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Numerical analysis / *Analyse numérique*

On a surprising instability result of Perfectly Matched Layers for Maxwell's equations in 3D media with diagonal anisotropy

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Abstract. The analysis of Cartesian Perfectly Matched Layers (PMLs) in the context of time-domain electromagnetic wave propagation in a 3D unbounded anisotropic homogeneous medium modelled by a diagonal dielectric tensor is presented. Contrary to the 3D scalar wave equation or 2D Maxwell's equations some diagonal anisotropies lead to the existence of backward waves giving rise to instabilities of the PMLs. Numerical experiments confirm the presented result.

Résumé. Dans cette note nous nous intéressons à l'analyse de stabilité de la méthode de couches absorbantes parfaitement adaptées (PMLs) pour la propagation d'ondes électromagnétiques en régime transitoire dans un milieu anisotrope décrit par un tenseur diélectrique diagonal. Contrairement aux cas de l'équation d'ondes scalaire 3D et des équations de Maxwell 2D, certaines anisotropies diagonales mènent à l'existence d'ondes inverses qui provoquent des instabilités de la méthode PML. Ce résultat est illustré par des simulations numériques.

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Nous nous intéressons à la simulation numérique de la propagation des ondes électromagnétiques, décrite par des équations de Maxwell, dans un milieu non borné tridimensionnel (voir (1) ci-dessous). Afin de borner artificiellement le domaine de calcul, une technique largement utilisée proposée initialement dans [6] et [7], consiste à appliquer les couches absorbantes parfaitement adaptées (PMLs). Cette méthode est efficace et très populaire car simple à implémenter. Toutefois il est connu que la méthode PML classique en coordonnées cartésiennes ne fonctionne

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pas lorsqu'il existe des ondes inverses dans la direction d'une des couches, i.e. des ondes pour lesquelles les projections de la vitesse de groupe et de la vitesse de phase dans cette direction sont opposées (voir la définition (9) pour plus de détails). Plus précisément, il a été démontré dans [2] que l'absence d'ondes inverses dans la direction de la couche est une condition nécessaire de stabilité des PMLs en régime transitoire.

Dans cette note nous nous concentrons sur des milieux anisotropes avec un tenseur diélectrique diagonal, modélisant par exemple certains types de cristaux. Ces cristaux sont appelés matériaux biréfringents ou bi-axiaux (voir [8] pour plus de détails). Pour ces modèles à anisotropie diagonale, peut-il y avoir existence d'ondes inverses et par conséquent des instabilités des PMLs ? La réponse est non pour l'équation des ondes scalaire 2D ou 3D et les équations de Maxwell 2D (qui peuvent se réduire à la résolution d'une équation scalaire), modèles pour lesquels la condition nécessaire de stabilité proposée dans [2] est toujours vérifiée. Dans ces derniers cas il serait même possible de montrer un résultat de stabilité des PMLs classiques en s'inspirant des techniques développées dans [10] et [5]. Cependant, de façon inattendue, dans le cas des équations de Maxwell 3D avec un tenseur diélectrique diagonal, certaines anisotropies mènent à l'apparition d'instabilités des PMLs (voir Figure 2). Ce dernier cas est contre-intuitif et nous expliquons ce phénomène dans cette note. Le résultat est formulé dans le théorème suivant :

Théorème 1. *Soit $\underline{\underline{\varepsilon}}$ un tenseur diélectrique diagonal avec les coefficients ε_i, $i = 1,2,3$. Si*

$$\min(\varepsilon_2, \varepsilon_3) < \varepsilon_1 < \max(\varepsilon_2, \varepsilon_3) \tag{1}$$

alors il existe des ondes inverses dans la direction $\boldsymbol{e}_1$. Sinon, il n'y a pas d'ondes inverses dans la direction $\boldsymbol{e}_1$.

En conséquence, la méthode PML est instable en régime transitoire si le milieu satisfait la condition (1). Les simulations numériques confirment l'apparition des instabilités dans ce cas (voir Figure 2). Notons que pour un tel milieu nous n'avons observé aucune instabilité numérique dans les deux autres directions, la justification théorique resterait à faire.

La preuve du théorème 1 n'est évidemment pas spécifique à la direction $\boldsymbol{e}_1$ et le résultat peut facilement être généralisé de la façon suivante : si les coefficients intervenant dans le tenseur diélectrique sont différents deux à deux alors la méthode PML est instable. Dans ce cas, il faudrait trouver une nouvelle stratégie pour borner le domaine de calcul car les méthodes de stabilisation des PMLs qui existent pour d'autres modèles ne semblent pas appropriées dans le cas présent (voir [10] pour l'acoustique en écoulement, [9] pour l'acoustique anisotrope, [11] pour les équations d'Euler linéarisées, [4] pour les modèles de métamatériaux dispersifs et [3] pour les plasmas froids fortement magnétisés).

1. Introduction

We are interested in simulating time-domain wave propagation in three-dimensional unbounded anisotropic media which can be described with Maxwell's equations. Since the medium is unbounded, one needs to introduce an equivalent or approximated formulation set in a bounded domain which is suitable for numerical purposes. The widely-used Perfectly Matched Layers (PML) method (see e.g. [6], [7]) consists in surrounding the computational domain by a layer which absorbs outgoing waves. PML techniques are very popular because they are efficient and easy to implement for a large class of problems. Moreover, their use requires no auxiliary knowledge (e.g. the fundamental solution) but only the PDE itself. However, it is well known that one can observe instabilities when classical Cartesian PMLs for anisotropic or dispersive media are used (see e.g. [2]).

In [2] a mathematical analysis has been performed and a necessary criterion of stability has been established: classical PMLs are unstable if there exist backward modes in one of the directions of the layer (a more precise mathematical definition is given below). In this note, we consider electromagnetic wave propagation in anisotropic media where the tensor of electric permittivity is diagonal. A typical example of such media is given by biaxial or birefringent crystals (see [8] for details). It is then natural to wonder, when considering models with diagonal anisotropy, do backward waves exist? The answer is no for the 2D and 3D scalar wave equation as well as for 2D Maxwell's equations (which can be reduced to the resolution of a scalar equation). But surprisingly backward waves do exist for 3D Maxwell's equations for a class of diagonal anisotropic dielectric tensors. This is counter-intuitive and a more detailed analysis follows.

We present first the problem statement and recall general considerations for the necessary stability criterion in Section 2, a detailed proof and numerical illustrations are given in Section 3.

2. Problem statement and reminders on PMLs

We consider electromagnetic wave propagation in an anisotropic medium described by Maxwell's equations (where we use the scaling $\varepsilon_0 = \mu_0 = 1$)

$$\underline{\underline{\varepsilon}}\partial_{tt}\boldsymbol{E}(t,\boldsymbol{x}) + \nabla\times\nabla\times\boldsymbol{E}(t,\boldsymbol{x}) = 0, \quad \boldsymbol{x} = (x_1,x_2,x_3)\in\mathbb{R}^3 \tag{1}$$

with compactly supported initial conditions $\boldsymbol{E}|_{t=0} = \boldsymbol{E}_0$, $\partial_t\boldsymbol{E}|_{t=0} = \boldsymbol{E}_1$, and with the tensor of electric permittivity $\underline{\underline{\varepsilon}}$ of the form

$$\underline{\underline{\varepsilon}} = \mathrm{diag}(\varepsilon_1,\varepsilon_2,\varepsilon_3), \quad \text{with } \varepsilon_j > 0, \quad j = 1,2,3.$$

In order to allow for numerical simulation of (1), we want to restrict the computations to a region of interest which includes the supports of the initial data. To do so, we surround the computational domain by a PML. Mathematically, there are different ways to present PMLs. One of them consists in considering equation (1) in the frequency domain. Inside this layer one modifies (1) by an appropriate complex frequency-dependent scaling aimed to ensure the exponential decay of the solution in space. The layer is then truncated and vanishing Dirichlet/Neumann boundary conditions are imposed on the external boundary.

In more detail, we consider the physical solution to (1) inside the domain $\boldsymbol{x}\in(-a,a)^3$, which we surround by the PML of width L. The computational domain is $(-a-L,a+L)^3$, and $(-a-L,a+L)^3\setminus(-a,a)^3$ is the truncated perfectly matched layer.

The PMLs are based on the analytic continuation (with respect to each variable) of the Fourier transform of the solution

$$\widehat{\boldsymbol{E}}(\omega,\boldsymbol{x}) := \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \mathrm{e}^{i\omega t}\boldsymbol{E}(t,\boldsymbol{x})\mathrm{d}t.$$

Now we introduce the change of variables applied to (1)

$$\widetilde{x}_j := \begin{cases} x_j - (i\omega)^{-1}\displaystyle\int_a^{x_j}\sigma_j(x_j')\mathrm{d}x_j', & |x_j|\geq a,\\ x_j, & |x_j|<a,\end{cases} \tag{2}$$

where the absorption functions $\sigma_j(x)$, $j=1,2,3$ are defined as follows

$$\sigma_j \in L^\infty((-a-L,a+L)), \text{ with } \sigma_j(x) := \begin{cases} 0, & \text{for } x\in(-a,a),\\ \sigma_j(x)\geq 0, & \text{otherwise.}\end{cases}$$

The PML method consists then in looking for the approximate solution $\widehat{\boldsymbol{E}}^\sigma(\omega,\boldsymbol{x})$ satisfying the following equation written in the frequency domain:

$$-\omega^2\underline{\underline{\varepsilon}}\widehat{\boldsymbol{E}}^\sigma(\omega,\boldsymbol{x}) + \nabla_\sigma\times\nabla_\sigma\times\widehat{\boldsymbol{E}}^\sigma(\omega,\boldsymbol{x}) = -i\omega\underline{\underline{\varepsilon}}\boldsymbol{E}_0 + \underline{\underline{\varepsilon}}\boldsymbol{E}_1, \quad \boldsymbol{x}\in(-a-L,a+L)^3, \tag{3}$$

$$\nabla_\sigma = \left(\gamma_1\partial_{x_1},\gamma_2\partial_{x_2},\gamma_3\partial_{x_3}\right)^T, \quad \gamma_j = \left(1-\frac{\sigma_j(x_j)}{i\omega}\right)^{-1}. \tag{4}$$

The above system is equipped with vanishing Dirichlet (or Neumann) boundary conditions at the boundary of the computational domain $(-a-L, a+L)^3$. We can notice that the dependence of (3) with respect to ω is rational. It is then classical to introduce auxiliary unknowns to come back to the time domain.

To analyse the stability of PMLs, we will follow the approach introduced in [2], by considering the time-domain PML system in each direction $\mathbf{e}_j$ with assumptions

$$a = 0, \quad L = \infty, \quad \sigma_j(x_j) \equiv \sigma_j = \text{const} > 0, \quad \sigma_l = 0 \text{ for all } l \neq j.$$

Let us remind this approach, which is based on the Kreiss stability analysis (cf. [12]). It relies on the plane-wave analysis of the system, i.e. on considering particular solutions of the form

$$\boldsymbol{U}(t, \boldsymbol{x}) = \widetilde{\boldsymbol{U}} e^{i(\omega t - \mathbf{k} \cdot \boldsymbol{x})}, \quad \widetilde{\boldsymbol{U}} \in \mathbb{C}^3,$$

where $\boldsymbol{U}(t, \boldsymbol{x})$ is a vector associated with the physical variable $\boldsymbol{E}^\sigma(t, \boldsymbol{x})$ and the auxiliary unknowns, and $\mathbf{k} = (k_1, k_2, k_3)$ is the wave vector. The PML system admits such solutions if and only if $\mathbf{k}$ and ω are related by the dispersion relation

$$F_\sigma(\omega, \mathbf{k}) = 0. \tag{5}$$

Considering this relation as an equation in ω allows to define the solutions $\omega_\sigma(\mathbf{k})$. Due to [12] the considered system is stable if and only if

$$\Im(\omega_\sigma(\mathbf{k})) \geq 0 \quad \forall\, \mathbf{k} \in \mathbb{R}^3. \tag{6}$$

One can write solutions $\omega_\sigma(\mathbf{k})$ as

$$\omega_\sigma(\mathbf{k}) = \omega(\mathbf{k}) + \Delta\omega_\sigma(\mathbf{k}),$$

where $\omega(\mathbf{k})$ are the so-called modes, i.e. solutions of the dispersion relation associated with the original system (1):

$$F(\omega, \mathbf{k}) = 0, \tag{7}$$

and $\Delta\omega_\sigma(\mathbf{k})$ are the perturbation terms. For non-dissipative models, the solutions $\omega(\mathbf{k})$ being real, the stability criterion (6) is therefore equivalent to

$$\Im(\Delta\omega_\sigma(\mathbf{k})) \geq 0 \quad \forall\, \mathbf{k} \in \mathbb{R}^3. \tag{8}$$

Expressing this criterion for all $\mathbf{k}$ is not a trivial task. However, in [2] a necessary stability condition for anisotropic non-dispersive media is given, expressing that (8) is satisfied for large $\mathbf{k}$. This condition can be related to properties of the modes of the original system $\omega(\mathbf{k})$. To formulate it, let us recall that the function $F(\omega, \mathbf{k})$ is polynomial in ω and $\mathbf{k}$, so that its solutions $\omega^{(n)}(\mathbf{k})$, $n = 1, \ldots, N$, can be chosen as N branches of analytic functions with respect to k_j, $j = 1, 2, 3$.

For a given mode $\omega^{(n)}(\mathbf{k})$, we can then define the *phase velocity* $\boldsymbol{v}_p^{(n)}$ and the *group velocity* $\boldsymbol{v}_g^{(n)}$:

$$\boldsymbol{v}_p^{(n)}(\mathbf{k}) = \frac{\omega^{(n)}(\mathbf{k})}{|\mathbf{k}|} \frac{\mathbf{k}}{|\mathbf{k}|}, \quad \boldsymbol{v}_g^{(n)}(\mathbf{k}) = \nabla_{\mathbf{k}} \omega^{(n)}(\mathbf{k}).$$

Considering a layer in the direction $\boldsymbol{e}_j$, the necessary stability condition of the PML method reads

$$\forall\, n = 1, \ldots, N \quad \forall\, \mathbf{k} \in \mathbb{R}^3 : (\boldsymbol{v}_p^{(n)}(\mathbf{k}) \cdot \boldsymbol{e}_j)(\boldsymbol{v}_g^{(n)}(\mathbf{k}) \cdot \boldsymbol{e}_j) \geq 0. \tag{9}$$

For example, if the PML is applied in $\boldsymbol{e}_1$ direction, the necessary stability condition reads for all $n = 1, \ldots, N$:

$$\frac{k_1}{\omega^{(n)}(\mathbf{k})} \frac{\partial \omega^{(n)}(\mathbf{k})}{\partial k_1} \geq 0 \quad \forall\, \mathbf{k} \in \mathbb{R}^3. \tag{10}$$

The modes $\omega^{(n)}(\mathbf{k})$ for which (9) holds are called forward in the $\boldsymbol{e}_j$ direction, otherwise they are called backward in the $\boldsymbol{e}_j$ direction. As shown in [2], this condition has a simple geometrical interpretation, expressing the fact that along the dispersive surfaces (i.e. level sets of $\omega^{(n)}(\mathbf{k})$), the phase and the group velocities are oriented in the same direction with respect to the $\boldsymbol{e}_j$ direction.

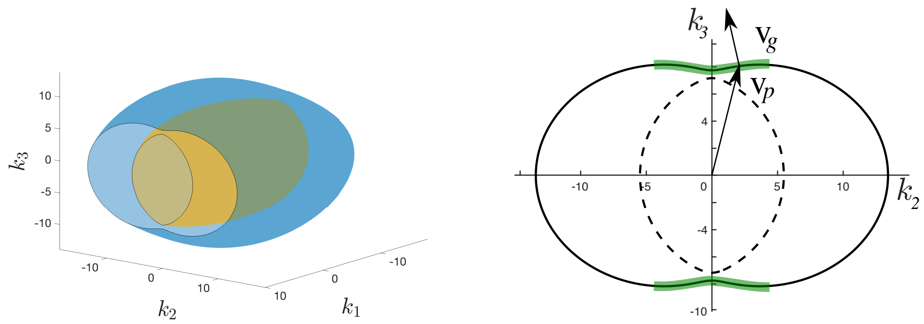

Figure 1. Solution of dispersion relation (3) for $\varepsilon_1 < \varepsilon_2 < \varepsilon_3$.

Since this condition is a necessary condition, we deduce that the existence of backward modes in the $\boldsymbol{e}_j$ direction leads to instabilities of PMLs in the same direction. In the following, we will analyse the stability of the PMLs for (1) relying on the criterion presented above.

3. Necessary condition on the tensor $\underline{\underline{\varepsilon}}$ for the PML stability

In this section, we are going to express the necessary stability condition of the PML method (9) in terms of the coefficients of the dielectric tensor $\underline{\underline{\varepsilon}}$. This result is obtained from an analysis of the dispersion relation associated with (1). The following result establishes the necessary stability condition of the PML applied for (1) in $\boldsymbol{e}_1$ direction:

Theorem 1. *Let $\underline{\underline{\varepsilon}}$ be a diagonal dielectric tensor with coefficients ε_i, $i = 1,2,3$. If*

$$\min(\varepsilon_2,\varepsilon_3) < \varepsilon_1 < \max(\varepsilon_2,\varepsilon_3) \tag{11}$$

then there exist backward propagating modes in the $\boldsymbol{e}_1$ direction. Otherwise there are no backward propagating waves in the $\boldsymbol{e}_1$ direction.

Proof. It is easily seen that a harmonic plane wave of the form $\boldsymbol{E}(t,\boldsymbol{x}) = \widetilde{\boldsymbol{E}}e^{i(\omega t-\mathbf{k}\cdot\boldsymbol{x})}$ is solution of (1) if and only if

$$\left(|\mathbf{k}|^2\mathbb{I} - \omega^2\underline{\underline{\varepsilon}} - \mathbf{k}\mathbf{k}^\top\right)\widetilde{\boldsymbol{E}} = 0.$$

This means that a non trivial solution $\widetilde{\boldsymbol{E}}$ exists if and only if the determinant $F(\omega,\mathbf{k})$ of the matrix $|\mathbf{k}|^2\mathbb{I} - \omega^2\underline{\underline{\varepsilon}} - \mathbf{k}\mathbf{k}^\top$ is zero, leading to the following dispersion relation

$$F(\omega,\mathbf{k}) = 0 \quad \text{with} \quad F(\omega,\mathbf{k}) := \varepsilon_1\varepsilon_2\varepsilon_3\omega^2 P(\omega,\mathbf{k}),$$

where $P(\omega,\mathbf{k})$ is a biquadratic polynomial in ω given by

$$P(\omega,\mathbf{k}) = -\omega^4 + \omega^2\left(k_1^2\frac{\varepsilon_2+\varepsilon_3}{\varepsilon_2\varepsilon_3} + k_2^2\frac{\varepsilon_1+\varepsilon_3}{\varepsilon_1\varepsilon_3} + k_3^2\frac{\varepsilon_1+\varepsilon_2}{\varepsilon_1\varepsilon_2}\right) - \frac{k_1^2+k_2^2+k_3^2}{\varepsilon_1\varepsilon_2\varepsilon_3}\sum_{i=1}^{3}\varepsilon_i k_i^2. \tag{12}$$

The four modes associated with

$$P(\omega,\mathbf{k}) = 0 \tag{13}$$

are denoted by $\omega_j^{\pm}(\mathbf{k}) := \pm\omega_j(\mathbf{k})$, $j = 1,2$. It is possible to prove that $\omega_j^{\pm}(\mathbf{k})$ define four almost everywhere different modes, in the case when $\varepsilon_i \neq \varepsilon_j$, for some $i \neq j$.

We have to check that all the modes $\omega_j^{\pm}(\mathbf{k})$ satisfy the condition (10). It is easy to see that it is equivalent to study the sign of the two quantities

$$C_j(\mathbf{k}) := k_1\frac{\partial\lambda_j(\mathbf{k})}{\partial k_1}, \quad j = 1,2, \tag{14}$$

where $\lambda_j(\mathbf{k}) := (\omega_j^{\pm}(\mathbf{k}))^2$ are defined from (13) as

$$\lambda_j(\mathbf{k}) = \frac{1}{2}\left(k_1^2\frac{\varepsilon_2+\varepsilon_3}{\varepsilon_2\varepsilon_3} + k_2^2\frac{\varepsilon_1+\varepsilon_3}{\varepsilon_1\varepsilon_3} + k_3^2\frac{\varepsilon_1+\varepsilon_2}{\varepsilon_1\varepsilon_2} + (-1)^j\sqrt{\Delta(\mathbf{k})}\right), \quad j=1,2, \tag{15}$$

and the discriminant $\Delta(\mathbf{k})$ is given by

$$\Delta(\mathbf{k}) = K(\mathbf{k})^2 + 4\frac{k_2^2k_3^2(\varepsilon_1-\varepsilon_2)(\varepsilon_1-\varepsilon_3)}{\varepsilon_1^2\varepsilon_2\varepsilon_3},$$

where

$$K(\mathbf{k}) = k_1^2\frac{\varepsilon_2-\varepsilon_3}{\varepsilon_2\varepsilon_3} + k_2^2\frac{\varepsilon_1-\varepsilon_3}{\varepsilon_1\varepsilon_3} + k_3^2\frac{\varepsilon_2-\varepsilon_1}{\varepsilon_1\varepsilon_2}. \tag{16}$$

Let us now consider two cases.

Case 1. $\varepsilon_1=\varepsilon_2$ **or** $\varepsilon_1=\varepsilon_3$**.** Without loss of generality we consider $\varepsilon_1=\varepsilon_2$. Then $\Delta(\mathbf{k}) = K(\mathbf{k})^2$ and $K(\mathbf{k}) = k_1^2\frac{\varepsilon_2-\varepsilon_3}{\varepsilon_2\varepsilon_3} + k_2^2\frac{\varepsilon_1-\varepsilon_3}{\varepsilon_1\varepsilon_3}$ so that

$$\lambda_1(\mathbf{k}) = \frac{k_1^2+k_2^2+k_3^2}{\varepsilon_1} \quad\text{and}\quad \lambda_2(\mathbf{k}) = \frac{k_1^2+k_2^2}{\varepsilon_3}+\frac{k_3^2}{\varepsilon_1},$$

from where by a straightforward computation, with (14), it follows that $C_j(\mathbf{k})\geq 0$ for $j=1,2$ and for all $\mathbf{k}\in\mathbb{R}^3$.

Case 2. $\min(\varepsilon_2,\varepsilon_3)<\varepsilon_1<\max(\varepsilon_2,\varepsilon_3)$**.** Again, without loss of generality, let us suppose that $\varepsilon_3<\varepsilon_1<\varepsilon_2$. By using the identity for $a,b,c>0 : (a+b+c)^2-4bc = (a+(\sqrt{b}-\sqrt{c})^2)(a+(\sqrt{b}+\sqrt{c})^2)$, we can easily deduce that $\Delta(\mathbf{k})\geq 0$ for all $\mathbf{k}\in\mathbb{R}^3$. Moreover, a direct computation yields

$$C_j(\mathbf{k}) = \frac{2k_1^2}{\varepsilon_2\varepsilon_3\sqrt{\Delta(\mathbf{k})}}\left((\varepsilon_2+\varepsilon_3)\sqrt{\Delta(\mathbf{k})} + (-1)^j(\varepsilon_2-\varepsilon_3)K(\mathbf{k})\right). \tag{17}$$

Because $\varepsilon_3<\varepsilon_1<\varepsilon_2$ we have $K(\mathbf{k})>0$, and thus $C_2(\mathbf{k})\geq 0$ for all $\mathbf{k}\in\mathbb{R}^3$. It remains to study the sign of $C_1(\mathbf{k})$.

Let us prove that there exists $\mathbf{k}^*\in\mathbb{R}^3$, such that $C_1(\mathbf{k}^*)<0$ (the result follows then from the continuity of C_1 with respect to $\mathbf{k}$). This is equivalent to showing the existence of $\mathbf{k}^* = (k_1^*,k_2^*,k_3^*)\in\mathbb{R}^3$ such that $k_1^*\neq 0$ and

$$(\varepsilon_2+\varepsilon_3)^2\Delta(\mathbf{k}^*) - (\varepsilon_2-\varepsilon_3)^2K(\mathbf{k}^*)^2 < 0. \tag{18}$$

By denoting $\widetilde{k}_2 = k_2((\varepsilon_1-\varepsilon_3)/\varepsilon_1)^{1/2}$ and $\widetilde{k}_3 = k_3((\varepsilon_2-\varepsilon_1)/\varepsilon_1)^{1/2}$, we show that

$$(\varepsilon_2+\varepsilon_3)^2\Delta(\mathbf{k}) - (\varepsilon_2-\varepsilon_3)^2K(\mathbf{k}) = \frac{4}{\varepsilon_2\varepsilon_3}\left[(k_1^2(\varepsilon_2-\varepsilon_3)+\widetilde{k}_2^2\varepsilon_2+\widetilde{k}_3^2\varepsilon_3)^2 - \widetilde{k}_2^2\widetilde{k}_3^2(\varepsilon_2+\varepsilon_3)^2\right].$$

If we choose $k_2^*>0$ and $k_3^*>0$, this quantity has the sign of:

$$k_1^2(\varepsilon_2-\varepsilon_3) + (\widetilde{k}_2\varepsilon_2-\widetilde{k}_3\varepsilon_3)(\widetilde{k}_2-\widetilde{k}_3).$$

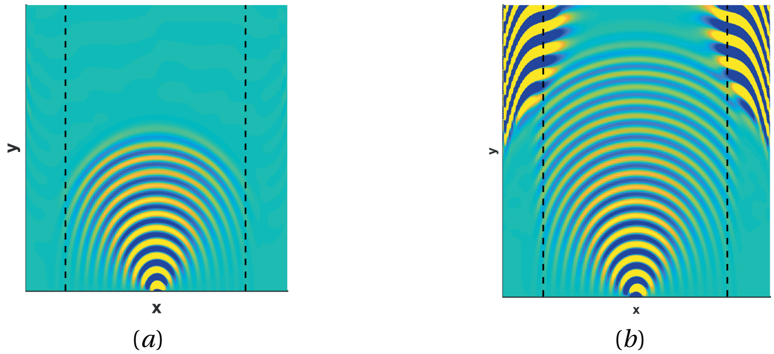

Figure 2. Snapshots of the electric field component $E_1(t,x,y,0)$ at (a) $t = 2.5$, (b) $t = 4$ for a medium with diagonal anisotropy defined by $\varepsilon_1 = 10, \varepsilon_2 = 20, \varepsilon_3 = 1$.

We deduce that for $\mathbf{k}^*$ chosen such that $k_2^* > 0$, $k_3^* > 0$, $\widetilde{k}_2^* - \widetilde{k}_3^* < 0$ and $\widetilde{k}_2^* \varepsilon_2 - \widetilde{k}_3^* \varepsilon_3 > 0$, namely

$$k_3^* \frac{(\varepsilon_2-\varepsilon_1)^{1/2}}{(\varepsilon_1-\varepsilon_3)^{1/2}} \frac{\varepsilon_3}{\varepsilon_2} < k_2^* < k_3^* \frac{(\varepsilon_2-\varepsilon_1)^{1/2}}{(\varepsilon_1-\varepsilon_3)^{1/2}},$$

and k_1^* small enough, (18) is satisfied. This finishes the proof. □

Remark 2. Since the proof is not specific to the $\boldsymbol{e}_1$ direction, we conclude that if $\varepsilon_1 \neq \varepsilon_2 \neq \varepsilon_3$, backward waves will exist in one of the axis directions, namely in the one that corresponds to $\boldsymbol{e}_j$ such that $\min_{k,k\neq j} \varepsilon_k < \varepsilon_j < \max_{k,k\neq j} \varepsilon_k$. On the other hand, if two of the coefficients of $\underline{\underline{\varepsilon}}$ are equal no backward waves exist.

Note that the criterion (9) being a necessary stability condition, the classical PML method is unstable in the time-domain for a medium satisfying condition (11). Numerical simulations confirm the instabilities of PML in the $\boldsymbol{e}_1$ direction (see Figure 2). Let us remark that in our numerical simulations we did not observe any instabilities appearing in the two other directions. A rigorous justification of this fact is out of scope of the present note.

Let us emphasize that the important (and surprising) result of the present study is that the classical Cartesian PML method may be unstable even in the case when the medium is described by a diagonal permittivity tensor. Since one faces instabilities in one of the coordinate directions if the medium satisfies the condition $\varepsilon_i \neq \varepsilon_j$ for $i \neq j$, an alternative approach to truncate the computational domain should be proposed. There exist several stabilisation techniques for some models with backward propagating modes, see [1] for some hyperbolic systems, [10] for advected acoustics, [9] for anisotropic acoustics, [11] for linear Euler equations, [4] for the models of dispersive metamaterials and [3] for strongly magnetized cold plasmas. However, because in the model we consider, for the same frequency both forward and backward propagating waves are present, those techniques seem to be inappropriate, and designing a new strategy remains an open question.

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