New Aspects of the Method of Lines

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Abstract—**A re-examination of the fundamentals of the Method of Lines (MoL) shows its close relation to the mode-matching technique, on which it is merely a variant with further approximations. It is obvious that the discretization of the differential operators should be avoided, because it has no advantage, and in fact only leads, to additional errors. This effect is demonstrated for a partially filled waveguide.**

I. Introduction

The method of lines (MoL) can be considered a well-established numerical procedure for the analysis of a variety of microwave and optical waveguide structures as well as plane wave scattering problems [1]–[5]. Its basic principle is the discretization of the wave equation in one or two dimensions and the analytical treatment in the remaining direction. In this letter, a comparison to the mode-matching technique is made, and it will be shown that both procedures use the same basis functions for the representation of the field quantities but different eigenvalues in the characteristic equation, which are not exact in the MoL because of the approximation of the operators. These fundamental features, which are not yet known to the practitioners, are demonstrated for a boundary value problem in Cartesian coordinates with discretization in one direction. The generalization to higher dimensions and other coordinate systems is straightforward.

II. Theory and Numerical Results

A typical boundary value problem occurring in the analysis of planar optical or microwave structures is depicted in Fig. 1. A structure that may be stratified in the y-direction with arbitrarily shaped metallizations in the interfaces is enclosed by lateral electric walls. For simplification, all coordinates and propagation constants are normalized with the free space wave number k_0.

Assuming a wave propagation $\exp(-jk_z z)$ the corresponding wave equation to be solved is

$$(D_x^2 + D_y^2 + \varepsilon_d)\psi_{e,h} = 0 \tag{1}$$

with

$$\begin{aligned} D_x^2 &= \frac{\partial^2}{\partial x^2} \\ D_y^2 &= \frac{\partial^2}{\partial y^2} \\ \varepsilon_d &= \varepsilon_r - \varepsilon_{re} \\ \varepsilon_{re} &= k_z^2 . \end{aligned} \tag{2}$$

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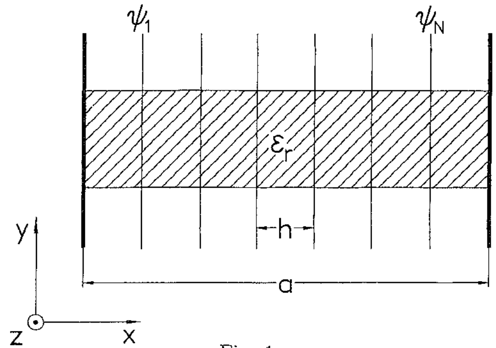

Fig. 1. Illustration of a typical boundary value problem occurring in planar optical or microwave analysis with discretization.

Herein, $\psi_{e,h}$ stands for the independent field components E_z or H_z, respectively. In the MoL the operator D_x^2 is replaced by its discretized form, the matrix $\boldsymbol{P}$, and also including the approximated boundary conditions, which in this case are of the Dirichlet type for E_z and of the Neumann type for H_z. The vector $\boldsymbol{\Psi}$ is transformed

$$\boldsymbol{\Psi} = \boldsymbol{T}\overline{\boldsymbol{\Psi}} \tag{3}$$

with

$$\boldsymbol{T}^{-1}\boldsymbol{P}\boldsymbol{T} = \boldsymbol{\lambda}^2 \tag{4}$$

to obtain a system of uncoupled ordinary differential equations

$$(\boldsymbol{I}D_y^2 - \boldsymbol{k}_y^2)\overline{\boldsymbol{\Psi}} = \boldsymbol{0} \tag{5}$$

with

$$\boldsymbol{k}_y^2 = \boldsymbol{\lambda}^2 - \varepsilon_d \boldsymbol{I} \tag{6}$$

To perform this diagonalization the related eigenvalue problem

$$(\boldsymbol{P} - \lambda^2 \boldsymbol{I}) \cdot \mathbf{t} = \mathbf{0} \tag{7}$$

has to be solved to obtain the elements of $\boldsymbol{\lambda}^2$ and the column vectors of the transformation matrix $\boldsymbol{T}$. With Dirichlet conditions on both sides and equidistant discretization, the elements of the eigenvalue and transformation matrix are

$$\lambda_i = \frac{2}{h} \sin \frac{i\pi}{2(N+1)} \tag{8}$$

$$T_{ij} = \sin \frac{ij\pi}{N+1} \quad i, j = 1, 2, \cdots, N. \tag{9}$$

Normalization factors have been omitted.

To compare with the mode-matching technique we use the modal expansions of the field in x-direction given by the

Fourier series

$$\psi(x, y) = \sum_{i=1}^{\infty} \tilde{\psi}_i(y) \sin k_{xi}x \quad k_{xi} = \frac{i\pi}{a} \tag{10}$$

suitable for the corresponding boundary conditions for E_z. A similar representation can be derived for H_z. From (1) follows an equivalent set of ordinary differential equations

$$(D_y^2 - k_{yi}^2)\tilde{\psi}_i = 0 \tag{11}$$

with

$$k_{yi}^2 = k_{xi}^2 - \varepsilon_d. \tag{12}$$

To set up a system equation that can then be solved numerically, a point-matching procedure [6] is applied to (10) at the equidistant points $x_j = h \cdot j$, $j = 1, 2, \cdots, N$, and the Fourier series is cut at $i = N$ according to the sampling theorem. In the following, this procedure will be called a discrete mode matching (DMM).

Under these conditions, the field components are

$$\begin{aligned}\psi_j &= \psi(x_j, y) \\ &= \sum_{i=1}^{N} \tilde{\psi}_i \sin \frac{ij\pi}{N+1}\end{aligned} \tag{13}$$

which is exactly the transformation following from (3) and (9) in the MoL. Now it is clear that the MoL uses a field representation with eigenmodes as full-domain basis functions, of which the number is equal to the number of discretization lines. Notice, however, that the eigenvalues in the characteristic equation (6) differ from those in the modal expansions (10). This fact has its reason in the approximation of the differential operator. With an increasing number of lines and thus $h \to 0$ we find from (9) using $h = (a/N+1)$

$$\begin{aligned}\lim_{N\to\infty} \lambda_i &= \frac{i\pi}{a} \\ &= k_{xi}\end{aligned} \tag{14}$$

if the sine-function is replaced by its argument for large N. In other words, the eigenvalues in the MoL are inexact and converge to the exact value, if the approximation of the operator is improved. This can also be seen from the recurrence relation

$$\boldsymbol{\lambda}_{k+1}^2 = \boldsymbol{\lambda}^2 \boldsymbol{\lambda}_k^2 [2(\boldsymbol{I} - \cos \boldsymbol{\lambda}_k)]^{-1} \tag{15}$$

presented in [7]. To compute the limit $\boldsymbol{\lambda}_g$ of the series, we make use of Cauchy's convergence theorem for each element i

$$\begin{aligned}\lim_{k\to\infty} |\lambda_{i,k+1} - \lambda_{i,k}| &= \lim_{k\to\infty} |\lambda_{i,k} - \lambda_{i,g}| \\ &= 0\end{aligned} \tag{16}$$

and with $\lambda_{i,k+1} = \lambda_{i,k} = \lambda_{i,g}$ we, of course, find from (9) and (15) the same limit

$$\begin{aligned}\lambda_{i,g} &= \frac{i\pi}{h(N+1)} \\ &= \frac{i\pi}{a}.\end{aligned} \tag{17}$$

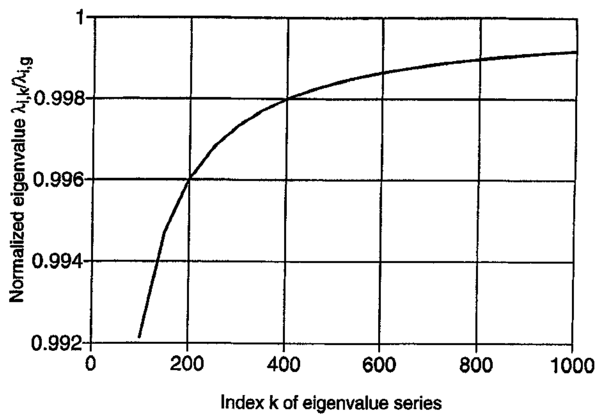

Fig. 2. Convergence of the eigenvalue series $\lambda_{i,k}$ according to [7] with $i = N+1$, $\lambda_{i,g} = \pi$.

Note the difference in the definition of λ_i in (9) and (15) by multiplication with h. The convergence behavior of (15) depends on i and is very slow for the worst case $i = N+1$ (Fig. 2).

For a further discussion of the precision that can be achieved with the MoL, we will investigate how the propagation constants of the modes of a waveguide filled with a stratified dielectric are obtained from the system equation. By means of an additional transformation, the waves are decomposed into modes TM and TE to y [8]. In the system equation

$$\overline{\overline{\boldsymbol{Y}}} \cdot \overline{\overline{\mathbf{E}}} = \mathbf{0} \tag{18}$$

the discretized and transformed tangential field components $\overline{\overline{\mathbf{E}}}$ in an arbitrary matching interface are thus multiplied with a diagonal matrix $\overline{\overline{\boldsymbol{Y}}}$. The solutions of (18) are obtained from

$$\begin{aligned}\det \overline{\overline{\boldsymbol{Y}}} &= \underbrace{\prod_{i=1}^{N+1} \overline{\overline{y}}_{ii}(k_{y,i-1})}_{\mathrm{TE}y} \cdot \underbrace{\prod_{i=N+2}^{2N+1} \overline{\overline{y}}_{ii}[k_{y,i-(N+1)}]}_{\mathrm{TM}y} \\ &= 0\end{aligned} \tag{19}$$

or

$$\overline{\overline{y}}_{ii}(k_{yj}) = 0 \tag{20}$$

with

$$i = 1, \cdots, 2N+1$$
$$k_{yj} = \begin{cases} \sqrt{k_{xj}^2 - \varepsilon_d} & \text{DMM} \\ \sqrt{\lambda_j^2 - \varepsilon_d} & \text{MoL} \end{cases} \tag{21}$$

and j according to the indices in (19) for TEy or TMy, respectively. Each equation i of (20) has an infinite number n of solutions corresponding to the propagation constants of the TEy_{jn} and TMy_{jn} modes. With the correct wave number k_{xj}, these are the characteristic equations from which k_z can also be obtained analytically. In the MoL the solutions depend on the discretization density and are exact only if $N \to \infty$ according to (14). Since $|\lambda_{j+1} - k_{xj+1}| > |\lambda_j - k_{xj}|$, they become more inaccurate for higher order modes, as can be seen from the convergence curves in Fig. 3. For a fair comparison, the same

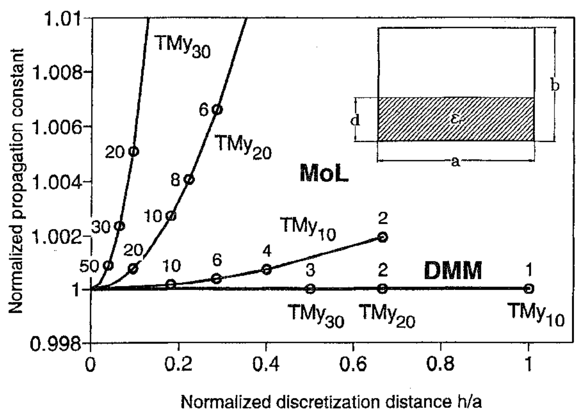

Fig. 3. Convergence of the normalized propagation constants of the fundamental and higher-order modes of a partially filled waveguide to their exact analytical values. $a/\lambda_0 = 2$, $b/a = 0.4$, $d/b = 0.2$, $\varepsilon_r = 2.55$. MoL: Method of lines, DMM: Discrete mode matching. The data labels indicate the number of E_z-lines.

algorithm for the numerical computation has been used for both methods. Only λ_j and k_{xj} have been interchanged.

III. Conclusion

The relation between the method of lines (MoL) and the mode-matching technique has been clarified. It has been found that both methods use the same modal representation of the field components, but in the MoL the differential operators are approximated, which results in an additional error increasing drastically for higher-order modes. In the mode-matching procedure or its discretized form (DMM) presented in this letter, the exact operators, boundary conditions, and spectral wave numbers are used. Since the eigenvalues used in the MoL converge to these exact quantities if the number of lines increases or the approximation of the operator is improved, the DMM always provides the more accurate results with the same analytical and computational effort. These recognitions are in a clear contradiction to what was claimed in [9]. Moreover, in the MoL the eigenvalues depend on the discretization scheme and have to be calculated numerically for a nonequidistant discretization [1]. From this point of view the diagonalization of the system of coupled ordinary differential equations by means of an appropriate equivalent transformation in the MoL, which seems to be a surprising property at first glance, turns out to be nothing but this well-known mathematical fact: the solution of the Helmholtz equation for separable boundary conditions will always separate.

If the eigensolutions are known analytically or can be obtained by means of a fast converging procedure, which is the usual case for most coordinate systems, the application of the MoL is not to be recommended because it only provides an additional error due to the unnecessary approximation of the operators. Avoiding the initial discretization and transformation process and using the exact wave numbers as eigenvalues from the beginning is, of course, the better choice.

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