Hybrid Analysis of Three-Dimensional Structures by the Method of Lines Using Novel Nonequidistant Discretization

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Abstract — **Many microwave structures contain various elements with very big difference in their size. Exact modeling of such structures with equidistant discretization requires considerable numerical effort and large memory capacity. Alternative formulas for nonequidistant discretization are proposed. New difference operators for nonequidistant discretization are given. The accuracy of these operators is compared with the previous ones used with the Method of Lines. Numerical results of two microwave filters are presented to check the accuracy of the new algorithm.**

I. Introduction

The method of lines (MoL) has been successfully applied to wide class of microwave, millimeterwave [1], [2] and optical devices, both two- and three- dimensional.

A great advantage of the MoL is the analytical calculation either in one or in two directions corresponding to 3–D or 2–D structures. For two-dimensional discretization, the analytical solution is performed in the direction of propagation, so that the length of the structure has no influence on computational effort [3].

Such influence have, however, the dimensions of the cross–section. In case of big differences between the size of individual elements of the cross-section, (e. g. substrate, air bridges, width of conductors and intermediate gaps), fine discretization must be used for exact modeling the small parts. Equidistant discretization for a whole such cross-section leads to very high number of lines and therefore increases significantly the computing time and memory requirements. For that reason, to reduce the number of lines, the nonequidistant discretization can be used [1], [4].

However, this possible remedy for too high number of lines has some disadvantages. It was observed, that the convergence curve in case of nonequidistant discretization is not as smooth as in the equidistant case and the accuracy of the first and second derivative is much lower compared with the equidistant discretization. Therefore, the discretization distance should be changed only gradually; the distance between lines can increase, when the field concentration decreases.

The alternative formulas for difference operators in case of nonequidistant discretization, which were partially developed by authors and partially adopted from Gordon, Lee, Mittra [5] have more advantages: they are second order accurate and they enable an abrupt change of the discretization distance. When the equidistant discretization is used, these formulas reduce themselves to the conventional ones.

The second derivatives are obtained, contrary to [5], as a product of the first ones. The accuracy of such formulation is second order with reference to the first derivatives.

With the proposed in this paper difference operators, scattering parameters of two microwave filters are calculated. The first is the narrow-band microstrip filter composed of two T–shaped port elements and two square-loop resonators. The second one is a filter with transmission zero above the passband due to cross coupling between first and third resonator.

II. Theory

In the MoL the structure is discretized with two (in case of 2–D discretization) or with four (for 3–D discretization) different line systems for electric and magnetic field components. This type of discretization has many advantages, which have been reported e. g. in [1]. One of the consequences of such discretization is, that the first derivative of one of the field components is calculated on the lines on which the other field component is discretized.

The conventional difference formulas for the first and second derivative of a magnetic or electric field component F are

$$\left.\frac{\partial F}{\partial x}\right|_i = \frac{F_{i+1} - F_i}{h_i} \qquad (1)$$

$$\left.\frac{\partial^2 F}{\partial x^2}\right|_i = \frac{F_{i-1} - 2F_i + F_{i+1}}{h_i^2} \qquad (2)$$

where h_i denotes the distance between the lines in x direction.

In the nonequidistant discretization scheme used previously with the MoL, the difference operators for the first and second derivatives are calculated from two and three consecutive lines respectively [4]. However, as it has been shown in [5] the accuracy of such formulation in case of nonequidistant discretization is low. While for the equidistant discretization the difference operators for the first and second derivative have second order accuracy, in

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nonequidistant case both difference operators have first and zeroth order accuracy respectively. Nevertheless, the authors have found, that if the first derivative is in the middle between two lines from which it is approximated, always second order accuracy is achieved. It can be easily proved. Assuming parabolic change of the field component F in the vicinity of i-th line (Fig. 1) according to:

$$F = F_i + a_1 (x - x_i) + a_2 (x - x_i)^2 \qquad (3)$$

The first derivative of F at a place $x - x_i = h_i/2$ can be written as

$$F'|_{h_i/2} = a_1 + a_2 h_i \qquad (4)$$

The field component F on the $i+1$-th line may be expressed as

$$F_{i+1} = F_i + a_1 h_i + a_2 h_i^2$$

The first derivative of F, calculated using eq. (1) is equal eq. (4), so the second order accuracy is obtained.

Therefore in the method of lines (the proposed formulas can be used with other FD methods as well), the nonequidistant discretization should be done as shown in Fig. 1.

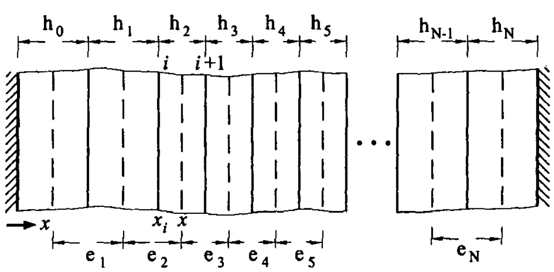

Fig. 1: Discretization scheme. $e_i = \frac{1}{2}(h_{i-1} + h_i)$

It should be stressed, that the lines for one of the field components (e. g. discretized on dashed lines) should be exactly in the middle between the other type of lines (solid). Thus, for the first derivative of the field component discretized on solid lines, one obtains:

$$\frac{\mathrm{d}\mathbf{F}_{\mathrm{DD}}}{\mathrm{d}x} = \boldsymbol{h}^{-1}\boldsymbol{D}_{\mathrm{DD}}\mathbf{F} = \overline{\boldsymbol{D}}_{\mathrm{DD}}\mathbf{F} \qquad (5)$$

where
$$\boldsymbol{h} = \mathrm{diag}\,(h_0, h_1, \ldots, h_{N-1}, h_N)$$

and $\boldsymbol{D}_{\mathrm{DD}}$ denotes the difference operator for central differences and Dirichlet-Dirichlet boundary conditions.

However, the other field component (discretized on solid lines) is not in the middle between dashed lines in case of nonequidistant discretization. For that reason eq. (5) has in this case only first oder accuracy.

As shown by Gordon *et al* [5], the first derivative in a small neighbourhood containing three consecutive lines x_{i-1}, x_i, x_{i+1} can be computed from:

$$\begin{aligned}\left(\frac{\mathrm{d}f}{\mathrm{d}x}(x)\right)_{\mathrm{num}} &= f(x_{i-1})\frac{(x - x_i) + (x - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + \\ &+ f(x_i)\frac{(x - x_{i-1}) + (x - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})} + \\ &+ f(x_{i+1})\frac{(x - x_i) + (x - x_{i-1})}{(x_{i+1} - x_i)(x_{i+1} - x_{i-1})}\end{aligned} \qquad (6)$$

This formula has second order accuracy and can be easily derived from eq. (3). It is adopted to the MoL and the first derivative for G, can be written as

$$\begin{aligned}\left.\frac{\partial G_{\mathrm{NN}}}{\partial x}\right|_i &= G_{i-1}\frac{2(h_i - h_{i+1})}{(h_{i-1} + h_i)(h_{i-1} + 2h_i + h_{i+1})} + \\ &+ G_i\frac{-2(h_{i-1} + 2h_i - h_{i+1})}{(h_{i-1} + h_i)(h_i + h_{i+1})} + \\ &+ G_{i+1}\frac{2(h_{i-1} + 3h_i)}{(h_i + h_{i+1})(h_{i-1} + 2h_i + h_{i+1})}\end{aligned} \qquad (7)$$

where G is the field component discretized on dashed lines or the first derivative of F which is calculated on dashed lines as well. Collecting all the derivatives in one matrix gives the difference operator $\overline{\boldsymbol{D}}_{\mathrm{NN}}$ for the field component discretized on dashed lines (with Neumann-Neumann boundary conditions).

It was found, that the formula (5), which was independently developed by the authors, match eq. (6).

The second derivatives are, however, not approximated by derivation of (6) like it was done in [5]. Instead of this, they are built as a product of the first derivatives. The accuracy of such formulation is, then, second order with reference to the first derivative and therefore better than that proposed in [5].

$$\boldsymbol{P}_{\mathrm{DD}} = \overline{\boldsymbol{D}}_{\mathrm{NN}}\overline{\boldsymbol{D}}_{\mathrm{DD}} \qquad \boldsymbol{P}_{\mathrm{NN}} = \overline{\boldsymbol{D}}_{\mathrm{DD}}\overline{\boldsymbol{D}}_{\mathrm{NN}} \qquad (8)$$

Thus, in case of nonequidistant discretization, the second derivative is approximated from four consecutive lines.

For 2–D discretization shown in Fig. 2, the general transmission line equations in discretized form are [6]

$$\frac{\mathrm{d}}{\mathrm{d}\bar{z}}\widehat{\mathbf{E}} = -\mathrm{j}\widehat{\boldsymbol{R}}_{\mathrm{H}}\widehat{\mathbf{H}} \qquad \frac{\mathrm{d}}{\mathrm{d}\bar{z}}\widehat{\mathbf{H}} = -\mathrm{j}\widehat{\boldsymbol{R}}_{\mathrm{E}}\widehat{\mathbf{E}} \qquad (9)$$

The new nonequidistant difference operators cannot be normalized, as it was done with the old ones [4]. Therefore, the relation $\boldsymbol{D}_{\mathrm{DD}} = -\boldsymbol{D}^{\mathrm{t}}_{\mathrm{NN}}$ is no more valid (the boundary conditions are dual for both types of lines). Accordingly, the matrices $\boldsymbol{R}_{\mathrm{E,H}}$ are given by:

$$\widehat{\boldsymbol{R}}_{\mathrm{E}} = \begin{bmatrix} \widehat{\boldsymbol{D}}^{\circ}_{\bar{x}}\widehat{\boldsymbol{\mu}}_z^{-1}\widehat{\boldsymbol{D}}^{\bullet}_{\bar{x}} + \widehat{\boldsymbol{\epsilon}}_y & -\widehat{\boldsymbol{D}}^{\circ}_{\bar{x}}\widehat{\boldsymbol{\mu}}_z^{-1}\widehat{\boldsymbol{D}}^{\circ}_{\bar{y}} \\ -\widehat{\boldsymbol{D}}^{\bullet}_{\bar{y}}\widehat{\boldsymbol{\mu}}_z^{-1}\widehat{\boldsymbol{D}}^{\bullet}_{\bar{x}} & \widehat{\boldsymbol{D}}^{\bullet}_{\bar{y}}\widehat{\boldsymbol{\mu}}_z^{-1}\widehat{\boldsymbol{D}}^{\circ}_{\bar{y}} + \widehat{\boldsymbol{\epsilon}}_x \end{bmatrix} \qquad (10)$$

$$\widehat{\boldsymbol{R}}_{\mathrm{H}} = \begin{bmatrix} \widehat{\boldsymbol{D}}^{\circ}_{\bar{y}}\widehat{\boldsymbol{\epsilon}_z^{-1}}\widehat{\boldsymbol{D}}^{\bullet}_{\bar{y}} + \widehat{\boldsymbol{\mu}}_x & \widehat{\boldsymbol{D}}^{\circ}_{\bar{y}}\widehat{\boldsymbol{\epsilon}_z^{-1}}\widehat{\boldsymbol{D}}^{\circ}_{\bar{x}} \\ \widehat{\boldsymbol{D}}^{\bullet}_{\bar{x}}\widehat{\boldsymbol{\epsilon}_z^{-1}}\widehat{\boldsymbol{D}}^{\bullet}_{\bar{y}} & \widehat{\boldsymbol{D}}^{\bullet}_{\bar{x}}\widehat{\boldsymbol{\epsilon}_z^{-1}}\widehat{\boldsymbol{D}}^{\circ}_{\bar{x}} + \widehat{\boldsymbol{\mu}}_y \end{bmatrix} \qquad (11)$$

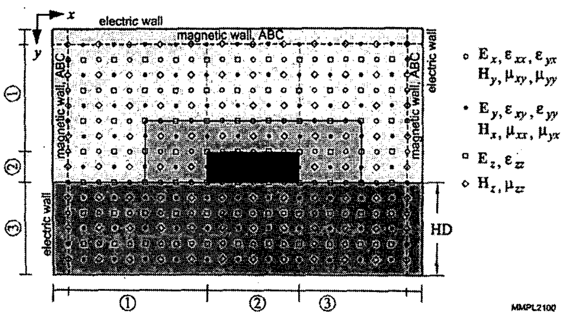

Fig. 2: Cross–section of a general planar structure with discretization points.

Combining eqs. (9) results in

$$\frac{\mathrm{d}^2}{\mathrm{d}\bar{z}^2}\widehat{\mathbf{E}} - \widehat{\boldsymbol{R}}_{\mathrm{H}}\widehat{\boldsymbol{R}}_{\mathrm{E}}\widehat{\mathbf{E}} = 0 \qquad \frac{\mathrm{d}^2}{\mathrm{d}\bar{z}^2}\widehat{\mathbf{H}} - \widehat{\boldsymbol{R}}_{\mathrm{E}}\widehat{\boldsymbol{R}}_{\mathrm{H}}\widehat{\mathbf{H}} = 0 \quad (12)$$

It should be noted, that multiplying both $\widehat{\boldsymbol{R}}_{\mathrm{E,H}}$ matrices, all terms which have four difference operators cancel.

III. Results

To compare the accuracy of the old and the new nonequidistant difference operators, the first and second derivatives of $\sin(x), x \in [0; \pi/2]$ and $e^{-x}, x \in [0; 1.5]$ functions were calculated. The $\sin(x)$ function was discretized with sinusoidal decrease of discretization distance whereas the e^{-x} function was discretized with the geometrical increase of the discretization distance with an extra abrupt change of discretization distance between two lines.

The results presented in Fig. 3 show the difference between the first and second derivatives of the both functions obtained by using the new and old difference operators and the analytical values. As seen, the numerical error of the new proposed nonequidistant difference operators is much lower. Especially in case of abrupt changes in the discretization distance, which are frequently unavoidable, the new difference operators have much better accuracy.

With the new nonequidistant difference operators scattering parameters of two microwave filters were computed. Both filters have big difference between the width of microstrips and the intermediate gaps. One of them has additionally big differences in thickness of the layers.

The first analyzed filter is a printed microstrip filter composed of T–shaped port elements and loop resonators (Fig. 4). The magnitude of scattering parameters (Fig. 5) is in very good agreement with measured and calculated results [7].

The second analyzed filter is a filter with transmission zero above the passband due to cross coupling between first

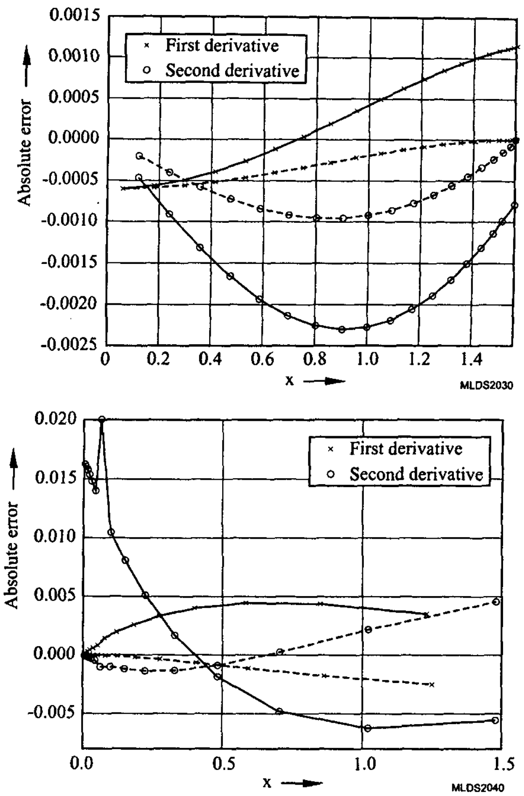

Fig. 3: Absolute numerical error of the new and the old nonequidistant difference operators. Discretized functions: $\sin(x)$ (upper) and e^{-x} (lower). Solid line – old difference operators, dashed line – new difference operators.

and third resonator (Fig. 6). For this filter the obtained results (Fig. 7) are also in very good agreement with results reported by Melcón *et al* [8].

IV. Conclusion

Alternative difference operators for nonequidistant discretization were proposed and substantiated. These operators enable to calculate the first and second derivatives with second order accuracy, whereas the old formulas provide first and zeroth order accuracy. With the new operators, an abrupt change in the discretization distance can be made. There is no need to model structures with gradually changed discretization distance only. The discretization process is therefore simplify.

The proposed formulas reduce themselves to the standard ones when the equidistant discretization is used. They can be used not only with the MoL, but also with other FD methods.

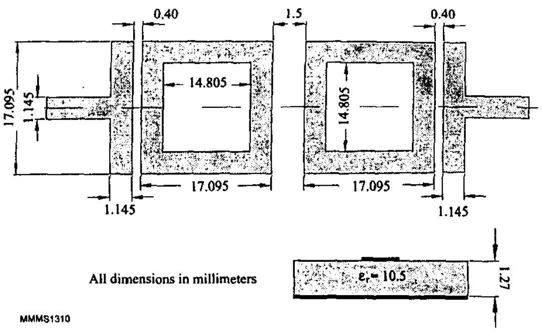

Fig. 4: Printed microstrip filter composed of T-shaped port elements and loop resonators.

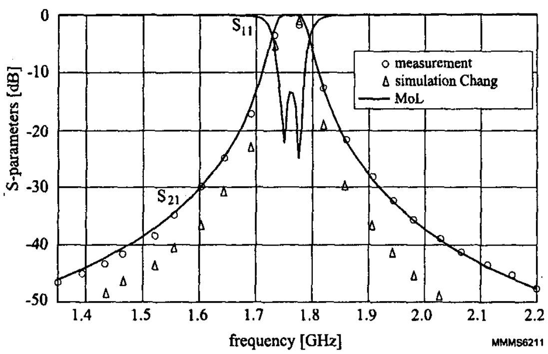

Fig. 5: Scattering parameters for the filter shown in Fig. 4.

It has been shown, that using one type of lines in the middle between the other type, one of the first derivatives can be approximated from two neighboring lines only, with second order accuracy.

It has been demonstrated, that the proposed algorithm makes the modeling of many microwave structures much more accurate and efficient.

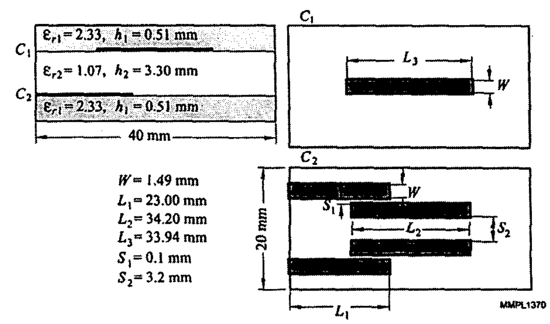

Fig. 6: Filter with transmission zero above the passband due to cross coupling between first and third resonator.

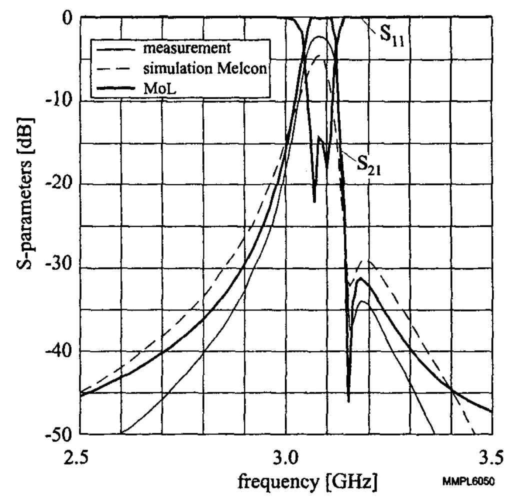

Fig. 7: Scattering parameters for the filter shown in Fig. 6.

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