# Unstructured-Grid Spectral Method for 3D Maxwell's Equations with Well-Posed PML 

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## 1 INTRODUCTION

Recent interests in the modeling of large-scale broadband electromagnetic problems have made the use of high-order and spectral time-domain methods more attractive because of their high efficiency and accuracy [1]-[5]. However, the analysis of stability of these numerical methods is often complicated significantly because of the presence of complex boundary conditions.

Recently, a penalty term is introduced by Hesthaven [2] [4] in spectral methods to impose the boundary conditions weakly rather than strongly as is classically done, thus removes many problems associated with the analysis of stable and accurate pseudospectral approximations. The methods are known as spectral penalty methods. The numerical stability and spectral convergence for these schemes have been established in a rigorous manner.

In order to model electromagnetic waves in an unbounded physical domain by a spectral method, a well-posed perfectly matched layer (PML) ABC [6] is used to absorb outgoing waves in this paper. The grid employed consists of unstructured tetrahedral elements, thus can easily model an arbitrary geometry. Furthermore, the penalty method enables an easy treatment at the interfaces between adjacent elements compared with the finite-element method.

## 2 Formulation

In order to model electromagnetic waves in an unbounded physical domain, the following 3D well-posed PML Maxwell's equations [6] are used to develop spectral penalty methods.

$$
\begin{align*}
& \frac{\partial(\mu \widetilde{\mathbf{H}})}{\partial t}+\nabla \times \widetilde{\mathbf{E}}=-A \widetilde{\mathbf{H}}-B \mathbf{H}^{(1)}  \tag{1}\\
& \frac{\partial(\epsilon \widetilde{\mathbf{E}})}{\partial t}-\nabla \times \widetilde{\mathbf{H}}=-C \widetilde{\mathbf{E}}-D \mathbf{E}^{(1)}-G \mathbf{E}^{(2)}-\mathbf{J} . \tag{2}
\end{align*}
$$

where $A, B, C, D, G$ are diagonal matrices defined as $A=\mu P, \quad B=\mu Q, \quad C=\sigma I+$ $\epsilon P, \quad D=\sigma P+\epsilon Q, \quad G=\sigma R$. Here $I$ denotes identity matrix and $P=\operatorname{Diag}\left[\omega_{y}+\omega_{z}-\right.$ $\left.\omega_{x}, \omega_{x}+\omega_{z}-\omega_{y}, \omega_{x}+\omega_{y}-\omega_{z}\right], Q=\operatorname{Diag}\left[\left(\omega_{x}-\omega_{y}\right)\left(\omega_{x}-\omega_{z}\right),\left(\omega_{y}-\omega_{x}\right)\left(\omega_{y}-\omega_{z}\right),\left(\omega_{z}-\right.\right.$ $\left.\left.\omega_{x}\right)\left(\omega_{z}-\omega_{y}\right)\right]$, and $R=\operatorname{Diag}\left[\omega_{y} \omega_{z}, \omega_{x} \omega_{z}, \omega_{x} \omega_{y}\right] . \widetilde{\mathbf{E}}=\mathbf{E}+\bar{\omega} \mathbf{E}^{(1)}, \widetilde{\mathbf{H}}=\mathbf{H}+\bar{\omega} \mathbf{H}^{(1)}$, $\bar{\omega}=\operatorname{Diag}\left[\omega_{x}, \omega_{y}, \omega_{z}\right]$, and $\mathbf{E}^{(1)}, \mathbf{E}^{(2)}, \mathbf{H}^{(1)}$ satisfy the following equations

$$
\begin{equation*}
\frac{\partial \mathbf{E}^{(1)}}{\partial t}=\widetilde{\mathbf{E}}-\bar{\omega} \mathbf{E}^{(1)}, \quad \frac{\partial \mathbf{E}^{(2)}}{\partial t}=\mathbf{E}^{(1)}, \quad \frac{\partial \mathbf{H}^{(1)}}{\partial t}=\widetilde{\mathbf{H}}-\bar{\omega} \mathbf{H}^{(1)} . \tag{3}
\end{equation*}
$$

To simplify matters, let us express the above Maxwell's euqations in a conservation form

$$
\begin{equation*}
\frac{\partial \mathbf{q}}{\partial t}+\nabla \cdot F(q)=\mathbf{S} \tag{4}
\end{equation*}
$$

where the state vector $\mathbf{q}$, the flux $F(q)=\left[F_{1}(\mathbf{q}), F_{2}(\mathbf{q}), F_{3}(\mathbf{q})\right]^{T}$, and the source term $\mathbf{S}$ are defined as follows

$$
\mathbf{q}=\left[\begin{array}{c}
\epsilon \mathbf{E} \\
\mu \mathbf{H}
\end{array}\right], \quad F_{i}(\mathbf{q})=\left[\begin{array}{c}
-\mathbf{e}_{\mathbf{i}} \times \mathbf{H} \\
\mathbf{e}_{\mathbf{i}} \times \mathbf{E}
\end{array}\right], \quad \mathbf{S}=\left[\begin{array}{c}
\mathbf{S}_{\mathbf{E}} \\
\mathbf{S}_{\mathbf{H}}
\end{array}\right]=\left[\begin{array}{c}
-C \widetilde{\mathbf{E}}-D \mathbf{E}^{(1)}-G \mathbf{E}^{(2)}-\mathbf{J} \\
-A \widetilde{\mathbf{H}}-B \mathbf{H}^{(1)}
\end{array}\right]
$$

Here $\mathbf{e}_{\mathbf{i}}$ denotes the three Cartesian unit vectors.
In order to construct a 3D spectral penalty method on an unstructured grid consisting of a number of arbitrary tetrahedra, a standard tetrahedron $\mathbf{I}$ of vertices $\mathbf{v}_{I}=$ $[-1,-1,-1]^{T}, \mathbf{v}_{I I}=[1,-1,-1]^{T}, \mathbf{v}_{I I I}=[-1,1,-1]^{T}$ and $\mathbf{v}_{I V}=[-1,-1,1]^{T}$ is introduced as a reference element. A standard tetrahedron $\mathbf{I}$ in coordinates $\xi=(\xi, \eta, \zeta)$ can be mapped into an arbitrary tetrahedron $\mathbf{D}$ in Cartesian coordinates $\mathbf{x}=(x, y, z)$ by the linear mapping. An instance of such mapping is illustrated in Fig. 1. Within the standard tetrahedron I, a set of nodal points $\left\{\xi_{j}\right\}$ can be introduced to achieve spectral accuracy for interpolation and spatial derivatives within the element (see [5] for details).


Figure 1: Mapping between the physical tetrahedron and the standard tetrahedron including the nodal sets for a 2nd-order interpolation.

By polynomial collocation methods, the unknown fields $\mathbf{E}$ and $\mathbf{H}$ in each tetrahedron of the unstructured grids is assumed to be well approximated as

$$
\begin{equation*}
\mathbf{E}(\mathbf{x}, t) \approx \sum_{j=0}^{N} \mathbf{E}_{j}(t) L_{j}(\mathbf{x}), \mathbf{H}(\mathbf{x}, t) \approx \sum_{j=0}^{N} \mathbf{H}_{j}(t) L_{j}(\mathbf{x}) \tag{5}
\end{equation*}
$$

where $\mathbf{E}_{j}(t)=\mathbf{E}\left(\mathbf{x}_{j}, t\right), \mathbf{H}_{j}(t)=\mathbf{H}\left(\mathbf{x}_{j}, t\right)$, and $L_{j}(\mathbf{x})$ is the 3 D multivariate Lagrange interpolation polynomial of order $n$ associated with $\xi_{j}$ whose total number is given by $N=\frac{1}{6}(n+1)(n+2)(n+3)$ to allow the polynomial basis to be complete.

Since simply performing time integration of (3) within each element does not ensure the correct boundary conditions between adjacent elements, the appropriate jump conditions must be taken into account. The change of the flux between elements can be obtained by by Rankine-Hugonoit jump conditions to satisfy the following relations [7]

$$
\hat{\mathbf{n}} \cdot[F]=\left\{\begin{array}{l}
\left(Z^{+}+Z^{-}\right)^{-1} \hat{\mathbf{n}} \times\left(Z^{+}[\mathbf{H}]-\hat{n} \times[\mathbf{E}]\right)  \tag{6}\\
\left(Y^{+}+Y^{-}\right)^{-1} \hat{\mathbf{n}} \times\left(-Y^{+}[\mathbf{E}]-\hat{n} \times[\mathbf{H}]\right)
\end{array}\right.
$$

where $[\mathbf{E}]=\mathbf{E}^{+}-\mathbf{E}^{-}$and $[\mathbf{H}]=\mathbf{H}^{+}-\mathbf{H}^{-}$measure the jumps in the field values across the interface and superscripts ' + ' and '-' refer to the values from neighbor and local element, respectively. Here parameters $Z^{ \pm}$denote the impedances and $Y^{ \pm}$denote the conductances of the medium. Eq. (6) will act as the penalizing boundary term in the following spectral penalty method for Maxwell's equations.

By the spectral penalty method, Maxwell's equations are satisfied in the following Galerkin-like way with the penalty term mentioned above

$$
\begin{equation*}
\int_{\mathbf{D}}\left(\frac{\partial \mathbf{q}}{\partial t}+\nabla \cdot F-\mathbf{S}\right) L_{i}(\mathbf{x}) d \mathbf{x}=\oint_{\delta \mathbf{D}} L_{i}(\mathbf{x}) \hat{\mathbf{n}} \cdot[F] d \mathbf{x} \tag{7}
\end{equation*}
$$

Substituting Eq.(5) into the above equation, we have an element-wise expression for the electric field

$$
\begin{equation*}
\frac{d \mathbf{E}}{d t}=\left(M^{\epsilon}\right)^{-1} \mathbf{V} \times \mathbf{H}+\left(M^{\epsilon}\right)^{-1} M \mathbf{S}_{\mathbf{E}}+\left.\left(M^{\epsilon}\right)^{-1} F\left(\hat{\mathbf{n}} \times \frac{Z^{+}[\mathbf{H}]-\hat{\mathbf{n}} \times[\mathbf{E}]}{Z^{+}+Z^{-}}\right)\right|_{\delta \mathbf{D}} \tag{8}
\end{equation*}
$$

and likewise for the magnetic field

$$
\begin{equation*}
\frac{d \mathbf{H}}{d t}=\left(M^{\mu}\right)^{-1} \mathbf{V} \times \mathbf{E}+\left(M^{\epsilon}\right)^{-1} M \mathbf{S}_{\mathbf{H}}-\left.\left(M^{\mu}\right)^{-1} F\left(\hat{\mathbf{n}} \times \frac{Y^{+}[\mathbf{E}]+\hat{\mathbf{n}} \times[\mathbf{H}]}{Y^{+}+Y^{-}}\right)\right|_{\delta \mathbf{D}} \tag{9}
\end{equation*}
$$

where $M_{i j}^{\epsilon}=\left(L_{i}(\mathbf{x}), \epsilon(\mathbf{x}) L_{j}(\mathbf{x})\right)_{\mathbf{D}}, M_{i j}^{\mu}=\left(L_{i}(\mathbf{x}), \mu(\mathbf{x}) L_{j}(\mathbf{x})\right)_{\mathbf{D}}, M_{i j}=\left(L_{i}(\mathbf{x}), L_{j}(\mathbf{x})\right)_{\mathbf{D}}$, $\mathbf{V}_{i j}=\left(L_{i}(\mathbf{x}), \nabla L_{j}(\mathbf{x})\right)_{\mathbf{D}}, F_{i j}=\left(L_{i}(\mathbf{x}), L_{l}(\mathbf{x})\right)_{\delta \mathbf{D}}$. Eqs.(8)-(9) and Eqs.(3) can be easily integrated by time-advancing techniques such as Runge-Kutta methods.

For the special case of PEC walls, the field jumps are given by $[\mathbf{E}]=-2 \mathbf{E}^{-}, \quad[\mathbf{H}]=0$, to enforce the correct boundary conditions and the material parameters by $Z^{+}=Z^{-}$. Besides introducing attenuation coefficient into PMLs, PEC boundary conditions are enforced on the outer boundary of the PMLs to truncate the computational domain.

## 3 Numerical Results

The radiation of an electric dipole source located at the center of a dielectric sphere in free space is carefully studied. The sphere is of the radius of 0.3 m with relative permittivity 0.5 and relative permeability 2 . The dipole is polarized along $+z$ direction and has a time-function of the first derivative of Blackman-Harris window function with the central frequency 600 MHz . The free space is truncated by a cube of each side of length 0.4 m which is covered by PMLs with thickness of 0.1 m . After meshing the computational domain with unstructured grid with tetrahedra, a 3rd-order spectral penalty method with the fivestep four-order low storage Runge-Kutta time-advancing technique is exploited to model the electromagnetic radiation. The surface mesh of the sphere is shown in the right figure in Fig. 2. The results shown as in the left figure in Fig. 2 illustrate that the numerical results agree well with analytical solution and the PMLs works well in absorbing outgoing waves.

## 4 Conclusions

A spectral penalty method for the solution of 3D Maxwell's equations with well-posed PML has been developed to model the electromagnetic waves in unbounded physical region. Numerical results of the radiation of an electric dipole source located at a sphere center show an excellent agreement with analytical solution. Other numerical results also illustrate the high accuracy and geometry flexibility of spectral penalty method. The well-posed PML can be successfully introduced into the spectral penalty methods and works very well in absorbing outgoing waves.






Figure 2: Comparison of numerical results with analytical solution (a): $E_{z}$ received at $(0.0 \mathrm{~m}, 0.0 \mathrm{~m}, 0.35 \mathrm{~m}) ;(\mathrm{c}): E_{x}$ received at $(0.25 \mathrm{~m}, 0.25 \mathrm{~m}, 0.3 \mathrm{~m}) ;(\mathrm{e}): E_{z}$ received at $(0.25 \mathrm{~m}, 0.25 \mathrm{~m}, 0.3 \mathrm{~m}) ;(\mathrm{b})(\mathrm{d})(\mathrm{f}):$ their relative errors, respectively.

## References

[1] Q. H. Liu, "The PSTD algorithm: A time-domain method requiring only two cells per wavelength," Microwave Opt. Technol. Lett., vol. 15, pp.158-165, 1997.
[2] J. S. Hesthaven, "Spectral penalty methods," Applied Numerical Mathematics, vol. 33, pp.23-41, 2000.
[3] J. S. Hesthaven, and T. Warburton, "Nodal High-Order Methods on Unstructured Grids I. Time-Domain Solution of Maxwell's Equations," J. Comput. Phys, vol.181, pp.186221, 2002.
[4] J. S. Hesthaven, and C. H. Teng "Stable spectral methods on tetrahedral elements," SIAM J. Sci. Comput., vol.21, pp.2352-2380, 2000.
[5] J. S. Hesthaven, "From electrostatics to almost optimal nodal sets for polynomial interpolation in a simplex," SIAM J. Numer. Anal., vol.35, pp.655-676, 1998.
[6] G.-X. Fan, and Q. H. Liu, "A well-posed PML absorbing boundary condition for lossy media," IEEE Antennas and Propagat. Soc. Intl. Symp., vol. 3, pp. 2-5, Jul. 2001.
[7] A. H. Mohammadian, V. Shankar, and W. F. Hall, "Computation of electromagnetic scattering and radiation using a time-domain finite-volume discretization procedure," Comput. Phys. Communications, vol.68, pp.175-196, 1991.

