Difficulties faced by Yee’s scheme in photonics problems

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Abstract. Popular Yee’s scheme for the FDTD method faces a number of difficulties for problems in layered media: if dielectric permittivity is discontinuous, the accuracy strongly deteriorates, if magnetic permeability is also discontinuous at the same points, the scheme does not allow to perform computation. We provide rigorous mathematical explanation of these difficulties and show them to have fundamental nature. For problems involving dielectric media interfaces, we propose technique allowing to improve the accuracy.

1. Introduction
Numerical computation of optical structures are performed for experiment interpretation, verification of theoretical models, design of new structures with given properties etc (see, e.g., [1]–[3]). Presence of media interfaces is a specific feature of such problems. At the interfaces, the material parameters are not smooth; on the contrary, they undergo hopping variation. This leads to knees in the solution; e.g., the phenomenon of light refraction described by the Snellius law is well-known. Such solutions are generalized (i.e., not classical). Numerical computation of such solutions is a considerable mathematical problem.

Majority of real problems is considered in non-stationary formulation. The most popular numerical technique for such problems is the finite-difference time-domain (FDTD) method [4], [5]. However, if media interfaces are present, the method faces serious difficulties. Firstly, for dielectric interfaces (i.e., if the dielectric permittivity ε is discontinuous), the calculation accuracy strongly deteriorates. This phenomenon has been described in references earlier (see, e.g., [6]). Secondly, the FDTD method is actually inapplicable if both magnetic permeability μ and dielectric permittivity ε encounter a jump. The error is enormous and decreases very slowly as mesh step tends to zero. Nowadays, more than 2000 publications are dedicated to the FDTD method, however, these fundamental disadvantages have not been overcome.

In the present work, we provide a rigorous mathematical explanation of the mentioned problems. We show that near the interface between non-magnetic media with different dielectric permittivities, the order of accuracy of Yee’s scheme decreases to 1. This is due to non-physical oscillations of the numerical solution caused by non-monotonicity of the scheme. We propose techniques allowing to decrease the non-monotonicity sufficiently. If both ε and μ are
discontinuous at the interface, the calculation divergence appears because the stencil of Yee’s scheme involves more than 1 spatial step.

2. Yee’s scheme
A large number of the FDTD method modifications has been proposed (both explicit and implicit, see, e.g., [5]). However, all of them are reduced to approximation of the Maxwell’s equations in Yee’s cell [7]. The steps is time for fields $E$ and $H$ are performed by turn (with half-step temporal shift); the spatial meshes for these fields are also shifted by half of the spatial step. For one-dimensional case, the stencil is given in Fig. 1.

![Figure 1. Stencil of one-dimensional Yee’s scheme. Filled markers correspond to $E_z$ nodes, empty ones are for $H_y$.](image1)

For the scheme to converge, all values should be continuous and smooth within the stencil. Suppose $\varepsilon$ is hopping at the interface and $\mu$ is continuous. We can place integer node at the interface point. Therefore, within the $E$ field stencil all functions are continuous and the scheme provides convergence. However, the $E$ field refracts at the interface and the calculation of the corresponding $H$ value involves two values of $E$, i.e., before and after the refraction. The values required for the $H$ field determination. Therefore, the accuracy of this calculation deteriorates sufficiently. The convergence is preserved but with decreased order of accuracy.

Similar situation takes place if the interface features hopping $\mu$ and continuous $\varepsilon$. In this case, we place a semi-integer node at the interface. Then, the discontinuity is knowingly not inside the $H$ field stencil, however, the $E$ field becomes unsmooth. Convergence is achieved but the order of accuracy is also decreased.

Suppose both $\varepsilon$ and $\mu$ are discontinuous at the interface. If we place an integer node of the $E$ field at this point then the $\mu$ jump is inside the $H$ stencil. Thereby, for the latter enormous error appears which does not decrease as the mesh step decreases. This causes large error of the $E$ field which also tends to zero very slowly or does not tend at all. If we place semi-integer node of the $H$ field at the interface then the $\varepsilon$ jump turn out inside the $E$ field stencil. In this case, error does not tend to zero on meshes affordable in practical computations. Thereby, Yee’s scheme is in principle inapplicable for media with interfaces at which both $\varepsilon$ and $\mu$ are discontinuous.

3. Non-monotonicity
By definition, finite-difference scheme is monotonous if a monotonous exact solution corresponds to monotonous numerical solution [8]. Otherwise, the scheme is called non-monotonous. In photonics problems, all solutions are not monotonic functions because they correspond to running waves. However, if a scheme is non-monotonous then in addition to real oscillations the numerical solution features fictitious non-physical short-wave or long-wave oscillations which introduce considerable error. Their amplitude decreases as mesh step tends to zero; however,
these oscillations may disappear slower than the errors caused by other factors (e.g., the approximation inaccuracies). In this case, the error due to non-monotonicity dominates.

Scheme non-monotonicity reveals for heterogenous media and especially if interfaces are present. Our analysis shows that Yee’s scheme is non-monotonous. This reason is the cause of poor accuracy of this scheme for problems with media interfaces. The non-monotonicity of Yee’s scheme has a fundamental origin which is discussed below.

The vector Maxwell equations written out componentwise are reduced to a system of transfer equations. For a linear transfer equation, the Godunov theorem is known [9]. From this theorem, the following corollary can be formulated:

Statement: Two-layer linear monotonous scheme for a system of hyperbolic equations cannot possess the order of accuracy larger or equal 2.

We would like to remind that scheme is called two-layer if its stencil involves two temporal moments for each value. Yee’s scheme, obviously, falls under the terms of this corollary. Therefore, its non-monotonicity cannot be eliminated completely and one can only decrease the amplitude of non-physical oscillations.

To illustrate Yee’s scheme non-monotonicity, we have computed transition of a plane wave through silicon slab with \( \varepsilon = 11.56 \). The calculations are performed on a set of meshes; steps of each mesh are twice as small as the steps of the previous mesh. The results are presented in Fig. 2. The “air-Si” and “Si-air” interfaces are depicted by dashed lines. The pulse shape before hitting the slab is shown by dotted line. Solid lines correspond to solution at the moment when the incident wave has left the slab and the reflected one has already escaped the domain.

One can see that the solution on all meshes possesses non-physical oscillations which are evidence of the scheme non-monotonicity. On coarse meshes with large step, they introduce considerable error. As the step decreases, the non-monotonicity amplitude also decreases, but does not disappear completely.

4. Dielectric interfaces

In references, numerous approaches providing the second order of accuracy have been proposed. For example, quite often, the interface is smeared; i.e., the discontinuous material parameters are replaced with some continuous (smoothed) dependencies [10], [11]. This leads to considerable decrease of reflection, i.e., distorts spectral properties of the structure.

\[
\varepsilon(x) = \varepsilon_l + (\varepsilon_r - \varepsilon_l) \tanh[(x - x_0)/\Delta], \quad x \in [0,1].
\]

Here, \( \Delta \) is a characteristic smearing width, \( x_0 = 0.5 \) is the interface position.
The incident wave moves from left to right and has pulse shape similar that of Fig. 2. We detect amplitude of reflected wave. The reflection coefficient $R$ equals the amplitude of the reflected wave divided by the amplitude of incident wave. Fig. 3 shows the dependence of this coefficient on $\Delta$ (blue line). The scale of the abscissa axis is logarithmic to cover broad range of $\Delta$. For comparison, we show the reflection from true (i.e., discontinuous) interface (red line) which is well known from theory $R_{\text{theor}} = (\sqrt{\varepsilon_r} - \sqrt{\varepsilon_l})/(\sqrt{\varepsilon_r} + \sqrt{\varepsilon_l}) = 0.382 \ldots$

One can see that interface smearing decreases the reflection; and the broader is the smearing, the stronger it affects reflection. Narrow smearing $\Delta \sim 0.01$ only slightly distorts the reflection. However, the medium is still strongly heterogeneous and the amplitude of non-physical oscillations is still large. Broad enough smearing $\Delta \sim 0.1$ weakens the non-monotonicity but introduces catastrophically large distortion into reflection; this is unacceptable.

In work [12], [13], the second order of accuracy is achieved by moving the mesh node near the interface. However, if the $\varepsilon$ jump is large, this procedure loses robustness. The step adjacent to the interface becomes so small that accurate numerical calculation of derivatives requires increased digit capacity. Also, in [13], effective value $\varepsilon_{\text{eff}}$ has to be introduced in the vicinity of the interface. Such alteration of the initial problem may lead to non-physical results as we have seen above. We propose to use mesh thickening approach [14]. Its application to electrodynamics problems is described in detail elsewhere [15] – [17].

5. Conclusion

Yee’s scheme of the FDTD method is extremely popular due to its simplicity and efficiency. Each year, a large number of works is published on application of the scheme in various problems and on improvements and generalizations of the scheme. These improvements are palliative and do not eliminate the main shortcomings of the scheme, so essentially new approaches are required.

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References

[1] Barsukova M G, Musorin A I, Shorokhov A S et al // APL Photonics 4, 016102 (2019)
[2] Okhlopkov K I, Shafrin P A, Ezhov A A et al // ACS Photonics, doi:10.1021/acsphotonics.8b01386
[3] Shibanuma T, Matsui T, Roschuk T et al // ACS Photonics 2017, Vol. 4, P. 489.
[4] Tadlove A and Hagness S C, Computational Electrodynamics: the Finite Difference Time-Domain Method. Artech House, 2005
[5] Tadlove A, Johnson S G, Oskooi A, Advances in FDTD Computational Electromagnetics: Photonics and Nanotechnology. Artech House, 2013.
[6] Cangellaris A C, Wright D B // IEEE Trans. Antennas Propag. 1991. Vol. 39. P. 1518.
[7] Yee K S // IEEE Trans. Antennas Propag. 1966. Vol. 14. P. 302.
[8] Kalitkin N N and Koryakin P V, Numerical methods. Vol. 2. Methods for mathematical physics. Moscow, Academia, 2013 [in Russian]
[9] Godunov S K // Math. Sbornik. 1959. Vol. 47, P. 271. Translated US Joint Publ. Res. Service, JPRS 7226, 1969.
[10] Hwang K P, Cangellaris A C // IEEE Microw. Wireless Compon. Lett. 2001. 11, N 4. P. 158.
[11] Hiroto T, Shibata Y, Lui W W et al. // IEEE Microwave Guided Wave Lett. 2000. 10. P. 359.
[12] Chu Q X, Ding H // IEEE Trans. Magn., 2006, Vol. 27. P. 3141.
[13] Chu Q X, Ding H // Microwave Opt. Techn. Lett. 2007, Vol. 49, P. 3007.
[14] Kalitkin N.N., Alshin A.B., Alshina E.A. et al. Computations on semi-uniform meshes, Moscow, Fizmatlit, 2005 [in Russian]
[15] Dombrovskaya Zh O, Bogolyubov A N // Memoirs of the Faculty of Physics, Lomonosov MSU, 2017, No. 4, P 174302 [in Russian].
[16] Dombrovskaya Zh O, Bogolyubov A N // Bull. Russ. Acad. Sci.: Physics, 2017, Vol. 81, No. 1. P. 106
[17] Dombrovskaya Zh. O. // Simul. Analysis Information Syst., 2016, Vol. 23, No 5. P. 539-547 [in Russian].