Higher Order Approximation for the Difference Operators in the Method of Lines

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Abstract—**In this paper a new general formalism for improving the convergence of the Method of Lines (MoL) is presented. The procedure reduces the discretization error to an order of higher than $O(h^4)$. The convergence behaviour is demonstrated for a rib waveguide for optical frequencies.**

I. Introduction

THE METHOD of lines (MoL) [1] — a special FDM — has been proven to be very useful for the analysis integrated microwave [2] and integrated optical wave[3] structures. In the MoL the equations are discretized only as far as necessary, and all other calculations are analytical. The structures may consist of many layers, especially in the coordinate direction in which the analytical calculations are made. In [4] up to 80 layers are used to model diffused waveguides. The procedure guarantees a high numerical precision with an acceptable computational expense. The MoL distinguishes itself by stationary behavior [5] and belongs to the DFT [6].

Customarily the difference operators are derived from Taylor expansions that are truncated after the quadratic term [7], [8]. A fourth order approximation for planar microwave structures was first investigated in[9]. The authors of [10], [11] explicitely give higher order approximations for the necessary first derivative, too. These authors claim that different transformation matrices are necessary for the second and the fourth order approximations. It will be shown in this paper that this is not the case. In fact in [10], [11] also the same matrices are used in both cases. Only the amplitudes of the eigenvectors are changed. By this way the important orthonormality is lost unnecessarily. In [12] it was shown how higher order approximations can be combined with interface conditions at dielectric steps.

This paper presents a new possibility to obtain higher order approximations by a recurrence relation. The order of the new approximation is higher than the fourth order approximation. Because of the special form an exact degree cannot be given. The obtained results are valid not only for the MoL in a cartesian coordinate system but also in a cylindrical coordinate system [13]–[15]. By using higher order approximations it is possible either to minimize the computational effort or to get smaller calculation errors with the same computational effort.

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II. Theory

To solve the wave equation in the MoL, one of the second order differential operators $\frac{\partial^2\psi}{\partial u^2}$, where u stands for x, y, z, φ or other suitable coordinates, has to be replaced by a suitable difference operator. From the Taylor series expansion for ψ on the line i (ψ is the scalar component of the vector potential or one of the two field components from which the total field is obtained) one obtains

$$\left(2\frac{h^2}{2!}\frac{\partial^2\psi}{\partial u^2} + 2\frac{h^4}{4!}\frac{\partial^4\psi}{\partial u^4} + 2\frac{h^6}{6!}\frac{\partial^6\psi}{\partial u^6} + 2\frac{h^8}{8!}\frac{\partial^8\psi}{\partial u^8} + \ldots\right)_i = \psi_{i-1} - 2\psi_i + \psi_{i+1} \tag{1}$$

or, in an other form.

$$h^2\frac{\partial^2}{\partial u^2} \cdot \left\{1 + 2\frac{h^2}{4!}\frac{\partial^2}{\partial u^2}\left[1 + \frac{4!}{6!}h^2\frac{\partial^2}{\partial u^2}\left(1 + \frac{6!}{8!}h^2\frac{\partial^2}{\partial u^2}(\ldots)\right)\right]\right\}\psi = -P \cdot \psi_i \tag{2}$$

$-P \cdot \psi_i$ is an abbreviation for the right side of (1). P should be the scheme of numbers $\{-1, 2, -1\}$. Concentrating only on the operators, we obtain

$$h^2\frac{\partial^2}{\partial u^2} = \frac{-P}{\left\{1 + 2\frac{h^2}{4!}\frac{\partial^2}{\partial u^2}\left[1 + \frac{4!}{6!}h^2\frac{\partial^2}{\partial u^2}\left(1 + \frac{6!}{8!}h^2\frac{\partial^2}{\partial u^2}(\ldots)\right)\right]\right\}} \tag{3}$$

We can interpret (3) as a recurrence relation to improve the approximation for the necessary difference operator. Starting with the normally used second order approximation

$$h^2\frac{\partial^2}{\partial u^2} \longrightarrow -\boldsymbol{P} \tag{4}$$

we obtain after the first recursion

$$h^2\frac{\partial^2}{\partial u^2} \to -\boldsymbol{P}\left\{\boldsymbol{I} - \frac{2!}{4!}\boldsymbol{P}\left[\boldsymbol{I} - \frac{4!}{6!}\boldsymbol{P}\left(\boldsymbol{I} - \frac{6!}{8!}\boldsymbol{P}(\ldots)\right)\right]\right\}^{-1} \tag{5}$$

If $\boldsymbol{P}$ has the eigenvalue matrix $\boldsymbol{\lambda}^2$, we obtain the new eigenvalue matrix $\boldsymbol{\lambda}_1^2$ by

$$\boldsymbol{\lambda}_1^2 = \boldsymbol{\lambda}^2\left\{\boldsymbol{I} - \frac{1}{12}\boldsymbol{\lambda}^2\left[\boldsymbol{I} - \frac{1}{30}\boldsymbol{\lambda}^2\left(\boldsymbol{I} - \frac{1}{56}\boldsymbol{\lambda}^2(\ldots)\right)\right]\right\}^{-1} \quad (6)$$

To obtain all field components, we need the difference operator for the differential quotient of the first order as well. By a similiar procedure starting from the line between the lines i and $i+1$ (that is, from the line system of the other component necessary for the expansion of the field or the dual boundary problem) we obtain, analog to (1)

$$h\frac{\partial\psi}{\partial u} + 2\frac{(h/2)^3}{3!}\frac{\partial^3\psi}{\partial u^3} + 2\frac{(h/2)^5}{5!}\frac{\partial^5\psi}{\partial u^5} + 2\frac{(h/2)^7}{7!}\frac{\partial^7\psi}{\partial u^7} + \ldots = \psi_{i+1} - \psi_i \quad (7)$$

or for the operator

$$h\frac{\partial}{\partial u} = D\left\{1+\frac{h^2}{2^2 3!}\frac{\partial^2}{\partial u^2}\left[1+\frac{3!}{2^2 5!}h^2\frac{\partial^2}{\partial u^2}\left(1+\frac{5!h^2}{2^2 7!}\frac{\partial^2}{\partial u^2}(\ldots)\right)\right]\right\}^{-1} \quad (8)$$

D stands for the number scheme $\{-1, 1\}$. The dual problem must be introduced for the approximations of the 2nd order differential operators on the right hand side. The higher order approximations obtained in this way are appropriate to the higher order approximations of the second order differential quotient. For the $\boldsymbol{\delta}$-matrices [1] we obtain

$$\boldsymbol{\delta}_1 = \boldsymbol{\delta}\left\{\boldsymbol{I} - \frac{\boldsymbol{\lambda}^2}{4\cdot 3!}\left[\boldsymbol{I} - \frac{\boldsymbol{\lambda}^2 3!}{4\cdot 5!}\left(\boldsymbol{I} - \frac{\boldsymbol{\lambda}^2 5!}{4\cdot 7!}\left(\boldsymbol{I} - \frac{\boldsymbol{\lambda}^2 7!}{4\cdot 9!}(\ldots)\right)\right)\right]\right\}^{-1} \quad (9)$$

If $\boldsymbol{\delta}$ has the subscript e, (see [1]) $\boldsymbol{\lambda}^2$ must also have the subscript e. If the order in the product of the braces and $\boldsymbol{\delta}$ is changed, then $\boldsymbol{\lambda}^2$ must obtain the subscript of the dual problem.

The two equations (6) and (9) could be rewritten in the following form

$$\boldsymbol{\lambda}_1^2 = \boldsymbol{\lambda}^2\boldsymbol{\lambda}^2\left\{2\boldsymbol{I} - 2\left[\boldsymbol{I} - \frac{1}{2!}\boldsymbol{\lambda}^2 + \frac{1}{4!}\boldsymbol{\lambda}^4 - + \ldots\right]\right\}^{-1} = \frac{\boldsymbol{\lambda}^2\boldsymbol{\lambda}^2}{2(\boldsymbol{I} - \cos\boldsymbol{\lambda})} \quad (10)$$

$$\boldsymbol{\delta}_1 = \boldsymbol{\delta\lambda}\left\{2\left[\left(\frac{\boldsymbol{\lambda}}{2}\right) - \frac{1}{3!}\left(\frac{\boldsymbol{\lambda}}{2}\right)^3 + \frac{1}{5!}\left(\frac{\boldsymbol{\lambda}}{2}\right)^5 - + \ldots\right]\right\}^{-1} = \frac{\boldsymbol{\delta\lambda}}{2\sin\frac{\boldsymbol{\lambda}}{2}} \quad (11)$$

For the product of the $\boldsymbol{\delta}$ matrices we obtain

$$\boldsymbol{\delta}_1^t\boldsymbol{\delta}_1 = \frac{\boldsymbol{\lambda}^2\boldsymbol{\lambda}^2}{4\sin^2\frac{\boldsymbol{\lambda}}{2}} = \frac{\boldsymbol{\lambda}^2\boldsymbol{\lambda}^2}{2(\boldsymbol{I} - \cos\boldsymbol{\lambda})} = \boldsymbol{\lambda}_1^2 \quad (12)$$

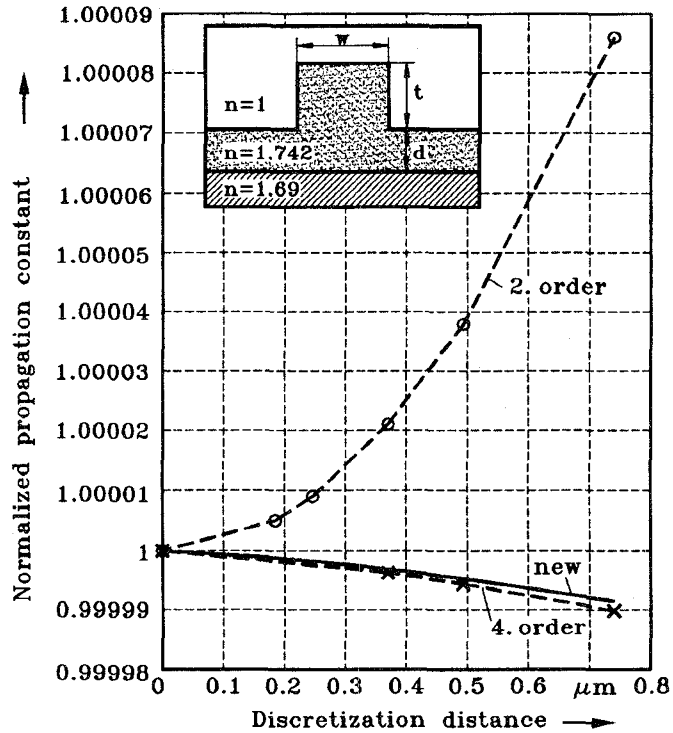

Fig. 1. Convergence curves of the normalized propagation constant for a rib waveguide (cross-section inserted) with the dimensions: $\lambda_0 = 1.55\ \mu m, k_0 d = 5,\ t/d = 1, w/d = 6$. Equations (10) and (11) are used for the new curve.

$\boldsymbol{\lambda}^2$ must have the same subscript as $\boldsymbol{\delta}$. If the order of the product on the left hand side is changed, the subscript of $\boldsymbol{\lambda}^2$ must be that of the dual problem.

Because of the identity in (12), the new results fit in the scheme known for $\boldsymbol{\delta}$ and $\boldsymbol{\lambda}$ [1], [17]. It should be mentioned that by setting the bracket in (3) equal to 1, the result in [7] is obtained. The same result can be obtained by expanding the trigonometric functions in (7), (9).

From the results obtained for the first step, recurrence relations can be written in the following form

$$\boldsymbol{\lambda}_{k+1}^2 = \boldsymbol{\lambda}^2\boldsymbol{\lambda}_k^2\{2(\boldsymbol{I} - \cos\boldsymbol{\lambda}_k)\}^{-1} \quad (13)$$

$$\boldsymbol{\delta}_{k+1}^2 = \boldsymbol{\delta\lambda}_k\left\{2\sin\frac{\boldsymbol{\lambda}_k}{2}\right\}^{-1} \quad (14)$$

These recurrence relations are given for completeness. Numerically the first step in (10), (11) is sufficient. The new approximation for the eigenvalues does not change the eigenvectors as can be seen from (5). This is true for the fourth order approximation too.

III. Numerical Results and Final Remarks

To verify the new equations, the convergence behaviour of the propagation constant of the quasi TE mode for a rib waveguide is analyzed.

Fig. 1 shows the propagation constant normalized with the extrapolated value against the discretization distance. The comparison of the curves demonstrates the increase of exactness. As can be seen, especially noteworthy is the improvement in comparison to the second order approximation. In comparison to the fourth order approximation the further improvement is small in this example.

The main importance of the new approximation lies in the relations in (10)–(12). Especially the product relation in (12) is important. Using these relations for the new approximation the whole apparatus developed for the second order approximation [1] can be used. This is not the case for the tradional fourth order approximation. But the result in (12) gives us an idea to construct new self-consistent approximations for the fourth order, too. This can be done by using the squareroot of $\boldsymbol{\lambda}^2$ for $\boldsymbol{\delta}$ (and choosing the suitable sign [1]) or using the higher order $\boldsymbol{\delta}$ and construct the $\boldsymbol{\lambda}^2$ by a suitable product. For the case of a microstrip cross section, the edge parameter value p =0.2735 was found.

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