

A NEW FINITE-DIFFERENCE TECHNIQUE FOR HIGHER-ORDER MODES
IN ARBITRARILY SHAPED WAVEGUIDES

M. J. Beaubien and A. Wexler
University of Manitoba
Winnipeg, Canada

To design new waveguide shapes and to assess their performance in larger systems, propagation constants and field patterns must be found. The following examples are typical of studies requiring knowledge of higher-order modes:

- a) bandwidth considerations - the upper limit is set by the inception of higher-order modes;
- b) waveguide discontinuity analysis - a set of modes is required to solve scattering problems¹; and
- c) multimode launching and propagation studies - applications include prediction of undesirable linear accelerator resonances, multimode techniques in aerial improvement², etc.

One of the most promising techniques appears to be the finite-difference method. In a very enlightening paper, Davies and Mulwyk³ illustrated the power and usefulness of the method. The cross-section of an arbitrary waveguide was divided into a mesh of squares each having sides of length h . The transverse form of the Helmholtz equation

$$(\nabla_t^2 + k_c^2)\phi(x,y) = 0, \quad (1)$$

where ∇_t^2 is the transverse Laplacian and k_c is the cutoff propagation constant, was written in the finite-difference form

$$\phi_1 + \phi_2 + \phi_3 + \phi_4 - 4\phi_0 + (k_c h)^2 \phi_0 = 0. \quad (2)$$

ϕ_0 is a typical node potential of the mesh and ϕ_1 to ϕ_4 are adjacent node potentials. Instead of defining the potential $\phi(x,y)$ at all points (x,y) , the potential ϕ_i is defined only at discrete points i . Equation (2) was evaluated at every node point with appropriate modification to include boundary conditions. These are that $\phi_i = 0$ for TM modes and that the normal derivative

$$\left[\frac{\partial \phi}{\partial n} \right]_i = 0$$

for TE modes. The resulting set of equations was written in matrix form

$$(A - \lambda I)\phi = 0 \quad (3)$$

where the square matrix of coefficients is denoted by A and Φ is the eigenvector consisting of all node potentials ϕ_i . Equation (3) is the standard form of a matrix eigenvalue problem where λ is the eigenvalue

$$\lambda = \frac{\langle \Phi, h \rangle}{\langle \Phi, \Phi \rangle}^2 \quad (4)$$

Equation (3) can be solved, for dominant and higher-order modes, by direct methods which require sufficient immediate-access computer store for all elements in matrix A . The order of this matrix is equal to the number of nodes. This then restricts the number of node points to about 100 with a consequent upper limit to the maximum attainable accuracy.

On the other hand, because the matrix is very sparse, there is no sense in storing anything but the non-zero elements. An even more economical method is to generate the matrix row-by-row as required, thus saving nearly all store for the vector Φ . This increases vastly the number of nodal points feasible. Iterative methods of solution must then be used. Davies and Mulwyk used up to 20,000 equations in solving a variety of waveguide shapes from the rectangular to a complicated club-shaped guide. They reported cutoff propagation constants with estimated accuracies of better than 0.1 percent. Starting with a first estimate to the eigenvalue $\lambda^{(1)}$, the corresponding $\Phi^{(1)}$ was found by the "Successive Point Overrelaxation" iterative method⁴. Using $\Phi^{(1)}$, an improved eigenvalue $\lambda^{(2)}$ was calculated from the Rayleigh quotient

$$\lambda^{(k+1)} = \frac{\Phi^{(k)}^T A \Phi^{(k)}}{\Phi^{(k)}^T \Phi^{(k)}} \quad (5)$$

k is the number of the successive eigenvalue estimate. The transpose is indicated by T . The advantage of Equation (5) is that it is stationary at the solution point and so approximate potential values ϕ_i yield a more accurate eigenvalue estimate. Using the new eigenvalue, a second and better estimate of the field potential is found, and so on until sufficient accuracy is obtained.

The disadvantage of this iteration technique is that it fails to converge for higher-order eigenvalues. Therefore, it is applicable to the dominant mode only and rarely, in cases of guide symmetry, to the second mode. There are two methods, described by Fadeeva⁵, for the solution of higher-order modes. Unfortunately, evaluation of each successive mode involves all previously determined lower-order modes. Inaccuracies accumulate and computations soon become useless.

Even if convergence were always guaranteed, degradation of accuracy with mode order must be expected due to the increased number of oscillations over the cross-section relative to a given mesh size. This increased discretization error occurs because the mesh appears coarser for higher-order modes.

It happens that for rectangular sections an exact analytic solution to the finite-difference eigenvalue problem exists⁶ and so the magnitude of this source of error can be demonstrated in this particular case. Consider TM modes in a rectangular guide with sides π and $(11/7)\pi$. An exact fit with mesh size $h = \pi/7$ yields 60 nodal equations. Solving the finite-difference

equations exactly, and knowing the solution to the continuous problem, discretization error in propagation constants of the first five modes are 0.8, 1.2, 2.6, 3.0, and 2.8 percent respectively. Halving the mesh size, thus yielding 273 equations, places the direct method beyond the capability of present-day computers. With this number of equations, the above errors are reduced to 0.1, 0.3, 0.7, 1.0, and 0.7 percent. Clearly, these errors can be offset by supplying more boundary and field information at smaller discrete intervals. In complicated guides, we must expect much less accuracy due mainly to imperfect fitting of the mesh to the boundary shape and to field singularities at internal corners⁷. The problem is that, for higher-order modes in particular, large numbers of equations are required. The only realistic method of solution is by iteration, and that usually fails to converge.

Iteration fails to converge for higher-order modes because the matrix $(A - \lambda I)$ is not positive definite for $\lambda > \lambda_1$. (λ_1 is the matrix eigenvalue corresponding to the first mode.) To allow iteration to succeed, the problem was reformulated as follows. The solution of the matrix eigenvalue equation

$$(A - \lambda I)(A - \lambda I)\phi = 0 \quad (6)$$

is satisfied by the same eigenvectors and eigenvalues as Equation (3). Eigenvalues of the new matrix $C = (A - \lambda I)^2$ are equal to the square of those of matrix $B = (A - \lambda I)$. C is therefore positive definite for all approximations to λ except at solution points λ_1 , where it is positive semidefinite. The iteration method used here is therefore guaranteed to converge for symmetric matrices. For slightly nonsymmetric matrices, which occur in TE problems, experimental verification of convergence has been obtained for the squared system.

In order to solve Equation (6) by successive overrelaxation, one must know matrix C . Certainly, direct squaring is impossible as the computer cannot keep $n^2 = (20,000)^2$ elements in its immediate-access store. If it could, a direct method of solution might be used in preference to iteration. Also, it appears to be a difficult task to square a large matrix and keep track of all new element locations and values so that only non-zero elements need to be stored. This will also waste computer store. As with the non-squared system, the most efficient method is to do row-by-row matrix generation, thus reserving nearly all store for ϕ . It turns out that this is possible for the finite-difference form of the Helmholtz equation and an algorithm was developed to do this while paying due regard to boundary conditions. The squared system yields linear equations of the form

$$-2e(\phi_1 + \phi_2 + \phi_3 + \phi_4) + 2(\phi_5 + \phi_6 + \phi_7 + \phi_8) + (\phi_9 + \phi_{10} + \phi_{11} + \phi_{12}) + (e^2 + 4)\phi_0 = 0 \quad (7)$$

$$\text{where } e = 4 - \lambda. \quad (8)$$

The ϕ values are node potentials in the vicinity of the central potential ϕ_0 . Equation (7) is modified slightly near boundaries.

Solution was obtained primarily as previously described. To speed convergence for a fine mesh, a number of eigenvalues and eigenvectors were found using a coarse one. These easily obtained solutions were then used to initiate iteration with a finer mesh. The approximate eigenvalues were used

as starting points and the values of the potential function at newly defined nodes were approximated by Taylor series interpolation between nodes of the coarse mesh.

An L-shaped region was chosen as an example of an arbitrary shape. Propagation constants for different mesh sizes for the TM case are given in the table. Field plots of constant E_z contours, for the first four modes, are illustrated in the figure.

k_c for TM Modes in an L-Shaped Guide ($h = \pi/7$)

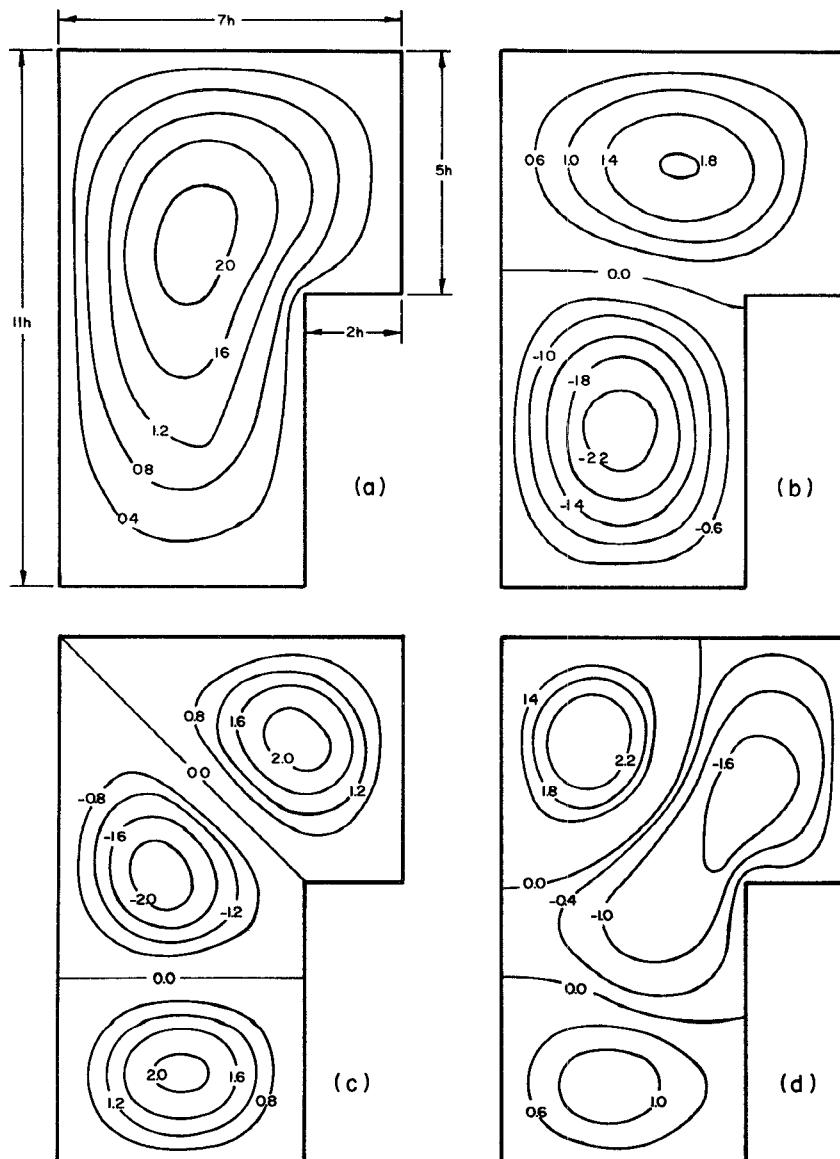
Mode	<u>h</u>	<u>h/2</u>	<u>h/4</u>	<u>h/8</u>	<u>h/16</u>
1	1.424487	1.428048	1.427770		
2	1.754002	1.773439	1.778203	1.779571	
3	2.184215	2.229285	2.240601	2.243657	2.245344
4	2.383168	2.427498	2.437205	2.439827	2.440858

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Constant E_z contours for the first four TM modes.