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Long-time behavior of PML absorbing boundaries for layered periodic structures

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ABSTRACT

In this work we consider a special case of the Perfectly Matched Layer (PML) divergence which is observed by the simulation of the planar periodic structures such as photonic crystal slabs or antenna arrays. This divergence is caused by an excitation of long-living artefact evanescent waves in these structures by an incident external pulse. We study the application of the known remedies to this problem: increasing the distance between the structure and PML, employing the κ parameter, employing non-PML absorbers. We also suggest a new simple and effective solution, where the usual PML is backed by an additional absorbing layer.

Perfectly matched layers (PMLs) [5,13] provide an efficient domain truncation technique for the computational electromagnetics, in particular, for the finite-difference time-domain (FDTD) method. These layers are composed of an artificial material that absorbs incoming waves regardless of their incidence angle and frequency. The effect of PML may be understood as a complex coordinate stretching [11]:

$$\frac{\partial}{\partial x} \rightarrow \left(\kappa_x(x) + i\frac{\sigma_x(x)}{\omega}\right)^{-1} \frac{\partial}{\partial x}, \tag{1}$$

transforming propagating waves $e^{ik_x x}$ in the x direction into decaying waves $e^{i\kappa k_x x - \sigma k_x x}$. The quantity $\sigma > 0$ controls the directional decay rate while $\kappa \geqslant 1$ is analogous to a gradual change of the spatial mesh step. Theoretically PML guarantees zero reflection from an interface with the computational domain. However, in the discretized implementation of the PML equations some unwanted features appear, like frequency-dependent reflection and even divergence. These issues have been extensively studied in the literature (e.g. see [3] and references therein), and may be summarized as the following practical rules for the use of PML [13]. PMLs should be placed at some distance L from the scatterers in the computational domain. The thickness d of PML should be around 10 space steps for the Yee scheme. To reduce numerical reflection σ_x and κ_x should increase gradually with x to some maximal values $\sigma_{\max}$ and $\kappa_{\max}$ at the PML depth. There were proposed different profiles for the spatial dependence of $\sigma_x(x)$ and $\kappa_x(x)$. It was shown, that by choosing appropriate profile one can control the character of the PML reflectance decrease with the increase of its thickness [1,9].

The setups where evanescent waves are present (e.g. waveguides) require special care because the evanescent waves are poorly absorbed by PMLs [6]. In particular, the choice $\kappa \neq 1$ may be employed to reduce the evanescent wave reflection, however then the overall reflection is greater [13]. There are cases, where PMLs cause gain instead of absorbtion: this happens for geometries where the wave group and phase velocities have different signs. It is suggested to use thick non-PML physical absorbers for these metamaterials [11]. There are different PML implementations which may be classified into split-field type and unsplit type. Mathematically strong well-posedness is proven for certain unsplit PMLs, while the split-field type is only weakly well-posed [2]. However, the PML divergence manifested in the exponential or linear growth of the fields in the PML with time is observed for some discretized forms of PMLs regardless their type [3]. In the following we consider the simulation setups where the long-time growth is observed for traditional PMLs and where it is crucial for the success of the simulation. We note that unlike the cases of PML-vacuum interface considered in [3], the divergence in our case is connected with the presence of the scattering structure and of the periodic boundary conditions (PBCs) in the transverse directions.

Calculation of the optical properties of the planar layered periodic structures with the FDTD method is performed by the simulation of the time-limited plane wave pulse propagation through the structure. The transmitted and reflected waves are then analyzed numerically. In the case of the normal wave incidence a single unit cell with PBCs may be simulated (Fig. 1), whereas the inclined incidence requires special FDTD algorithms [4,14], but analogous computational setups. In these setups PMLs are used for terminating the non-periodical directions of the domain. They absorb the

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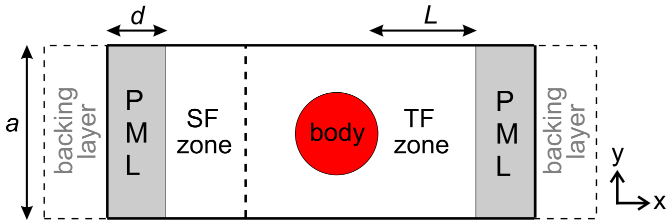

Fig. 1. FDTD simulation setup for a layered periodic structure. The incident wave is generated by the TF/SF method and propagates in the x direction, PBCs are applied in the y and z directions.

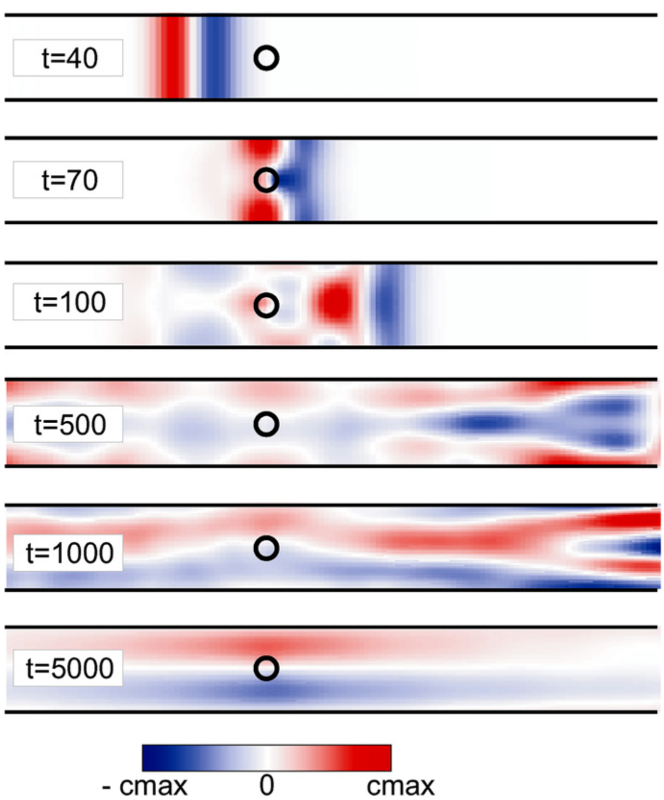

Fig. 2. Onset of a long-living standing wave in the structure composed of an array of infinite dielectric rods. The color-bar range is cmax$(t \leqslant 100) = 1.5$, cmax$(t = 500) = 0.01$, cmax$(1000 \leqslant t \leqslant 5000) = 0.02$.

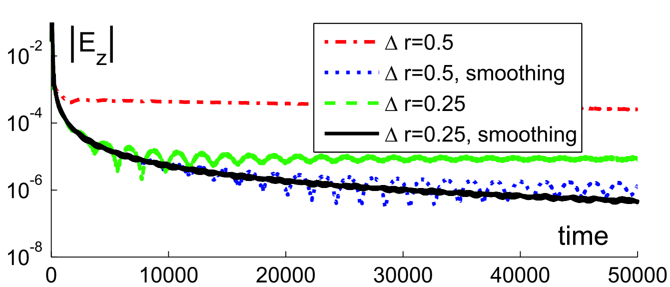

Fig. 3. Time dependence of the electric field at the axis of the rod (Fig. 2) for different spatial mesh resolutions Δr for the usual staircase model and the subpixel smoothing (no PMLs). The data is running-averaged with the window of $\Delta T = 100$.

reflected and transmitted waves modeling their withdrawal to the infinity. Total exit of the radiation from the structure determines the simulation time.

We found that when performing this kind of FDTD simulations with the structures formed by purely dielectric scatterers the incident pulse excites artefact waves with the amplitude several orders of magnitude less than the one of the incident wave. Let

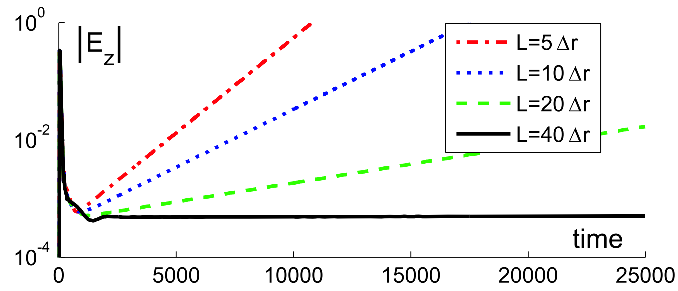

Fig. 4. Time dependence (running average $\Delta T = 100$) of the electric field at the axis of the rod (Fig. 2) for different distances between PML and the structure L. Mesh step $\Delta r = 0.5$.

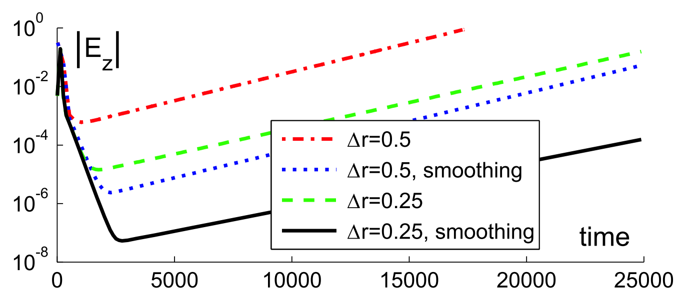

Fig. 5. Same as Fig. 4 for different Yee mesh resolutions Δr ($L = 5$).

us demonstrate the excitation of the long-living spurious waves by the 2D example structure consisting of an array of infinite dielectric ($\varepsilon = 5$) rods with the radius $R = 1$ and the distance $a = 10$ between the neighbors (Fig. 1). Here and in all other simulations mentioned below we assume the speed of light to be $c = 1$ and employ the Berenger's incident pulse [13] of the duration $\tau = 40$. To consider the spurious waves first separately from PMLs we perform the time stepping in the very elongated domain until the radiation reaches the PMLs which are placed far from the structure ($L = 100{,}000$). We use a 2D FDTD simulation with the Yee scheme and spatial mesh step of Δr. Note that we intentionally shift the rod axis to $0.25\Delta r$ from the Yee cell center in the y direction to create asymmetry in the computational domain. This asymmetry is usually present in real applications. The associated numerical error manifests itself as a standing wave with the period of a in the y direction (Fig. 2). The main part of the radiation leaves the structure during the time ~ 200, then the remaining spurious signal becomes a standing wave (see Fig. 2 at $t = 5000$) and continues to oscillate with slowly decaying amplitude. The rate of decay can be increased by decreasing Δr (Fig. 3), so this wave may be attributed to the discretization error and in the analytical limit $\Delta r \to 0$ it is absent. Note that subpixel smoothing methods [10,8] aimed at reducing the staircase effects may be used to further decrease this error (Fig. 3).

In some cases the interaction of the artefact waves with PMLs may lead to their slow exponential growth. The artefact wave is stabilized by the transverse PBCs and may be regarded as a wave evanescent in the PML direction. The extent of this wave may be greater than the PML thickness. Let us consider the interaction of the spurious wave with PML by varying the distance L between the PMLs and the structure. The calculations were performed both for uniaxial and convolutional PML implementations [13] with thickness of PML $d = 5$ (10 mesh cells for $\Delta r = 0.5$) and gave identical results. We used the fourth power polynomial grading of the PML losses σ, σ^* with depth and reflection factor $R = 1e{-}8$, which are traditional optimal settings. As seen from Fig. 4, the decrease of L leads to the exponential growth of the spurious standing wave. De-

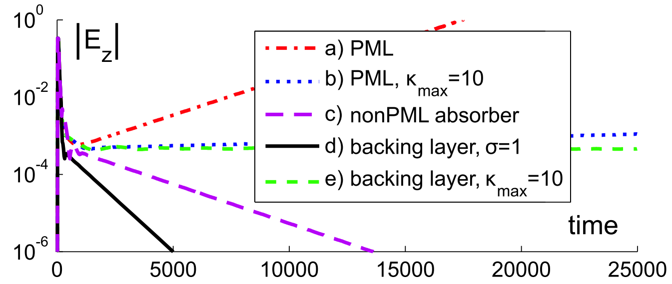

Fig. 6. Same as Fig. 4 ($L = 5$) for different absorbing layers: a): usual 10-cells thick PML; b): the same as a) with gradually changing κ_x; e): 100-cells thick physical absorber with gradually changing σ; d): a) + 10-cells of type-1 backing layer with $\sigma = 1$; e): a) + 10 cells of type-2 backing layer with $\kappa_{\max} = 1$.

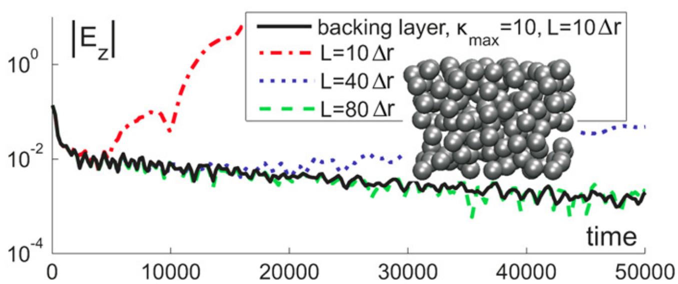

Fig. 7. 3D Yee FDTD calculation (mesh step $\Delta r = 0.5$) of the transmission through disordered dielectric media. Time dependence of the electric field at the center of computational domain (running average $\Delta T = 100$) is shown for 10-cells thick PMLs of different distance from structure to PML L and 10-cells thick type-2 backing layer.

crease of the mesh step Δr and applying subpixel smoothing does not influence this growth, but only delays the onset time (Fig. 5).

Usually the time required for the artefact wave to reach the amplitude of the incident pulse is much greater than the simulation time. However for structures with complex geometry like multilayered photonic crystals or disordered media the radiation undergoes multiple reflections and the radiation exit time becomes rather long. The exponential divergence of PML manifested at long times prevents from obtaining the correct transmittance properties from the FDTD simulation. This kind of divergence is not connected with the FDTD implementation and we reproduced it by a number of open-source codes: Electromagnetic Template Library [15] (http://fdtd.kintechlab.com), Meep package [12] and MATLAB FDTD code, supplemented to the Taflove's book [13].

We found several possible solutions to the mentioned problem. The introduction of the κ parameter helps to substantially suppress the error growth rate (Fig. 6). However, this leads to the reflection increase from PML [13], and for our test 2D setup this reflection for the main part of the pulse becomes 10^{-3} in amplitude compared to 10^{-6} for the usual PML. The second way is the application of a thick physical (non-PML) absorber with gradually changing loss parameter σ [11]. For the same fourth power loss profile this method required at least 100 mesh cells thick absorber, thus substantially increasing the number of computations. The third way which appeared to have the optimal effect consists in placing additional backing layer after the usual PML (Fig. 1). We studied two types of the baking layers: 1) physical absorber with constant loss or 2) additional PML layer with gradually changing κ_x and constant σ_x equal to $\sigma_{\max}$ of the underlying PML. In both cases the backing layer of 10 mesh cells was sufficient to suppress divergence. The main pulse is attenuated in the usual PML, thus the proposed setup does not spoil the reflection properties. The study of the transmission and reflection spectra for the structure has shown that the backing layer had no influence on the physical solution. We also tested the baking layers on a realistic 3D problem of a normal wave transmission through a layer of disordered dielectric balls ($\varepsilon = 5$) of radius $R = 1$. The thickness of the dielectric structure was $D = 13.8$ and the dielectric filling factor was $f = 0.2$. For modeling of the disorder we used a large supercell with the transverse dimensions of $D_t = D$. Introduction of a 10-cells thick backing layer of type 2 with gradually changing κ_x as well as increasing the distance to PML to 80 mesh steps lead to similar PML convergence (Fig. 7). Note that the type-1 backing layer with physical loss σ of the same thickness did not lead to the desired effect.

To conclude we mention that application of the additional absorber layers to the back of PMLs may efficiently suppress PML divergence caused by the spurious evanescent waves characterizing the transmission FDTD setups. Backing layers can also improve the accuracy in hybrid transfer-matrix FDTD calculations [7] for the transverse Bragg frequencies that are poorly absorbed by the PML. This work is partially supported by the research program 1 of the Russian Academy of Science and by the Russian Federal Agency for Science and Innovations (contract 02.523.11.3014).

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