Optimum Mesh Grading for Finite-Difference Method

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Abstract— **The coarseness error of the finite-difference (FD) method is studied analyzing a typical planar waveguide and a rectangular coaxial geometry. Results for equidistant and graded mesh are compared in terms of accuracy and numerical efforts. Because of the field singularities involved a graded mesh proves to be superior compared to the equidistant case. A grading strategy with optimum efficiency is presented. Furthermore, the results show that the most significant improvement in accuracy can be obtained by incorporating the edge behavior into the FD scheme.**

I. Motivation

NOWADAYS numerical methods for electromagnetic simulation constitute an indispensable tool for solving microwave engineering problems. Among the different approaches, the finite-difference (FD) method in time domain (FDTD) has received great attention due to its flexibility and its direct relationship with Maxwell's equations. Commonly, discretization follows the central difference scheme according to Yee [1]. As well known, this scheme exhibits second-order accuracy as long as an equidistant mesh is used. In the case of mesh grading, this characteristic deteriorates to the first order. In the past, several approaches were proposed to overcome this limitation (e.g., [2]). But this is accomplished at the expense of other properties such as flexibility.

In the discussions on this topic, however, one fact needs to be emphasized that appears to be not as generally known as the above-mentioned ones: In the derivation of the second-order accuracy behavior, one assumes regular, i.e. bounded, fields. If the discretized domain contains field singularities, the order of accuracy is determined by the singularity rather than by the inherent order of accuracy (see, e.g., finite-element (FE) method [3]). Such singularities occur at each metallic corner. In the case of planar microwave circuits, for instance, the field behavior near the corners or edges dominates the overall behavior. Hence, it becomes questionable whether the second-order rule provides a good estimation for practical applications.

In this context, the paper contributes results on three aspects:

1) The accuracy of the FD method in the presence of field singularities is studied in detail.
2) Information is provided how to choose discretization in order to optimize the tradeoff between accuracy and numerical efforts.

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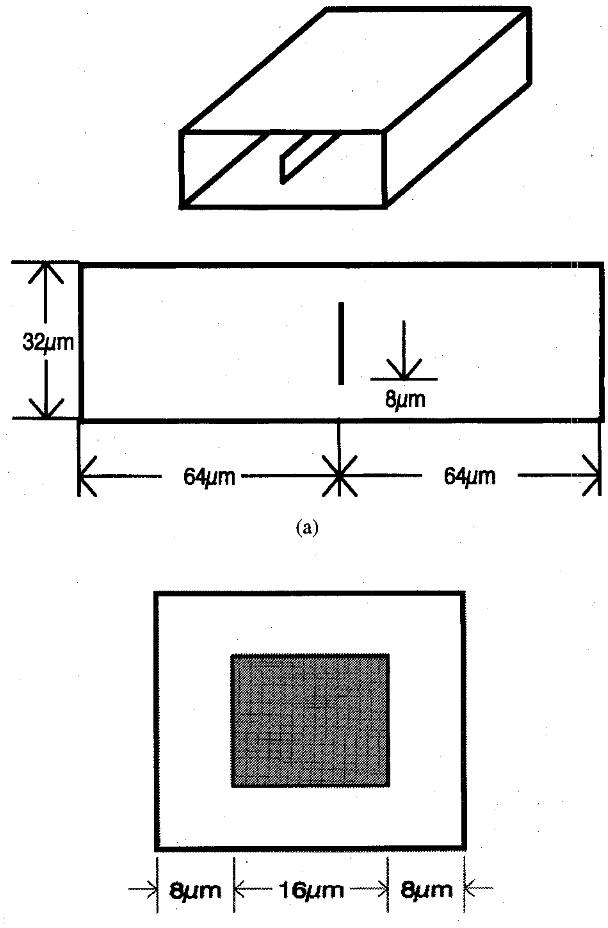

Fig. 1. The waveguide cross sections under consideration. (a) Slot-line type of structure with infinitely thin center conductor (b) Square coaxial geometry (center conductor and enclosure are ideally conducting).

3) The improvement when including the edge behavior into the FD scheme is shown.

One should note that our considerations focus on the so-called coarseness error, i.e., the error caused by the limited spatial resolution. There are, of course, other sources of error, e.g., the dispersion due to discretization, which, however, are beyond the scope of this paper.

II. Method of Analysis and Meshing

In order to determine accuracy one needs to treat a structure for which the results are analytically known or can be derived by other highly accurate methods. On this reason, we choose the waveguide problems depicted in Fig. 1.

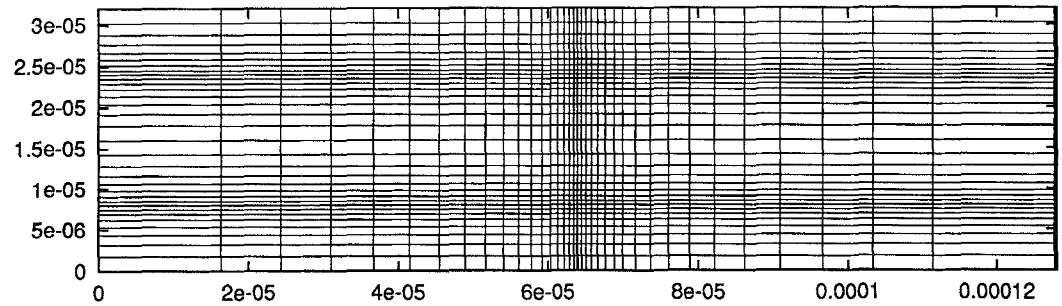

Fig. 2. Example for discretization by a graded mesh (cross section of structure in Fig. 1(a) with smallest cell size $\Delta s_{min} = 0.5\mu$m, grading according to a geometric series with factor $q = \sqrt[4]{2}$, all dimensions in meter).

With respect to the intended investigations, the structures offer the following desirable properties:

1) In Fig. 1(a), the fields concentrate in the slots. Thus, it represents a good example for the situation in planar circuits where the field behavior in a slot region determines the characteristics (e.g., CPW, slot-line, coupled microstrip). Fig. 1(b) shows a similar geometry, but with a thick center conductor and thus a different order of edge singularity (square coaxial cable).
2) The geometry of both structures is symmetrical and relatively simple. Therefore, the influence of the field singularity can be separated and it is not clouded by other effects.
3) The waveguides support a pure TEM fundamental wave. Thus, the characteristic impedance Z is well defined and may be used as an indicator for overall accuracy. On the other hand, the outer boundaries form a rectangular waveguide. Hence higher-order modes can be investigated at the same time.
4) Assuming the lateral walls of structure (a) to be removed the characteristic impedance of the TEM mode can be derived analytically by conformal mapping. For type (b) and the higher-order mode of type (a), a mode-matching approach [8] is used as a reference.

The dimensions are chosen so that the slot geometry corresponds to the situation typical for MMIC's and that the cut-off frequencies for the higher-order modes are sufficiently high.

For analysis, we employ FD methods both in time (FDTD [4]) and frequency domain (FDFD [5]). In the FDTD case, a three-dimensional (3-D) treatment is applied exciting the structure with a Gaussian pulse, whereas in the FDFD case a two-dimensional (2-D) eigenvalue problem is solved. The time step Δt in the FDTD analysis is chosen to be 0.9 the value at the stability limit. Comparing the results of both methods we found that the deviations are of minor importance and do not affect the following investigations.

In order to separate the influence of the different mesh parameters we proceed as follows:

1) An equidistant mesh is used starting with a cell size of $\Delta s = \Delta x = \Delta y = 8\mu$m. Subsequently, its value is reduced to 4μm, 2μm, etc.
2) A graded mesh is applied with the smallest cell size Δs_{min} located at the corners of the inner conductor. Starting from these points, the cell size is increased successively by a constant factor q. Hence, the cell sizes follow a geometric series. Fig. 2 illustrates this strategy for the case of Fig. 1(a).

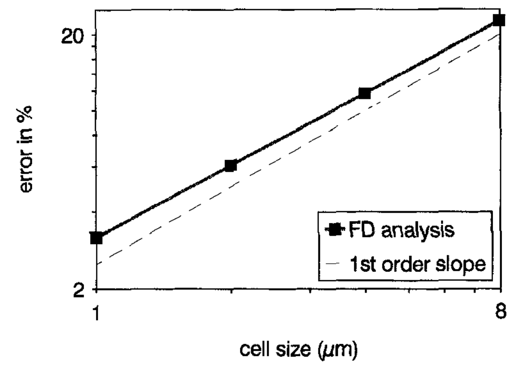

Fig. 3. Percentage error in characteristic impedance Z of the waveguide according to Fig. 1(a) versus cell size for an equidistant mesh (the relative error refers to the analytical value $Z = 94.2\Omega$ obtained by conformal mapping).

III. Results

A. Infinitely Thin Center Conductor (TEM mode)

First, the equidistant case with infinitely thin center conductor, Fig. 1(a), under TEM-mode excitation will be considered. In Fig. 3, the error is plotted as a function of the cell size.

Clearly, one observes a first-order behavior (the same finding applies to the phase constant β of the higher-order mode – see Section III-D). At the first glance, this may be surprising since one expects a second-order characteristic.

The discrepancy is caused by the field singularity. The investigated structure with an infinitely thin strip exhibits an edge singularity of the order 0.5 (i.e., $E \sim 1/\sqrt{r}$ with E denoting the normal electric field and r the distance from the edge). Incorporating this behavior into the FD equations, the resulting field approximation may be checked by a simple treatment. One finds a rule $\Delta E \sim \Delta s^{0.5}$ that is worse than $\Delta Z \sim \Delta s^1$ as observed in Fig. 3. Presumably, certain errors cancel out when calculating the impedance Z from the fields.

Second, a graded mesh is applied (see Fig. 2) and the influence of both the smallest cell size Δs_{min} and the grading factor q is studied.

Fig. 4 illustrates the results. It presents curves varying q with Δs_{min} kept constant. The error ΔZ in characteristic impedance Z is plotted against the number n of cells in

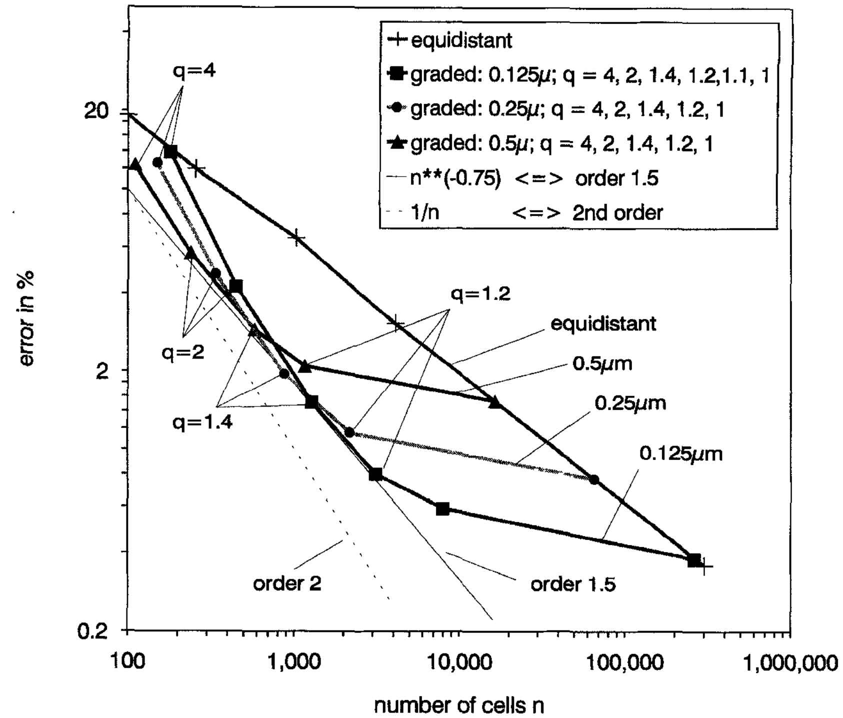

Fig. 4. Error of characteristic impedance Z against number of cells n required: comparison between equidistant and graded mesh with $\Delta s_{min} = 0.5\mu$m, 0.25μm, and 0.125μm and the grading factor q varied as given in the inset (for other data see Fig. 3).

the cross-section, which corresponds to the computer efforts involved (note that n scales with $(\Delta s)^{-2}$, i.e., a first-order characteristic with error $\Delta Z \sim \Delta s$ is equivalent to $\Delta Z \sim n^{-0.5}$). The aim of the diagram in Fig. 4 is to provide information on an application-oriented figure of merit, that is which accuracy can be achieved for a given number of cells, or, vice versa, which is the numerical expense for a given accuracy. In other words, the nearer a curve to the origin of the diagram the more effective the discretization.

The results demonstrate clearly that mesh grading leads to considerable improvement in efficiency. For the structure considered, the graded mesh outperforms the equidistant case even for q values as large as 4. Regarding the order of accuracy, a value of about 1.5 is achieved compared to 1 for the equidistant mesh. Hence, due to the singularity effect, the grading yields a better order of accuracy than possible by an equidistant mesh. Furthermore, the curves in Fig. 4 indicate that there is an optimum choice for the grading factor q. Independent of the smallest cell size, a value q in the range $1.2\ldots2$ yields the best results in terms of efficiency. For larger values of q, accuracy degrades due to poor resolution. For $q \to 1$, on the other hand, the increase in mesh size does not lead to an equivalent improvement in accuracy because the uniform mesh behavior is recovered. This characteristic is illustrated by Fig. 5 where the mesh size n as well as the error are plotted against the grading factor q.

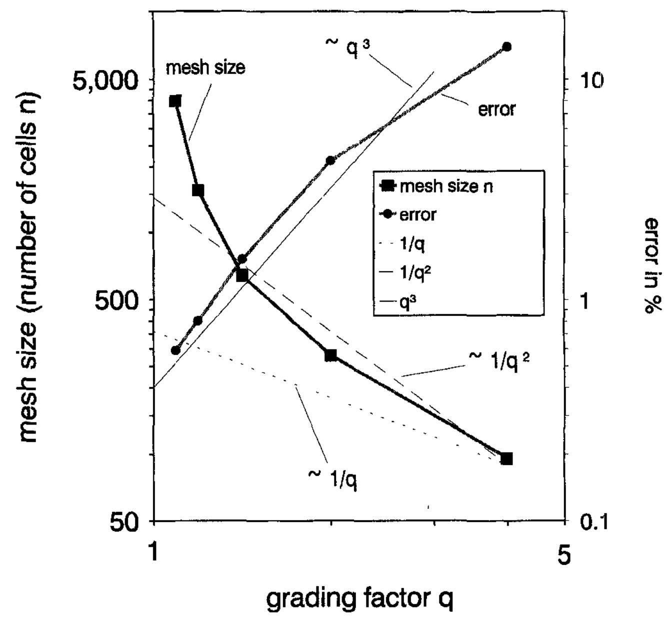

Fig. 5. Mesh size n and error in Z against grading factor q for $\Delta s_{min} = 0.125\mu$m (other data identical to Fig. 3).

B. Thick Center Conductor

Fig. 6 provides information on the error characteristics for the structure of Fig. 1(b). This different type of waveguide is treated in order to generalize the results of the previous section, i.e., to check whether the findings for the structure in Fig. 1(a) remain valid for type (b) as well. Because of the square cross-section of the center conductor only 90^o edges are involved. Hence, the order of singularity is weaker than for version (a) ($E \sim r^{-1/3}$).

Comparing the results with those for the infinitely thin strip (Fig. 4) two important features can be observed:

1) The slope of the curve for the equidistant mesh is different. The behavior follows a $n^{-2/3}$ rule, which corresponds to an error order $\Delta Z \sim (\Delta s)^{4/3}$ compared

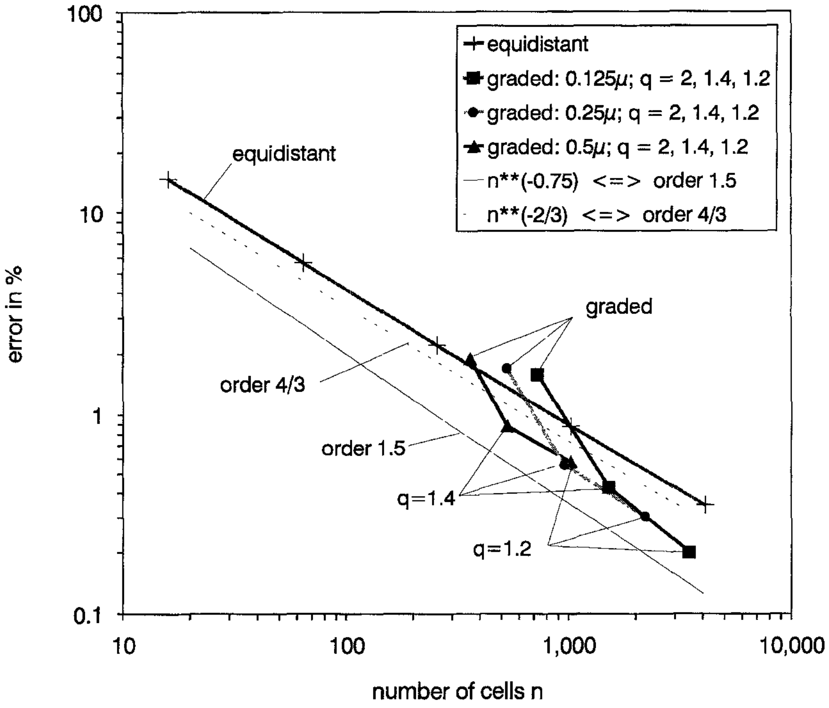

Fig. 6. Data of Fig. 4 for the square coaxial geometry of Fig. 1(b): Error of characteristic impedance Z against number of cells n (equidistant discretization and graded mesh with $\Delta s_{min} = 0.5\mu$m, 0.25μm, 0.125μm, and the grading factor q varied as given in the inset; the relative error refers to the value $Z = 36\ 82\Omega$ obtained by mode-matching method [8]).

with $\Delta Z \sim \Delta s$ for the infinitely thin strip in Fig. 4. This finding supports the afore-mentioned statement that the order of accuracy is determined by the field singularities rather than by the common second-order characteristic of the central-difference scheme.

2) The improvement that can be achieved by mesh grading is less pronounced than in Fig. 4. For $q \geq 2$, the equidistant mesh even turns out to be more efficient than the graded one. These differences probably can be attributed to the fact that in the case of the square coaxial geometry the influence of the edge singularities on the overall waveguide properties is not as significant as in the case of Fig. 1(a).

The important point, however, is not that the influence of the singularity is weaker than for Fig. 1(a) but that the general dependence on grading factor q closely resembles the case treated before: q values in the range $1.2 \ldots 1.4$ lead to optimum numerical efficiency. Also, as in Fig. 4, the order of accuracy that can be achievd by mesh grading approaches the value 1.5. This means: The optimum choice of the meshing parameters does not critically depend on the type of singularity or on the individual structure. As a consequence, guide lines may be derived that apply to a very general class of structures. This, of course, is very important for practical application.

C. Improved FD Treatment of Edge Singularities

The results shown before, particularly those for the thin strip of Fig. 1(a), point out the significance of the field description at the metallic edges. Therefore, when seeking a formulation with improved accuracy one has to concentrate on the singularity rather than on the regular domains. As was shown in [6], the singular behavior can be explicitly incorporated into the FD equations. The treatment is based on the integral form of Maxwell's equations over the elementary cells (i.e., a finite-integration scheme, which, however, in most cases yields equations identical to common FD theory). Due to the integral formulation it is possible to take into account a field singularity of known order explicitly in the FD equations for the elementary cells adjacent to the edge. The modifications can be implemented easily into the FD code and do not increase the numerical expense (see also [7]). This approach was applied to the structure of Fig. 1(a) in order to assess the improvement in accuracy.

In Fig. 7 the results are compared to the conventional FD formulation. First, it has to be stated that the modified version yields better accuracy for all data calculated. In the case of an equidistant mesh, the error is reduced dramatically by a factor of about 5. For the graded mesh, the improvement depends on the factor q. Again, $q = 1.2 \ldots 1.4$ leads to best efficiency. As can be expected, the error reduction that can be achieved by mesh grading is less than for the conventional FD formulation since the singularity effects are accounted for *a priori*.

D. Higher-Order Mode

So far, the investigations are confined to the TEM mode. Hence, the question arises whether the findings apply to other modes as well. For this reason, we consider the first higher-order mode of the structure of Fig. 1(a). Instead of the characteristic impedance, the propagation constant β is studied at a sufficiently high frequency ($f = 1.5$ THz, this value might appear to be unrealistically high but it can easily be reduced by scaling up the waveguide dimensions). A high-accuracy mode-matching analysis serves as a reference ($\beta = 21\,153.0$).

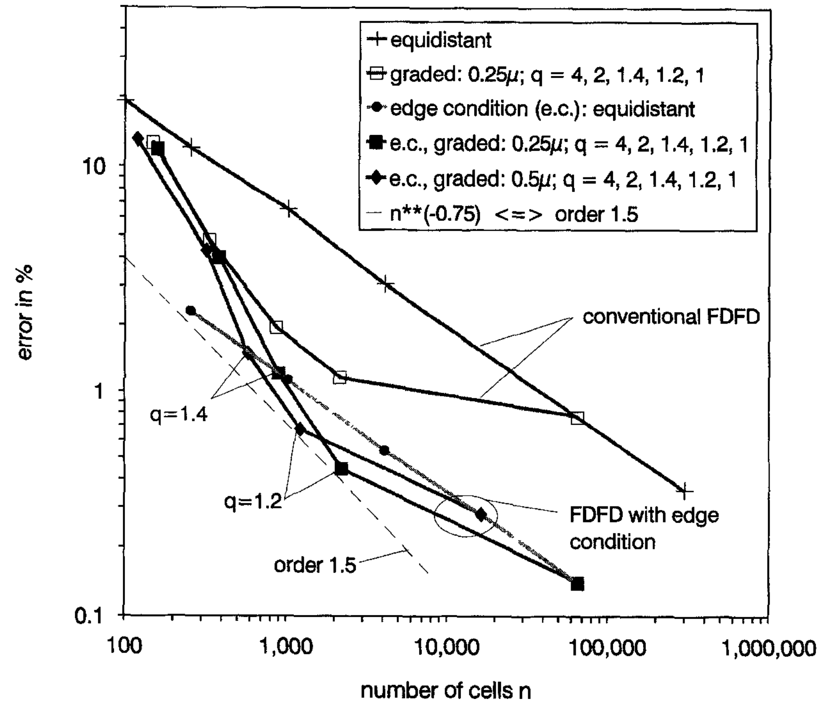

Fig. 7. Data of Fig. 4 when using modified FD equations accounting for the edge singularity [6]: Error of characteristic impedance Z against number of cells n for both equidistant and graded mesh (with $\Delta s_{min} = 0.5\mu$m, 0.25μm, and the grading factor q varied as given in the inset); other data as in Fig. 3.

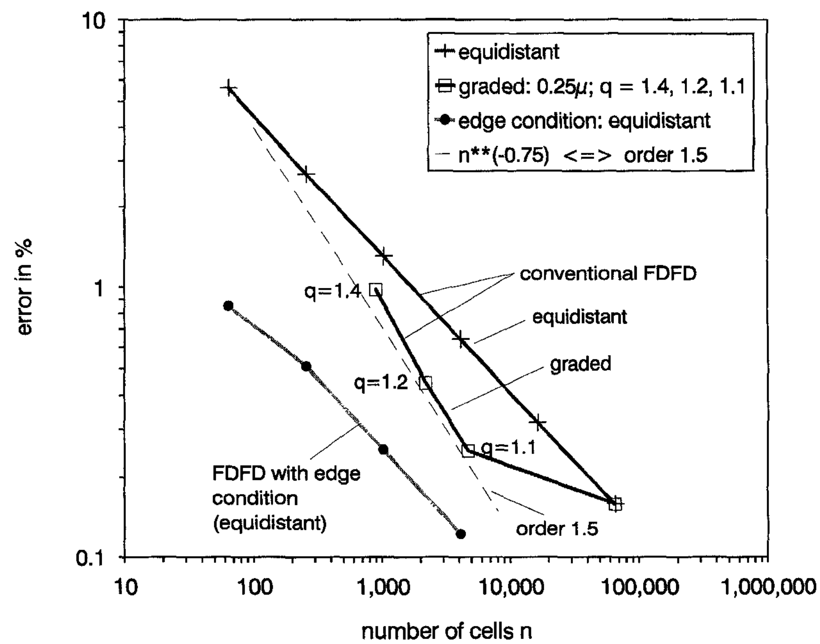

Fig. 8. Data of Fig. 7 for the first higher-order mode of the structure in Fig. 1(a): Error of propagation constant β against number of cells n for conventional FD approach with both equidistant and graded mesh and for the modified version including the edge singularity (equidistant case); $\Delta s_{min} = 0.25\mu$m, grading factor $q$varied as given in the inset; reference value $\beta = 21\,153.0$ at $f = 1.5$THz calculated by mode-matching technique [8]; other data as in Fig. 7.

Fig. 8 presents the results. This figure clearly demonstrates that:

1) The propagation constant β behaves as the characteristic impedance in the TEM situation, i.e., its second order accuracy deteriorates to a first -order characteristic due to the singularity (for the unperturbed rectangular waveguide it is of second order);
2) as in the preceding sections, the graded mesh proves to be superior to the equidistant gridding. Again, a grading factor q of about 1.2 leads to best performance;
3) including the edge condition according to Section III-C greatly improves accuracy.

This makes clear that the results of the TEM case hold for higher-order modes as well.

IV. Conclusion

From the results presented the following conclusions with regard to the FD analysis of planar circuits and fin-line structures can be drawn.

1) The well-known second-order error behavior of the FD method refers only to regular fields and does not hold at field singularities. For the infinitely thin strip, we find only a first-order behavior in characteristic impedance and propagation constant. This means that the overall accuracy is determined primarily by the spatial resolution at the metallic edges and corners.
2) Although the introduction of mesh grading increases the principal FD error from second to first order, it yields a much better overall accuracy than the equidistant version for a given mesh size. This is due to the improved field resolution near the singularities.
3) If one uses a graded mesh with a constant ratio q relating the neighboring discretization steps, one has two degrees of freedom: the smallest cell size Δs_{min} and the grading factor q. Our investigations indicate that choosing q in the range $1.2 \ldots 1.4$ yields optimum efficiency independent of the minimum cell size. This finding applies for higher-order waveguide modes equally.
4) For structures with strong singularities (e.g., of the CPW and slot-line type) a significant improvement in accuracy can be achieved by incorporating the edge singularity into the FD equations [6]. Error reductions up to a factor of more than 5 are found. Such an approach can be easily implemented if the order of singularity is known. This is the case for the common 2-D waveguide problems (see, e.g., [9]). One should mention, however, that problems are encountered when dealing with 3-D geometries, because there is no a-priori-knowledge available concerning the order of singularity at metallic corners. This has to be investigated further.

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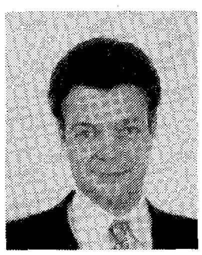

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