GENERALISED UNSPLIT E-H PML WITH JEC TECHNIQUE FOR DISPERSIVE MEDIA

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1- Introduction

Different approaches propose the introduction of dispersive models to the FDTD method. They are generally divided into three categories: Z-transform method, ADE method (Equation Differential Auxiliary) and RC method (Convolution Recursive). The three methods offer now second-order precision. This is true particularly for the PLRC [1] and JEC [2] techniques, which belong to the RC method. This latest is very efficient for its computation time and memory occupation. Moreover its extension to multiple-pole susceptibility function is straigthforward. On the other hand, open dispersive media can be simulated in the FDTD method thanks to the PML absorber. Fan & Liu [3] have described an approach, which is infortunately depending on dispersive model (Debye, Drude, Lorentz). Teixera & Chew [4] have proposed a general formulation using the PLRC technique, but the algorithm becomes complex and the split components for **E**, **H**, **D** and **B,** and the recursive accumulator, raise drastically the computation time and the memory size.

What we propose is a simple and general approach based on the complex coordinate stretched PML theory [5] that are combined with the JEC technique (J-E Convolution) in 3D-space to simulate opened-space linear dispersive media. The constitutive parameters of the PML are applied uniquely on the **D-B** induction vectors. In consequence the influence of the PML absorber is independent of the constitutive parameters of the dispersive or conductive media. As a result, the components of the **E-H** field vectors are unsplit and the algorithm treating the different media in the inner region is preserved in the PML region. In the following section, the JEC technique is summarizing for a general dispersive medium including Debye and Lorentz models. The third section develops the new general PML-JEC absorber for dispersive media. Then an effective algorithm is proposed to calculate the split components of **D** and **B** only in the PML region. To illustrate the effectiveness of the proposed algorithm, numerical result with Lorentz and Debye dispersive media is given in the last section.

2- The JEC technique

The JEC technique as proposed in [2] is generalised here and presented concisely by considering the general dispersive model in the time domain:

$$\varepsilon(t)=\varepsilon_0\varepsilon_\infty\delta(t)+\varepsilon_0\chi_r(t)$$
$$\text{with } \chi_r(t)=\left[A_1\cos(\omega_1 t)+B_1\cos(\omega_1 t)\right]e^{-\alpha_1 t}U(t) \tag{1}$$

The coefficients A_1, B_1 and α_1 are real and constant. The equivalent Debye model is obtained by setting ω_1=0 and B_1=0 and the equivalent Lorentz model by setting A_1=0. To update $\chi(t)$ in a corresponding discrete recursive form, the general relation (1) can be written in the following complex form:

$$\hat{\chi}_r(t)=\hat{G}_1 e^{-\hat{\gamma}_1 t}U(t) \tag{2}$$

where $\chi_r(t)=\Re e\{\hat{\chi}_r(t)\}$; $\hat{\gamma}_1=\alpha_1+i\omega_1$; $\hat{G}_1=A_1+iB_1$ and $U(t)$ the Heaviside function

The complex permittivity is introduced to the Maxwell-Faraday equation in the time domain:

$$\text{rot}\mathbf{H}(\mathbf{t})=\partial_t\mathbf{D}(\mathbf{t})+\sigma_e\mathbf{E}(\mathbf{t})$$
$$\text{where } \mathbf{D}(\mathbf{t})=\varepsilon_0\varepsilon_\infty\mathbf{E}(\mathbf{t})+\varepsilon_0\chi_r(t)\otimes\mathbf{E}(\mathbf{t}) \tag{3}$$

Using (2) to derive **D(t)**, one can show that (3) becomes:

$$\mathrm{rot}\mathbf{H}(t) = \varepsilon_0 \varepsilon_\infty \partial_t \mathbf{E}(t) + (\varepsilon_0 A_1 + \sigma_e)\mathbf{E}(t) + \mathbf{J}(t) \tag{4}$$

where $A_1 = \Re e(\hat{G})$ and **J**(t) is a density current defined by:

$$\mathbf{J}(t) = -\varepsilon_0 \Re e\left\{\hat{G}_1 \hat{\gamma}_1 e^{-\hat{\gamma}_1 t}\right\} \otimes \mathbf{E}(t) \tag{5}$$

To perform the convolution operation, a discrete rectangular rule summation is applied to (5), A complex expression is then derived with a recursive form and a second-order precision for each **J** component [2]. Here the recursive form becomes:

$$\hat{J}^{n+\frac{1}{2}} = \varepsilon_0 e^{-\hat{\gamma}_1 \Delta t} \hat{J}^{n-\frac{1}{2}} - \varepsilon_0 \hat{G}_1 \hat{\gamma}_1 e^{-\hat{\gamma}_1 \frac{\Delta t}{2}} E^n \Delta t \tag{6}$$

The update of **E** components is obtained from (4):

$$E^{n+1} = \frac{1}{\varepsilon_\infty + \frac{\Delta t}{2}\left(A + \sigma_e/\varepsilon_0\right)} \left\{\left(\varepsilon_\infty - \frac{\Delta t}{2}\left(A + \sigma_e/\varepsilon_0\right)\right) E^n - \frac{\Delta t}{\varepsilon_0} \Re e\left(\hat{J}^{n+\frac{1}{2}}\right) + \frac{\Delta t}{\varepsilon_0}(\mathbf{n} \cdot \mathrm{rot}\mathbf{H})^{n+\frac{1}{2}}\right\} \tag{7}$$

The algorithm update is explicit and its extension to multiple-pole dispersion model is straightforward. We should mention that an added storage is required for each component of **J** to treat (6). Further, if the model is Debye type, the equation (6) becomes real instead of complex.

3- Generalised unsplit E-H PML for dispersive media

The general theory of PML ABC is deduced from the complex coordinate stretching [5]. Some degrees of freedom in the Maxwell's equations are added to achieve the reflectionless absorption of the wave inside the PML region. In the frequency domain, the modified Maxwell's equations in the complex coordinate stretching PML formulation with the convention $e^{i\omega t}$ are:

$$\nabla_s \times \mathbf{E} = -i\omega \mathbf{B} \quad \text{and} \quad \nabla_s \times \mathbf{H} = i\omega \varepsilon_0 \varepsilon_\infty \mathbf{E} + (\varepsilon_0 A_1 + \sigma_e)\mathbf{E} + \mathbf{J} \tag{8}$$

The second equation takes into account the dispersive media as given in (4) and (5). ∇_s is defined as:

$$\nabla_s = \hat{x}\frac{1}{s_x}\partial_x + \hat{y}\frac{1}{s_y}\partial_y + \hat{z}\frac{1}{s_z}\partial_z \quad \text{and} \quad s_l = a_l + i\frac{\Omega_l}{\omega} \;\; (l=x,y,z) \tag{9}$$

The s_l are frequency dependent complex stretching variable. The real variables a_l and Ω_l are functions of the PML space profile and are introduced to attenuate without reflection the evanescent and propagating waves respectively. To well separate the influence of the variables s_l from the different media, a vector $\mathbf{D_1}$ is introduced such as:

$$i\omega \mathbf{D_1} = i\omega \varepsilon_0 \varepsilon_\infty \mathbf{E} + (\varepsilon_0 A_1 + \sigma_e)\mathbf{E} + \mathbf{J} \tag{10}$$

$$\text{so } \nabla_s \times \mathbf{H} = i\omega \mathbf{D}_1 \tag{11}$$

Now, before to transpose equations in the time domain, $\mathbf{D_1}$ and **B** are split in three components ($\mathbf{D_{1sx}}$+ $\mathbf{D_{1sy}}$+$\mathbf{D_{1sz}}$ and $\mathbf{B_{sx}}$+$\mathbf{B_{sy}}$+$\mathbf{B_{sz}}$ respectively) to facilitate manipulation and each component is defined from (8), (9) and (11) in the time domain as $\mathbf{B_{sz}}$ and $\mathbf{D_{1sz}}$:

$$a_z \partial_t \mathbf{B_{sz}} + \Omega_z \mathbf{B_{sz}} = -\partial_z \hat{\mathbf{z}} \times \mathbf{E} \tag{12-a}$$

$$a_z \partial_t \mathbf{D_{1sz}} + \Omega_z \mathbf{D_{1sz}} = +\partial_z \hat{\mathbf{z}} \times \mathbf{H} \tag{12-b}$$

By circular permutation, the other components are deduced. From (10), a new time domain equation is obtained:

$$\partial_t \mathbf{D_1} = \varepsilon_0 \varepsilon_\infty \partial_t \mathbf{E} + (\varepsilon_0 \mathbf{A_1} + \sigma)\mathbf{E} + \mathbf{J} \tag{13}$$

Equations (12) and (13) can be written easily in the discrete space. For example, the update of split components B_{yz}, D_{1yz} and unsplit components E_y is given:

$$B_{yz}^{n+\frac{1}{2}} = ab_z \cdot B_{yz}^{n-\frac{1}{2}} - bb_z \cdot \left[\Delta E_x^n / \Delta z\right] \; ; \; D_{1yz}^{n} = ad_z \cdot D_{1yz}^{n-1} + bd_z \cdot \left[\Delta H_x^{n+\frac{1}{2}} / \Delta z\right] \tag{14-a}$$

$$E_y^{n+1} = ae_y E_y^n + be_y \left\{ \Delta t \left(D_{1yx}^{n+1} + D_{1yz}^{n+1} - D_{1yx}^{n} - D_{1yz}^{n} \right) - J_y^{n+\frac{1}{2}} \right\} \quad (14\text{-b})$$

ab_z, ad_z, bb_z and bd_z are coefficients depending on the variables a_z and Ω_z. The PML algorithm with the update of the $\mathbf{D_1}$-**B** components (14-a) is clearly independent of the media (with or without electrical losses). Coupled with the JEC technique, The PMLs can absorb outgoing wave from any Debye or Lorentz dispersive media with one or multiple poles. This original algorithm consists to update 12 subcomponents for $\mathbf{D_1}$ and **B** and 6 components for **E** and **H**. We will show in the next section that the number of the $\mathbf{D_1}$-**B** subcomponent update can be further reduced. Noting that the components of **B** are not necessary except if a dispersive magnetic medium is present. However, the use of **B** avoids the split components of **H**. The magnetic media are not considered in this paper but the JEC technique can be applied to them with a magnetic model similar to (1).

4- Efficient PML algorithm

Enhancements can be introduced to above algorithm to reduce the number of subcomponent update for $\mathbf{D_1}$ and **B** in considering that the absorption contribution of each component s_l operates separately from the others. In addition the absorption contribution of s_z is limited to the xoy (inf and sup) PML regions including corner and edge zones (fig.1). Same thing is true for the variable s_x associated to the yoz PML region and the variable s_y associated to the zox PML region. So, for each PML region, only 4 split components of $\mathbf{D_1}$ and **B** are useful for absorption. For example, with xoy PML region, only the components D_{1xz}, D_{1yz}, B_{xz} and B_{yz} are needed for the absorption contribution of s_z. Hence, with the treatment of all 6 PML regions, we obtain automatically the update of 12 $\mathbf{D_1}$-**B** split components in the PML corner zones (intersection between three regions) and the update of 8 $\mathbf{D_1}$-**B** split components in the PML edge zones (intersection between two regions). So the algorithm can be performed as following:

a- Update **E** components everywhere even in the PML region with classical algorithm (included dispersive media with current density **J**) as (7). For Example:
   $E_y(i,j,k) = ae_y(i,j,k)*E_y(i,j,k)+ be_y(i,j,k)*(DH_x(i,j,k)*d\_dz(k) -(DH_z(i,j,k)* d\_dx(i) -J_y)$
   where $d\_dz(k) = 1/Dz$ and $d\_dx(i) = 1/Dx$ if index k or i is in the inner region else zero if index k or i is in the PML region.
b- Update $\mathbf{D_1}$ components as (14-a) and add them to **E** components (only 4 $\mathbf{D_1}$-**B** split components in each PML region). For example in the xoy PML region:
   $D_{1yz}(i,j,k) = ad_z(k)* D_{1yz\,prev}(i,j,k)+ bd_z(k)*DH_x(i,j,k)$
   $E_y(i,j,k) = E_y(i,j,k)+ be_y(i,j,k)*Dt*(D_{yz}(i,j,k)-D_{yz\,prev}(i,j,k))$
   The parameter Δt can be suppressed by including it in $bd_z(k)$ and avoiding one supplementary operation. $D_{yz\,prev}$ is the D_{yz} component of the previous time step and it must be stored in a temporary variable.
c- Update **H** components similarly to (a)
d- Update **B** components and add them to **H** components similarly to (b)

Added memory cost of the PML is reduced to minimum with 4 storages for each PML region. Notice that the dispersive or conductive media in the PML do not add supplementary storage.

5- Validation

The PML-JEC algorithm is validated successfully with Lorentz, Drude and Debye dispersive media in 3D-space. Relative error due to PML termination with Lorentz and Debye dispersive media is presented here. In both cases, the reference is calculated on 25 processors with a large domain (235*235*130 cells) terminated by 16-cell PML absorber. The first case is a dipole radiating above a 2-pole Lorentz medium that penetrates in the PML (fig.2-a) with 6 observation points placed near the PML absorber. Relative error (fig 2-b) is always less than –60dB. The second case is a plane wave with 30° incident angle (fig.3-a) penetrating in a 2-pole Debye medium in which a cylindrical metal is buried. Error relative from two observation points placed near PML Corners is also less than –55dB.

6- Conclusion

A general and efficient PML-JEC absorber is described. The **E-H** components are unsplit so the algorithm for the dispersive media can be applied in the PML region without modification. Wave Absorption inside each 6 PML region is accomplished due to only 4 added split component of $\mathbf{D_1}$ and **B**. Simple algorithm is derived and it should mention that the new PML do not add complex code for the data parallelism and no more communications between the processes are necessary.

Fig 1: xoy PML region, cell size nx*ny*npml

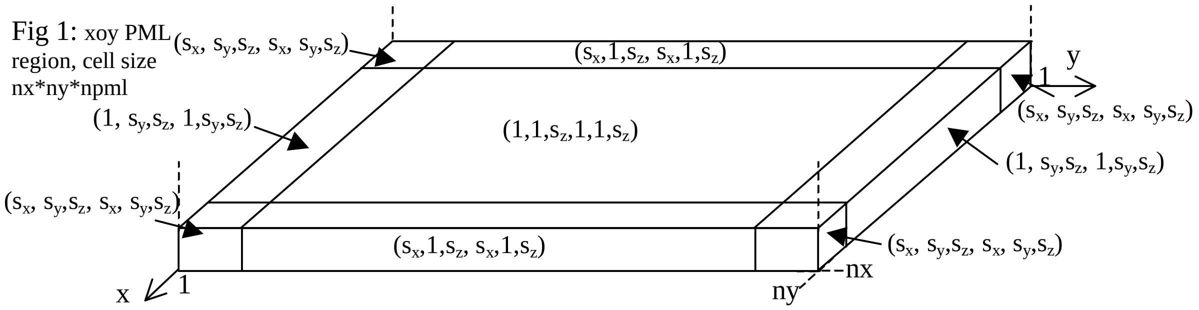
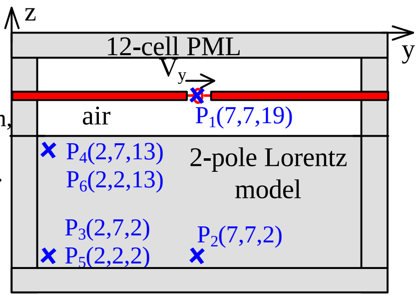


Fig 2-a: A voltage driven dipole above a Lorentz medium, gaussian pulse, fmax = 80 GHz. The field are probed at 6 points.



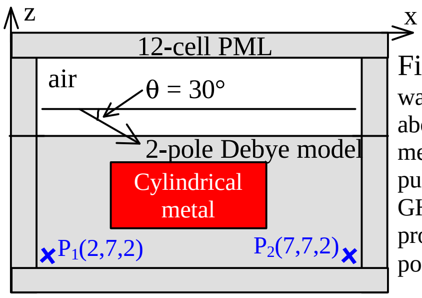


Fig 3-a: Plane wave source above a Debye medium, gaussian pulse, fmax = 10 GHz. Fields are probed at 2 points.

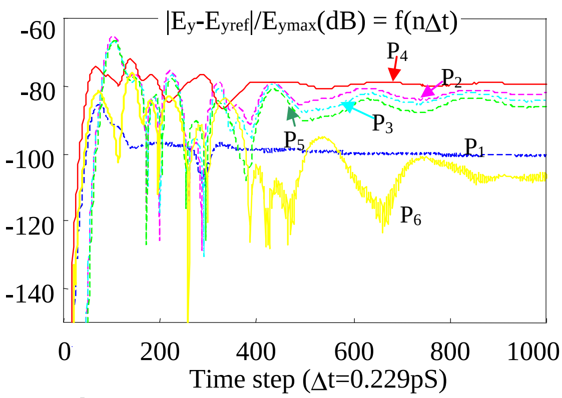


Fig 2-b: relative error due to a 12-cell PML termination of 2-pole Lorentz medium

Lorentz poles : $\varepsilon_\infty = 3.5$; $\varepsilon_s = 5.5$

$\omega_1 = 2\pi*20*10^9$ $\omega_2 = 2\pi*50*10^9$

$\delta_1 = 0.05\ \omega_1$; $G_1 = 0.4$ $\delta_2 = 0.1\ \omega_1$; $G_2 = 0.4$

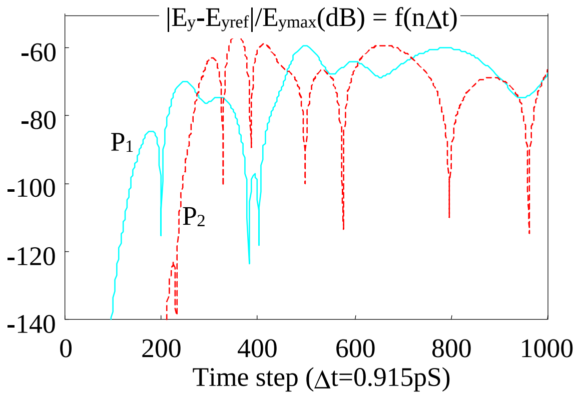


Fig 3-b: relative error due to a 12-cell PML termination of 2-pole Debye medium

Debye poles : ε_∞ 12.3 ; $\varepsilon_s = 5.5$

$G_1(\varepsilon_s-\varepsilon_\infty) = 15.0$ $G_2(\varepsilon_s-\varepsilon_\infty) = 8.0$

$\tau_1 = 3.98nS$ $\tau_2 = 19.9pS$

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