the height is 39 mm. The coordinates of the center point of the resonant ring is [-45.25 mm, 0 mm, -21.5 mm]. The geometry of this resonant ring is exhibited in Fig. 5.11. The dipole source location is [-105 mm, -20 mm, 11.25 mm] and the observation point is located at [155 mm, 20 mm, 11.25 mm].

A tetrahedron mesh is preferred for the resonant ring part because it can capture the geometry details better; for the other parts, a structured brick mesh is preferred for its efficiency in meshing the coarse geometry where high-order basis functions can be adopted. Therefore, the hybrid DGTD method is a good option for this case, and
the mesh is shown in Fig. 5.12. It is divided into three subdomains, and the second one contains the resonant ring, so it uses a dense mesh with first-order tetrahedrons. The other two subdomains use bricks. For the \textbf{EH} scheme, the orders of the basis functions for the three subdomains are $E_4H_3$, $E_2H_1$, $E_4H_3$, respectively; and for the \textbf{EB} scheme, the basis functions are $E_3B_3$, $E_1B_1$ and $E_3B_3$, respectively. The source type is a Blackman-Harris window (BHW) pulse with the characteristic frequency of 1 GHz. The temporal integration is 5000 steps with fourth-order ExRK scheme, and the time step interval is 2 ps.

Comparison of $E_z$ component at the observation point between the conventional FDTD method, \textbf{EH} and \textbf{EB} scheme DGTD methods is shown in Fig. 5.13. The numerical resonant frequencies can be extracted from the spectrum of the received signals, which are shown in Fig. 5.14. The x-coordinates of the black stars are the resonant frequencies from the high accuracy FDTD, which is used as reference. The comparison of the first eight resonant frequencies are listed in Table 5.3. The \textbf{EB} and \textbf{EH} scheme DGTD methods both agree well with FDTD. Four significant digits are kept after the decimal point, both schemes have same accuracy for the first six modes. However, for the 7th and the 8th modes, the \textbf{EB} scheme DGTD method has a smaller error, which means it has a better performance in suppressing the dispersion. In addition, the \textbf{EB} scheme DGTD method is advantageous in DoFs and memory overhead.

5.3.4 \textit{Multiscale Ground Penetrating Radar Simulation}

Ground penetrating radar (GPR) is broadly used in earth science, engineering and societal applications, such as research in fluvial sedimentology, aeolian dune sands, archaeology, landmine and unexploded ordnance (UXO) detection, and so on. The most popular tool for forward modeling in GPR for the complex environment is the FDTD method (Teixeira et al., 1998; Lampe et al., 2003). However, the model is
Table 5.3: Resonant frequencies from \textbf{EH} scheme DGTD method, \textbf{EB} scheme DGTD method and FDTD. Unit (GHz)

<table>
<thead>
<tr>
<th>Scheme</th>
<th>FDTD</th>
<th>\textbf{EH} scheme DGTD</th>
<th>\textbf{EB} scheme DGTD</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st mode</td>
<td>1.2605</td>
<td>1.2573 (0.254%)</td>
<td>1.2573 (0.254%)</td>
</tr>
<tr>
<td>2nd mode</td>
<td>1.5076</td>
<td>1.5076 (0)</td>
<td>1.5076 (0)</td>
</tr>
<tr>
<td>3rd mode</td>
<td>1.8341</td>
<td>1.8311 (0.164%)</td>
<td>1.8311 (0.164%)</td>
</tr>
<tr>
<td>4th mode</td>
<td>2.1607</td>
<td>2.1546 (0.282%)</td>
<td>2.1546 (0.282%)</td>
</tr>
<tr>
<td>5th mode</td>
<td>2.5513</td>
<td>2.5452 (0.239%)</td>
<td>2.5452 (0.239%)</td>
</tr>
<tr>
<td>6th mode</td>
<td>2.6123</td>
<td>2.6062 (0.234%)</td>
<td>2.6062 (0.234%)</td>
</tr>
<tr>
<td>7th mode</td>
<td>2.8289</td>
<td>2.8137 (0.537%)</td>
<td>2.8198 (0.321%)</td>
</tr>
<tr>
<td>8th mode</td>
<td>3.0243</td>
<td>3.0090 (0.506%)</td>
<td>3.0151 (0.304%)</td>
</tr>
</tbody>
</table>

Table 5.4: Computation Resource Comparison between \textbf{EH} and \textbf{EB} scheme DGTD methods.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>DoFs</th>
<th>CPU Time (s)</th>
<th>Memory (MB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>\textbf{EH} scheme DGTD</td>
<td>61632</td>
<td>712.31</td>
<td>578</td>
</tr>
<tr>
<td>\textbf{EB} scheme DGTD</td>
<td>26487</td>
<td>152.49</td>
<td>125</td>
</tr>
</tbody>
</table>

usually significantly simplified, and the wideband antennas are modeled not very accurately due to the structured grids from FDTD. Therefore, the proposed \textbf{EB} scheme DGTD method is employed to simulate the forward process of the simplified GPR model with the antennas and carrying cart.

The whole geometry structure of the GPR is shown in Fig. 5.15. Two wideband biconical antennas (Jol, 2008), which are installed on a four-wheel metal cart, are used as the transmitting and receiving antennas. The structure is shown in Fig. 5.16, where the radius of the biconical antenna is 40 mm, and the gap between the two parts is excited with a lumped voltage port. The ground is modeled with 2 layers. The top layer is a dry soil with the relative permittivity of 2.4 and conductivity of 0.005 S/m, and one landmine is buried in it. The bottom layer is a wet soil with the relative permittivity of 4 and conductivity of 0.02 S/m, and a thin metal plate
is buried in it. This plate is tilted with a normal vector of \([-0.212012, -0.148453, -0.965926]\), and the thickness is 2 mm. The interface between the top and bottom soil layers is also tilted, the normal vector is \([0.115560 0.074289 -0.990519]\). This case can be used to simulate the clutter from the metal piece when detecting landmine in the ground. The clearance between the two hemi-spheres of the antenna is 2 mm. The whole simulation scale is 1 m, so the multiscale factor is 500. The perfectly matched layer is used outside the physical domain. The mesh of the case is shown in Fig. 5.17. The lumped port part, the cart and the antennas are meshed with first-order tetrahedrons, while the air around the cart is meshed with fourth-order bricks. The two soil layers are meshed with unstructured fifth-order hexahedrons instead of bricks due to the tilted interface.

Note that the thin metal plate is modeled as an infinite thin PEC face in the EB scheme DGTD method. We can construct an object with the same medium of the background (the tilted artificial box in the bottom layer shown in Fig. 5.17(f)). One of the six faces of the artificial box is just located at the position of the metal plate, and this face is defined as PEC. In this way, the metal plate, which will result in quite dense mesh in FDTD, is converted to a face boundary condition in EB scheme DGTD method. This treatment will not introduce poor-quality (highly twisted) or small elements. And the error from this approximation is negligible, but the DoFs can be reduced significantly. This is an obvious advantage of the unstructured methods (finite element method and spectral element method) over FDTD.

The whole case is divided into 18 subdomains, the comparison of the results is shown in Fig. 5.18. The excitation source is a first-order Blackman-Harris window (BHW) pulse with the characteristic frequency of 1 GHz. High accuracy conventional non-uniform FDTD is used as a reference. The result from EB scheme DGTD method agrees well with the reference. The comparison of computational resource is listed in Table 5.5. High-order brick and hexahedron elements efficiently reduce the
total number of unknowns and tetrahedrons can preserve the fine geometries with an acceptable mesh density (12 points per wavelength with first-order tetrahedrons). In the EB scheme DGTD method, implicit-explicit Runge-Kutta method is employed for temporal integration. Tetrahedron meshed parts use implicit time stepping to break the limitation of the CFL condition (Courant et al., 1967), and the brick and hexahedron meshed parts use explicit time stepping to save memory. However, in conventional FDTD, the small size of the lumped port, the tilted soil interface and metal plate all require dense mesh, which will lead to a very small time step interval. This is the reason for the 2.04 times gain of the EB scheme DGTD method in CPU time. The memory consumption of EB scheme DGTD method is higher than FDTD. The reason lies in that FDTD is a matrix-free algorithm and the FDTD code we use allow non-uniform mesh to save DoFs, meanwhile, the geometry structure of GPR case is not very complex, the advantage of hybrid mesh in the EB scheme DGTD method has not been fully exerted.

Table 5.5: Computational Resource Consumption Comparison between EB scheme DGTD and FDTD methods for GPR case

<table>
<thead>
<tr>
<th></th>
<th>FDTD</th>
<th>EB scheme DGTD</th>
<th>Gain</th>
</tr>
</thead>
<tbody>
<tr>
<td>DoFs (million)</td>
<td>422</td>
<td>1.33</td>
<td>317</td>
</tr>
<tr>
<td>CPU Time (h.)</td>
<td>8.1</td>
<td>3.97</td>
<td>2.04</td>
</tr>
<tr>
<td>Memory (GB)</td>
<td>8.39</td>
<td>11.1</td>
<td>0.76</td>
</tr>
</tbody>
</table>

5.3.5 Multiscale Antenna Coupling on a tank

The coupling of two monopole antennas on a tank is simulated with the proposed EB scheme DGTD method. This is a multiscale problem as some parts, such as the gap between the hull and skirt, the gap between the wheels and the track and the monopole antennas as shown in Fig. 5.19, are very small in size compared to the whole computational region. The geometry size of the tank (antennas and gun
included) is about 10 m × 4 m × 2.5 m, and the smallest size in this model is the radius of the monopole antennas, which is only 1 mm. Therefore, the multiscale factor is about 10000. The transmitting monopole antenna is fed by a lumped port, and the excitation source is the first-order Blackman-Harris window (BHW) pulse with the characteristic frequency of 66.5 MHz.

The EB scheme well-posed perfectly matched layer (PML) is adopted to simulate the open boundary condition. The thickness of the PML is 1.2 m in all directions, and each direction uses one fifth-order brick element. For the physical region, three big air cubes are segmented and meshed with fifth-order bricks. The brick mesh in these volumes will decrease the DoFs significantly. The other parts of physical region are meshed with first-order tetrahedrons as these volumes contain complex structures, where relatively small elements are needed to capture the fine structure. Especially for the parts which causes the multiscale characteristic of this problem (e.g., the antenna part), we need to segment them from other parts and mesh them with very small elements, and use non-conformal mesh to connect with the neighbor parts. The mesh is shown in Fig. 5.20.

The whole case is divided into 19 subdomains. The IMRK time integration is used for the subdomains with small tetrahedrons, and the EXRK time integration applies for the subdomains meshed with bricks and relatively big tetrahedrons. The reference is from the conventional FDTD method with a dense non-uniform grid. The comparison of the scattered voltage and S parameters between the proposed EB scheme DGTD method and FDTD is shown in Fig. 5.21. The agreement between these two methods is good; however, it is obvious from Table 5.6 that the new EB scheme DGTD method is more efficient than FDTD in both memory consumption and the CPU time. The reason for the advantage in CPU time mainly attributes to the efficient IMEXRK time integration scheme. As this case has many curved faces and geometry-small structures, the EB scheme DGTD method can have much fewer
unknowns than FDTD, thus costing less memory.

Table 5.6: Computational Resource Consumption Comparison between EB scheme DGTD and FDTD methods

<table>
<thead>
<tr>
<th></th>
<th>FDTD</th>
<th>EB scheme</th>
<th>DGTD</th>
<th>Gain</th>
</tr>
</thead>
<tbody>
<tr>
<td>DoFs (million)</td>
<td>876</td>
<td>1.02</td>
<td>858.8</td>
<td></td>
</tr>
<tr>
<td>CPU Time (h.)</td>
<td>14.33</td>
<td>8.62</td>
<td>1.66</td>
<td></td>
</tr>
<tr>
<td>Memory (GB)</td>
<td>15.8</td>
<td>8.77</td>
<td>1.81</td>
<td></td>
</tr>
</tbody>
</table>
Figure 5.7: Comparison between EB scheme DGTD method and EH scheme DGTD method with the reference FDTD results: (a) Total voltage of Port 1; (b) Scattered voltages of Ports 1 and 2; (c) $S_{11}$ and $S_{12}$. 
Figure 5.8: Geometry of the bedroom.

Figure 5.9: Mesh of the cylinder chair.
Figure 5.10: Comparison between the EB scheme DGTD method and FDTD. (a) Transient $E_z$ component at the receiver; (b) Signal magnitude of $E_z$ in the frequency domain.
Figure 5.11: Geometry of the resonant ring cavity.

Figure 5.12: Mesh of the resonant ring cavity.

Figure 5.13: $E_z$ component of the time domain signal at the observation point (155 mm, 20 mm, 11.25 mm).
Figure 5.14: The resonant frequencies obtained from high accuracy FDTD, EH and EB scheme DGTD methods.

Figure 5.15: Geometry of a ground penetrating radar case.

Figure 5.16: Geometry of the biconical antenna in the GPR.
Figure 5.17: Multiscale mesh for the GPR case in Fig. 5.15. (a) Brick mesh of the air around the cart; (b) Tetrahedron mesh of the cart and the antenna parts; (c) Tetrahedron mesh of the lumped port part; (d) Tetrahedron mesh of the landmine part; (e) Hexahedron mesh of top layer soil; (f) Hexahedron mesh of bottom layer soil.
Figure 5.18: Calculated signals at the antenna ports. (a) Scattered voltage of lumped port 1 (transmitter); (b) Scattered voltage of lumped port 2 (receiver); (c) scattering parameter S11; (d) scattering parameter S21.

Figure 5.19: Geometry of the tank and some fine structures.
Figure 5.20: Multiscale mesh for the tank case in Fig. 5.19. (a) Brick mesh of the PML Region; (b) Brick mesh of the three air cubes; (c) Tetrahedron mesh of the volume around the tank; (d) Tetrahedron mesh of the monopole antenna.
Figure 5.21: (a) Scatter voltage comparison; (b) S parameter comparison.
Anisotropic DGTD method

The weak form of the EB scheme Maxwell’s equations after testing are (Ren et al., 2013):

\[
\int_V \Phi_i \cdot (\frac{\partial \bar{\varepsilon} E_i}{\partial t} + \bar{\sigma}_e E_i + J^i) dV = \int_V \nabla \times \Phi_i \cdot \bar{\mu}^{-1} B^i dV + \int_S \Phi_p^i \cdot (\hat{n}_i \times \bar{\mu}^{-1} B^t) dS \tag{6.1}
\]

\[
\int_V \Psi_i \cdot (\frac{\partial B^i}{\partial t} + \bar{\sigma}_m \bar{\mu}^{-1} B^i + M^i) dV = - \int_V \nabla \times \Psi_i \cdot E^i dV - \int_S \Psi_i \cdot (\hat{n}_i \times E^t) dS
\]

\[
= - \int_V \Psi_i \cdot \nabla \times E^i dV + \int_S \Psi_i \cdot (\hat{n}_i \times E^t) dS - \int_S \Psi_i \cdot (\hat{n}_i \times E^t) dS
\]

\[
= - \int_V \Psi_i \cdot \nabla \times E^i dV + \int_S \Psi_i \cdot (\hat{n}_i \times E^t) dS, \tag{6.2}
\]

where $\bar{\varepsilon}$, $\bar{\mu}$, $\bar{\sigma}_e$, and $\bar{\sigma}_m$ are all tensors denoting the material’s permittivity, permeability, electric and magnetic conductivities, respectively. $J$ and $M$ are the imposed electric and magnetic current density sources. The testing curl-conforming and divergence-conforming basis functions, $\Phi$ and $\Psi$, can be found in (Ren et al., 2015; Tobón et al., 2015; Peterson et al., 1998). Index $i$ denotes the quantities of the local
subdomain, while \( j \) denotes adjacent ones. Note that integration by parts is applied once in (6.1). As we perform the curl operation on curl-conforming basis functions, integration by parts is applied twice in (6.2). Note that similar techniques are also used for nodal DG finite element and spectral element methods for hyperbolic systems (Hesthaven and Warburton, 2004; Kopriva and Gassner, 2010; Hesthaven and Warburton, 2002).

6.1 EB Scheme Anisotropic Riemann Solver

The terms \( \hat{n} \times \bar{\mu}^{-1}B \) and \( \hat{n} \times E \) in the surface integration parts in (6.1) and (6.2) are the numerical fluxes, where \( E \) and \( B \) are the total fields. The numerical fluxes are introduced to relax the tangential intensity fields continuity condition. Because this relatively strict condition requires solving the whole linear system together (Silvester and Ferrari, 1996), it hinders domain decomposition. The key point of the DG method is how to calculate this flux, and many methods have been proposed, such as the central flux (Bernacki et al., 2006), Riemann solver (upwind flux) (Mohammadian et al., 1991), Lax-Friedrichs flux (Svärd et al., 2005), penalty method (Montseny et al., 2008), etc. Riemann solver is known to be the more accurate than the central flux, Lax-Friedrichs and penalty methods because the other three can be regarded as simplified versions of the Riemann solver.

Riemann solver is a one-dimensional eigen-problem with the plane incident wave assumption along the normal direction of an interface. To evaluate the upwind flux in an anisotropic medium, the constitutive parameters \( \bar{\epsilon} \) and \( \bar{\mu} \) need to be represented in local coordinate, \( i.e., \bar{\epsilon}_l = \mathbf{T} \bar{\epsilon} \mathbf{T}^{-1} \) and \( \bar{\mu}_l = \mathbf{T} \bar{\mu} \mathbf{T}^{-1} \), the transformation matrix \( \mathbf{T} \) is as follows:

\[
\begin{bmatrix}
\hat{x} \\
\hat{y} \\
\hat{z}
\end{bmatrix} = \mathbf{T}^{-1} \begin{bmatrix}
\hat{t}_1 \\
\hat{t}_2 \\
\hat{n}
\end{bmatrix}
\]

(6.3)
where \((\hat{x}, \hat{y}, \hat{z})\) and \((\hat{t}_1, \hat{t}_2, \hat{n})\) are global and local coordinates, respectively.

The anisotropic medium Riemann solver for the \textbf{EH} scheme is derived in (Alvarez et al., 2012). Here we just briefly summarize this for reference. Using the fractional-step procedure (LeVeque, 2002), the nabla operator is split into the normal and surface derivatives:

\[
\nabla = \frac{\partial}{\partial n} \hat{n} + \nabla_s \tag{6.4}
\]

Maxwell’s equations can be split into two subproblems, one is a total continuous problem which does not need flux, and the other is a 2D conservation law where a Riemann problem needs to be solved. The subproblem of conservation law is only related with the tangential components of the fields as shown below:

\[
\frac{\partial \mathbf{H}_t}{\partial t} + \bar{\mu}^{-1} \, t \frac{\partial}{\partial n} \hat{n} \times \mathbf{E}_t = 0 \tag{6.5}
\]

\[
\frac{\partial \mathbf{E}_t}{\partial t} - \bar{\epsilon}^{-1} \, t \frac{\partial}{\partial n} \hat{n} \times \mathbf{H}_t = 0 \tag{6.6}
\]

\[
\bar{\mu}^{-1} = \begin{bmatrix}
\mu'_{11} & \mu'_{12} \\
\mu'_{21} & \mu'_{22}
\end{bmatrix} \tag{6.7}
\]

\[
\bar{\epsilon}^{-1} = \begin{bmatrix}
\epsilon'_{11} & \epsilon'_{12} \\
\epsilon'_{21} & \epsilon'_{22}
\end{bmatrix} \tag{6.8}
\]

where \(\mathbf{E}_t = [\mathbf{E}_{t1}, \mathbf{E}_{t2}]^T\), \(\mathbf{H}_t = [\mathbf{H}_{t1}, \mathbf{H}_{t2}]^T\), \(T\) denotes the transposition and

\[
\bar{\mu}^{-1} = \begin{bmatrix}
\mu'_{l,t} & \mu'_{l,tn} \\
\mu'_{l,nt} & \mu'_{l,nn}
\end{bmatrix} \tag{6.9}
\]

\[
\bar{\epsilon}^{-1} = \begin{bmatrix}
\epsilon'_{l,t} & \epsilon'_{l,tn} \\
\epsilon'_{l,nt} & \epsilon'_{l,nn}
\end{bmatrix} \tag{6.10}
\]

After defining \(\mathbf{q} = [\mathbf{H}_{t1}, \mathbf{H}_{t2}, \mathbf{E}_{t1}, \mathbf{E}_{t2}]^T\), the system becomes an eigenproblem

\[
\frac{\partial \mathbf{q}}{\partial t} = \mathbf{A} \frac{\partial \mathbf{q}}{\partial n} \tag{6.11}
\]
By diagonalizing the matrix $A$, the impedance and admittance matrices of the anisotropic Riemann solver are

$$
Z = R C_2^{-1} R^{-1} D_2^{-1} \tilde{C}_{t,t}^{-1}
$$

(6.12)

$$
Y = \bar{\mu}_{t,t}^{-1} D_2 R C_2^{-1} R^{-1} D_2^{-1}
$$

(6.13)

where the system matrix $A$, and intermediate matrices $R, C_2, D_2$ can be found in (Alvarez et al., 2012).

Utilizing (6.12) and (6.13), a more detailed expression with the coordinate transformation matrix $T$ is shown as below:

$$
(\hat{n}^i \times \hat{\mu}^{-1} B^i) = T^{-1} (Z^i + Z^j)^{-1} [Z^j T (\hat{n}^i \times (\hat{\mu}^i)^{-1} B^i) + Z^j T (\hat{n}^i \times \hat{n}^i \times (E^j - E^i))]
$$

(6.14)

$$
(\hat{n}^i \times E^i) = T^{-1} (Y^i + Y^j)^{-1} [Y^j T (\hat{n}^i \times E^j) + Y^j T (\hat{n}^i \times \hat{n}^i \times ((\hat{\mu}^j)^{-1} B^j - (\hat{\mu}^i)^{-1} B^i))]
$$

(6.15)

where $\bar{\mu}^i$ and $\bar{\epsilon}^i$ are relative permeability and permittivity of the $i$th subdomain, respectively. The Riemann solver (6.14) and (6.15) can be explained from the right to the left in a simple way. The flux from one side (for example, $(\hat{n}^i \times (\hat{\mu}^j)^{-1} B^j)$ in (6.14) is from the adjacent subdomain) is first transformed to the local coordinates of the interface by $T$. Then the flux is partially distributed (left multiplied by $(Z^i + Z^j)^{-1} Z^j$) into the other side according to the impedances (or admittances) of both sides, and then distributed flux is transformed back to the global coordinates. The coordinate transformation matrices $T$ and $T^{-1}$ are requisite in general. In an isotropic medium, we do not use them because the admittance and impedance are scalars instead of tensors, thus $T$ and $T^{-1}$ are canceled by each other in (6.14) and (6.15).
The system matrices in (6.1) and (6.2) from the volume integration have the same expressions as those for an isotropic medium except that the constitutive parameters are tensors. The matrices from surface integration, which are related to the Riemann solver, are different from those in an isotropic medium case:

\[
(L^{ij}_{eb})_{pq} = \langle \Phi^i_p, T^{-1}(Z_i + Z_j)^{-1}(Z_j T(\delta\hat{n} \times \hat{n}) \times (\bar{\mu}^{-1})^{-1}\Psi^j_q))\rangle_{S_{ij}} \quad (i \neq j) \tag{6.16}
\]

\[
(L^{ij}_{be})_{pq} = -\langle \Psi^i_p, T^{-1}(Y_i + Y_j)^{-1}(Y_j T(\delta\hat{n} \times \hat{n}) \times \Phi_q^j))\rangle_{S_{ij}} \quad (i \neq j) \tag{6.17}
\]

\[
(L^{ii}_{eb})_{pq} = \sum_{j=1}^{N} \langle \Phi^i_p, T^{-1}(Z_i + Z_j)^{-1}(Z_j T(\delta\hat{n} \times \hat{n}) \times (\bar{\mu}^{-1})^{-1}\Psi^j_q))\rangle_{S_{ij}} \tag{6.18}
\]

\[
(L^{ii}_{be})_{pq} = \sum_{j=1}^{N} \langle \Psi^i_p, T^{-1}(Y_i + Y_j)^{-1}(Y_j T(\delta\hat{n} \times \hat{n}) \times \Phi_q^j))\rangle_{S_{ij}} \tag{6.19}
\]

\[
(L^{ij}_{ec})_{pq} = \langle \Phi^i_p, T^{-1}(Z_i + Z_j)^{-1}T(\delta\hat{n} \times \hat{n}) \times (\bar{\mu}^{-1})^{-1}\Psi^j_q))\rangle_{S_{ij}} \quad (i \neq j) \tag{6.20}
\]

\[
(L^{ij}_{bc})_{pq} = -\langle \Psi^i_p, T^{-1}(Y_i + Y_j)^{-1}T(\delta\hat{n} \times \hat{n}) \times (\bar{\mu}^{-1})^{-1}\Psi^j_q))\rangle_{S_{ij}} \quad (i \neq j) \tag{6.21}
\]

\[
(L^{ii}_{ec})_{pq} = \sum_{j=1}^{N} \langle \Phi^i_p, T^{-1}(Z_i + Z_j)^{-1}T(\delta\hat{n} \times \hat{n}) \times \Phi_q^j))\rangle_{S_{ij}} \tag{6.22}
\]

\[
(L^{ii}_{bc})_{pq} = \sum_{j=1}^{N} \langle \Psi^i_p, T^{-1}(Y_i + Y_j)^{-1}T(\delta\hat{n} \times \hat{n}) \times \Phi_q^j))\rangle_{S_{ij}} \tag{6.23}
\]

where \(S_{ij}\) is the interface between the \(i\)th and \(j\)th subdomains, and \(\langle f, g \rangle_{S_{ij}} = \int_{S_{ij}} f^T g \, ds\). Subscripts \(p\) and \(q\) are the local indexes of basis functions.

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6.2 EB Scheme Anisotropic Perfectly Matched Layer

A non-convolutional, unsplit Maxwellian perfectly matched layer is proposed to match an arbitrary anisotropic medium. This PML can be viewed as an extension of the work in (Fan and Liu, 2003). First, we introduce the complex coordinate-stretching variables to Maxwell’s equations while assuming the permeability, permittivity, electric conductivity and magnetic conductivity are arbitrary tensors

\[ \partial \eta \rightarrow \left[ 1 + \frac{\omega_{\eta}(\eta)}{j\omega} \right] \partial \eta \quad (\eta = x, y, z) \quad (6.24) \]

where \( \omega_{\eta} \) is the attenuation coefficient in the direction \( \eta \) (\( \eta = x, y, z \)). For simplicity, we just consider the \( z \) component of both sides of Faraday’s law and Ampere’s law as below:

\[ \frac{\partial (\bar{\epsilon}E)_z}{\partial t} = \frac{\partial (\bar{\mu}^{-1}B)_y}{\partial x} - \frac{\partial (\bar{\mu}^{-1}B)_x}{\partial y} - (\bar{\sigma}, \bar{E})_z \quad (6.25) \]

\[ \frac{\partial \bar{B}_z}{\partial t} = \frac{\partial \bar{E}_x}{\partial y} - \frac{\partial \bar{E}_y}{\partial x} - (\bar{\sigma}_m\bar{\mu}^{-1}B)_z \quad (6.26) \]

With (6.24) and the transformation \( \frac{\partial}{\partial t} \rightarrow j\omega \), (6.25) and (6.26) can be expanded in the frequency domain as:

\[ j\omega (\bar{E})_z + (\omega_x + \omega_y)(\bar{E})_z + (\bar{\sigma}_e)\frac{\omega_x\omega_y(\bar{E})_z + (\omega_x + \omega_y)(\bar{\sigma}_e)E_z}{j\omega} + \frac{\omega_x\omega_y(\bar{\sigma}_e)E_z}{(j\omega)^2} \]

\[ = \frac{\partial}{\partial x} (1 + \frac{\omega_y}{j\omega})(\bar{\mu}^{-1}B)_y - \frac{\partial}{\partial y} (1 + \frac{\omega_x}{j\omega})(\bar{\mu}^{-1}B)_x \quad (6.27) \]

\[ j\omega B_z + (\omega_x + \omega_y)B_z + (\bar{\sigma}_m\bar{\mu}^{-1}B)_z + \frac{\omega_x\omega_yB_z + (\omega_x + \omega_y)(\bar{\sigma}_m\bar{\mu}^{-1}B)_z}{j\omega} \]

\[ + \frac{\omega_x\omega_y(\bar{\sigma}_e\bar{\mu}^{-1}B)_z}{(j\omega)^2} = \frac{\partial}{\partial x} (1 + \frac{\omega_y}{j\omega})E_y - \frac{\partial}{\partial y} (1 + \frac{\omega_x}{j\omega})E_x \quad (6.28) \]
Denote $\frac{\partial \mathbf{E}^{(1)}}{\partial t} = \tilde{\mathbf{E}}$, $\frac{\partial \mathbf{E}^{(2)}}{\partial t} = \mathbf{E}^{(1)}$, $\frac{\partial \mathbf{B}^{(1)}}{\partial t} = \tilde{\mathbf{B}}$, $\frac{\partial \mathbf{B}^{(2)}}{\partial t} = \tilde{\mathbf{B}}$ and define the auxiliary variables as

$$\tilde{\mathbf{E}}_\eta = \mathbf{E}_\eta + \omega_\eta \mathbf{E}^{(1)}_\eta \quad (\eta = x, y, z) \quad (6.29)$$

$$(\tilde{\mu}^{-1} \tilde{\mathbf{B}})_\eta = (\tilde{\mu}^{-1} \mathbf{B})_\eta + \omega_\eta (\tilde{\mu}^{-1} \mathbf{B}^{(1)})_\eta \quad (\eta = x, y, z) \quad (6.30)$$

$$\mathbf{\Lambda}_0 = \text{diag}\{\omega_x, \omega_y, \omega_z\} \quad (6.31)$$

Equations (6.27) and (6.28) can be transformed back to the time domain

$$\frac{\partial (\tilde{\mathbf{E}}_z)}{\partial t} + (\tilde{\sigma}_e \tilde{\mathbf{E}})_z + (\omega_x + \omega_y) (\tilde{\mathbf{E}})_z - (\tilde{\sigma}_e \mathbf{\Lambda}_0 \tilde{\mathbf{E}})_z + \omega_x \omega_y (\tilde{\sigma}_e \mathbf{E}^{(2)})_z + (\omega_x + \omega_y) (\tilde{\sigma}_e \mathbf{E}^{(1)})_z$$

$$- (\tilde{\sigma}_e \mathbf{\Lambda}_0 \mathbf{E}^{(1)})_z + (\tilde{\sigma} \mathbf{\Lambda}_0 \tilde{\mathbf{E}}^{(1)})_z + \omega_x \omega_y (\tilde{\mathbf{E}}^{(1)})_z - (\omega_x + \omega_y) (\tilde{\sigma} \mathbf{\Lambda}_0 \mathbf{E}^{(1)})_z$$

$$= \frac{\partial (\tilde{\mu}^{-1} \mathbf{B})_y}{\partial x} - \frac{\partial (\tilde{\mu}^{-1} \mathbf{B})_x}{\partial y} \quad (6.32)$$

$$\frac{\partial \tilde{\mathbf{B}}_z}{\partial t} + (\tilde{\sigma}_m \tilde{\mu}^{-1} \tilde{\mathbf{B}})_z + (\omega_x + \omega_y) \tilde{\mathbf{B}}_z - (\tilde{\sigma}_m \mathbf{\Lambda}_0 \tilde{\mu}^{-1} \tilde{\mathbf{B}})_z + \omega_x \omega_y (\tilde{\sigma}_m \mathbf{\tilde{\mu}^{-1} B}^{(2)})_z$$

$$+ (\omega_x + \omega_y) (\tilde{\sigma}_m \tilde{\mu}^{-1} \mathbf{B}^{(1)})_z - (\tilde{\sigma}_m \mathbf{\Lambda}_0 \tilde{\mu}^{-1} \mathbf{B}^{(1)})_z + (\tilde{\mu} \mathbf{\Lambda}_0 \mathbf{\tilde{\mu}^{-1} B}^{(1)})_z + \omega_x \omega_y \mathbf{B}^{(1)}$$

$$- (\omega_x + \omega_y) (\tilde{\mu} \mathbf{\Lambda}_0 \tilde{\mu}^{-1} \mathbf{B}^{(1)})_z = \frac{\partial \tilde{\mathbf{E}}_x}{\partial y} - \frac{\partial \tilde{\mathbf{E}}_y}{\partial x} \quad (6.33)$$

Similarly to (6.25) and (6.26), we can obtain the equations for the $x$ and $y$ components. After defining diagonal matrices:

$$\mathbf{\Lambda}_1 = \text{diag}\{\omega_y + \omega_z, \omega_z + \omega_x, \omega_x + \omega_y\} \quad (6.34)$$

$$\mathbf{\Lambda}_2 = \text{diag}\{\omega_y \omega_z, \omega_z \omega_x, \omega_x \omega_y\} \quad (6.35)$$

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the \( \mathbf{EB} \) scheme compact form of Maxwell’s equations in the PML region is as follows:

\[
\nabla \times \tilde{\mathbf{E}} = -\frac{\partial \tilde{\mathbf{B}}}{\partial t} - (\tilde{\sigma}_m \tilde{\mu}^{-1} + \Lambda_1 + \tilde{\mu} \Lambda_0 \tilde{\mu}^{-1}) \tilde{\mathbf{B}}
\]

\[-\Lambda_2 \tilde{\sigma}_m \tilde{\mu}^{-1} \mathbf{B}^{(2)} - (\Lambda_1 \tilde{\sigma}_m \tilde{\mu}^{-1} - \tilde{\sigma}_m \Lambda_0 \tilde{\mu}^{-1}
\]

\[+ \tilde{\mu} \Lambda_0 \tilde{\mu}^{-1} - \Lambda_1 \tilde{\mu} \Lambda_0 \tilde{\mu}^{-1} + \Lambda_2) \mathbf{B}^{(1)}\]

(6.36)

\[
\nabla \times \tilde{\mu}^{-1} \tilde{\mathbf{B}} = \frac{\partial \tilde{\mathbf{E}}}{\partial t} + (\tilde{\sigma}_e + \Lambda_1 \tilde{\epsilon} + \tilde{\epsilon} \Lambda_0) \tilde{\mathbf{E}} + \Lambda_2 \tilde{\sigma}_e \mathbf{E}^{(2)}
\]

\[+ (\Lambda_1 \tilde{\sigma}_e - \tilde{\sigma}_e \Lambda_0 + \tilde{\epsilon} \Lambda_0^2 - \Lambda_1 \tilde{\epsilon} \Lambda_0 + \Lambda_2 \tilde{\epsilon}) \mathbf{E}^{(1)}\]

(6.37)

and the auxiliary equations are

\[
\frac{\partial \mathbf{E}^{(1)}}{\partial t} = \tilde{\mathbf{E}} - \Lambda_0 \mathbf{E}^{(1)}
\]

(6.38)

\[
\frac{\partial \mathbf{E}^{(2)}}{\partial t} = \mathbf{E}^{(1)}
\]

(6.39)

\[
\frac{\partial \mathbf{B}^{(1)}}{\partial t} = \tilde{\mathbf{B}} - \tilde{\mu} \Lambda_0 \tilde{\mu}^{-1} \mathbf{B}^{(1)}
\]

(6.40)

\[
\frac{\partial \mathbf{B}^{(2)}}{\partial t} = \mathbf{B}^{(1)}
\]

(6.41)

The auxiliary equations (6.38)-(6.41) in PML are totally local and the profile parameters are only related with the volume integration, not with the Riemann solver. Therefore, the upwind flux aforementioned applies to not only the physical regions but also the PML regions. The extra work in the PML regions, which includes calculating the additional damping terms in Maxwell’s equations and updating the auxiliary ordinary differential equations, is not cumbersome. The system equations in PML regions are:
\[
M^i_{ee} \frac{d\tilde{\epsilon}^i}{dt} = K^i_{eb} \tilde{b}^i + R^i_{ee} \tilde{\epsilon}^i + S^i_{ee}(e^{(1)})^i + T^i_{ee}(e^{(2)})^i + \sum_{j=1}^{N} L^i_{eb} \tilde{b}^j + \sum_{j=1}^{N} L^i_{ee} \tilde{\epsilon}^j \tag{6.42}
\]

\[
M^i_{bb} \frac{d\tilde{b}^i}{dt} = K^i_{be} \tilde{\epsilon}^i + R^i_{bb} \tilde{b}^i + S^i_{bb}(b^{(1)})^i + T^i_{bb}(b^{(2)})^i + \mathbf{m}^i + \sum_{j=1}^{N} L^i_{be} \tilde{\epsilon}^j + \sum_{j=1}^{N} L^i_{bb} \tilde{b}^j \tag{6.43}
\]

\[
M^i_{ee} \frac{d(e^{(1)})^i}{dt} = M^i_{ee} \tilde{\epsilon}^i + T^i_{ee}(e^{(1)})^i \tag{6.44}
\]

\[
M^i_{bb} \frac{d((b^{(1)})^i}{dt} = M^i_{bb} \tilde{b}^i + T^i_{bb}(b^{(1)})^i \tag{6.45}
\]

where \( \tilde{\epsilon}, e^1, e^{(2)}, \tilde{b}, b^{(1)} \) and \( b^{(2)} \) are the unknown vectors. The mass and stiffness matrices \( (M_{ee}, M_{bb}, K_{be} \text{ and } K_{eb}) \) can be found in (Ren et al., 2015), except the difference that the constitutive parameters are tensors. \( \mathbf{L} \) matrices are defined in \( (6.16)-(6.23) \). The damping matrices are listed below:

\[
(R_{ee})_{pq} = -\langle \Phi_p, (\bar{\sigma}_e + \Lambda_1 \bar{\epsilon} + \bar{\epsilon} \Lambda_0) \Phi_q \rangle_{V_e} \tag{6.46}
\]

\[
(S_{ee})_{pq} = -\langle \Phi_p, (\Lambda_1 \bar{\sigma}_e - \bar{\sigma}_e \Lambda_0 + \bar{\epsilon} \Lambda_0^2 - \Lambda_1 \bar{\epsilon} \Lambda_0 + \Lambda_2 \bar{\epsilon}) \Phi_q \rangle_{V_e} \tag{6.47}
\]

\[
(T_{ee})_{pq} = -\langle \Phi_p, \Lambda_2 \bar{\sigma}_e \Phi_p \rangle_{V_e} \tag{6.48}
\]

\[
(R_{bb})_{pq} = -\langle \Psi_p, (\bar{\sigma}_m \bar{\mu}^{-1} + \Lambda_1 + \bar{\mu} \Lambda_0 \Lambda^{-1}) \Psi_q \rangle_{V_e} \tag{6.49}
\]
\[(S_{bb})_{pq} = -\langle \Psi_p, (\Lambda_1 \bar{\sigma} - \bar{\sigma} \Lambda_0 + \bar{\epsilon} \Lambda_0^2 - \Lambda_1 \bar{\epsilon} \Lambda_0 + \Lambda_2 \bar{\epsilon}) \Psi_q \rangle \nabla_e \quad (6.50)\]

\[(T_{bb})_{pq} = -\langle \Psi_p, \Lambda_2 \bar{\sigma} m \bar{\mu}^{-1} \Psi_q \rangle \nabla_e \quad (6.51)\]

The time integration scheme can be the leap-frog, the explicit fourth order Runge-Kutta (RK4), or the explicit-implicit RK4 schemes. As time stepping is not the main point of this paper, it is not shown here, but can be found in (Chen et al., 2011; Ren et al., 2015, 2013). The following numerical results employs the explicit RK4 scheme.

To remove of the potential late-time instability in classical anisotropic PML, Meza-Fajardo and Papageorgiou introduced the multiaxial PML (M-PML) in a split form for FDTD in elastic wave propagation (Meza-Fajardo and Papageorgiou, 2008). M-PML is further discussed and developed in (Zeng et al., 2011; Meza-Fajardo and Papageorgiou, 2010). The idea of M-PML is to add small damping profiles in all directions. Only slight modification is needed to obtain M-PML from classical PML as shown in Fig. 6.1. The attenuation in the direction \(\eta (\eta = x, y, z)\) is described by \(\omega_\eta\). In classical PML, damping only exists in the directions where the coordinates are beyond the physical region. For example, the \(x\) coordinate of area 1 is beyond the range of the physical region, while the \(y\) coordinate is within it. Thus the damping profile only exists in the \(x\) direction. However, in M-PML, the damping profiles in area 1 include both \(x\) and \(y\) components as functions of \(x\). We denote them as \(\omega_x(x)\) and \(\omega_y(x)\), respectively. The additional term \(\omega_x(x)\) can be proportional to \(\omega_y(x)\) and the ratio is defined as \(r(y, x)\). For area 2, the damping profiles are \(\omega_x(y)\) and \(\omega_y(y)\). The damping profiles in the corner area are added from adjacent areas 1 and 2. See Fig. 6.1(b).

In a 3D Maxwellian problem, a ratio matrix \(R\) can be defined to obtain the
Figure 6.1: Attenuation parameters in (a) Classic PML; (b) Multiaxial PML.

M-PML requires simply replacing $\omega_\eta$ in (6.31), (6.34) and (6.35) with $\omega'_\eta$ based on the classical PML. Note that the M-PML is not a perfectly matching condition (Meza-Fajardo and Papageorgiou, 2012), and a small spurious numerical reflection exists between physical region and M-PML. However, we can set the non-diagonal elements in $\mathbf{R}$ small, which means the additional damping from M-PML is small compared to the dominant damping terms from classical PML. But this additional damping plays an important role in stability in anisotropic media as will be shown.

$$
\begin{bmatrix}
\omega'_x \\
\omega'_y \\
\omega'_z
\end{bmatrix} = \mathbf{R}
\begin{bmatrix}
\omega_x \\
\omega_y \\
\omega_z
\end{bmatrix}
= 
\begin{bmatrix}
1 & r(x, y) & r(x, z) \\
r(y, x) & 1 & r(y, z) \\
r(z, x) & r(z, y) & 1
\end{bmatrix}
\begin{bmatrix}
\omega_x \\
\omega_y \\
\omega_z
\end{bmatrix}
$$

(6.52)
in the numerical parts in this paper. Usually, \( r(\xi, \zeta) = 0.05 \) \((\xi, \zeta = x, y, z, \; \xi \neq \zeta)\) is enough from our numerical experiments.

### 6.3 Numerical Results

#### 6.3.1 Case 1: PEC cavity filled with two full anisotropic media

The transient response of a PEC cavity filled with two full-tensor anisotropic lossy media is studied and compared to Comsol, which, to our knowledge, is the only commercial software able to handle full-tensor anisotropic media easily. The edge length of the cubic cavity is \( l = 2 \text{ m} \), and the cavity center is the origin. An electric dipole source polarized along the \((1, 1, 1)\) direction and an observation point are located at \((-0.2, -0.2, -0.2) \text{ m}\) and \((0.6, 0.6, 0.6) \text{ m}\), respectively. The excitation signal is the Black-Harris window (BHW) pulse with the characteristic frequency of 155 MHz.

The interface between the two media are tilted as shown in Fig. 6.2(a). The relative permittivities, relative permeabilities and conductivities are as follows:

\[
\mathbf{\epsilon}_r, 1 = \begin{bmatrix} 3.1253 & -0.8283 & 0.6657 \\
-0.8283 & 1.5524 & -0.7651 \\
0.6657 & -0.7651 & 2.3223 \end{bmatrix}
\]

\[
\mathbf{\epsilon}_r, 2 = \begin{bmatrix} 1.0302 & -0.1099 & 0.1310 \\
-0.1099 & 3.1612 & 0.9997 \\
0.1310 & 0.9997 & 2.8087 \end{bmatrix}
\]

\[
\mathbf{\mu}_r, 1 = \begin{bmatrix} 2.3125 & -0.3750 & -0.7578 \\
-0.3750 & 2.2500 & 0.2165 \\
-0.7578 & -0.3750 & 1.4375 \end{bmatrix}
\]

\[
\mathbf{\mu}_r, 2 = \begin{bmatrix} 1.2500 & 0.2165 & 0.3750 \\
0.2165 & 2.6875 & -0.5413 \\
0.3750 & -0.5413 & 2.0625 \end{bmatrix}
\]
\[
\sigma_1 = \begin{bmatrix}
0.0014 & -0.0005 & 0.0001 \\
-0.0005 & 0.0016 & -0.0001 \\
0.0001 & -0.0001 & 0.0010 \\
\end{bmatrix}
\]

\[
\sigma_2 = \begin{bmatrix}
0.0010 & 0 & 0 \\
0 & 0.0011 & 0.0003 \\
0 & 0.0003 & 0.0019 \\
\end{bmatrix}
\]

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure6_2.png}
\caption{PEC cavity filled with two different full-tensor anisotropic media. (a) Geometry, and (b) mesh.}
\end{figure}

In the DGTD method, the cavity is divided into two subdomains with the interface between subdomains chosen exactly the same as the medium interface. Thus, the Riemann solver has to deal with two different anisotropic media, which is a relatively more stringent test than a homogeneous medium. Three schemes used are \( E_nB_n \), \( E_nH_n \) and \( E_nH_{n+1} \), where \( n \) is the order of the basis functions. \( n \) is 4 and 2 for hexahedrons and tetrahedrons, respectively. Fig. 6.3 and Fig. 6.4 and shows the excellent agreement between \( E_nB_n \), \( E_nH_{n+1} \) schemes based DGTD methods and Comsol for all the six components of the electric and magnetic field intensities. Therefore, the \( EB \) scheme anisotropic Riemann solver is effective and accurate. However, the result from \( E_nH_n \) scheme DGTD method is incorrect. This means the conclusion from the isotropic medium DGTD method still holds for the anisotropic case, that is, the \( EB \) scheme is free of spurious modes with same order of basis functions for \( E \) and \( B \)
$\mathbf{B}$, while the $\mathbf{EH}$ scheme has to use mixed orders of basis functions for $\mathbf{E}$ and $\mathbf{H}$ (Chen et al., 2011). Therefore, the $\mathbf{E}_n\mathbf{B}_n$ scheme is preferred as it has less DoFs than $\mathbf{E}_n\mathbf{H}_{n+1}$.

Figure 6.3: Comparison between DGTD methods and Comsol for a cavity filled with two anisotropic media. (a) $\mathbf{E}_x$; (b) $\mathbf{E}_y$; (c) $\mathbf{E}_z$. 

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Figure 6.4: Comparison between DGTD methods and Comsol for a cavity filled with two anisotropic media. (a) $H_x$; (b) $H_y$; (c) $H_z$.

6.3.2 Case 2: M-PML for full-anisotropic medium

The field distribution in an infinite homogenous full anistropic medium due to an electric dipole source is studied to test the proposed M-PML. The physical region is $1.167 \text{ m} \times 1.167 \text{ m} \times 1.167 \text{ m}$ cube truncated by M-PML with $r(\xi, \zeta) = 0.05$ ($\xi, \zeta = x, y, z, \xi \neq \zeta$). The relative permittivity and permeability of the medium are as follows:

\[
\epsilon_r = \begin{bmatrix}
1.3750 & -0.0777 & -0.4779 \\
-0.0777 & 1.0161 & 0.0990 \\
-0.4779 & -0.0990 & 1.6089 \\
\end{bmatrix}
\]
\[ \mu_r = \begin{bmatrix} 1.9375 & 0.2296 & 0.0765 \\ 0.2296 & 1.1562 & -0.2812 \\ 0.0765 & -0.2812 & 1.9062 \end{bmatrix} \]

The dipole source is located at (-0.13, -0.08, -0.1)m, with the polarization of (1, 1, 1). The dipole receiver is located at (0.22, 0.14, 0.07) m. The excitation function is BHW pulse with the central frequency of 138.75 MHz. Fig. 6.5 gives out the mesh. The M-PML is composed of 5th order cubes with the edge length of 0.8333 m (the top half of the PML region is set transparent to reveal the mesh of physical region in Fig. 6.5(a)), while the physical region are discretized by 4th order cubes with the edge length of 0.625 m. Thus the mesh is non-conformal between the two regions, which is more obvious from top view in Fig. 6.5(b).

![Figure 6.5: (a) Mesh of the physical region and M-PML; (b) Top View.](image)

As PML is not provided in the transient solver of Comsol, scattering boundary condition (SBC) is used. Also, we choose the result of a large cavity with the same anisotropic medium as reference. Before the reflected wave arrives, the field recorded by the receiver is the same as that in free space. Fig. 6.6 demonstrates the numerical results from PML, M-PML, Comsol SBC and large cavity.

The agreement between DGTD methods with classical PML, M-PML and DGTD with large cavity is very good until the reflected wave reach the receiver. That means both PML and M-PML has absorbed the coming wave effectively with very small
Figure 6.6: Comparison between results from DGTD method with PML, M-PML, Comsol with SBC and large PEC cavity. (a) 0 − 100 ns; (b) Zoom to 0 − 20 ns.

reflection, the relative errors (compared to large cavity results before the reflected wave arrives) are shown in Fig. 6.7. As the M-PML is ’imperfect’, a relatively large reflection can be observed between 10 ns and 20 ns. However, the largest relative error is only 0.38%, which means the reflection of the M-PML is -48.4 dB, it is accurate enough in engineering requirement.

Figure 6.7: The relative errors of results from PML and M-PML compared to the reference result from a large cavity.

Another key characteristic to evaluate the material based absorbing boundary condition is the late-time instability. The stability of the M-PML and classical PML are compared. If the observation window is prolonged to 380 ns, the instability of the classical PML can be found from Fig. 6.8, however, the M-PML is stable. Besides
simply recording the field intensity, the total energy inside the whole physical region is a more obvious way in evaluation of the stability. For the transient problems, if the total energy increases after the time support of the excitation pulse, it is a proof of instability. As illustrated in Fig. 6.9, the energy of the physical region with classical PML has increased after 110 ns, while for the M-PML case, the energy decays monotonously in the late time. We have tested 0.4 million time steps and the M-PML is always stable. Thus M-PML is an effective and stable absorbing boundary condition for arbitrary anisotropic medium in DGTD method.

**Figure 6.8:** Late time stability performance of M-PML and PML.

**Figure 6.9:** The total energy in the physical region. (a) PML; (b) M-PML.
6.3.3 Case 3: Fully space-time separated TF/SF technique for plane wave illumination in anisotropic medium with M-PML

Before showing the numerical results, a fully space-time separated TF/SF technique we proposed for the plane incident wave with non-conforming mesh will be explained with details. The physical region is illuminated by plane wave and truncated with M-PML (or classical PML, note that all the following processings for TF/SF technique also apply to classical PML). We use the scattered and total fields as the unknowns for the M-PML and the physical regions, respectively. The TF/SF interface is just the same as the shared face between M-PML and physical region, and the meshes across the TF/SF interface could be non-conformal with different kinds of elements.

A 2D sketch of this technique is illustrated in Fig. 6.10. Every basis function has a controlling point, where the value of the basis function is maximal. Assume
the $i$th subdomain is a physical subdomain, and the $j$th one is its adjacent M-PML subdomain. The unknown vectors for the $i$th and $j$th subdomains are $v_i = [e_{i,1}, \ldots, e_{i,m}, b_{i,1}, \ldots, e_{i,n}]^T$ and $v_j = [e_{j,1}, \ldots, e_{j,k}, h_{j,1}, \ldots, h_{j,l}]^T$, where $T$ denotes the transpose of a vector, $e$ and $b$ are the unknowns for E and B, and the DoFs for the $i$th and $j$th subdomains are $(m+n)$ and $(k+l)$, respectively. As M-PML region uses scattered field, the incident plane wave needs to be added. The incident wave is projected to the basis functions in the $j$th subdomain, and forms an 'incident vector' $v_{j,\text{inc}} = [e_{\text{inc},1}, \ldots, e_{\text{inc},k}, b_{\text{inc},1}, \ldots, b_{\text{inc},l}]^T$, where $e_{\text{inc},p} = \langle E_{\text{inc}}, \Phi_{j,p} \rangle$ and $b_{\text{inc},p} = \langle B_{\text{inc}}, \Psi_{j,p} \rangle$. $E_{\text{inc}}$ and $B_{\text{inc}}$ are the incident electric and magnetic intensities, while $\Phi$ and $\Psi$ are the basis functions for E and B.

Note that in general anisotropic media, the ordinary wave and extraordinary waves have different wave speeds and wave vectors. The following TF/SF technique applies for both cases. Assume the wave speed in this anisotropic medium is $c$ (either ordinary wave speed or extraordinary wave speed), $f(t)$ is the time function of the plane wave, and $r_{i,p}$ is the distance from the $p$th controlling point in the $i$th subdomain to the plane wave front at the time $t = 0$. Then the time-delay matrix is defined as

$$F_i = \begin{bmatrix} f(t - \frac{r_{i,1}}{c}) & \cdots & \cdots & f(t - \frac{r_{i,m+n}}{c}) \end{bmatrix} \quad (6.53)$$

and the system equation for the local subdomain with the TF/SF technique is

$$M_i \frac{d\mathbf{v}_i}{dt} = L_{ii} \mathbf{v}_i + \sum_j L_{ij} \mathbf{v}_j + F_i \sum_j L_{ij} \mathbf{v}_{j,\text{inc}} \quad (6.54)$$

That means the time at which to add the incident wave is controlled by the locations of the controlling points in the local subdomain, and it has no relation with any information from the adjacent subdomains. However, the quantity of flux
added to the local subdomain is determined by the upwind flux (Riemann solver) and the incident field vector. This requires the information from both local and adjacent subdomains. Fig. 6.10 gives an example of the 2D case. The local (physical) subdomain and the adjacent (M-PML) subdomain are discretized with the 2nd order triangles and rectangles respectively for illustration purpose, although this method is implemented in 3D for high order basis functions. Before the wave front reaches the controlling point (the round point) of the edge basis function (the upward solid arrow) in element 1, the incident wave does not need to be added, even though it is projected onto the basis functions in the M-PML subdomains. For example, the upward dashed arrow in Fig. 6.10 represents a basis function in element 2 in the M-PML region, and the plane wave arrives at the its controlling point (square point) earlier than the round point in element 1. But the flux cannot be added to the basis function (upward solid arrow) in element 1 until the wave front reaches the round point, even though the basis functions in elements 1 and 2 are coupled by the \( \mathbf{L} \) matrix. Similarly, when taking the M-PML as the local subdomain, the incident wave should be subtracted from the physical subdomain’s flux to obtain the scattered field for the boundary treatment.

Note that in equation (6.54), \( \sum_j L_{ij} v_{j, \text{inc}} \) is calculated only once when assembling the system matrices. At each time marching step, we only need to generate a new \( \mathbf{F}_i \), and the additional computation load is negligible. In this way, the spatial connection of the basis functions from different subdomains can be pre-stored when assembling, and it is independent of the time function of the incident plane wave. An advantage of this approach is the multiple functionalities of the shared interface: It plays the roles of the SF/TF interface, the Riemann solver interface, and the non-conforming mesh connector.

In the following, we use the same case of subsection B above, but change the
source to be BHW plane wave. It is in the \(xz\) plane, the normalized \(k\) vector is \([0.5, 0, 0.866]\). At \(t = 0\), the wave front is at the point \((-2.08333, 0, -2.08333)\) m. Use the TF/SF technique aforementioned, the 2D snapshots of \(B_x\) and \(E_y\) distribution on the surface \(y = 0\) are shown in Fig. 6.11. In these 2D figures, the wavefront is a straight line and the field distribution are changing very smoothly as a function of space, which is the characteristics of a plane wave. Fig. 6.12 shows the good agreement of the electric field intensity and magnetic flex density at the receiver between DGTD method and the analytical solution (Chew, 1995). Thus the DGTD with TF/SF technique, combined with M-PML, can provide an effective tool for simulating electromagnetic problems in unbounded anisotropic medium with plane wave illumination. It should be explained that the analytical solution in (Chew, 1995) is for frequency domain, we have transformed it to the time domain. In addition, as the anisotropic medium is non-dispersive, it also applies to wideband cases.

### 6.3.4 Negative refraction in bicrystals

Negative refraction, in which the group velocity is in the opposite direction of phase velocity, has attracted much attentions as this phenomenon provides the possibility to manufacturing super lens which can focus evanescent modes without missing image details (Pendry, 2000). The widely acquaintance method to achieve negative refraction is based on left-hand material (LHM)(Shelby et al., 2001). However, LHM is neither a sufficient or a necessary condition for achieving negative refraction (Krowne and Zhang, 2007). Here we want to numerically simulate the negative refraction of light-wave travelling in the \(YVO_4\) bicrystal via the proposed anisotropic DGTD method with an M-PML of \(r(\xi, \zeta) = 0.05\) \((\xi, \zeta = x, y, z; \xi \neq \zeta)\).

The \(YVO_4\) bicrystal in this case consists of two twinning halves (Zhang et al., 2003) (denoted as part A and B) as shown in Fig. 6.13. The arrows indicate the orientation of the uniaxis in part A and B, respectively. Both halves are nonmagnetic
and have the same permittivity in the principle coordinate system:

\[ \epsilon_r = \begin{bmatrix} 4.0671 & 0 & 0 \\ 0 & 4.0671 & 0 \\ 0 & 0 & 5.0661 \end{bmatrix} \]

Using coordinate transformation, the relative permittivities of parts A and B in global Cartesian coordinate systems are:

\[ \epsilon_{r,1} = \begin{bmatrix} 4.5666 & 0 & -0.4995 \\ 0 & 4.0671 & 0 \\ -0.4995 & 0 & 4.5666 \end{bmatrix} \]

\[ \epsilon_{r,2} = \begin{bmatrix} 4.5666 & 0 & 0.4995 \\ 0 & 4.0671 & 0 \\ 0.4995 & 0 & 4.5666 \end{bmatrix} \]

We assume the incident wave is propagating in +z direction within the XZ plane. For this bicrystal, an ordinary wave, whose electric field is in the y direction will travel in the material just as in one material (Zhang et al., 2003), not affected by the interface between parts A and B. We only consider extraordinary wave which can produce refraction.

In DGTD simulation for this case, we introduce the half space TF/SF condition as shown in Fig. 6.14, that is, the source added to the TF/SF interface A is the sum of the incident and reflected plane waves, while the source added to the TF/SF interface B is the transmitted plane wave. The M-PML is also divided into two halves, each half has the same material as the physical domain it is matched for. In this way, the source added to the whole SF/TF interface is the same as the plane wave in infinite half space, no approximation error will be introduced.

We define \( \theta \) as the angle between the normal direction of the surface and the \( \mathbf{k} \) vector. Unlike the isotropic medium, the direction of the \( \mathbf{k} \) vector in anisotropic medium is usually different from the Poynting vector, that is, the direction of the
phase velocity is different from the direction of energy propagation. Assume P is one point on TF/SF interface A, while Q is on TF/SF interface B. As shown in Fig. 6.15, generally, four waves exist when plane wave sponge on the interface between two different anisotropic media (Chew, 1995). They are ordinary and extraordinary waves traveling in $+z$ (transmitted waves) and $-z$ (reflected waves) direction, respectively (wave 2 3 5 and 6 in Fig. 6.15). Therefore, the sum of waves 1, 2, 4 and 5 should be added to Point P, and the sum of waves 3 and 6 should be added to Q as the boundary condition for this anisotropic half space case. As we only consider the extraordinary wave, the ‘incident’ electric field can be written in a compact form for points P and Q, $\mathbf{E}_P = f(t-t_1)\mathbf{E}_1 + f(t-t_2)\mathbf{E}_2$ and $\mathbf{E}_Q = f(t-t_3)\mathbf{E}_3$, where $f$ is the time function of the pulse. If the materials and $\theta$ are given, $\mathbf{k}_A$, the phase velocity $v_{p,A}$ and $\mathbf{E}_1$ in material A could be calculated. $\mathbf{k}_B$, $\mathbf{E}_2$ and $\mathbf{E}_3$ can be obtained from the state-variable approach for layered medium (Chew, 1995; Morgan et al., 1987) because $\mathbf{k}_s$ (in this case $\mathbf{k}_s = \mathbf{k}_x$), which is the horizontal component of $\mathbf{k}$, is known and keep unchanged across the interface due to phase matching. Then the phase velocity in material B is known because $v_{p,B} = \omega/|\mathbf{k}_B|$. It is obvious from Fig. 6.15 that $t_1 = l_1/v_{p,A}$, $t_2 = (l_2 + OP)/v_{p,A}$ and $t_3 = (l_2 + OQ)/v_{p,B}$, where $l_1$ and $l_2$ are the distances from points P and O to the wavefront at $t = 0$. Similarly, we can obtain $\mathbf{H}_P$ ($\mathbf{B}_P$) and $\mathbf{H}_Q$ ($\mathbf{B}_Q$).

In the DGTD numerical simulation, the incident BHW pulse plane wave has the central frequency $f_c = 563.9 \text{ THz}$. The sizes of both of the twining parts A and B are $4\lambda \times 4\lambda \times 4\lambda$, and the thickness of the PML is $\lambda$ in all the directions, where $\lambda = \frac{1}{f_c}$. All the cubes in the mesh are 4th order element with the edge length of $\lambda$.

In the following, we will use three cases to show both normal refraction and neg-ative refraction. The incident angles of the $\mathbf{k}$ vectors are $\theta = -10^\circ$, $\theta = 35^\circ$ and $\theta = 0^\circ$, respectively. As the $z$ component of the Poynting vector ($S_z$) is continuous across the interface ($z = 0$), the $x$ component of the Poynting vector ($S_x$) deter-
mines whether it is normal refraction or negative refraction. If $S_x$ has a sign change across the interface, the incident and refraction energy flows lie on the same side of the normal of the interface, this phenomenon is negative refraction, otherwise, it is normal refraction. In Fig. 6.16(a), 6.16(c) and 6.16(e), it can be observed that $S_x$ is always negative value, and in Fig. 6.17(a), 6.17(c) and 6.17(e), $S_x$ is always positive, therefore, they both represent the normal refractions. However, in Fig. 6.18(c), $S_x$ changes from negative value to positive value, which represents the negative refraction. These conclusions can be also drawn from the vector arrows for Poynting vectors, such as Fig. 6.18(d). In the area ($z < 0$), the angle of the energy propagation is $\phi = -6.2557^\circ$, while in the area ($z > 0$), the angle of the energy propagation is $\phi = 6.2498^\circ$. However, for the first and second normal refraction cases, the angles of the Poynting vector have the same sign, as shown in Fig. 6.16(b), 6.16(d), 6.16(f) and Fig. 6.17(b), 6.17(d), 6.17(f).

Fig. 6.19 records the Poynting vector directions of a point on the wave front versus time for the aforementioned three cases. The point is located at (0, 0, -6$l$) at the time $t = 0$. In Fig. 6.19(c), the Poynting vector of this wave front point changes from a negative angle in medium A to a positive angle in medium B, so it is negative refraction, while Fig. 6.19(a) and Fig. 6.19(b) show normal refractions. In addition, no reflected waves are found, which agrees with the description of zero reflection of this bycrystal in (Krowne and Zhang, 2007).

More different $\theta$ have been tested, and the comparison between the numerical results and the analytical solutions are shown in Fig. 6.20. The incident and refractive angles of the energy flows agree very well, the errors are all less than 1%. In Fig. 6.20, the whole 2D surface is divided into 4 quadrants by the dashed lines. A point lies in the first or the third quadrant represents normal refraction, while a point in the second or fourth quadrant represents negative refraction. For this $YVO_4$ bicrystal, the negative refraction occurs when the incident angle (respect to energy)
is within the region $[-12.34^\circ, 0^\circ]$. 
Figure 6.11: Snapshots of $B_x$ and $E_y$ on the surface $y = 0$. (a) $B_x$ at 14.4 ns; (b) $B_x$ at 18 ns; (c) $B_x$ at 21.6 ns; (d) $B_x$ at 25.2 ns; (e) $E_y$ at 14.4 ns; (f) $E_y$ at 18 ns; (g) $E_y$ at 21.6 ns; (h) $E_y$ at 25.2 ns.
Figure 6.12: Comparison between DGTD method and analytical solution for plane wave traveling in anisotropic medium. (a) $E_x$; (b) $E_y$; (c) $E_z$; (d) $B_x$; (e) $B_y$; (f) $B_z$.

Figure 6.13: YVO4 bicrystal with two halves.
Figure 6.14: Modeling YVO$_4$ bicrystal using half space TF/SF and M-PML.

Figure 6.15: Reflection and refraction on the interface.
Figure 6.16: Positive Refraction ($\theta = -10^\circ$). (a) $x$ component of Poynting vector at $t = 4$ fs; (b) Poynting vector at $t = 4$ fs; (c) $x$ component of Poynting vector at $t = 6$ fs; (d) Poynting vector at $t = 6$ fs; (e) $x$ component of Poynting vector at $t = 8$ fs; (f) Poynting vector at $t = 8$ fs.
Figure 6.17: Positive Refraction ($\theta = 35^\circ$). (a) $x$ component of Poynting vector at $t = 5.28$ fs; (b) Poynting vector at $t = 5.28$ fs; (c) $x$ component of Poynting vector at $t = 7.04$ fs; (d) Poynting vector at $t = 7.04$ fs; (e) $x$ component of Poynting vector at $t = 8.8$ fs; (f) Poynting vector at $t = 8.8$ fs.
Figure 6.18: Positive Refraction ($\theta = 0^\circ$). (a) $x$ component of Poynting vector at $t = 3.52$ fs; (b) Poynting vector at $t = 3.52$ fs; (c) $x$ component of Poynting vector at $t = 5.28$ fs; (d) Poynting vector at $t = 5.28$ fs; (e) $x$ component of Poynting vector at $t = 7.04$ fs; (f) Poynting vector at $t = 7.04$ fs.
Figure 6.19: Poynting vector directions of a point on the wavefront versus time. (a) $\theta = -10^\circ$; (b) $\theta = 35^\circ$; (c) $\theta = 0^\circ$.

Figure 6.20: Numerical and analytical incident and refractive angles.
7

Summary and Future Work

7.1 Summary

In this work, the main stream numerical methods in computational electromagnetics are first reviewed, and the necessity of the DGTD method for the multiscale problems are stressed.

The DGTD method we propose are advantageous in three aspects. First, compared to the conventional element level DG, this new DGTD allows multiple elements in the same subdomain, thus the total DoF can be reduced significantly and implicit time stepping are achievable to shorten the total CPU time. Second, this DGTD method use multiple kinds of elements, low order elements (usually tetrahedrons) are used to mesh the geometry fine parts, and high order elements (hexahedrons) are employed to mesh the coarse parts to maximize the efficiency. Third, non-conformal mesh can not only allow different kinds of elements but also sharp change of the element size, therefore the DoF can be further decreased.

The previous research on the subdomain level DG is based on the EH scheme both on the primal mesh. This scheme works well with different order of basis
functions for $E$ and $H$ at the cost of introducing wasted unknowns. If same order of basis functions for $E$ and $H$ are used, it will have the problem of spurious modes. The root reason is $E$ and $H$ should be on the primal and dual meshes respectively to approximate the discrete Hodge, previous research puts them both on the primal mesh which will introduce the spurious modes. However, the $E$ and $B$ are compatible with each other even if they are both on the primal mesh with same order of basis functions. Therefore, the $EB$ scheme has much less DoFs, thus some large cases which are difficult for $EH$ scheme can be simulated.

In the $EB$ scheme DGTD method, both curl-conforming and divergence-conforming basis functions are used or proposed for multiple kinds of elements, including the hexahedron, the tetrahedron and the prism. The $EB$ scheme upwind flux is proposed to calculate the numerical flux between adjacent subdomains. Maxwellian long-time stable ordinary partial differential equation based PML are proposed to absorbing the outgoing wave to simulate the unbounded problems. The effectiveness and efficiency of the proposed DGTD is illustrated by the numerical results and multiscale problems are solved successfully with the $EB$ scheme DGTD method.

The $EB$ scheme DGTD method is further extended to arbitrary anisotropic media, it allows arbitrary permittivities, permeabilities and conductivities of full tensors. The anisotropic $EB$ scheme upwind flux is obtained via operator split method and eigen analysis. The anisotropic time domain Maxwellian ordinary partial differential equation based PML is extended from isotropic version and multi-axial MPL is introduced to obtain long time stability. The anisotropic Riemann solver is tested with imhomogeneous anistropic media and shown be effective. The anisotropic M-PML is long time stable and absorb the outgoing wave effectively. Also the half space TF/SF boundary condition is brought forward. The negative refraction in YVO$_4$ bicrystal is simulated with the anisotropicDGTD and half space TF/SF condition for the first time with numerical methods.
To sum up, the subdomain level compatible \textbf{EB} scheme DGTD method is more effective and more efficient than the \textbf{EH} scheme. Its advantage in the CPU time over the conventional element level DGTD method is obvious. For the problem with a large multiscale factor, the memory consumption can be also less than the element level DGTD method. It is a powerful simulation tool in the time domain.

The main contribution by the authors are as follows:

- Proposed the \textbf{EB} scheme for DGTD method.
- Found the root reason of advantage of \textbf{EB} scheme DGTD method over the \textbf{EH} scheme DGTD method.
- New basis functions for the field variables $B$.
- \textbf{EB} scheme upwind flux for DGTD method.
- \textbf{EB} scheme ODE based Maxwellian late time stable non-convolutional unsplit PML for DGTD method.
- \textbf{EB} scheme upwind flux for anisotropic DGTD method.
- \textbf{EB} scheme ODE based Maxwellian non-convolutional unsplit PML for anisotropic DGTD method.
- Introduced Multi-axial PML (MPML) into electromagnetics.
- Modify the MPML to an unsplit form.
- Proposed the non-conformal space-time separated Total Field / Scattered Field (TF/SF) boundary condition for time domain plane incident wave.
- Proposed the half space (TF/SF) boundary condition.
• Studied and compared the accuracy, convergence for the **EB** scheme and **EH** scheme SETD and FETD method.

• Simulated the multiscale problem with **EB** scheme DGTD method effectively and efficiently.

• Simulated the negative refraction in $YVO_4$ bicrystal with the proposed **EB** scheme anistropic DGTD method.

### 7.2 Future Work

A few active aspects can be studied and developed in the following research of DGTD method. They are:

• Parallalization of the DGTD method using MPI to model very large scale problems.

• Study the direct solver for the sparse matrices in the DGTD method to solve the system more efficiently.

• Implement the adaptive hp refinement DGTD method with the hierarchical basis functions.

• More efficient implicit time stepping scheme for the DGTD method.

• Theoretical study of the multiaxial Perfectly Matched Layer and quantify the ratio matrix.

• Further study the dispersion relationship and apply **EB** scheme DGTD method for modeling the dispersive media.

• The DGTD method can be applied to more applications, such as modeling graphene, ionosphere and etc.
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3. Ren, Q.; Sun, Q.; Tobn, L.; Zhan Q.; Liu, Q.H. ”Hybrid EB Scheme Based Spectral Element-Finite Element Discontinuous Galerkin Time Domain Method for Multiscale Electromagnetic Simulations” (Under review)
4. Ren, Q.; Zhan, Q.; Liu, Q.H. "Discontinuous Galerkin Time Domain (DGTD) Method with Multiaxial Perfectly Matched Layer (M-PML) for Arbitrary Anisotropic Medium” (Under review)


8. Sun, Q.; Tobón, L.; Ren, Q.; Hu, Y; Liu, Q.H. "A new DG-FETD implicit time stepping scheme based on E and B fields for sequentially ordered systems” (Accepted).

9. Sun, Q.; Ren, Q.; Zhan, Q; Liu, Q.H. "New 3D Hybrid Finite Difference/Finite Element DGTD Method with Non-Conformal Meshes” (Submitted).

10. Sun, Q.; Ren, Q.; Zhan, Q; Liu, Q.H. "Efficient Explicit-Implicit Hybrid FDTD-SETD-FETD for Electromagnetic Modeling” (In preparation).

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