Journal of Computational Physics 230 (2011) 2369–2377

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Short note

Distinguishing correct from incorrect PML proposals and a corrected unsplit PML for anisotropic, dispersive media

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ARTICLE INFO

Article history:
Received 27 September 2010
Accepted 2 January 2011
Available online 9 January 2011

Keywords:
Perfectly matched layer
Computational electromagnetism
FDTD

ABSTRACT

We show that some previous proposals for perfectly matched layer (PML) absorbers in anisotropic media or for waveguides at oblique incidence are not, in fact true PMLs; in previous work we similarly showed a failure of several PML proposals for periodic media (photonic crystals). We therefore argue that a more careful validation scheme is required for PML proposals, in contrast to past authors who have typically checked only that reflections are small for a fixed resolution, and suggest a simple validation scheme that can be readily applied to any PML proposal regardless of derivation or implementation. We demonstrate this test for a corrected, unsplit-field PML valid for anisotropic, dispersive media, implemented in both planewave-expansion and finite-difference time-domain (FDTD) methods.

1. Introduction

A perfectly matched layer (PML) is an artificial absorbing medium that is commonly used to truncate computational grids for simulating wave equations (e.g. Maxwell's equations), and is designed to have the property that interfaces between the PML and adjacent media are reflectionless in the exact wave equation [1,2]. Previously, we found certain instances where past "PML" proposals [3–7] for inhomogeneous media (photonic crystals [8]) were not in fact reflectionless in the exact wave equation [9]. In this paper, we demonstrate a similar failure of a prior unsplit-field PML proposal for anisotropic media [10] and also of proposals of PMLs for oblique waveguides [11,12]. We have argued that such errors are easily overlooked because all PML implementations use an absorption that gradually increases from the absorber interface (in order to mitigate discretization effects) [2] – such an "adiabatic absorber" performs arbitrarily well, even if it is not a PML, as long as the absorber is sufficiently thick [9]. Although many previous papers "validate" their PML proposals by checking whether the reflection is low for a given resolution [13–18] and/or decreases with PML thickness [1,19], the true test of a PML is to verify that the reflections systematically vanish as the resolution is increased (approaching the exact wave equation). However separating reflected and incident waves can be cumbersome in complex inhomogeneous and/or anisotropic media.

In this paper, we suggest an equivalent testing procedure that involves simply computing the difference between two computations as a function of resolution (identical except for different PML thicknesses); the mathematical foundations for this procedure are derived from our previous work [9], which applied a related procedure to study the effect of smoothness rather than resolution and correctness. In particular, we apply this validation procedure to demonstrate a problem with a previous proposal for an unsplit PML in anisotropic media [10]; in our previous work [9], we identified a failure of PML in periodic media by a different method (exact reflection computations) that is not as easily generalized. As an alternative, we

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0021-9991/$ - see front matter
doi:10.1016/j.jcp.2011.01.006

formulate (via complex coordinate-stretching) and validate a corrected unsplit-field uniaxial PML for arbitrary anisotropic, dispersive, and conducting media in the time domain. Although there exist other correct alternatives for PML in anisotropic media [13–16,18–24] (including correct split-field proposals [21,13,15] by the same authors as the later incorrect unsplit-field formulation), our unsplit PML formulation has the appeal of a simple correction to previous UPML-like proposals that were correct for isotropic media [25,26,10]. We demonstrate this PML formulation both for a planewave method in frequency domain and for a finite-difference time-domain method (with a free-software implementation [27]). In the time domain, the frequency-dependence of the PML response is well known to require additional storage (e.g. auxiliary fields) [2], but we show that our scheme involves requirements at least as good as previous correct split-field PML proposals for anisotropic media [13–16,20–23]. (Anisotropic media are becoming increasingly widespread in computational electromagnetism, both for anisotropic metamaterials [28–30] and even for nominally isotropic media, where in the latter case accurate subpixel averaging requires the discretization to use effective anisotropic media at material boundaries [31–33].) Also, we previously suggested the inapplicability of standard PMLs for dielectric waveguides incident upon the absorbing medium at an oblique angle [9] and we now explicitly demonstrate this failure using a similar testing procedure.

There are several nearly equivalent formulations of PMLs. Berenger's original formulation [1] split the wave solution into the sum of two new artificial field components. A more physically intuitive formulation was subsequently proposed [25,26] by showing that an equivalent effect can be obtained using a special uniaxial anisotropic medium ("UPML") introduced into the ordinary ("unsplit") Maxwell equations. Although these original PML derivations were for homogeneous media, in which the reflections were explicitly computed and set to zero, a more elegant and general derivation was proposed [34,35], in which the PML is viewed as a complex "coordinate stretching" where Maxwell's equations are analytically continued to complex coordinates (transforming oscillating solutions into exponential decays). This coordinate-stretching viewpoint is equivalent to the split-field approach [34], and is also equivalent to the anisotropic-media PML formulation [36] (where the latter can be viewed as a special case of the "transformational optics" approach of Ward and Pendry to coordinate transformation in electromagnetism [28]). The coordinate-stretching viewpoint is even applicable to deriving PML in inhomogeneous media, as long as the media are invariant along the PML direction [9], although there are certain "backward-wave" inhomogeneous media where PML fails for other reasons [37]. Subsequent refinements include the incorporation of a real as well as imaginary coordinate stretching in order to attenuate evanescent waves [38], shifting the zero-frequency pole in order to better attenuate low-frequency waves (CFS-PML) [2,17,39], and implementation of the latter by a recursive-convolution technique (CPML) [18].

The same coordinate-stretching approach is applicable to derive reflectionless PMLs for arbitrary anisotropic media. Several such proposals employed the split-field approach [20–23,13–16] or convolutional approach [18,19,24] to obtain time-domain equations, and split-field PMLs were also derived for homogeneous anisotropic media by directly computing the reflection coefficients at the PML interface [20,14,23]. The transformational-optics approach also leads to a simple uniaxial anisotropic PML medium in the frequency domain [40], and in this paper we point out that the same approach also yields a straightforward time-domain PML for anisotropic and dispersive media, although in time domain a new factorization is required in order to efficiently implement the frequency dependence. Zhao et al., in addition to proposing correct split-field PMLs for anisotropic media [21,13,15], also proposed an unsplit-field PML for anisotropic media in which the PML is encapsulated in conductivity factors for the equation updating the **D** field from $\nabla \times \mathbf{H}$, separate from the (unmodified) constitutive relation giving **E** from **D** [10]. However, we show in this paper that the Zhao unsplit-PML proposal relies on a commutation of the coordinate-stretch matrix and the material tensor which is not generally correct in anisotropic media, and as a result the absorber is not reflectionless in the limit of high resolution. The reflections are often small enough not to be noticed, however, especially if the anisotropy is weak, which is why this problem may not have been obvious in previous work. We also demonstrate that previous suggestions of PMLs for oblique waveguides [11,12] are also invalid as the material function (and hence Maxwell's equations) is not invariant along the PML direction. We had noted this possibility in the past [9] and now explicitly demonstrate the PML failure and suggest a simple workaround using a pseudo-PML [9].

PML is simplest to derive in frequency domain (for linear media with arbitrary dispersion and anisotropy), where the fields all have time-dependence $e^{-i\omega t}$. An ordinary PML in Cartesian coordinates is derived by a complex coordinate stretching, where each coordinate is stretched by a factor

$$s_{x,y,z} = \kappa_{x,y,z} + \frac{i\sigma_{x,y,z}}{\omega}, \tag{1}$$

where $\kappa \geqslant 1$ (a *real* coordinate stretching used to attenuate evanescent waves [38]) and $\sigma > 0$ is the PML "conductivity." (The CFS variant of PML replaces ω with $\omega + i\alpha$ in order to shift the $\omega = 0$ pole below the real axis [2,17,18,39].) For example, to terminate the cell in the x direction, only σ_x is not unity. These coordinate stretchings can be absorbed into Maxwell's equations as a change in ε and μ, thanks to the general transformation-optics principle [28]. In particular, the original permittivity tensor ε in the PML region is replaced by an effective tensor $\tilde{\varepsilon}$ given by (as derived in the general anisotropic case [32, Appendix] and also derived for the specific case of PML with a diagonal coordinate stretching [40])

$$\tilde{\varepsilon} = \frac{\mathcal{J}\varepsilon(\omega)\mathcal{J}^{\mathrm{T}}}{\det\mathcal{J}}, \tag{2}$$

where $\mathcal{J} = \mathrm{diag}\left(s_x^{-1}, s_y^{-1}, s_z^{-1}\right)$ is the Jacobian matrix of the coordinate stretching. There is also an identical transformation of the magnetic permeability μ, but for simplicity we focus here on ε.

An *isotropic* tensor $\varepsilon(\omega)$ commutes with $\mathcal{J}$, and as a result one can simply multiply ε by $\mathcal{J}\mathcal{J}^{\mathrm{T}}/\det\mathcal{J} = \mathrm{diag}(s_y s_z/s_x, s_x s_z/s_y, s_x s_y/s_z) = \Sigma$. One can then separate Ampere's law $\nabla\times\mathbf{H} = -i\omega\tilde{\varepsilon}\mathbf{E}$ into two parts: a time-derivative part $\nabla\times H = -i\omega\Sigma\mathbf{D}$ with a PML conductivity Σ, and an "unmodified" constitutive relation $\mathbf{D} = \varepsilon(\omega)\mathbf{E}$. In this way, the PML-dependent parts are separated from the material properties ε derived from the non-PML regions. This approach was dubbed a "material-independent PML" by Zhao with an unsplit-field [10] formulation (where Zhao denoted Σ by $\hat{\varepsilon}^D$). Zhao's unsplit-field PML proposal is henceforth referred to as the ZUML.

However, it is clear in Eq. (2) that an arbitrary anisotropic ε (with off-diagonal entries) cannot in general be commuted with $\mathcal{J}$, and therefore the transformation to $\Sigma\varepsilon$ is *no longer* equivalent to a complex coordinate stretching. Therefore, one would not expect the ZUML to be a true reflectionless PML in the limit of the exact wave equation, and this is precisely what we observe in our numerical validation below. Instead, for anisotropic media one should use the uncommuted form of Eq. (2) [40], and we discuss below how this can be implemented in the time-domain with appropriate auxiliary fields to capture the frequency dependence, while retaining the UPML-like unsplit-field structure and the "material-independent" property of an unmodified constitutive relation in one subcomputation.

2. Adiabatic absorbers and PML reflections

All adiabatic absorbers, whether PML or not, are characterized by a continuous conductivity or absorption-strength profile $\sigma(x)$, which becomes more gradual as the absorber is made thicker. Outside the absorbing regions, where $\sigma = 0$, the wave equation and thus the solution are unchanged, and it is only inside the absorbing region ($\sigma > 0$) that the oscillating solution becomes exponentially decaying. In the exact wave equation for a true PML, this transition occurs with no reflections, no matter how fast σ changes, even if σ changes discontinuously. In practice, even for a true PML, there are reflections whenever σ changes abruptly, due to discretization effects, and this is mitigated by smoothly turning on σ over some distance L [2]. It turns out that the reflection characteristics of any smoothly turned-on absorption, whether PML or not, have certain universal characteristics determined by the smoothness of $\sigma(x)$ [9], and these characteristics are central to understanding absorbing-layer behaviors and validation. The reflections from both PML and non-PML absorbers consist of two parts: round-trip and transition reflections.

The first component is the *round-trip* reflection (also called the "theoretical reflection" in the case of a PML [1]) that arises when waves enter the absorbing region and undergo exponential decay before reflecting off the hard-wall (e.g. Dirichlet) boundaries at the edge of the computational cell. This "round-trip" reflection R_{RT} is a measure of how much of the incident wave is *not* absorbed by the absorbing region and is exponentially small:

$$R_{\mathrm{RT}} \sim e^{-4\frac{k_x}{\omega}\int_0^L \sigma(x')dx'}, \tag{3}$$

where the absorption profile starts at $x = 0$, and the factor of 4 is because the reflection is proportional to the round-trip (2L) field squared, and k_x is the propagation constant in the x direction.

The second component of the overall reflection is the *transition* reflection R_{T} at the interface of the absorbing and adjacent non-absorbing media, which is nonzero even for PML at a finite resolution. Let us define $\sigma(x)$ in the absorbing region ($x \in [0,L]$) by $\sigma(x) = \sigma_0 s(x/L)$, where $s(u)$: $[0,1] \mapsto [0,1]$ is a dimensionless profile and σ_0 is an overall amplitude. σ_0 can be chosen to achieve some theoretical maximum round-trip absorption R_{RT} for normal-incident waves in a medium of index n (so that $k_x = \omega n$), obtaining $\sigma_0 = -\ln R_{\mathrm{RT}}/[4nL\int_0^1 s(u')du']$ from Eq. (3). For $x < 0$, outside the PML, $\sigma = 0$, i.e. $s(u < 0) = 0$. As L is made longer and longer for a fixed $s(u)$, the PML profile σ turns on more and more gradually [both because $s(u)$ is stretched out and because σ_0 decreases], and the numerical reflections decrease. Previously, we demonstrated for any absorber (PML or not) the fundamental connection between the smoothness of $s(u)$ and the rate of decrease of transition reflection with L, derived from coupled-mode theory [9]. For example, the transition reflections scale as $R_{\mathrm{T}} \sim 1/L^{2d+2}$ for the common case of a monomial profile $s(u) = u^d$. Throughout the remainder of this paper, we set the estimated round-trip reflection R_{RT} to be negligibly small ($<10^{-25}$) and focus solely on the transition reflection. The consequence of a PML is to make the coefficient of the $R_{\mathrm{T}}(L)$ relation smaller, with the coefficient vanishing for infinite resolution [9].

Not only does this mean that the transition reflections can rapidly vanish for a thick enough absorber, even without PML, but it also suggests a simple way to validate a PML. In particular, the *difference* $R(L_1) - R(L_2)$ between the reflections for two simulations with identical interiors but different PML thicknesses L_1 and L_2, with the same R_{RT}, must also effectively vanish in the limit of infinite resolution. At a finite resolution, the difference is dominated by the transition reflections, which vanish for the exact wave equation, leaving at most small differences in round-trip reflections due to phase factors – in principle, the difference should decrease with resolution until it reaches some floor proportional to R_{RT}, but in practice for the purpose of validation we choose R_{RT} to be small enough that we never reach this floor. In contrast, for an absorber that is not a PML, the difference should converge at high resolution to some nonzero value determined by the transition reflections in the exact wave equation, independent of (and much larger than) R_{RT}. Moreover, we need not compute the reflections explicitly: if we simply subtract the interior *fields* from the two simulations, the difference is due entirely to the reflections and must vanish in the same way (for a PML) as resolution increases. Note that, to perform as rigorous a test as possible of the PML, it is desirable to employ a simulation involving waves incident upon the PML with a wide range of angles; this is achieved below using a point-dipole source.

On the other hand, the reflections and field differences will vanish (at a fixed resolution, for negligible round-trip reflections) as $L \to \infty$ for *any* adiabatic absorber, whether or not it is a PML. In particular, if L_2 is $L_1 = L$ plus some constant difference ΔL (i.e., $L_2 = L + \Delta L$) for a monomial profile $s(u) = u^d$, then the reflection difference vanishes as $\sim 1/L^{2d+4}$ for any absorber, while the reflection itself vanishes as $\sim 1/L^{2d+2}$ [9]. Such an adiabatic absorber is a fall-back option when no PML is available [9,37,41], but it also means that a failure of a putative PML may be obscured by the use of a sufficiently thick absorbing region.

3. Validation of anisotropic PML proposals

We apply this idea to illustrate the failure of incorrect PML formulations in anisotropic media, first considering a frequency-domain simulation: we compute the frequency-domain response to a time-harmonic current source [8, Appendix D] with a planewave expansion method (PWFD) solved by an iterative bi-conjugate gradient algorithm [42] in two dimensions (2d). We perform two simulations with identical parameters except for the absorber thickness L, and compute the difference of the electric fields at the same (arbitrarily chosen) point $\mathbf{x}$ in the interior of both simulations, defining a *field convergence factor*

$$\frac{\left|\mathbf{E}^{(L+\Delta L)}(\mathbf{x}) - \mathbf{E}^{(L)}(\mathbf{x})\right|^2}{\left|\mathbf{E}^{(L)}(\mathbf{x})\right|^2}. \tag{4}$$

(More generally, we could use any overall norm of the difference in the interior fields of the computation, but the fields at a single point suffice so long as they are not identically zero at that point.) We use thicknesses L and $L + \Delta L$, where ΔL is some nonzero difference (here chosen to be $\Delta L = \lambda$, the vacuum wavelength of the point-dipole source). Fig. 1 shows the results of these two-dimensional PWFD simulations for uniform isotropic (vacuum) and anisotropic media (ε formed from an isotropic diagonal tensor with eigenvalues $\{12, 1, 12\}$ and principal axes rotated 45° about the y and z axes); the differences between a correct PML, ZUML, and a non-PML absorber (consisting of just a scalar electric conductivity) are stark. In the correct PML formulation, the reflection from the boundaries converges to zero as resolution is increased towards the continuum limit, whereas the non-PML absorber in the uniform medium saturates to a *constant* nonzero reflection (the Fresnel reflection coefficient from the exact Maxwell equations). The ZUML is clearly a non-PML absorber for anisotropic media, with nonzero reflection in the continuum limit, as predicted above from the fact that its derivation is not equivalent to an analytic continuation of Maxwell's equations.

As predicted in the previous section, Fig. 2 demonstrates that all absorption profiles (whether PML or not) exhibit the same characteristic power-law scaling with L, determined only by the differentiability d of the profile. The impact of a true PML is to improve the constant factor in this relationship, although ZUML is actually not too bad in this respect at low resolution (and gets even better for milder anisotropy). This illustrates why merely checking whether the reflection is low for a given resolution [13–18] and/or decreases with PML thickness [1,19] can be a misleading test for the validity of a PML proposal.

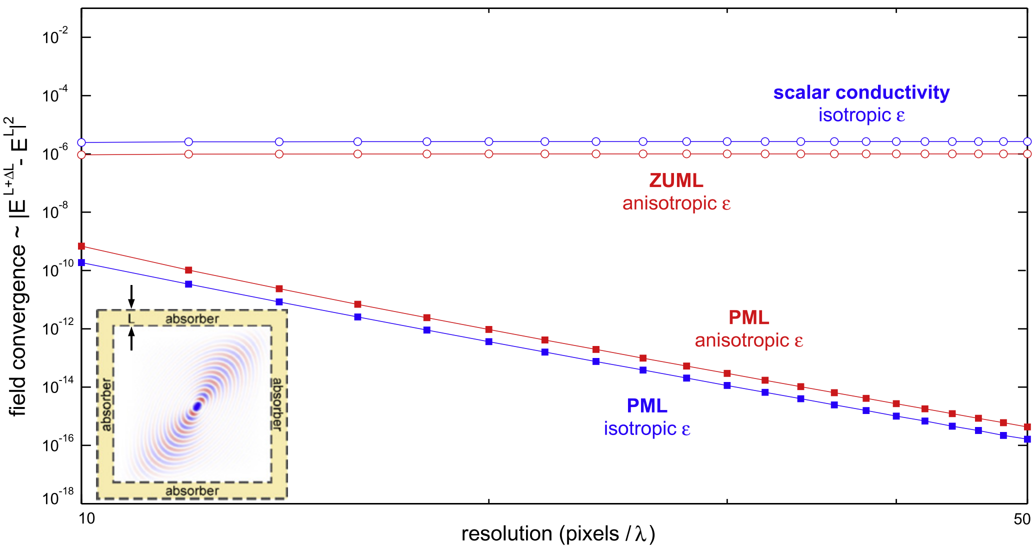

Fig. 1. Field convergence factor (a proxy for the reflection coefficient), Eq. (4) with $\Delta L = \lambda$, as a function of discretization resolution for both isotropic and anisotropic media with PML and non-PML (scalar conductivity) absorbing boundaries calculated using a planewave-expansion frequency-domain solver in 2d. The unsplit-field PML proposal by Zhao [10] is denoted "ZUML," and is seen not to be a true PML for the anisotropic medium where it fails to be reflectionless even in the limit of high resolution, similar to the scalar conductivity for an isotropic media. Inset: $Re[E_z]$ field profile of a point-dipole source located at the center of the anisotropic-media computational cell surrounded by an absorbing material (blue/white/red = positive/zero/negative). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

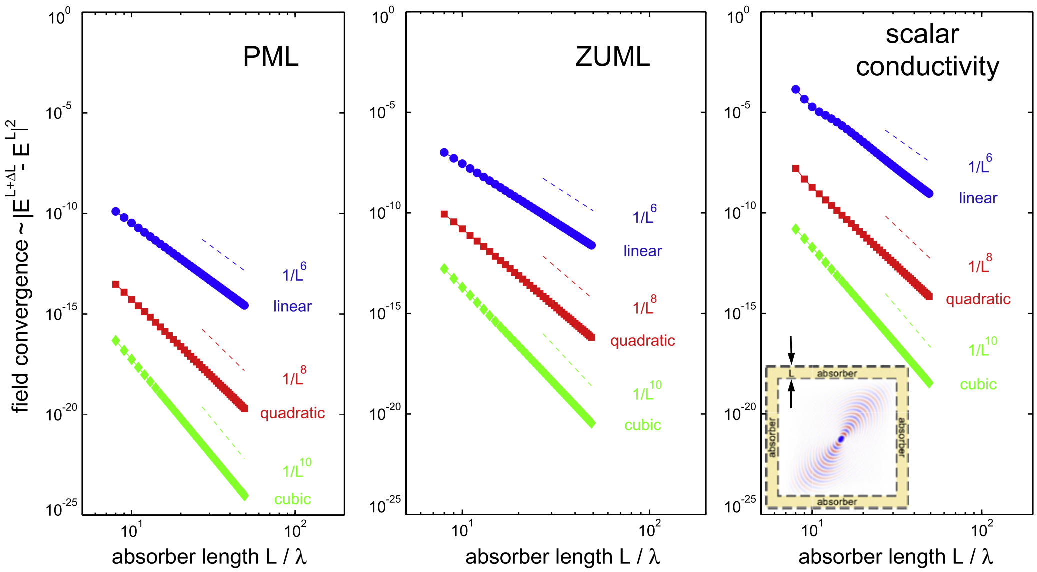

Fig. 2. Field convergence factor (a proxy for the reflection coefficient), Eq. (4) with $\Delta L = \lambda$, vs. absorber thickness L in anisotropic media computed using a 2d planewave frequency-domain solver at a resolution of 9 pixels/λ for various monomial absorber functions $s(u)$ ranging from linear [$s(u) = u$] to cubic [$s(u) = u^3$]. For comparison, the predicted asymptotic power laws are shown as dashed lines. Left plot for PML, middle for ZUML, and right for scalar electric conductivity. Inset: $\Re[E_z]$ field profile of a point-dipole source located at the center of the anisotropic-media computational cell surrounded by an absorbing material (blue/white/red = positive/zero/negative). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

4. PML formulation in time domain

As reviewed above, the coordinate-stretching derivation of PML is straightforward in the frequency domain. The subtlety is that the transformations/materials of PML are frequency-dependent, and so to express them in time domain involves the evolution of appropriate auxiliary differential equations. This complication did not arise in previous frequency-domain unsplit PML proposals for anisotropic media [40], and the anisotropy means that previous UPML time-domain schemes for isotropic media [26,10] are not directly applicable, so a new reformulation is required. (Equivalently, multiplication by a frequency-dependent susceptibility corresponds in the time domain to a convolution, leading to "convolutional PML" formulations [18]. Because the frequency dependence is in the form of a polynomial fraction in ω, it can be implemented with finite auxiliary storage by a recursive "IIR" filter [43].) The emphasis is on keeping the number of auxiliary differential equations (and the resulting memory and computational costs) to a minimum, while not making the PML region too complicated compared to the non-PML regions. As the treatment of ε and μ are identical except for interchange of **D** with **B** and **E** with **H** (and a sign flip from Ampere's to Faraday's law), we only describe the ε and $d\mathbf{D}/dt$ equations (Ampere's law) here.

The most convenient ODEs to discretize are first-order ODEs. For example, $a = s \cdot b = (1 + i\sigma/\omega) \cdot b$ gives $-i\omega a = -i\omega b + \sigma b$, which corresponds to the first-order ODE $\frac{da}{dt} = \frac{db}{dt} + \sigma b$. For more general scaling factor, such as the $s = \kappa + \sigma/(-i\omega + \alpha)$ that appears in shifted-pole PML [2,17,39], $a = s \cdot b$ still leads to a simple first-order ODE $\frac{da}{dt} + \alpha a = \kappa \frac{db}{dt} + (\sigma + \kappa\alpha)b$. (In the language of digital signal processing, this factorization into first-order ODEs is equivalent to the "cascade" form of a recursive/IIR filter [43].)

So, before we proceed to time domain, we want to *factorize* $\nabla \times \mathbf{H} = -i\omega\tilde{\mathbf{D}}$ where $\tilde{\mathbf{D}} = \tilde{\varepsilon}(\omega)\mathbf{E}$ into terms with only *one* factor of s (or σ/ω) each (or ratios of single s factors). In doing so, we are free to change the definition of **D** and introduce new auxiliary fields as desired, since the fields in the PML region are not physical. A key trick is the factorization:

$$\frac{\mathcal{J}}{\det\mathcal{J}} = s_x s_y s_z \begin{pmatrix} s_x^{-1} & & \\ & s_y^{-1} & \\ & & s_z^{-1} \end{pmatrix} = \begin{pmatrix} s_y & & \\ & s_z & \\ & & s_x \end{pmatrix} \begin{pmatrix} s_z & & \\ & s_x & \\ & & s_y \end{pmatrix} = \mathcal{S}_1 \mathcal{S}_2. \tag{5}$$

Using this factorization, and defining new auxiliary fields, **U** and **W**, we can factorize Eq. (2) into the following equivalent form (giving the same relationship between **H** and **E**):

$$\tilde{\mathbf{D}} = \mathcal{S}_1 \underbrace{\mathcal{S}_2 \underbrace{\varepsilon(\omega) \underbrace{\mathcal{J}^T \mathbf{E}}_{\mathbf{W}}}_{\mathbf{U}}}_{\mathbf{D}} \tag{6}$$

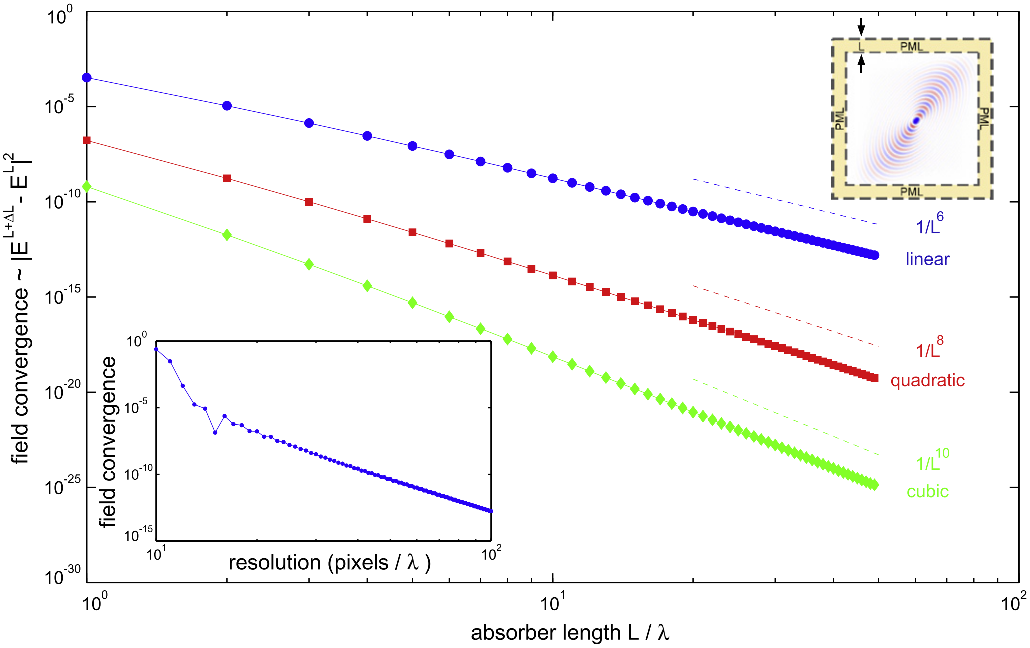

Fig. 3. Field convergence factor (a proxy for the reflection coefficient), Eq. (4) with $\Delta L = \lambda$, vs. absorber thickness L for the corrected UPML formulation calculated using the finite-difference time-domain (FDTD) method for various monomial absorber functions. For comparison of the slopes, the predicted asymptotic power laws are shown as dashed lines. Lower-left inset: field convergence factor versus discretization resolution for the corrected UPML formulation in FDTD, demonstrating that it converges to zero: a true PML. Upper-right inset: $\Re[E_z]$ field profile of a point-dipole source located at the center of the anisotropic-media computational cell surrounded by a PML absorbing material (blue/white/red = positive/zero/negative). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

where now $\nabla \times \mathbf{H} = -i\omega\mathcal{S}_1\mathbf{D}, \mathbf{D} = \mathcal{S}_2\mathbf{U}, \mathbf{U} = \varepsilon(\omega)\mathbf{W}$ and $\mathbf{W} = \mathcal{J}^T\mathbf{E}$. Each of these is first-order in time and therefore straightforward to implement in the time domain, noting that the computation of **W** from **U** is identical to the computation of **E** from **D** in the non-PML regions (including any auxiliary fields needed to implement a dispersive ε by standard techniques [2]). As an example of the finite-difference equations that result from this factorization, consider the z component of the electric field within an x-directed PML boundary region for a nondispersive isotropic medium: one first updates D_z at timestep $n + 1$ via $D_z^{n+1} = (1 + \sigma\Delta t/2)^{-1}[(1 - \sigma\Delta t/2)D^n + \Delta t(\nabla \times \mathbf{H}^{n+0.5})_z]$, then U_z from $U_z^{n+1} = D_z^{n+1}$, then W_z from $W_z^{n+1} = \varepsilon^{-1}U_z^{n+1}$, then E_z from $E_z^{n+1} = W_z^{n+1}$. In fact, because of the many s factors that are unity in a typical (unidirectional) PML region, many of the auxiliary field components can be omitted in those regions in order to save computation time and storage (as quantified in the Appendix A).

In contrast, for isotropic, nondispersive ε, the standard UPML approach [25,26] corresponds to the factorization $\tilde{\varepsilon}(\omega) = \mathcal{S}_1\varepsilon\mathcal{S}_2\mathcal{J}$, where one has commuted $\mathcal{J}$ with ε (similar to the ZUML). Then one updates Maxwell's equations via $\nabla \times \mathbf{H} = -i\omega\mathcal{S}_1\mathbf{D}, \mathcal{J}^{-1}\mathbf{D} = \varepsilon\mathcal{S}_2$, both of which are first-order in time.

As shown in Fig. 3, the factorization of Eq. (5) (as implemented in our free-software FDTD package [27]) preserves the correctness of the PML that was demonstrated above in the frequency domain. In particular, the inset shows the field-difference converging with resolution, whereas the main graph of Fig. 3 reaffirms the expected scalings with absorber thickness L for various absorption profiles $s(u)$ $(u, u^2$, and $u^3)$. In the time domain, using the value of the field at a single time instant in Eq. (4) may not adequately capture the reflections from the boundaries (since we may "miss" the reflection if we choose an unlucky time). Instead we employ a discrete-time Fourier transform (DTFT) of the fields (accumulated during the simulation [27]) in response to a Gaussian-pulse dipole source, evaluated at the center frequency of the pulse (here denoted by the corresponding vacuum wavelength λ).

Other valid alternatives include the split-field approach, which has been correctly derived for anisotropic media without invalid commutations [13–16,20–23], or in general any coordinate-transformation approach that is not absorbed into the materials but is left as a transformation of the derivatives [18]. The computational expense of our unsplit formulation is at least as good as that of the split-field methods (see Appendix A), while the viewpoint of simply factorizing transformed materials has a certain aesthetic appeal and appears to be the simplest correction to the standard UPML approaches.

5. PML failure for oblique waveguides

We suggested previously that PML is inapplicable to the case of an oblique waveguide since the material function is not analytic in the direction of the PML [9]. Several authors in the past had made claims that ordinary PML formulations were

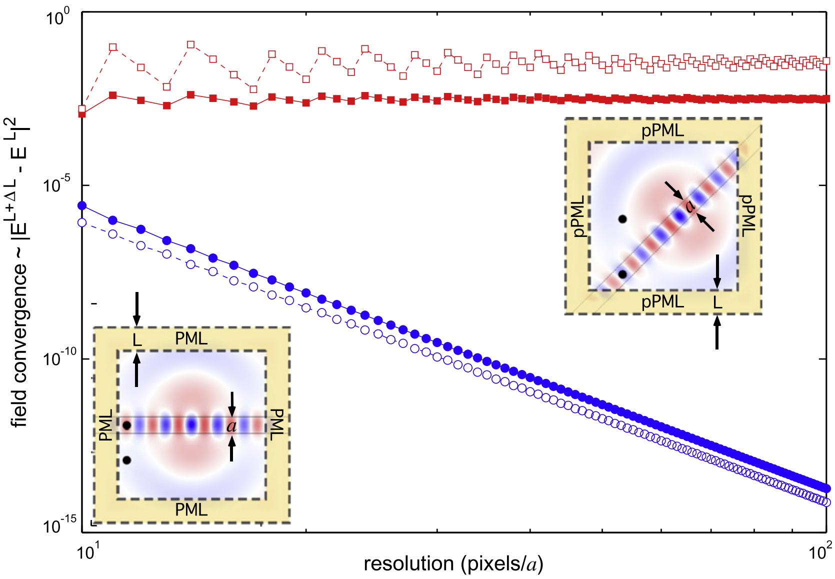

Fig. 4. Oblique waveguide PML resolution test in FDTD: field convergence factor (a proxy for the reflection coefficient), Eq. (4) with $\Delta L = a$ (= waveguide thickness) versus resolution. Results were computed using a waveguide of width a oriented 45° (upper line, red squares; upper inset) and perpendicular (bottom line, blue circles; lower inset) to the PML interface with an E_z point dipole source placed within the center of the waveguide and a monitor point chosen adjacent to the absorbing boundaries. Filled and open symbols correspond to field monitor points inside and outside the waveguide, respectively (with positions indicated by black dots in the insets). Insets show electric fields $\Re[E_z]$ (blue/white/red = positive/zero/negative). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

valid for such circumstances [11,12], but in fact were apparently employing adiabatic non-PML absorbers with sufficient thicknesses to mitigate the reflections. (We have dubbed this approach of using unmodified "PML" equations in cases where they are inapplicable, relying on adiabatic absorption to compensate for failure of the PML, a "pseudo-PML" or pPML [9].) Using the same resolution test we presented above, we can now explicitly demonstrate the failure of PML in this example, in comparison to the case of a working PML for a waveguide that is normally incident on the PML region. Fig. 4 shows the saturated reflection from a pseudo-PML absorber in the continuum limit as resolution is increased. Note that the exact position of the monitor point for the field-convergence factor makes very little difference (a small constant factor), since the failure of PML will generally produce reflected waves throughout the computational cell; this is demonstrated by the filled and open symbols in Fig. 4, which compare the results for monitor points inside and outiside the waveguide, respectively. In problems where such a waveguide channel cannot be rotated to an orientation normal to the PML, it is possible that some additional (real) coordinate transformation could be used to *locally* rotate the waveguide into the correct direction, absorbing the coordinate transformation into the materials ε and μ [28]. (However, care must be taken that such a coordinate transformation not introduce new variation along the PML direction that itself spoils the PML.) Such a problem-dependent solution is outside the scope of this paper.

6. Concluding remarks

We have presented a straightforward method to verify the correctness of any proposed PML formulation irrespective of its implementation that simply involves computing the difference between two computations as a function of resolution. Such a validation procedure is useful, we have argued, since any adiabatic absorber (PML or not) can be made to have sufficiently low reflection so that its deviation from a true PML may be overlooked. Several researchers had made claims of working PMLs in the past for anisotropic media, periodic media, and oblique waveguides that we have shown turn out to be just instances of adiabatic pseudo-PML absorbers. For anisotropic media, we derived a corrected PML formulation as a simple re-factorization of typical UPML proposals. In the case of oblique-incidence waveguides, a possible workaround is the use of a pseudo-PML absorber (sacrificing two or three orders of magnitude in the constant factor compared to a true PML, but this sacrifice can be compensated by a thicker absorber). A true PML solution for the oblique-waveguide problem, especially one that handles multiple waveguides incident at different angles on the same boundary, may be an interesting problem for future research. A validation scheme such as the one presented here, which is not fooled by reflections that are simply low but are not converging to zero with resolution, seems increasingly relevant as the PML concept is applied to more and more geometries, material systems, wave equations, and computational schemes.

Acknowledgements

This work was supported in part by the Materials Research Science and Engineering Center program of the National Science Foundation under Grant Nos. DMR-9400334 and DMR-0819762, by the Army Research Office through the Institute for Soldier Nanotechnologies under contract DAAD-19-02-D0002.

Appendix A

We now compare the computational cost (in terms of only the number of auxiliary variables required) of our proposed UPML formulation for anisotropic media in the time domain to that of other correct PML implementations based on the split-field approach [14,22]. We leave out in this comparison the convolutional PML (CPML) formulation since the shifted pole requires an extra auxiliary variable [18]. Let us consider for nondispersive, anisotropic media the example of a PML in a single direction x (neglecting the case of corners of the computational cell where multiple PML directions overlap), considering only the **E** and **D** updates since the **H** and **B** updates have an identical form (exactly doubling the storage requirements). Our UPML formulation presented in this paper nominally requires two additional auxiliary vector fields **U** and **W** (amounting to an extra six individual field components) in the PML regions. (Note that, for anisotropic media, separate **D** and **E** fields must be stored even in non-PML regions [27] because the $\mathbf{E} = \varepsilon^{-1}\mathbf{D}$ update must be non-local on the Yee grid for stability [44].) However, in a unidirectional PML region, only s_x is non-unity, we need only store two auxiliary field components (W_x and U_y) from Eq. (6), whereas $W_{\{y,z\}} = E_{\{y,z\}}$ and $U_{\{x,z\}} = D_{\{x,z\}}$ and need not be stored explicitly.

Exactly the same amount of auxiliary storage is required in a split-field PML formulation, as long as appropriate simplifications are made. To review, the split-field formulation can be derived from a coordinate stretching in which ∇ is replaced by $\tilde{\nabla}$, where $\tilde{\nabla}_k = \frac{1}{s_k}\frac{\partial}{\partial x_k}$. Then, the **D** update equation $-i\omega\mathbf{D} = \tilde{\nabla} \times \mathbf{H}$ is split into three equations:

$$-i\omega s_k \mathbf{D}^{(k)} = (\nabla \times \mathbf{H})^{(k)}, \tag{7}$$

where $\mathbf{D} = \sum_k \mathbf{D}^{(k)}$ and $(\nabla \times \mathbf{H})^{(k)}$ denotes the terms of $\nabla \times \mathbf{H}$ that only have $\frac{\partial}{\partial x_k}$ derivatives. With the usual stretch factor $s_k = 1 + i\sigma_k/\omega$, Eq. (7) contains only first-order terms in $-i\omega$ so it readily converts to a first-order equation in the time domain. The electric field is given by the unmodified constitutive relation $\mathbf{E} = \varepsilon^{-1}\mathbf{D}$. Just as in our unsplit-field PML, this ostensibly requires two auxiliary fields since **D** is split into three fields. However, several simplifications occur. First, the $D_k^{(k)}$ component of each auxiliary field can be omitted since $(\nabla \times \mathbf{H})_k$ has no x_k derivative: since only two components of each auxiliary field are stored, this corresponds to a total of 6 components. Furthermore, if only s_1 is non-unity, then the $\mathbf{D}^{(2)}$ and $\mathbf{D}^{(3)}$ auxiliary fields can be combined into a single equation for $\mathbf{D}^{(2)} + \mathbf{D}^{(3)}$, leading to a total of 5 components that need to be stored, or 2 additional components, just as for our unsplit formulation above. One complication should be noted, however. In counting the storage requirements, we have assumed that **D** is not stored explicitly in the PML regions, but is rather computed as needed from $\mathbf{D}^{(k)}$. In this case, however, the implementation of the $\mathbf{E} = \varepsilon^{-1}\mathbf{D}$ update must be modified in the PML region to account for the splitting (noting that the splitting is different in each PML region if we exploit the optimizations above). This complicates the implementation compared to our unsplit-field formulation, in which the same implementation of the constitutive relations can be used in the PML and non-PML relations (simply passing different arrays for the components to swap **W** for **E** and so on).

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