Enhanced FDTD Edge Correction for Nonlinear Effects Calculation

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Introduction

The electromagnetic field in the vicinity of sharp edges needs a special treatment in numeric calculation whenever accurate, fast converging results are necessary. One of the fundamental works concerning field singularities has been proposed in 1972 [1] and states that the electromagnetic energy density must be integrable over any finite domain, even if this domain contains singularities. It is shown, that the magnetic field $\vec{H}(\varrho,\varphi)$ and electric field $\vec{E}(\varrho,\varphi)$ are proportional to $\propto \varrho^{(t-1)}$ for $\varrho \to 0$. The variable ϱ is the distance to the edge and t has to fulfill the integrability condition and thus is restricted to $0 < t < 1$. This result is often used to reduce the error corresponding to the singularity without increasing the numerical effort [2 - 5]. For this purpose, a correction factor K is estimated by inserting the proportionality into the wave equation. It is shown, that this method improves the accuracy of the result significantly, however the order of convergence is often not studied. In [4] a method to modify the material parameters in order to use analytic results to improve the numeric calculation is presented. In this contribution we will - inspired by the scheme given in [4] - develop a new method to estimate a correction factor for perfect conducting materials (PEC) and demonstrate the improvement of the results compared to the standard edge correction. Therefore analytic results (comparable to [1]) are consequently merged with the scheme in [4].
The main goal of this work is the calculation of the second harmonic generation (SHG) in the wave response of so-called metamaterials [6]. Frequently these structures contain sharp metallic edges with field singularities at the interfaces which have a strong impact on the SHG signals. Thus, an accurate simulation of singularities is highly important. However, the following approach can also be applied to many other setups, and one of them is shown in the example below.

1 Edge Correction

In order to derivate the correction factor, the setup shown in Fig. 1(a) is investigated. The Laplacian differential equation $\nabla^2\Phi(\varrho,\varphi) = 0$ is solved by standard analytic approaches in cylindrical coordinates. Using the gradient operator the electric field

$$E_\varrho = \sum_{n=0}^{\infty} E_n \varrho^{\left(\frac{\pi(n+1)}{\beta}-1\right)} \sin\left(\frac{\pi(n+1)}{\beta}\varphi\right) \tag{1}$$

$$E_\varphi = \sum_{n=0}^{\infty} E_n \varrho^{\left(\frac{\pi(n+1)}{\beta}-1\right)} \cos\left(\frac{\pi(n+1)}{\beta}\varphi\right) \tag{2}$$

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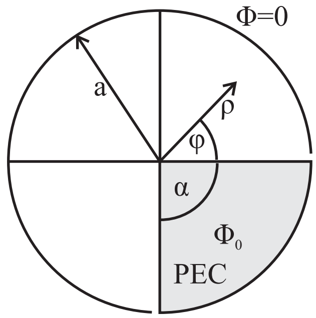
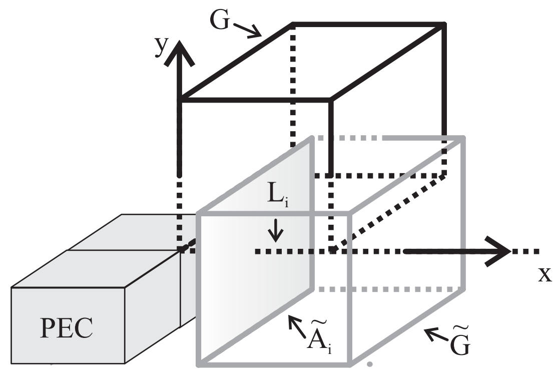


(a) Boundary Value Problem.



(b) FIT Scheme.

Figure 1: Setup for the analysis of edge singularities (a) and example FIT grid with used nomenclatur (b). The grid flux $\widehat{\widehat{d}}_i$ is defined on the dual Grid $\widetilde{G}$, the grid voltage $\widehat{e}_i$ corresponds to the primary grid G.

can be derived. Within these equations E_n depends only on the chosen parameters of the setup (Φ_0, a) and the variable n. Thus E_n is independent of ϱ and φ. The constant β is defined as $2\pi - \alpha$. It is obvious, that singular expressions only occur when $n = 0$ and $\pi/\beta < 1$.
Following the idea of [4], a detailed look at the calculation scheme is necessary. For the sake of compact notation, the notation of the finite integration technique (FIT [7]) is used. The electric flux density $\vec{D}$ is linked with the electric field strength $\vec{E}$ via the material parameters $\vec{D} = \varepsilon \vec{E}$. However, in FIT this is expressed by the material matrix $\mathbf{M}_\varepsilon$

$$\widehat{\widehat{\mathbf{d}}} = \mathbf{M}_\varepsilon \widehat{\mathbf{e}}. \tag{3}$$

Evaluating equation (3) for a certain grid-edge i in $\vec{e}_x$ direction that belongs to the edge in Fig. 1(b) and linking the grid flux with the grid voltage leads to following Matrix entry and equation:

$$M_{\varepsilon_i} = \frac{\Delta\widetilde{y}\Delta\widetilde{z}}{\Delta x}\varepsilon, \quad \widehat{\widehat{d}}_i = \frac{\Delta\widetilde{y}\Delta\widetilde{z}}{\Delta x}\varepsilon\, \widehat{e}_i. \tag{4}$$

Here $\Delta\widetilde{y}$ and $\Delta\widetilde{z}$ are the dual grid lengths in y and z direction, Δx is the primary grid length in x direction.
Writing down the same expressions using the results from the analytic calculation (index a) (where E_x and D_x are the results we derived from the analytic approach transformed in cartesian coordinates):

$$\widehat{e}_{a_i} = \int_{\Delta x} E_x(x, y = 0)dx, \quad \widehat{\widehat{d}}_{a_i} = \int_{\Delta\widetilde{y}}\int_{\Delta\widetilde{z}} D_x(x = \frac{\Delta x}{2}, y)dzdy \tag{5}$$

Since $D_x = \varepsilon E_x$ is valid for the analytic approach, this leads to a permittivity entry ε_{a_i} at the material matrix which is based on the analytic field information:

$$\varepsilon_{a_i} = \frac{\widehat{\widehat{d}}_{a_i}}{\widehat{e}_{a_i}} = \varepsilon\Delta\widetilde{z}\frac{\int_{\Delta\widetilde{y}} E_x(x = \frac{\Delta x}{2}, y)dy}{\int_{\Delta x} E_x(x, y = 0)dx} = M_{\varepsilon_i} K_i. \tag{6}$$

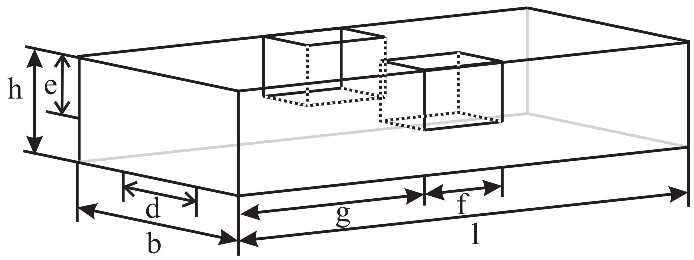


Figure 2: Setup - air filled waveguide with PEC implants. The dashed lines mark the edges where a correction factor is performed.

Thus a factor K_i is derived which can be multiplied by the material matrix entry M_{ε_i} giving us the possibility to use the analytic information about the field distribution at an edge within the standard implementation. Due to the fact, that singular expressions only occur for $n = 0$ one can reduce the sum within equation (1) and equation (2) to the terms for $n = 0$ [2]. All constant expressions can be canceled out and the correction factor is independent of all variables that are necessary to set up the static boundary value problem. Since φ depends on x and y, the angular dependence has to be considered when the integrals are solved numerically. This distinguishes the formulas from former approaches where the angle has been chosen constant as $\varphi = \pi$ for the correction in $\vec{e}_x$ direction. Similar correction factors can be derived for the $\vec{e}_y$ direction as well as for the $\vec{H}$ and $\vec{B}$ field.

2 Numerical Example

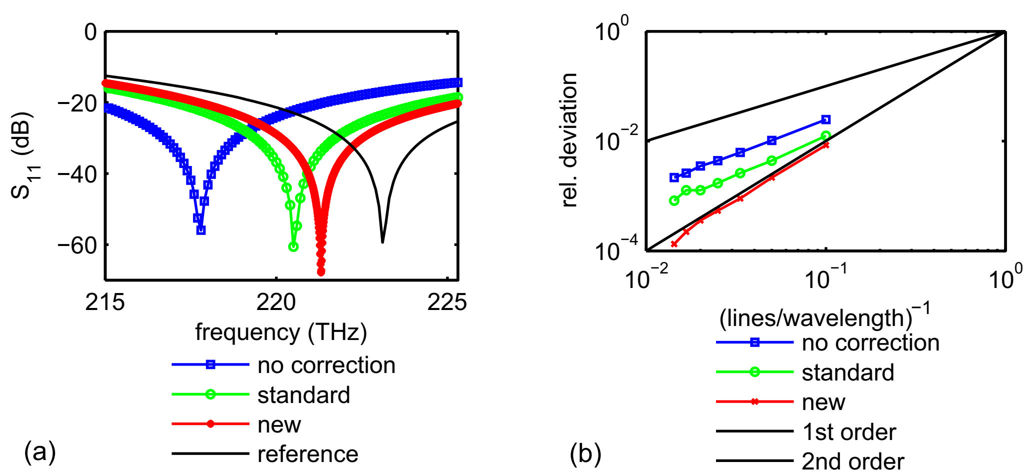


Figure 3: (a) Reflection coefficient S_{11}(10 lines/wavelength). (b) Relative deviation to the reference result (resonance frequency).

First testings have been performed using a 2D static setup (step capacitor). As expected, the resulting error can be decreased significantly - even compared to the standard edge correction. The setup shown here is a full 3D calculation of a rectangular waveguide - excited by a TE mode from the right side (see Fig. 2). Within this waveguide, two PEC bricks are implanted in order to have a resonant structure and metallic edges in the calculation domain. The parameters are chosen as $l = 2.4$ μm, $h = 0.4$ μm, $b = 0.8$ μm, $d = 0.32$ μm, $e = 0.24$ μm, $f = 0.4$ μm and $g = 1.0$ μm.

The reflection coefficients are calculated and show a clear spike at the resonant point. As reference result, a commercial FIT tool (CST Microwave Studio Suite 2009 [5]) with built-in edge correction and a very dense mesh is used. The frequency range is chosen to be 200THz - 300THz and all advanced mesh properties beside the singularity correction are switched off. The result curves in Fig. 3 show a second order convergence and an improvement of the total error compared to a calculation using the standard correction factor and a calculation without correction.

3 Conclusion

An edge correction has been developed providing a considerable enhancement of the accuracy in electromagnetic field calculation. This edge correction is based on a modification of the material parameters in the vicinity of the edge. For non equidistant grids the integrals in equation (6) have to be calculated for each gridpoint corresponding to the edge which requires a slightly increased effort in the preprocessing. However, beside the modification of the material matrix, the calculation algorithm has been retained unchanged. Thus the numerical effort for the time step iteration loop stays the same. Further examples concerning linear and nonlinear problems will be presented at the conference.

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