Application of Davidenko's Method to the Solution of Dispersion Relations in Lossy Waveguiding Systems

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Abstract—**Davidenko's method is a reduction of Newton's method for the numerical solution of n-coupled nonlinear algebraic equations into n-coupled first-order differential equations in a dummy variable. This algorithm is useful for the solution of dispersion relations of electromagnetic waves propagating in lossy waveguiding structures, particularly layered geometries containing one or more gyrotropic layers. In this class of problems, Newton-based numerical techniques are not always satisfactory and Davidenko offers an alternative which is efficient and reliable and which relaxes the extent of the restriction placed on the initial guess to be sufficiently close to the solution. Presented are Davidenko's method, its application to lossy-waveguide dispersion relations, and an example where the algorithm was applied successfully.**

I. Introduction

PROBLEMS DEALING with electromagnetic-wave propagation in multilayered media usually require numerical solutions of the dispersion relation which leads to the modal spectrum ($\omega - \beta$ diagram) of the waveguiding geometry being studied. These dispersion relations, although in general are complicated expressions, are also mathematically well behaved. That is, in the frequency intervals of interest, they are smooth and have smooth derivatives except at a finite number of points. Therefore, the use of simple and well-developed numerical techniques such as Newton's method and others [1] suffices in many cases of interest.

Complications can arise, however, when the need to include losses in the mathematical formulation of the problem make the dispersion relation a complex transcendental equation in a complex variable. In this case, an extension of Newton's method into the two-dimensional case could, in principle, be used.

Indeed, programs based on Newton's method are available [1], [2] for the solution of n nonlinear algebraic equations in n unknowns such as those from the IMSL library [3].

These methods, however, do not always produce satisfactory results. The author has found empirically that this is particularly so when the multilayer structure under study includes gyrotropic layers, i.e., gyroelectric, such as a solid-state plasma (semiconductor or metal), or gyromagnetic, such as a ferrite material [4]–[7].

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In this paper, an alternative method is presented which, although expandable to the n-dimensional case, has proven very successful when $n = 2$, namely, in the case of a complex transcendental dispersion relation in a complex variable. The method is generally attributed to Davidenko [8], and its usefulness has recently been brought to the attention of the chemical engineering community by W. E. Schiesser [9].

No attempt is made here to find the reasons for the failure of other algorithms in the class of problems mentioned above or to make a rigorous comparison between them and Davidenko's. Davidenko's method is simply recommended here whenever readily available routines based on Newton or quasi-Newton methods fail.

II. Davidenko's Method

The basic idea behind Davidenko's method is to reduce Newton's method for a system of n nonlinear algebraic equations in n unknowns to a set of n first-order ordinary differential equations (ODE's) in a dummy variable t.

The basic ideas underlying Davidenko's method can best be explained by considering the one-dimensional case [9]. From a practical point of view, it must be said that the complications inherent in the use of this algorithm over, say, Newton's method are only justified in the case of two or more systems of equations. In the one-dimensional case, root-finders based on derivative-free algorithms such as the secant or the bisection methods are faster and easier to implement and many times even preferable to Newton's method.

Let

$$f(x) = 0 \tag{1}$$

be a nonlinear algebraic equation in the variable x. Newton's method applied to this equation is simply

$$\frac{df(x_n)}{dx}\Delta x_n = -f(x_n) \tag{2}$$

where Δx_n is a correction term for x_n

$$x_{n+1} = x_n + \Delta x_n \tag{3}$$

and n denotes the iteration number. That is, we expect that the point x_{n+1} is closer to the solution than the point x_n. Substituting (3) in (2), we obtain the more familiar form of

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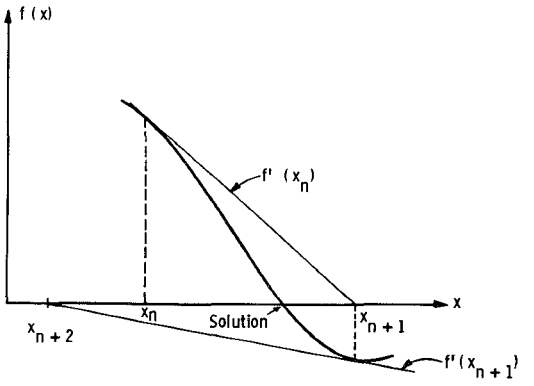

Fig. 1. Starting at a certain point x_n, Newton's method gives us x_{n+1}. However, as in the case illustrated here, a successive application of Newton's method does not take us nearer the solution but to a point (x_{n+2}) farther away. In other words, the algorithm does not converge unless our initial guess happens to be in a region very close to the solution.

Newton's method

$$x_{n+1} = x_n - \frac{f(x_n)}{df(x_n)/dx} \tag{4}$$

or

$$\frac{df(x_n)}{dx} = \frac{0 - f(x_n)}{x_{n+1} - x_n}. \tag{5}$$

Equation (5) is just the equation of a straight line through the points $(x_n, f(x_n))$ and $(x_{n+1}, 0)$. In other words, the next point in the iteration process, i.e. x_{n+1}, is taken to be the intersection of the straight line tangent to $f(x)$ at the point x_n with the x-axis (see Fig. 1). Hence, Newton's algorithm has a step size Δx_n defined by (2).

However, as is the case of Fig. 1, the initial guess may lay outside the region where Newton's method converges. Or, in other words, the correction term Δx_n may be excessive for the initial guess point chosen because $df(x_n)/dx$ (the Jacobian determinant in the n-dimensional case) is too small, as indicated by (4). This restriction placed on the initial guess of having to lie in a region sufficiently small around the solution can be relaxed if we reduce the size of the correction Δx_n by including a factor ϵ in (2), i.e.,

$$\frac{df(x_n)}{dx}\Delta x_n = -\epsilon f(x_n) \tag{6}$$

where $0 < \epsilon < 1$. Rewriting this equation as

$$\frac{\Delta x_n}{\epsilon} = -\frac{f(x_n)}{df(x_n)/dx} \tag{7}$$

and taking the limit when $\epsilon \to 0$, Δx_n is then replaced by a differential correction term, assuming that $f(x)$ is continuous in the vicinity of x_n. That is, (7) becomes (relabelling ϵ as dt)

$$\frac{dx}{dt} = -\frac{f(x)}{df/dx} \tag{8}$$

where t is now a scalar independent variable which is introduced merely to construct the algorithm and has no basis in the original problem, Equation (1).

With these considerations in mind we can now go back to Fig. 1, where we see that we have devised a way to approach a root of $f(x) = 0$ from an initial guess (the initial condition $x(0)$ of differential equation (8)) in infinitesimal steps of size dx corresponding to increments dt of the dummy variable t, arriving at the root after a long "time" t, i.e., for $t \to \infty$. Thus, the original problem $f(x) = 0$ is a particular case of (8) for $t \to \infty$. That is, the value of x which satisfies $f(x) = 0$ also satisfies (8) for $t \to \infty$. Indeed, from(8), we see that

$$\frac{dx}{dt} = -\frac{f(x)}{df/dx} = \frac{dx}{d(lnf)}$$

which implies that

$$f(x) = Ae^{-t}$$

A being an integration constant. For $t \to \infty$, we have $f(x) = 0$.

Equation (8) can be extended to the n-dimensional case, namely,

$$\frac{dx}{dt} = -(\boldsymbol{J})^{-1}\boldsymbol{f}(\boldsymbol{x}) \tag{9}$$

where $\boldsymbol{J}$ is the Jacobian matrix for the n nonlinear algebraic set of equations in n unknowns

$$\begin{aligned} f_1(x_1, x_2 \cdots x_n) &= 0 \\ f_2(x_1, x_2 \cdots x_n) &= 0 \\ &\vdots \quad\quad \vdots \\ f_n(x_1, x_2 \cdots x_n) &= 0 \end{aligned}$$

or, in matrix form,

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{O}$$

with $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$, where T stands for transposed matrix.

Equation (9) is the basic form of Davidenko's method and can be considered as a system of n initial-value ordinary differential equations that can be integrated subject to an initial condition $\boldsymbol{x}(0)$. This initial condition vector is the counterpart of the initial trial solution in Newton's method [5], [9].

From the point of view of the implementation of this algorithm into a computer program, it must be noted that there exist many successful algorithms and published computer programs available [1]–[3], [9] for solving systems of first-order ordinary differential equations. The asymptotic solutions at $t \to \infty$ could be found to the desired degree of precision by comparing the difference between the results of integration up to two consecutive intervals, i.e., the quantity $|x(t + \Delta t) - x(t)|$ to a number δ representing the desired precision. When

$$|x(t + \Delta t) - x(t)| \leqslant \delta$$

the integration can be stopped.

It must be added here that the algorithm has exponential convergence with respect to t [9].

III. Application of Daivdenko's Method to a Lossy Electromagnetic Wave Propagation Problem

The dispersion relation of a lossy waveguiding system, a complex transcendental equation with complex roots, can be generally expressed as

$$F(\omega;\gamma)=0 \tag{10}$$

with $\gamma=\alpha+j\beta$, where the unknowns are α and β, the real and imaginary parts of the propagation constant γ, respectively.

We wish to solve (10) for different values of the parameter ω, the angular frequency. Equation (10) can be treated as a set of two nonlinear algebraic equations in two unknowns by writing it as the set

$$\begin{aligned}\mathrm{Re}\left[F(\omega;\gamma)\right]&\equiv G(\omega;\alpha,\beta)=0\\ \mathrm{Im}\left[F(\omega;\gamma)\right]&\equiv H(\omega;\alpha,\beta)=0.\end{aligned} \tag{11}$$

In this case, it is possible to express the Jacobian matrix of the system and its inverse in closed form, since the dispersion function $F(\omega;\gamma)$ is an analytic complex function on the γ-plane except at a finite number of points. The Cauchy–Riemann relations are then satisfied, that is, from (11)

$$\begin{aligned}G_\alpha&=H_\beta\\ G_\beta&=-H_\alpha\end{aligned} \tag{12}$$

where $G_\alpha\equiv\partial G/\partial\alpha$, etc. The Jacobian matrix is

$$J=\begin{bmatrix}G_\alpha & G_\beta\\ H_\alpha & H_\beta\end{bmatrix}$$

or, using (12)

$$J=\begin{bmatrix}G_\alpha & G_\beta\\ -G_\beta & G_\alpha\end{bmatrix}. \tag{13}$$

On the other hand, using the properties of analytic functions (12), we have

$$\frac{\partial F}{\partial\gamma}\equiv F_\gamma=G_\alpha+jH_\alpha=G_\alpha-jG_\beta. \tag{14}$$

That is

$$\begin{aligned}G_\alpha&=\mathrm{Re}\left[F_\gamma\right]\\ G_\beta&=-\mathrm{Im}\left[F_\gamma\right].\end{aligned} \tag{15}$$

From (13) and (15), the determinant of the Jacobian matrix is

$$\det J=G_\alpha^2+G_\beta^2=|F_\gamma|^2 \tag{16}$$

and, using (15) and (16), the inverse Jacobian matrix is

$$J^{-1}=\frac{1}{\det J}\begin{bmatrix}G_\alpha & -G_\beta\\ G_\beta & G_\alpha\end{bmatrix}=\frac{1}{|F_\gamma|^2}\begin{bmatrix}\mathrm{Re}\left[F_\gamma\right] & \mathrm{Im}\left[F_\gamma\right]\\ -\mathrm{Im}\left[F_\gamma\right] & \mathrm{Re}\left[F_\gamma\right]\end{bmatrix}. \tag{17}$$

We can now write the formal expression of Davidenko's method (9) with

$$x=(\alpha,\beta)^T$$

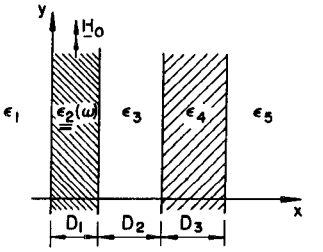

Fig. 2. Five-region canonical waveguiding structure whose dispersion relation was solved using Davidenko's method.

and

$$f=(G,H)^T$$

namely,

$$\frac{d}{dt}\begin{bmatrix}\alpha\\ \beta\end{bmatrix}=-J^{-1}\begin{bmatrix}G\\ H\end{bmatrix}$$

or, using (11) and (17)

$$\begin{aligned}\frac{d\alpha}{dt}&=-\frac{1}{|F_\gamma|^2}\left(\mathrm{Re}\left[F\right]\mathrm{Re}\left[F_\gamma\right]+\mathrm{Im}\left[F\right]\mathrm{Im}\left[F_\gamma\right]\right)\\ \frac{d\beta}{dt}&=+\frac{1}{|F_\gamma|^2}\left(\mathrm{Re}\left[F\right]\mathrm{Im}\left[F_\gamma\right]-\mathrm{Im}\left[F\right]\mathrm{Re}\left[F_\gamma\right]\right).\end{aligned} \tag{18}$$

Equation (18), a system of two coupled first-order ODE's, is the expression of the problem $F(\omega;\gamma)=0$ (10) in terms of Davidenko's algorithm. The solution of (18) for $t\to\infty$ (large t) will give us α and β for a given frequency ω to the desired precision. Notice that the right-hand side of both equations need only be expressed in terms of the dispersion function F and its derivative with respect to γ, F_γ. Furthermore, F_γ, although a complicated expression, can always be written in closed form. The real and imaginary parts of F and F_γ need not be found explicitly since they will be calculated numerically. Equation (18) can then be solved using any quality integrator with automatic step-size adjustment [1]–[3], [9].

IV. Example of the Use of Davidenko's Method

Davidenko's method was tested in the case of a five-layer waveguiding structure where one of the layers is gyroelectric. The following example is included here for the sake of completeness although it has already been presented in [7]. It is hoped, however, that the reader will find its inclusion here convenient and the comments on the method's practical implementation useful. For more details on the problem studied see [6] and [7].

Fig. 2 shows a diagram of the geometry studied. It is assumed infinite in the y- and z-directions. Propagation of electromagnetic waves is in the z-direction. The gyroelectric layer is presumed to be a semiconductor biased by a magnetic field $\vec{H}_0$ along the y-direction. It is char-

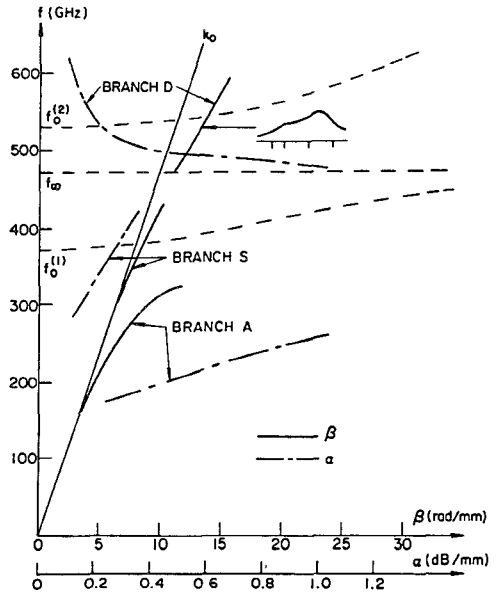

Fig. 3. Sample dispersion diagram for the five-region canonical structure. Nonreciprocal device isolation. Forward propagation. Parameters:

$$\omega_p = 10^{13},\ \omega_c = 10^{12},\ \tau = 8\times 10^{-12},$$
$$\epsilon^{(0)} = 13,\ \epsilon_4 = 4,\ \epsilon_1 = \epsilon_3 = \epsilon_5 = 1,$$
$$D_1 = 50\ \mu m,\ D_2 = D_3 = 100\ \mu m.$$

acterized by the dielectric tensor

$$\epsilon(\omega) = \begin{bmatrix} \xi & 0 & -j\eta \\ 0 & \zeta & 0 \\ j\eta & 0 & \xi \end{bmatrix}$$

where ξ, ζ, and η are complex functions of frequency, the biasing field, the carrier concentration, the dc dielectric constant of the semiconductor and an imaginary term, the carrier collision frequency, which accounts for the losses in the semiconductor [6]. The other four regions in Fig. 2 are isotropic dielectrics of different constants. The losses are significant in this problem.

The dispersion relation is a complicated expression in the complex variable $\gamma = \alpha + j\beta$, the propagation constant. It has the form [7]

$$F(\omega;\gamma) = e^{-2k_2D_1} - \frac{e^{k_4D_3}\left(R_1e^{k_3D_2} + R_2e^{-k_3D_2}\right) + e^{-k_4D_3}\left(R_3e^{k_3D_2} + R_4e^{-k_3D_2}\right)}{e^{k_4D_3}\left(R_5e^{k_3D_2} + R_6e^{-k_3D_2}\right) + e^{-k_4D_3}\left(R_7e^{k_3D_2} + R_8e^{-k_3D_2}\right)} = 0 \tag{19}$$

where R_i, $i = 1,\ldots,8$ and k_l, $l = 2,3,4$, are complex functions of γ, ω, the semiconductor's parameters and the dielectric constants of the other four regions. D_1, D_2, and D_3 are the layer thicknesses (Fig. 2).

Equation (19) was solved using Davidenko's method. The coupled differential equations (18) were solved using RKF45—a subroutine for solving initial value problems in ODE's which is based on Runge–Kutta formulas developed by E. Fehlberg in 1970 and implemented by L. F. Shampine and H. A. Watts in 1974 [1]. The subroutine and the accompanying computer program used to perform the calculations were written in FORTRAN language.

Other algorithms for integration of (18) could be used as well. See, for example, the papers by W. E. Schiesser [9] and by P. T. Boggs [10].

A sample calculation of the roots of (19) as a function of frequency is presented in Fig. 3 for the case in which a dielectric ($\epsilon_4 = 4$) layer is placed at a certain distance from the semiconducting layer. Both regions are surrounded by air. The parameters characterizing the semiconductor are given in the figure caption. Their physical significance is explained in [6].

Three modes or branches are depicted in the figures. Higher order thickness modes were found in the region $f_0^{(1)} < f < f_\infty$ and above $f_0^{(2)}$ [6]. These are not included in the figure. Each of the branches has an attenuation constant and a phase constant. The straight line labeled k_0 corresponds to the electromagnetic-wave propagation in vacuum.

The problem was solved rapidly and efficiently using Davidenko's method. Earlier attempts at solving this problem using a quasi-Newton algorithm from the IMSL library [3] (Muller's method) were unsuccessful because of the great difficulty of finding roots in most regions of the $\omega - \beta$ diagram. Furthermore, the initial guess was very critical, and a great deal of time was spent trying different ones in order to calculate only one point in the $\omega - \beta$ diagram. These problems were completely eliminated with Davidenko's method, when only one initial guess in the approximate vicinity of the root would, in most cases, suffice. Many more cases involving different combinations of parameters were then studied using this algorithm, which led to the useful conclusions presented in [6] and [7].

V. Conclusions

Davidenko's method is a reduction of the Newton–Raphson numerical method for solving n-coupled nonlinear algebraic equations into a set of n simultaneous first-order differential equations in a dummy variable. In this paper, we have shown the usefulness of this method for problems of electromagnetic-wave propagation in multi-layer waveguiding structures where one of the layers is gyroelectric and lossy. However, very similar dispersion relations are obtained when a gyromagnetic medium is used instead, as well as in more complicated problems which could be modeled using combinations of layered geometries with or without gyrotropic regions. An example of this can be found in the analysis of open dielectric waveguides for millimeter and optical wavelengths [11].

The method was shown to be particularly useful when losses are included and is recommended for those lossless problems in which the use of Newton's method proves unsatisfactory.

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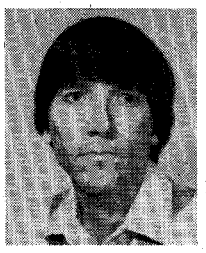

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