High Order Explicit Convolution Free Time-domain Finite Element PML Implementation

Neilen Marais and David B. Davidson*

Abstract — **This paper presents a simple, convolution free, uni-axial perfecly matched layer (UPML) implementation applicable to high-order, explicit finite element time-domain (FETD) solvers. While implementing the UPML for the general FETD case is fairly complex, a simple FDTD-inspired implementation can be derived for the special case of diagonalised Cartesian hexahedra (also called Lobatto-cells). The FDTD description is not directly applicable to Lobatto-cells; analysis in a discrete differential-forms framework results in a suitable FEM description. The resulting semi-discrete form is discretised in time using the leapfrog central-difference method, although an approximation (also present in the FDTD implementation) is made to avoid the need for time-convolution.**

1 Introduction

In common with all PDE based methods, finite element methods (FEM) requires domain truncation methods to make the simulation of finite structures embedded in open regions possible. Berenger's perfectly matched layer (PML) [1] method, first used finite difference time domain (FDTD) context, is an attractive domain termination scheme. While its application to FDTD and frequency domain FEM formulations is fairly straight forward, general PML implementation for finite element time domain (FETD) methods is not: implementations based on the vector-wave equation (curl-curl form) are formidably complex while potentially suffering from instability [2]; coupled Maxwell's equation implementations are more straight forward [3], but in general requires the storage of several auxiliary variables to avoid the need for numerical time-convolution.

In the special case of lumped Cartesian hexahedra [4], their specific properties allow an efficient and straight-forward extention of the uniaxial PML (UPML) to higher order explicit FETD in a manner inspired by the FDTD example [5, §7.8]. When used in an implicit/explicit hybrid [6] with a hexahedral/tetrahedral hybrid discretisation [7], good geometrical modelling and computational efficiency can be comibed.

*Department of Electrical and Electronic Engineering University of Stellenbosch, South Africa nmarais@gmail.com, davidson@sun.ac.za

2 Analysis

2.1 Continuum UPML Absorber

The UPML method describes the absorber as a dispersive, electrically and magnetically lossy, anisotropic material with a characteristic impedance that is matched to its surroundings. The frequency-domain Maxwell's equations in a UPML region matched to free-space is written as:

$$\nabla \times \vec{H} = j\omega\epsilon \bar{\bar{s}} \vec{E}, \tag{1}$$

$$\nabla \times \vec{E} = -j\omega\mu \bar{\bar{s}} \vec{H}, \tag{2}$$

where

$$\bar{\bar{s}} = \begin{bmatrix} \frac{s_y s_z}{s_x} & & \\ & \frac{s_x s_z}{s_y} & \\ & & \frac{s_x s_y}{s_z} \end{bmatrix}, \tag{3}$$

and

$$s_u = \kappa_u + \frac{\sigma_u}{j\omega\epsilon_0}. \tag{4}$$

$\kappa_{x/y/z}$ are stretching factors that makes the medium electrically longer for values larger than 1. $\sigma_{x/y/z}$ are electric or magnetic conductivities[1] that cause the fields inside the PML region to attenuate. Setting $\sigma_x > 0$ causes the attenuation of waves travelling in the $\hat{x}$ direction. Note that the same $\bar{\bar{s}}$ is used for both (1) and (2) in order to match the medium to free-space.

We define for subsequent use:

$$\bar{\bar{s}}_x = \begin{bmatrix} s_x & & \\ & s_y & \\ & & s_z \end{bmatrix}. \tag{5}$$

By permuting the diagonal entries, we also have $\bar{\bar{s}}_y$ with diagonal s_y, s_z, s_x and similarly for $\bar{\bar{s}}_z$. Now,

$$\bar{\bar{s}} = \bar{\bar{s}}_x^{-1} \bar{\bar{s}}_y \bar{\bar{s}}_z, \tag{6}$$

but since all the matrices are diagonal, we can permute the application of $\bar{\bar{s}}_x^{-1}$, $\bar{\bar{s}}_y$ and $\bar{\bar{s}}_z$ in any order. Similar diagonal matrices can be defined for $\bar{\bar{\sigma}}_{x/y/z}$ and $\bar{\bar{\kappa}}_{x/y/z}$ such that

$$\bar{\bar{s}}_x = \bar{\bar{\kappa}}_x + \frac{\bar{\bar{\sigma}}_x}{j\omega\epsilon_0}. \tag{7}$$

[1] Applied to the $\vec{E}$ field, $\sigma_{x/y/z}$ is an electric conductivity, magnetic when applied to $\vec{H}$.

The FDTD convolution-free implementation now introduces two auxiliary fields. In the FDTD literature the physical fields are given as $\vec{E}$ and $\vec{H}$ and the auxiliary fields as $\vec{D}$ and $\vec{B}$. This is not quite accurate, since they are not the physical $\vec{D}$ and $\vec{B}$ fluxes; instead they are written $\tilde{D}$ and $\tilde{B}$ here, the tilde indicating their non-physical nature. They are defined as

$$\tilde{D} = \epsilon \overline{\overline{s}}_x^{-1} \overline{\overline{s}}_z \vec{E}, \qquad \tilde{B} = \mu \overline{\overline{s}}_x^{-1} \overline{\overline{s}}_z \vec{H}, \tag{8}$$

allowing the application of the material operator $\overline{\overline{s}}$ to be split into two steps. Together with (1, 2) this implies:

$$\vec{D} = \overline{\overline{s}}_y \tilde{D}, \qquad \vec{B} = \overline{\overline{s}}_y \tilde{B}. \tag{9}$$

The FDTD analysis proceeds to directly substitute these relations into the Cartesian component form, leading to expressions that have an obvious finite differences discretisation. Unfortunately it does not provide any insight into the FEM discretisation of the UPML.

A suitable FEM discretisation may be obtained by analysing the UPML as differential forms [8, 9]. I.t.o. the auxiliary field components, we have

$$j\omega \star_{s_y} \tilde{D} = dH, \tag{10}$$

$$j\omega \star_{s_y} \tilde{B} = -dE, \tag{11}$$

where $\star_{s_y}$ is a material Hodge operator. Given that H and E are 1-forms, the result of the differential operator d on the RHS is 2-form. For the LHS to also be 2-form, the material Hodge $\star_{s_y}$ has to operate on 1-forms, implying that $\tilde{D}$ and $\tilde{B}$ are 1-forms. For (8) to have consitent forms on both sides, ϵ and μ have to be combined with $\overline{\overline{s}}_z$ as single Hodge operators to form:

$$\tilde{D} = \star_{s_x^{-1}} \star_{\epsilon s_z} E, \qquad \tilde{B} = \star_{s_x^{-1}} \star_{\mu s_z} B. \tag{12}$$

2.2 Semi-discrete UPML

The standard semi-discretisation of Maxwell's equations discretises $\vec{E}$ as 'n discrete 1-form and $\vec{B}$ as a discrete 2-form, both defined on the primary lattice. The discrete forms implicitly define *twisted* lattice discretisations of $\vec{D}$ and $\vec{H}$ on the dual grid [9]. Some pertinent properties of the discrete differntial forms operators in 3-D space are:

- The discrete exterior derivative operator d operating on a 1-form (i.e. $\nabla\times$) results in 2-form on the same (i.e. *primary* or *twisted*) lattice.
- Hodge $\star$ operators define an isomorphism between between l-forms on one lattice (e.g. primary 1-form) and $(3-l)$-forms on the dual lattice (e.g. twisted 2-form).

Written in discrete forms notation, (10-12) become:

$$j\omega[\star_{s_y}]\{\tilde{d}\} = [C]^T\{h^\dagger\}, \tag{13}$$

$$j\omega[\star^\dagger_{s_y}]\{\tilde{b^\dagger}\} = -[C]\{e\}, \tag{14}$$

$$\{\tilde{d}\} = [\star_{s_x}]^{-1}[\star_{\epsilon s_z}]\{e\}, \tag{15}$$

$$\{\tilde{b^\dagger}\} = [\star^\dagger_{s_x}]^{-1}[\star^\dagger_{\mu s_z}]\{h^\dagger\}, \tag{16}$$

where the $\dagger$ superscript indicates twisted form quantities, $[C]$ is the incidence (i.e. exterior derivative) matrix, $[\star]$ is a discrete Hodge matrix and $\{\cdot\}$ represents discrete form degrees of freedom. Continuum Hodges, e.g. $\star_{s_x}$, operate on both electric and magnetic quantities, while in the discrete case there are separate Hodges defined for either primary grid or twisted forms.

Calculating the entries of the primary grid discrete Hodge operators is quite straight forward using the normal Galerkin Hodge process:

$$[\star_{\epsilon s_z}]_{ij} = \int_\Omega \vec{w}_i^{(1)} \cdot \epsilon \overline{\overline{s}}_z \vec{w}_j^{(1)}\, d\Omega, \tag{17}$$

and similarly for $[\star_{s_y}]$ and $[\star_z]$, where $\vec{w}_i^{(1)}$ are the primary grid 1-form basis functions used to expand the $\vec{E}$ field. Calculating the entries for the twisted form Hodge operators is not obvious since basis function expansions of the twisted forms are unknown. They can, however, be defined quite simply by using Galerkin duality [10, 11]. For example:

$$[\star^\dagger_{\mu s_z}] = [\star_{\mu^{-1} s_z^{-1}}]^{-1}, \tag{18}$$

with

$$[\star_{\mu^{-1} s_z^{-1}}]_{ij} = \int_\Omega \vec{w}_i^{(2)} \cdot \mu^{-1} \overline{\overline{s}}_z^{-1} \vec{w}_j^{(2)}\, d\Omega, \tag{19}$$

where $\vec{w}_i^{(2)}$ are the primary grid 2-form basis functions used to expand $\vec{B}$. Now we can rewrite (16) as

$$\{\tilde{b^\dagger}\} = [\star_{s_x^{-1}}][\star_{\mu^{-1} s_z^{-1}}]^{-1}\{h^\dagger\}, \tag{20}$$

and similarly for (14).

The standard frequency-domain FEM discretisation of the UPML material, is

$$\{d^\dagger\} = [\star_{\epsilon s}]\{e\} \tag{21}$$

$$\{b\} = [\star_{\mu^{-1} s^{-1}}]^{-1}\{h^\dagger\}, \tag{22}$$

where

$$[\star_{\epsilon s}]_{ij} = \int_\Omega \vec{w}_i^{(1)} \cdot \epsilon \overline{\overline{s}} \vec{w}_j^{(1)}\, d\Omega, \tag{23}$$

and a similar integral involving 2-form basis functions for $[\star_{\mu^{-1} s^{-1}}]$.

Assuming initially that $\bar{\bar{s}}$ and ϵ are constant, we can write[2]

$$[\star_{\epsilon s}] = \frac{\epsilon s_y s_z}{s_x}[L_x^{(1)}] + \frac{\epsilon s_z s_x}{s_y}[L_y^{(1)}] + \frac{\epsilon s_x s_y}{s_z}[L_z^{(1)}] \quad (24)$$

and a similar expression for $[\star_{\mu^{-1}s^{-1}}]$ where the $[L_u^{(l)}]$ matrices represent the metric of the l-form basis functions in the $\hat{u}$ direction:

$$[L_u^{(l)}]_{ij} = \int_\Omega (\hat{u} \cdot \vec{w}_i^{(l)}) \cdot (\hat{u} \cdot \vec{w}_j^{(l)})\, d\Omega. \quad (25)$$

It is quite clear that in general $[\star_{s_y}][\star_{s_x}]^{-1}[\star_{\epsilon s_z}] \neq [\star_{\epsilon s}]$. However, the $[L_u]$ matrices for Cartesian hexahedra have additional structure since the basis functions are defined in separate $\hat{x}$, $\hat{y}$ and $\hat{z}$ directed groups. Assuming the global degrees of freedom are numbered such that the $\hat{x}$, $\hat{y}$ and $\hat{z}$ directed groups are numbered in order, we have

$$[L_x^l] = \begin{bmatrix} [L_{xx}^l] & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (26)$$

and similarly for $[L_y^l]$ with $[L_{yy}^l]$ on the second diagonal block and $[L_z^l]$ with $[L_{zz}^l]$ on the third. Now we can write:

$$[\star_{\epsilon s_z}] = \epsilon s_z [L_{xx}^{(1)}] \oplus \epsilon s_x [L_{yy}^{(1)}] \oplus \epsilon s_z [L_{zz}^{(1)}]. \quad (27)$$

Considering only the x directed dofs we have

$$\begin{aligned} \left([\star_{s_z}][\star_{s_x}]^{-1}[\star_{\epsilon s_z}]\right)_x &= \left(s_y [L_{xx}^{(1)}] \frac{1}{s_x} [L_{xx}^{(1)}]^{-1} \epsilon s_z [L_{xx}^{(1)}] \right) \\ &= \frac{s_y s_z}{s_x} [L_{xx}^{(1)}] \\ &= \left([\star_{\epsilon s}]\right)_x, \end{aligned} \quad (28)$$

and similarly for the y and z blocks. The identity (28) depends on multiplication by the material properties being commutative; this is ensured by the choice of constant material properties and by the block-diagonal property of the $[L_u]$ matrices. However, when using the basis functions and approximate inner product as defined in [4], both the $[L_u]$ matrices and material operators can be written as diagonal matrices, implying commutative multiplication. In other words, when using these lumped Cartesian hexehedra, *the two-step material application is equivalent to the standard FEM discretisation.*

[2]Note, here s_x, s_y and s_z are the scalar quantities in (4), not to be confused with the the dyads $\bar{\bar{s}}_x$, etc. in (6)

2.3 Fully Discrete UPML

To make the UPML operational, time-domain expressions are required. If the time-domain expressions involve only first-derivatives of time, the standard central difference leap-frog time-discretisation can be used without the need for numerical convolution. Subsequently we assume diagonalised Cartesian hexahedra are used for the spatial discretisation. We consider the case where the material properties are element-wise constant as is normal for the FEM. Because of the block-diagonal nature of the matrices, we can analyse the $\hat{x}$, $\hat{y}$ and $\hat{z}$ basis sets independently; subsequently we will *only work with the $\hat{x}$ components*, since the analysis of the other components are similar. Also assuming diagonal $[L_u]$ matrices we can calculate the entries of the diagonal material operator matrices as e.g. (and similarly for the other material matrices)

$$[s_x]_{ii} = \frac{\sum_K^{\text{supp}(\vec{w}_i^{(1)})} s_x(K)}{\text{len}(\text{supp}(\vec{w}_i^{(1)}))}, \quad (29)$$

where $\text{supp}(\vec{w}_i^{()})$ is the support of basis function $\vec{w}_i^{()}$ and $\text{len}(\cdot)$ gives the number of elements.

We only treat the derivation of an update equation for (20), since none of the other update equations involve problematic time derivatives. Substituting the material defined above into (20), we have

$$\{\tilde{b}^\dagger\} = [s_x^{-1}][L_{xx}^{(2)}] \left([\mu^{-1} s_z^{-1}][L_{xx}^{(2)}] \right)^{-1} \{h^\dagger\}, \quad (30)$$

but since all the matrices are diagonal, we solve for $\{h^\dagger\}$ and get

$$\{h^\dagger\} = [s_x^{-1}]^{-1}[\mu^{-1} s_z^{-1}]\{\tilde{b}^\dagger\}. \quad (31)$$

Now we consider only a single equation defined for $\{h^\dagger\}_i$ and $\{\tilde{b}^\dagger\}$. Using the fact that discrete 2-forms can only have face or volume degrees of freedom, a given $\vec{w}_i^{(2)}$ can have support in at most 2 elements. We label the elements K_a and K_b. Now we have

$$\{h^\dagger\}_i = \frac{\frac{1}{s_x(K_a)} + \frac{1}{s_x K_b}}{\frac{1}{\mu K_a s_z(K_a)} + \frac{1}{\mu(K_b) s_z(K_b)}} \{\tilde{b}^\dagger\}_i. \quad (32)$$

This results in an expression that requires time-convolution to cast into the time-domain. If we make the following approximation:

$$\frac{1}{s(K_a)} + \frac{1}{s(K_b)} \simeq \frac{1}{(s(K_a) + s(K_b))/2}, \quad (33)$$

resulting in the much simpler form

$$\bar{\mu} \bar{s_z} \{h^\dagger\}_i = \bar{s_x} \{b^\dagger\}_i \quad (34)$$

where the overbar indicates the average value in K_a and K_b. Now we can write

$$\bar{\mu}(j\omega\bar{\kappa_z} + \bar{\sigma_z})\{h^\dagger\}_i = (j\omega\bar{\kappa_x} + \bar{\sigma_x})\{b^\dagger\}_i. \quad (35)$$

This is in fact the same form that the FDTD equations take [5, §7.8.1]. The approximation implied by (33) goes some ways to explaining the need for graded FDTD profiles; if the material parameters vary smoothly, (33) will be a resonable approximation. Transforming to the time-domain, we get

$$\bar{\mu}(\frac{\partial}{\partial t}\bar{\kappa_z} + \bar{\sigma_z})\{h^\dagger\}_i = (\frac{\partial}{\partial t}\bar{\kappa_x} + \bar{\sigma_x})\{b^\dagger\}_i. \quad (36)$$

This form contains only first derivatives, hence straight-forward time discretisation is possible using standard leap-frog central differencing and the semi-implicit [5, (3.26)] treatment of loss terms.

To make the UPML operational, the following procedure is followed: At whole time-steps (13) is solved for $\{\tilde{d}\}$ followed by solving (15) for $\{e\}$. At half time-steps, (14) is solved for $\{b^\dagger\}$, followed by solving (16) for $\{h^\dagger\}$. Since all the system matrices are diagonal, the solution is explicit. Above we assume that the equations have been converted to their time-domain equivalents.

3 Results

Results are shown for an infinitesimal dipole located at the centre of a 2x2x2m freespace cube with a cell-size of 1/7.5 m and a 5-cell UMPL termination with a cubic profile. The speed of light is normalised to 1m/s. The dipole is excited using a differentiated Gaussian pulse with a centre-frequency of 1 Hz, and the timestep 1/75 s.

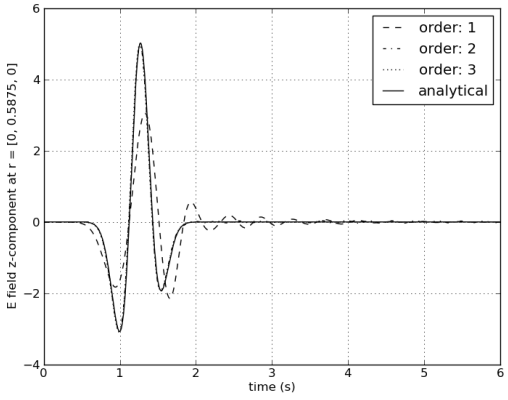

Figure 1: Comparison of 1st, 2nd and 3rd order UPML-terminated explicit FETD infintesimal dipole solutions with analytical result.

The 1st order result in fig. 1 shows a fairly poor transient response due to numerical dispersion caused by the rather coarse discretisation, and also a significant reflected wave of ≈ -15 dB. The 2nd order result has an almost perfect transient response, and reflection of ≈ -45 dB. The 3rd order result improves the reflection to ≈ -62 dB. Note that they all use the same PML profile and size; the differences are due only to improvements in field discretisation.

4 Conclusion

The two-step FDTD UPML implementation was analysed using differential forms in order to produce a scheme suitable for FEM implementation. It was shown that this scheme is equivalent to the rigorous FEM discretisation when lumped Cartesian hexahedra are used. Results of an higher-order explicit FEM based on these elements and the UPML method derived here was presented, showing good absorber performance.

References

[1] J.-P. Berenger, "A perfectly matched layer for the absorption of electromagnetic waves," *Journal of Computational Physics*, vol. 114, pp. 185–200, Oct. 1994.

[2] T. Rylander and J.-M. Jin, "Perfectly matched layer in three dimensions for the time-domain finite element method applied to radiation problems," *IEEE Trans. Antennas Propagat.*, vol. 53, pp. 1489–1499, 2005.

[3] B. Donderici and F. L. Teixeira, "Conformal perfectly matched layer for the mixed finite element time-domain method," *IEEE Trans. Antennas Propagat.*, vol. 56, pp. 1017–1026, 2008.

[4] G. Cohen and P. Monk, "Gauss point mass lumping schemes for Maxwell's equations," *Numerical Methods for Partial Differential Equations*, vol. 14, pp. 63–88, 1998.

[5] A. Taflove and S. C. Hagness, Eds., *Computational Electrodynamics The Finite-Difference Time-Domain Method*, 3rd ed. Artech House, 2005.

[6] N. Marais and D. B. Davidson, "Efficient High-Order time domain hybrid Implicit/Explicit finite element methods for microwave electromagnetics," *Electromagnetics*, vol. 30, no. 1, p. 127, 2010.

[7] ——, "Conforming arbitrary order hexahedral/tetrahedral hybrid discretisation," *IET Electron. Lett.*, vol. 44, no. 24, pp. 1384–385, Nov. 2008.

[8] G. A. Deschamps, "Electromagnetics and differential forms," *Proc. IEEE*, vol. 69, no. 6, pp. 676–969, Jun. 1981.

[9] F. L. Teixeira and W. C. Chew, "Lattice electromagnetic theory from a topological viewpoint." *Journal of Mathematical Physics*, vol. 40, p. 169, 1999.

[10] B. He and F. Teixeira, "Geometric finite element discretization of Maxwell equations in primal and dual spaces," *Physics Letters A*, vol. 349, pp. 1–14, 2006.

[11] B. He and F. L. Teixeira, "Differential forms, Galerkin duality, and sparse inverse approximations in finite element solutions of Maxwell equations," *IEEE Trans. Antennas Propagat.*, vol. 55, pp. 1359–1368, 2007.