Adaptive mesh for computation of electromagnetic wave propagation through high refractive index dielectric structures

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Abstract. We consider spatial step selection for finite-difference solution of Maxwell's curl equations in presence of dielectric interfaces. If the contrast of the refractive indices is high, the wave number in optically thick medium decreases greatly and the fields oscillate fast. To improve accuracy, we propose a special quasi-uniform mesh which provides fine enough meshes in the vicinity of the interface and does not impose abundant computations in optically thin medium. The fundamental advantage of quasi-uniform meshes in finite-difference is the possibility to obtain the solution simultaneously with its error value. We describe the corresponding procedure.

1. Introduction
Recently, a great deal of attention is attracted to nanostructures consisting of high refractive index dielectric materials [1]. Important feature of such structures is presence of strong magnetic response. If size of the metaatoms is comparable with incident wavelength, magnetic resonance appears with magnitude comparable with that of electric resonance.

Solving such problems via finite-difference techniques (both, in time and frequency domains), one encounters two main mathematical difficulties. The first of them is presence of media interfaces, i.e. discontinuity of material parameters. The fields refract at the interface, i.e., they are not smooth functions.

The second difficulty is connected with sharp decreasing of wavelength in high refractive index materials compared with free space. To provide reasonable accuracy, spatial mesh should be fine enough, i.e., spatial solution period should include several (about 5 – 7) mesh steps. If the contrast of dielectric permittivities is large at the media interface, one should use very small step inside optically thick medium where the fields oscillate very fast. However, implication of such step in optically thin medium is unreasonable because the fields vary smoothly. Therefore, meshes adapted to the solution should be implied. The oscillation frequency changes at the media interface. Consequently, the adaptive mesh can be constructed a priori, i.e., before the computation. This fact simplifies consideration of the problem (in contrast to dynamically adapted meshes constructed in the process of solution).
Commonly, piece-wise uniform meshes are applied (see, e.g., [2], [3]) because they permit more simple theoretical investigation and, in particular, construction of a priori convergence estimates. Such meshes are knowingly better than uniform ones because they provide small step in optically thick medium and large step in optically thin domain.

However, at the point of transition from large step to small one, the accuracy might deteriorate. For example, in Yee’s scheme [4], adjacent large and small steps should be matched with each other to provide the second order of accuracy [5], [6]. On the other hand, small step should be adapted to the refractive index contrast. These requirements may contradict each other. Thereby, piece-wise uniform meshes are not optimal.

We propose another approach. It includes, firstly, implication of quasi-uniform meshes [7], [8] defined as smooth transformation of some uniform mesh. Secondly, calculations should be performed on a sequence of thickening meshes with decreasing step. This strategy provides a posteriori error estimates which almost coincide with actual accuracy. The approach is applicable to any finite-difference computation. We consider it on the example of the finite-difference time domain (FDTD) method.

2. Adaptive mesh

First of all, let us remind the definition of quasi-uniform meshes. These meshes were proposed by A. A. Samarskii and developed by N. N. Kalitkin and his collaborators. By definition, a quasi-uniform mesh \( \{x_j\} \) is obtained from uniform mesh \( \{\xi_j\} \), \( \xi_j - \xi_{j-1} = \text{const} \) via transformation \( x(\xi) \) which satisfies the following conditions:

(i) \( x(\xi) \) is smooth function,

(ii) \( x(\xi) \) monotonically increases,

(iii) \( x(\xi) \) transforms segment \( \xi \in [\alpha, \beta] \) into given interval \( x \in [a, b] \).

Step of a quasi-uniform mesh is defined as follows: \( h_j = (2/J) \cdot x'(\xi_{j+1/2}) \) where \( J \) is the total number of mesh steps. It is a generalization of a conventional definition \( h_j = x_{j+1} - x_j \). Note that the difference between two adjacent steps is \( \Delta h = h_j - h_{j-1} = O(h^2) \), i.e., the steps vary smoothly. This is the fundamental difference between arbitrary non-uniform mesh and quasi-uniform one.

The key point is to construct appropriate transformation \( x(\xi) \) which provides fine enough mesh in the regions where the field varies sharply and coarse mesh in regions of slight field variation. In the present work, we have constructed such a mesh for problems with dielectric interfaces. The approach is applicable to multidimensional case. However, for the sake of clarity, we describe it for a simple one-dimensional problem: normal incidence of a plane wave on an interface between homogeneous dielectric media with refractive indices \( n_l \) (left) and \( n_r \) (right).

Let the free-space wave number be \( k \). Let \( x \) be the spatial coordinate, the computational domain is \( x \in [-a, a] \) and the interface is situated at \( x = 0 \). For determinacy, suppose \( n_l < n_r \).

![Figure 1](image_url). Comparison of transformations \( x(\xi) \), filled markers are (1), empty ones are (2) from [10]).
For homogenous media, it is reasonable to select constant step since the wave number remains constant. Therefore, constant step value is reasonable, and the transformation \( x(\xi) \) is linear. The step value is \( h_{l,r} = [k^2\alpha^2 \text{Re} n_{l,r}]^{-1}\Delta\xi \), where \( \Delta\xi = (\beta - \alpha)/J \). If media interfaces are present, the physical picture changes. The wave reaches the interface and partially reflects. In front of the interface, the field amplitude increases. At the interface, the fields refract, i.e., \( E \) and \( H \) undergo sharp bend. To the right of the interface, the fields travel with reduced wavelength \( \lambda/(\text{Re} n_r) \). Therefore, in the immediate vicinity of the interface, the step should smoothly decrease from \( h_l \) to \( h_r \), i.e., the relation of steps at \( x = 0 \) and \( x = -1 \) equals \( \text{Re} n_r/\text{Re} n_l \). The outlined requirements are met by the following transformation \( x(\xi) \):

\[
x(\xi) = a\{\text{th}[C(\xi + 1)(1 + (\xi + 1)^2)/3] - 1\}, \quad -1 \leq \xi \leq 0
\]

\[
x(\xi) = h_r\xi, \quad 0 \leq \xi \leq \beta
\]

(1)

Here, \( \beta = a^2 k \text{Re} n_r \). The coefficient \( C \) is introduced to provide \( x'(0)/x'(-1) = \text{Re} n_r/\text{Re} n_l \). The left part of the transformation \( x(\xi) \) (i.e., for \(-1 \leq \xi \leq 0\)) was proposed in [9] for stationary diffusion problems. We generalize it for non-stationary hyperbolic problems where the wave number may abruptly change due to refractive index variation. The proposed mesh can be generalized to describe metal-dielectric interfaces where the fields only slightly penetrate into the skin layer. However, this is beyond the scope of the present work.

Let us compare the proposed mesh (1) with the known transformations on the example of [10]. In the mentioned work, the following quasi-uniform mesh was proposed:

\[
x(\xi) = A + (B + C\xi)^n.
\]

(2)

Here, \( A, B, C \) are adjusting parameters. The dependence of \( \xi \) on \( x \) for transformations (1) and (2) is presented in Fig. 1. One can see that the mesh (2) redundantly increases the number of nodes relatively far from the interface in the domain where the fields vary smooth.

3. Mesh refinement

Calculation on a single mesh does not allow to estimate the accuracy in principle. To control convergence, one has to perform calculations on a set of meshes with decreasing step, e.g., twice from mesh to mesh. This strategy provides a posteriori error estimates which do not require any a priori information on the solution and its derivatives. This strategy should be implied in all numerical computations. The procedure is as follows.

Firstly, let us perform calculations on several refining meshes. At each refinement, the number of steps is doubled and the value of each step becomes 2 times smaller. In result, we construct a sequence of numerical solutions which tend to some limiting solution.

Secondly, using this sequence, we can calculate estimate of the actual error via the Richardson method [11]. Let \( E_N \) and \( E_{2N} \) be the values of the electric field on meshes with \( N \) and \( 2N \) nodes, respectively. The error estimate \( \delta E_{2N} \) for \( E_{2N} \) is given by the following formula:

\[
\delta E_{2N} = (E_{2N} - E_N)/(2^p - 1),
\]

(3)

here, \( p \) is the order of accuracy. The estimate is based on the fact that we know the rate of error decreasing as meshes are thickened. The estimate is asymptotically exact: the larger is \( N \), the closer is the estimate to the actual accuracy of the computation [8]. Practically, the value (3) almost coincides with the real accuracy. This estimate does not involve any suppositions on the exact solution. Therefore, it is applicable for any mesh calculation if the steps are small enough to provide the error decreasing according to theoretical order of accuracy.

Thirdly, let us exclude the error (3) from the solution, i.e., perform extrapolation refinement of the solution. To do so, we use the following formula

\[
\bar{E}_{2N} = E_{2N} - \delta E_{2N}.
\]

(4)
This refinement increases the order of accuracy by 1 because it eliminates the principal term in the scheme residual.

The described approach is universal and can be applied to any mesh method if we know its order of accuracy. In finite-difference computations of electrodynamics problems, this strategy was implied for the first time in [12] – [14].

It worth noting that the idea of extrapolation (i.e., to subtract the error estimate from the approximate solution) has been proposed for point source method approaches (see, e.g., [15], [16]). However, firstly, this group of methods essentially differs from the finite-difference techniques and is beyond the scope of the present work.

Secondly, the accuracy estimates for the point source methods are majorant (while the Richardson estimate is asymptotically accuracy). Therefore, extrapolation permits only to decrease the principle term of the error but cannot eliminate this term completely. The accuracy of such extrapolation depends on how close is the convergence estimate to the real value of the error. For simple model problems, the estimate is reasonably close to the real error and extrapolation allows to enhance the accuracy. However, for complicated problems (e.g., scattering on multiple particles with sophisticated shape) the estimation can be rather far from the real error (if the latter is overcautious). In this case, the extrapolation does not improve the result and an even deteriorate the accuracy.

In the Richardson approach for finite-difference schemes, the mentioned difficulty can be overcome via additional mesh refinement due to asymptotical properties of the accuracy estimation.

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